

Information and Entropy in Quantum Theory

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Abstract

Recent developments in quantum computing have revived interest in the notion of information as a foundational principle in physics. It has been suggested that information provides a means of interpreting quantum theory and a means of understanding the role of entropy in thermodynamics. The thesis presents a critical examination of these ideas, and contrasts the use of Shannon information with the concept of 'active information' introduced by Bohm and Hiley.

We look at certain thought experiments based upon the 'delayed choice' and 'quantum eraser' interference experiments, which present a complementarity between information gathered from a quantum measurement and interference effects. It has been argued that these experiments show the Bohm interpretation of quantum theory is untenable. We demonstrate that these experiments depend critically upon the assumption that a quantum optics device can operate as a measuring device, and show that, in the context of these experiments, it cannot be consistently understood in this way. By contrast, we then show how the notion of 'active information' in the Bohm interpretation provides a coherent explanation of the phenomena shown in these experiments.

We then examine the relationship between information and entropy. The thought experiment connecting these two quantities is the Szilard Engine version of Maxwell's Demon, and it has been suggested that quantum measurement plays a key role in this. We provide the first complete description of the operation of the Szilard Engine as a quantum system. This enables us to demonstrate that the role of quantum measurement suggested is incorrect, and further, that the use of information theory to resolve Szilard's paradox is both unnecessary and insufficient. Finally we show that, if the concept of 'active information' is extended to cover thermal density matrices, then many of the conceptual problems raised by this paradox appear to be resolved.

Contents

1	Introduction	10
2	Information and Measurement	13
2.1	Shannon Information	13
2.1.1	Communication	15
2.1.2	Measurements	16
2.2	Quantum Information	17
2.2.1	Quantum Communication Capacity	17
2.2.2	Information Gain	18
2.2.3	Quantum Information Quantities	20
2.2.4	Measurement	22
2.3	Quantum Measurement	24
2.4	Summary	29
3	Active Information and Interference	30
3.1	The Quantum Potential as an Information Potential	31
3.1.1	Non-locality	31
3.1.2	Form dependence	32
3.1.3	Active, Passive and Inactive Information	33
3.2	Information and interference	34
3.2.1	The basic interferometer	35
3.2.2	Which way information	37
3.2.3	Welcher-weg devices	39
3.2.4	Surrealistic trajectories	43
3.2.5	Conclusion	48
3.3	Information and which path measurements	48
3.3.1	Which path information	49
3.3.2	Welcher-weg information	52
3.3.3	Locality and teleportation	55
3.3.4	Conclusion	59

3.4	Conclusion	62
4	Entropy and Szilard's Engine	64
4.1	Statistical Entropy	65
4.2	Maxwell's Demon	67
4.2.1	Information Acquisition	68
4.2.2	Information Erasure	69
4.2.3	"Demonless" Szilard Engine	72
4.3	Conclusion	76
5	The Quantum Mechanics of Szilard's Engine	79
5.1	Particle in a box	81
5.2	Box with Central Barrier	82
5.2.1	Asymptotic solutions for the HBA, $V \gg E$	86
5.3	Moveable Partition	87
5.3.1	Free Piston	88
5.3.2	Piston and Gas on one side	90
5.3.3	Piston with Gas on both sides	93
5.4	Lifting a weight against gravity	98
5.5	Resetting the Engine	102
5.5.1	Inserting Shelves	103
5.5.2	Removing the Piston	106
5.5.3	Resetting the Piston	106
5.6	Conclusions	111
5.6.1	Raising Cycle	112
5.6.2	Lowering Cycle	113
5.6.3	Summary	114
6	The Statistical Mechanics of Szilard's Engine	116
6.1	Statistical Mechanics	117
6.2	Thermal state of gas	120
6.2.1	No partition	121
6.2.2	Partition raised	121
6.2.3	Confined Gas	122
6.2.4	Moving partition	123
6.3	Thermal State of Weights	128
6.3.1	Raising and Lowering Weight	128
6.3.2	Inserting Shelf	131
6.3.3	Mean Energy of Projected Weights	132

6.4	Gearing Ratio of Piston to Pulley	134
6.4.1	Location of Unraised Weight	135
6.5	The Raising Cycle	135
6.6	The Lowering Cycle	141
6.7	Energy Flow in Popper-Szilard Engine	144
6.8	Conclusion	150
7	The Thermodynamics of Szilard's Engine	152
7.1	Free Energy and Entropy	153
7.1.1	One Atom Gas	154
7.1.2	Weight above height h	156
7.1.3	Correlations and Mixing	157
7.2	Raising cycle	160
7.3	Lowering Cycle	165
7.4	Conclusion	168
8	Resolution of the Szilard Paradox	169
8.1	The Role of the Demon	170
8.1.1	The Role of the Piston	170
8.1.2	Maxwell's Demons	172
8.1.3	The Significance of Mixing	173
8.1.4	Generalised Demon	179
8.1.5	Conclusion	183
8.2	Restoring the Auxiliary	184
8.2.1	Fluctuation Probability Relationship	184
8.2.2	Imperfect Resetting	187
8.2.3	The Carnot Cycle and the Entropy Engine	199
8.2.4	Conclusion	201
8.3	Alternative resolutions	202
8.3.1	Information Acquisition	202
8.3.2	Information Erasure	204
8.3.3	'Free will' and Computation	207
8.3.4	Quantum superposition	210
8.4	Comments and Conclusions	215
8.4.1	Criticisms of the Resolution	215
8.4.2	Summary	217
9	Information and Computation	219
9.1	Reversible and tidy computations	219

9.1.1	Landauer Erasure	220
9.1.2	Tidy classical computations	223
9.1.3	Tidy quantum computations	224
9.1.4	Conclusion	227
9.2	Thermodynamic and logical reversibility	227
9.2.1	Thermodynamically irreversible computation	228
9.2.2	Logically irreversible operations	228
9.3	Conclusion	230
10	Active Information and Entropy	232
10.1	The Statistical Ensemble	232
10.2	The Density Matrix	235
10.2.1	Szilard Box	236
10.2.2	Correlations and Measurement	237
10.3	Active Information	238
10.3.1	The Algebraic Approach	239
10.3.2	Correlations and Measurement	242
10.4	Conclusion	248
A	Quantum State Teleportation	250
A.1	Introduction	250
A.2	Quantum Teleportation	251
A.3	Quantum State Teleportation and Active Information	252
A.4	Conclusion	255
B	Consistent histories and the Bohm approach	257
B.1	Introduction	257
B.2	Histories and trajectories	258
B.3	The interference experiment	260
B.4	Conclusion	264
C	Unitary Evolution Operators	265
D	Potential Barrier Solutions	268
D.1	Odd symmetry	270
D.1.1	$E > V$	270
D.1.2	$E = V$	271
D.1.3	$E < V$	272
D.1.4	Summary	273
D.2	Even symmetry	273

D.2.1	$E > V$	273
D.2.2	$E = V$	274
D.2.3	$E < V$	275
D.2.4	Summary	276
D.3	Numerical Solutions to Energy Eigenvalues	276
E	Energy of Perturbed Airy Functions	279
F	Energy Fluctuations	282
G	Free Energy and Temperature	285
H	Free Energy and Non-Equilibrium Systems	290

List of Figures

3.1	Basic Interferometer	35
3.2	Which-path delayed choice	39
3.3	Welcher-weg cavities	42
3.4	Surrealistic Trajectories	44
4.1	The Szilard Engine	68
4.2	Landauer Bit and Logical Measurement	70
4.3	Bit Erasure	72
4.4	The Popper version of Szilard’s Engine	73
4.5	The Cycle of the Popper-Szilard Engine	77
5.1	Superpositions of odd and even symmetry states	85
5.2	Asymptotic Values of Energy Levels	87
5.3	Motion of Piston	89
5.4	Airy Functions for a Mass in Gravitational Field	99
5.5	Splitting Airy Function at Height h	104
5.6	Correlation of Weights and Piston Position	109
5.7	The Lowering Cycle of the Popper-Szilard Engine	115
6.1	Mean Flow of Energy in Popper-Szilard Engine	147
7.1	Change in Entropy on Raising Cycle	164
7.2	Change in Entropy on Lowering Cycle	168
9.1	Distributed quantum computing	225
B.1	Simple interferometer	258
B.2	The CH ‘trajectories’.	259
B.3	The Bohm trajectories.	260
D.1	First six energy eigenvalues with potential barrier	277
D.2	Perturbation of Even Symmetry Eigenstates	278
D.3	Degeneracy of Even and Odd Symmetry Eigenstates	278

G.1 The Entropy Engine 288

List of Tables

4.1	The Controlled Not Gate	71
6.1	Work extracted from gas	126
7.1	Thermodynamic Properties of the Raising Cycle	164
7.2	Thermodynamic Properties of Lowering Cycle	167

Chapter 1

Introduction

In recent years there has been a significant interest in the idea of information as fundamental principle in physics[Whe83, Whe90, Zur90b, Per93, FS95, Fri98, Deu97, Zei99, Sto90, Sto92, Sto97, amongst others]. While much of this interest has been driven by the developments in quantum computation[Gru99, CN01] the issues that are addressed are old ones. In particular, it has been suggested that:

1. Information theory must be introduced into physical theories at the same fundamental level as concepts such as energy;
2. Information theory provides a resolution to the measurement problem in quantum mechanics;
3. Thermodynamic entropy is equivalent to information, and that information theory is essential to exorcising Maxwell's Demon.

The concept of information used in these suggestions is essentially that introduced by Shannon[Sha48] and it's generalisation to quantum theory by Schumacher[Sch95]. This concept was originally concerned with the use of different signals to communicate messages, and the capacity of physical systems to carry these signals, and is a largely static property of statistical ensembles.

A completely different concept of information was introduced by Bohm and Hiley[BH93] in the context of Bohm's interpretation of quantum theory[Boh52a, Boh52b]. This concept was much more dynamic, as it concerned the manner in which an individual system evolves.

In this thesis we will be examining some of these relationships between information, thermodynamic entropy, and quantum theory. We will use information to refer to Shannon-Schumacher information, and active information to refer to Bohm and Hiley's concept. We will not be examining the ideas of Fisher information[Fis25, Fri88, Fri89, FS95, Fri98, Reg98], although it is interesting to note that the terms that result from applying this to quantum theory bear a remarkable equivalence to the quantum potential term in the Bohm approach. Similarly, we will not be considering the recently introduced idea of *total* information due to Bruckner and Zeilinger[BZ99, BZ00a, BZ00b]. We will also leave aside the concept of *algorithmic* information[Ben82, Zur89a, Zur89b, Zur90a,

Cav93, Cav94], as this concept has only been defined within the context of classical Universal Turing Machines. To be meaningful for quantum systems this concept must be extended to classify quantum bit strings operated upon by a Universal Quantum Computer, a task which presents some considerable difficulties.

The structure of the thesis is as follows.

In Chapter 2 we will briefly review Shannon and Schumacher information, and the problems for interpreting information in a quantum measurement. Chapter 3 will introduce Bohm and Hiley's concept of active information, and will examine recent thought experiments[ESSW92] based upon the use of 'one-bit detectors' which criticises this interpretation. We will show that this criticism is unfounded.

Chapter 4 introduces the relationship between entropy and information, by reviewing the discussion of Szilard's Engine[Szi29]. This thought experiment has been used to suggest that an intelligent being (a Maxwell Demon) could reduce the entropy of a system by performing measurements on strings of bits.

Finally in Chapter 10 we will re-examine the concept of active information to see if it has any relevance to thermodynamics. We will find that recent developments of the Bohm interpretation[BH00] suggest that the problems surrounding the Szilard Engine may be viewed in a new light using the concept of active information. The fundamental conflict in interpreting thermodynamics is between the statistical ensemble description, and the state of the individual system. We will show that, by extending Bohm's interpretation to include the quantum mechanical density matrix we can remove this conflict in a manner that is not available to classical statistical mechanics and does not appear to be available to other interpretations of quantum theory.

With regard to the three issues raised above, therefore, we will have found that:

1. The introduction of information as a fundamental principle in physics certainly provides a useful heuristic device. However, to be fruitful a much wider concept of information than Shannon's seems to be required, such as that provided by Bohm and Hiley;
2. The use of Shannon-Schumacher information in a physical theory must presume the existence of a well defined measurement procedure. Until a measurement can be certain to have taken place, no information can be gained. Information theoretic attempts to resolve the quantum measurement problem are therefore essentially circular unless they use a notion of information that goes beyond Shannon and Schumacher;
3. Although Shannon-Schumacher information and Gibbs-Von Neumann entropy are formally similar they apply to distinctly different concepts. As an information processing system must be implemented upon a physical system, it is bound by physical laws and in an appropriate limit they become related by Landauer's Principle. Even in this limit, though, the different nature of the concepts persists.

Chapter 2

Information and Measurement

In this Chapter we will briefly review the concept of Shannon information[Sha48, SW49] and it's application to quantum theory.

Section 1 reviews the classical notion of information introduced by Shannon and it's key features. Section 2 looks at the application of Shannon information to the outcomes of quantum measurements[Kul59, Per93, Gru99, CN01]. We will be assuming that a quantum measurement is a well defined process. The Shannon measure may be generalised to Schumacher information, but the interpretation of some of the quantities that are constructed from such a generalisation remains unclear. Finally in Section 3 we will consider an attempt by [AC97] to use the quantum information measures to resolve the measurement problem, and show that this fails.

2.1 Shannon Information

Shannon information was original defined to solve the problem of the most efficient coding of a set of signals[SW49, Sha48]. We suppose that there is a source of signals (or sender) who will transmit a given message a with probability P_a . The message will be represented by a bit string (an ordered series of 1's and 0's). The receiver will have a decoder that will convert the bit string back into it's corresponding message. Shannon's theorem shows that the mean length of the bit strings can be compressed to a size

$$I_{Sh} = - \sum_a p_a \log_2 p_a \quad (2.1)$$

without introducing the possibility of errors in the decoded message¹. This quantity I_{Sh} is called the Shannon information of the source. As it refers to the length in bits, per message, into which the messages can be compressed, then a communication channel that transmits I_{Sh} bits per message has a signal capacity of I_{Sh} .

¹This assumes there is no noise during transmission.

This concept of information has no relationship to the meaning or significance that the sender or the receiver attributes to the message itself. The information content of a particular signal, $-\log_2 p_a$, is simply an expression of how likely, or unlikely the message is of being sent. The less likely the occurrence of a message, the greater information it conveys. In the limit where a message is certain to occur ($P_a = 1$), then no information is conveyed by it, as the receiver would have known in advance that it was going to be received. An extremely rare message conveys a great deal of information as it tells the receiver that a very unlikely state of affairs exists. In many respects, the Shannon information of the message can be regarded as measuring the 'surprise' the receiver feels on reading the message!

The most important properties of the Shannon information, however, are expressed in terms of conditional $I(\alpha|\beta)$ and mutual $I(\alpha : \beta)$ information, where two variables α and β are being considered. The probability of the particular values of $\alpha = a$ and $\beta = b$ simultaneously occurring is given by $P(a, b)$, and the joint information is therefore

$$I(\alpha, \beta) = - \sum_{a,b} P(a, b) \log_2 P(a, b)$$

From the joint probability distribution $P(a, b)$ we construct the separate probability distributions

$$\begin{aligned} P(a) &= \sum_b P(a, b) \\ P(b) &= \sum_a P(a, b) \end{aligned}$$

the conditional probabilities

$$\begin{aligned} P(a|b) &= \frac{P(a, b)}{P(b)} \\ P(b|a) &= \frac{P(a, b)}{P(a)} \end{aligned}$$

and the correlation

$$P(a : b) = \frac{P(a, b)}{P(a)P(b)}$$

This leads to the information terms²

$$\begin{aligned} I(\alpha) &= - \sum_{a,b} P(a, b) \log_2 P(a) \\ I(\beta) &= - \sum_{a,b} P(a, b) \log_2 P(b) \\ I(\alpha|\beta) &= - \sum_{a,b} P(a, b) \log_2 P(a|b) \\ I(\beta|\alpha) &= - \sum_{a,b} P(a, b) \log_2 P(b|a) \\ I(\alpha : \beta) &= - \sum_{a,b} P(a, b) \log_2 P(a : b) \end{aligned}$$

²These terms may differ by the minus sign from the definitions given elsewhere. The Shannon information as given represents the ignorance about the exact state of the system.

which are related by

$$\begin{aligned} I(\alpha|\beta) &= I(\alpha, \beta) - I(\beta) \\ I(\beta|\alpha) &= I(\alpha, \beta) - I(\alpha) \\ I(\alpha : \beta) &= I(\alpha, \beta) - I(\alpha) - I(\beta) \end{aligned}$$

and obey the inequalities

$$\begin{aligned} I(\alpha, \beta) &\geq I(\alpha) \geq 0 \\ I(\alpha, \beta) &\geq I(\alpha|\beta) \geq 0 \\ \min [I(\alpha), I(\beta)] &\geq -I(\alpha : \beta) \geq 0 \end{aligned}$$

We can interpret these relationships, and the α and β variables, as representing communication between two people, or as the knowledge a single person has of the state of a physical system.

2.1.1 Communication

If β represents the signal states that the sender transmits, and α represents the outcomes of the receivers attempt to decode the message, then $P(a|b)$ represents the reliability of the transmission and decoding³.

The receiver initially estimates the probability of a particular signal being transmitted as $P(b)$, and so has information $I(\beta)$. After decoding, the receiver has found the state a . Presumably knowing the reliability of the communication channel, she may now use Bayes's rule to re-estimate the probability of the transmitted signals

$$P(b|a) = \frac{P(a|b)P(b)}{P(a)}$$

On receiving the result a , therefore, the receiver has information

$$I(\beta|a) = \sum_b P(b|a) \log_2 P(b|a)$$

about the signal sent. Her information gain, is

$$\Delta I_a(\beta) = I(\beta|a) - I(\beta) \tag{2.2}$$

Over an ensemble of such signals, the result a will occur with probability $P(a)$. The mean information possessed by the receiver is then

$$\langle I(\beta|a) \rangle = \sum_a P(a) I(\beta|a) = I(\beta|\alpha)$$

So the conditional information $I(\beta|\alpha)$ represents the average information the receiver possesses about the signal state, given her knowledge of the received state, while the term $I(\beta|a)$ represents

³There are many ways in which the decoding may be unreliable. The communication channel may be noisy, the decoding mechanism may not be optimally designed, and the signal states may be overlapping in phase space

the information the receiver possesses given a specific outcome a . The mean information gain

$$\langle \Delta I(\beta|a) \rangle = \sum_a P(a) \Delta I_a(\beta) = I(\alpha : \beta)$$

The mutual information is the gain in information the receiver has about the signal sent. It can be shown that, given that the sender is also aware of the reliability of the transmission and decoding process, that the conditional information $I(\alpha|\beta)$ represents the knowledge the sender has about the signal the receiver actually receives. The mutual information can then be regarded as the symmetric function expressing the information both receiver and sender possess in common, or equivalently, the *correlation* between the state of the sender and the state of the receiver.

If the transmission and decoding processes are completely reliable, then the particular receiver states of α will be in a one-to-one correspondence with the signal states of β , with probabilities $P(a|b) = 1$. This leads to

$$\begin{aligned} I(\alpha) &= I(\beta) \\ I(\beta|\alpha) = I(\alpha|\beta) &= 0 \\ I(\alpha : \beta) &= -I(\alpha) \end{aligned}$$

It should be remembered that the information measure of complete certainty is zero, and it increases as the uncertainty, or ignorance of the state, increases. In the case of a reliable transmission and decoding, the receiver will end with perfect knowledge of the signal state, and the sender and receiver will be maximally correlated.

2.1.2 Measurements

The relationships above have been derived in the context of the information capacity of a communication channel. However, it can also be applied to the process of detecting and estimating a state of a system. The variable β will represent the *a priori* probabilities that the system is in a particular state. The observer performs a measurement upon the system, obtaining the result in variable α .

The initial states do not have to represent an exact state of the system. If we start by considering a classical system with a single coordinate x and its conjugate momentum p_x , the different states of β represent a partitioning of the phase space of the system into separate regions b , and the probabilities $P(b)$ that the system is located within a particular partition. The measurement corresponds to dividing the phase space into a partitioning, represented by the different states of α and locating in which of the measurement partitions the system is located.

We now find that the conditional information represents the improved knowledge the observer has of the initial state of the system (given the outcome of the measurement) and the mutual information, as before, represents the average gain in information about the initial state.

Note that if the measurement is not well chosen, it may convey no information about the original partitioning. Suppose the partitioning of β represents separating the phase space into the regions

$p_x > 0$ and $p_x < 0$, with equal probability of being found in either ($P(p_x > 0) = P(p_x < 0) = \frac{1}{2}$) and a uniform distribution within each region. Now we perform a measurement upon the *position* of the particle, separating the phase space into the regions $x > 0$ and $x < 0$. The probabilities are

$$\begin{aligned} P(p_x > 0|x > 0) &= \frac{P(x>0)p_x>0P(p_x>0)}{P(x>0)} = \frac{1}{2} \\ P(p_x < 0|x > 0) &= \frac{P(x>0)p_x<0P(p_x<0)}{P(x>0)} = \frac{1}{2} \\ P(p_x > 0|x < 0) &= \frac{P(x<0)p_x>0P(p_x>0)}{P(x<0)} = \frac{1}{2} \\ P(p_x < 0|x < 0) &= \frac{P(x<0)p_x<0P(p_x<0)}{P(x<0)} = \frac{1}{2} \end{aligned}$$

A measurement based upon the partition $x > 0$ and $x < 0$ would produce no gain in information. However, it is always possible to define a finer grained initial partitioning (such as dividing the phase space into the four quadrants of the x, p_x axes) for which the measurement increases the information available, and in this case would provide complete information about the location of the original partition.

If the measurement partition of α coincides with the partition of β then the maximum information about β will be gained from the measurement. In the limit, the partition becomes the finely grained partition where each point (p_x, x) in the phase space is represented with the probability density function $\Pi(p_x, x)$.

In classical mechanics the observer can, in principle, perfectly distinguish all the different states, and make the maximum information gain from a measurement. However, in practice, some finite partitioning of the phase space is used, owing to the physical limitations of measuring devices.

2.2 Quantum Information

When attempting to transfer the concept of information to quantum systems, the situation becomes significantly more complex. We will now review the principal ways in which the measure and meaning of information is modified in quantum theory.

The first subsection will be concerned with the generalisation of Shannon's theorem, on communication capacities. This produces the Schumacher quantum information measure. Subsection 2 will consider the Shannon information gain from making measurements upon a quantum system. Subsection 3 reviews the quantities that have proposed as the generalisation of the relative and conditional information measures, in the way that Schumacher information generalises the Shannon information. These quantities have properties which make it difficult to interpret their meaning.

2.2.1 Quantum Communication Capacity

The primary definition of information came from Shannon's Theorem, on the minimum size of the communication channel, in mean bits per signal, necessary to faithfully transmit a signal in the

absence of noise. The theorem was generalised to quantum theory by Schumacher [Sch95, JS94].

Suppose that the sender wishes to use the quantum states ψ_a to represent messages, and a given message will occur with probability p_a . We will refer to $I[\rho]$ as the Shannon information of the source. The quantum coding theorem demonstrates that the minimum size of Hilbert space H that can be used as a communication channel without introducing errors is

$$\text{Dim}(H) = 2^{S[\rho]}$$

where

$$\begin{aligned} \rho_a &= |\psi_a\rangle \langle \psi_a| \\ \rho &= \sum_a p_a \rho_a \\ S[\rho] &= -\text{Tr}[\rho \log_2 \rho] \end{aligned} \tag{2.3}$$

By analogy to the representation of messages in bits, a Hilbert space of dimension 2 is defined as having a capacity of 1 qbit, and a Hilbert space of dimension n , a capacity of $\log_2 n$ qbits.

If the signal states are all mutually orthogonal

$$\rho_a \rho_{a'} = \delta_{aa'} \rho_a^2$$

then

$$S[\rho] = -\sum_a p_a \log_2 p_a$$

If this is the case, then the receiver can, in principle, perform a quantum measurement to determine exactly which of the signal states was used. This will provide an information gain of exactly the Shannon information of the source.

However, what if the signal states are not orthogonal? If this is the case, then [Weh78]

$$S[\rho] < I[\rho]$$

It would appear that the signals can be sent, without error, down a smaller dimension of Hilbert space. Unfortunately, as the signal states are not orthogonal, they cannot be unambiguously determined. We must now see how much information can be extracted from this.

2.2.2 Information Gain

To gain information, the receiver must perform a measurement upon the system. The most general form of a measurement used in quantum information is the Positive Operator Valued Measure (POVM) [BGL95]. This differs from the more familiar von Neumann measurement, which involves the set of projection operators $|a\rangle \langle a|$ for which $\langle a | a^\theta \rangle = \delta_{aa'}$ and

$$\sum_a |a\rangle \langle a| = I$$

is the identity operator. The probability of obtaining outcome a , from an initial state ρ is given by

$$p_a = \text{Tr}[\rho |a\rangle \langle a|]$$

This is not the most general way of obtaining a probability measure from the density matrix. To produce a set of outcomes a , with probabilities p_a according to the formula

$$p_a = \text{Tr}[\rho A_a]$$

the conditions upon the set of operators A_a are that they be *positive*, so that

$$\langle w | A_a | w \rangle \geq 0$$

for all states $|w\rangle$, and that the set of operators sums to the identity

$$\sum_a A_a = I$$

For example, consider a spin- $\frac{1}{2}$ system, with spin-up and spin-down states $|0\rangle, |1\rangle$ respectively and the superpositions $|u\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ $|v\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ then the following operators

$$\begin{aligned} A_1 &= \frac{1}{2} |0\rangle \langle 0| \\ A_2 &= \frac{1}{2} |1\rangle \langle 1| \\ A_3 &= \frac{1}{2} |u\rangle \langle u| \\ A_4 &= \frac{1}{2} |v\rangle \langle v| \end{aligned}$$

form a POVM. A given POVM can be implemented in many different ways⁴, but will typically require an auxiliary system whose state will be changed by the measurement.

The signal states ρ_b occur with probability p_b . Using the same expression for information gain as in Equation 2.2 so we can now apply Bayes's rule as before, with

$$p(a|b) = \text{Tr}[A_a \rho_b]$$

to give the probability, on finding outcome a , that the original signal state was b

$$p(b|a) = \frac{p(b)\text{Tr}[A_a \rho_b]}{p(a)} \quad (2.4)$$

We now define the relative information, information gain and mutual information as before

$$\begin{aligned} I(\beta|a) &= \sum_b P(b|a) \log_2 P(b|a) \\ \Delta I_a(\beta) &= I(\beta|a) - I(\beta) \\ \langle I(\beta|a) \rangle &= \sum_a P(a) I(\beta|a) = I(\beta|\alpha) \\ \langle \Delta I(\beta|a) \rangle &= \sum_a P(a) \Delta I_a(\beta) = I(\alpha : \beta) \end{aligned}$$

⁴The example given here could be implemented by, on each run of the experiment, a random choice of whether to measure the 0-1 basis or u-v basis. This will require a correlation to a second system which generates the random choice. In general a POVM will be implemented by a von Neumann measurement on an extended Hilbert space of the system and an auxiliary[Per90, Per93].

It can be shown that the maximum gain in Shannon information, known as the Kholevo bound, for the receiver is the Schumacher information[Kho73, HJS⁺96, SW97, Kho98].

$$I[\alpha : \beta] \leq S[\rho]$$

So, although by using non-orthogonal states the messages can be compressed into a smaller volume, the information that can be retrieved by the receiver is reduced by exactly the same amount.

2.2.3 Quantum Information Quantities

The information quantity that results from a measurement is still defined in terms of Shannon information on the measurement outcomes. This depends upon the particular measurement that is performed. We would like to generalise the joint, conditional, and mutual information to quantum systems, and to preserve the relationships:

$$\begin{aligned} S[A|B] &= S[AB] - S[B] \\ S[B|A] &= S[AB] - S[A] \\ S[A : B] &= S[AB] - S[A] - S[B] \end{aligned}$$

This generalisation[AC95, Gru99, SW00, CN01, and references therein] is defined from the joint density matrix of two quantum systems ρ_{AB} .

$$\begin{aligned} \rho_A &= \text{Tr}_B [\rho_{AB}] \\ \rho_B &= \text{Tr}_A [\rho_{AB}] \\ S[AB] &= -\text{Tr} [\rho_{AB} \log_2 \rho_{AB}] \\ S[A] &= -\text{Tr} [\rho_{AB} \log_2 (\rho_A \otimes 1_B)] \\ &= -\text{Tr} [\rho_A \log_2 \rho_A] \\ S[B] &= -\text{Tr} [\rho_{AB} \log_2 (1_A \otimes \rho_B)] \\ &= -\text{Tr} [\rho_B \log_2 \rho_B] \\ S[A|B] &= -\text{Tr} [\rho_{AB} \log_2 \rho_{A|B}] \\ S[B|A] &= -\text{Tr} [\rho_{AB} \log_2 \rho_{B|A}] \\ S[A : B] &= -\text{Tr} [\rho_{AB} \log_2 \rho_{A:B}] \end{aligned} \tag{2.5}$$

where the matrices⁵

$$\rho_{A|B} = \lim_{n \rightarrow \infty} \left[\rho_{AB}^{1/n} (1_A \otimes \rho_B)^{1/n} \right]^n$$

⁵Where all the density matrices commute, then

$$\begin{aligned} \rho_{A|B} &= \rho_{AB} (\rho_A \otimes 1_B)^{-1} \\ \rho_{A:B} &= \rho_{AB} (\rho_A \otimes \rho_B)^{-1} \end{aligned}$$

in close analogy to the classical probability functions

$$\begin{aligned}\rho_{B|A} &= \lim_{n \rightarrow \infty} \frac{1}{n} \left[\rho_{AB}^{1/n} (\rho_A \otimes 1_B)^{1/n} \right]^n \\ \rho_{A:B} &= \lim_{n \rightarrow \infty} \frac{1}{n} \left[\rho_{AB}^{1/n} (\rho_A \otimes \rho_B)^{1/n} \right]^n\end{aligned}$$

However, these quantities display significantly different properties from Shannon information. The most significant result is that it is possible for $S[A] > S[AB]$ or $S[B] > S[AB]$. This allows $S[A|B], S[B|A] < 0$ and $-S[A : B] > S[AB]$ which cannot happen for classical correlations, and does not happen for the Shannon information quantities that come from a quantum measurement. A negative conditional information $S[A|B] < 0$, for example, would appear to imply that, given perfect knowledge of the state of B , one has 'greater than perfect' knowledge of the state of A !

The clearest example of this is for the entangled state of two spin- $\frac{1}{2}$ particles, with up and down states represented by 0 and 1:

$$\psi = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

This is a pure state, which has

$$S[AB] = 0$$

The subsystem density matrices are

$$\begin{aligned}\rho_A &= \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|) \\ \rho_B &= \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|)\end{aligned}$$

so that

$$S[A] = S[B] = 1$$

The conditional quantum information is then

$$S[A|B] = S[B|A] = -1$$

The significance that can be attributed to such a negative conditional information is a matter of some debate[AC95, AC97, SW00]. We have noted above that the Shannon information of a measurement on a quantum system does not show such a property. However, the Kholevo bound would appear to tell us that each of the quantities $S[A]$, $S[B]$ and $S[AB]$ can be the Shannon information gained from a suitable measurement of the system.

The partial resolution of this problem lies in the fact that, for quantum systems, there exist joint measurements which cannot be decomposed into separate measurements upon individual systems. These joint measurements may yield more information than can be obtained for separable measurements even in the absence of entanglement[GP99, Mas00, BDF⁺99, Mar01]. In terms of *measurements* the quantities of $S[AB]$, $S[A]$ and $S[B]$ may refer to information gains from mutually incompatible experimental arrangements. There is correspondingly no *single* experimental arrangement for which the resulting *Shannon* information will produce a negative conditional information.

2.2.4 Measurement

We have so far reviewed the existence of the various quantities that are associated with information in a quantum system. However, we have not really considered what we mean by the information gained from a quantum measurement.

In a classical system, the most general consideration is to assume a space of states (whether discrete digital messages or a continuous distribution over a phase space) and probability distribution over those states.

There are two questions that may be asked of such a system:

1. What is the probability distribution?
2. What is the state of a given system?

If we wish to determine the probability distribution, the means of doing this is to measure the state of a large number of equivalently prepared systems, and as the number of experiments increases the relative frequencies of the states approaches the probability distribution. So the measurement procedure to determine the state of the given system is the same as that used to determine the probability distribution.

For a quantum system, we must assume a Hilbert space of states, and a probability distribution over those states. Ideally we would like to ask the same two questions:

1. What is the probability distribution?
2. What is the state of a given system?

However, we find we a problem. The complete statistical properties of the system are given by the density matrix

$$\rho = \sum_a p_a \rho_a$$

where the state ρ_a occurs with probability p_a . We can determine the value of this density matrix by an *informationally complete* measurement⁶. However, this measurement does *not* necessarily tell us the states ρ_a or p_a . The reason for this is that the quantum density matrix does not have a unique decomposition. A given density matrix ρ could have been constructed in an infinite number of ways. For example, the following ensembles defined upon a spin- $\frac{1}{2}$ system

Ensemble 1

$$\begin{aligned}\rho_1 &= |0\rangle\langle 0| \\ \rho_2 &= |1\rangle\langle 1|\end{aligned}$$

⁶An informationally complete measurement is one whose statistical outcomes uniquely defines the density matrix. Such a measurement can only be performed using a POVM[BGL95, Chapter V]. A single experiment, naturally, cannot reveal the state of the density matrix. It is only in the limit of an infinite number of experiments the relative frequencies of the outcomes uniquely identifies the density matrix.

$$\begin{aligned}
p_1 &= \frac{1}{2} \\
p_2 &= \frac{1}{2}
\end{aligned}$$

Ensemble 2

$$\begin{aligned}
\rho_A &= |u\rangle \langle u| \\
\rho_B &= |v\rangle \langle v| \\
p_A &= \frac{1}{2} \\
p_B &= \frac{1}{2}
\end{aligned}$$

Ensemble 3

$$\begin{aligned}
\rho_1 &= |0\rangle \langle 0| \\
\rho_2 &= |1\rangle \langle 1| \\
\rho_A &= |u\rangle \langle u| \\
\rho_B &= |v\rangle \langle v| \\
p_1 &= \frac{1}{4} \\
p_2 &= \frac{1}{4} \\
p_A &= \frac{1}{4} \\
p_B &= \frac{1}{4}
\end{aligned}$$

with $|u\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ $|v\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$, all produce the density matrix $\rho = \frac{1}{2}I$, where I is the identity.

The informationally complete measurement will reveal the value of an unknown density matrix, but will not even reveal the probability distribution of the states that compose the density matrix, unless the different ρ_a states happen to be orthogonal, and so form the basis which diagonalises the density matrix (and even in this case, an observer who is ignorant of the fact that the signal states have this property will not be able to discover it).

To answer the second question it is necessary to have some *a priori* knowledge of the 'signal states' ρ_a . In the absence of *a priori* knowledge, the quantum information gain from a measurement has no objective significance. Consider a measurement in the basis $|0\rangle \langle 0|, |1\rangle \langle 1|$. With Ensemble 1, the measurement reveals the actual state of the system. With Ensemble 2, the measurement causes a wavefunction collapse, the outcome of which tells us nothing of original state of the system, and destroys all record of it. Without the knowledge of which ensemble we were performing the measurement upon we are unable to know how to interpret the outcome of the measurement.

This differs from the classical measurement situation. In a classical measurement we can refine our partitioning of phase space, until in the limit we obtain the probability density over the whole

of the phase space. If the classical observer starts assuming an incorrect probability distribution for the states, he can discover the fact. By refining his measurement and repeatedly applying Bayes's rule, the initially subjective assessment of the probability density asymptotically approaches the actual probability density. The initially subjective character of the information eventually becomes an objective property of the ensemble.

In a quantum system, there is no measurement able to distinguish between different distributions that combine to form the same density matrix. The observer will never be able to determine which of the ensembles was the actual one. If he has assumed the correct signal states ρ_a , then he may discover if his probabilities are incorrect. However, if his initial assumption about the signal states going into the density matrix are incorrect, he may never discover this.

It might be argued that the complete absence of *a priori* knowledge is equivalent to an isotropic distribution over the Bloch sphere⁷. An observer using such a distribution could certainly devise a optimal measurement, in terms of information gain [Dav78]. Although some information might be gained, the *a posteriori* probabilities, calculated from Bayes's rule, would be distributions over the Bloch sphere, conditional upon the outcome of the experiments. However, the outcomes of such a measurement would be same for each of the three ensembles above. The *a posteriori* probabilities continue to represent an assessment of the observer's knowledge, rather than a property of the ensemble of the systems.

On the other hand, we are not at liberty to argue that only the density matrix is of significance. If we *are* in possession of *a priori* knowledge of the states composing the density matrix, we will construct very different measurements to optimise our information gain, depending upon that knowledge. The optimal measurement for Ensemble 2 is of the projectors $|u\rangle\langle u|$ and $|v\rangle\langle v|$, while for Ensemble 3 a POVM must be used involving all four projectors. All of these differ from the optimal measurement for an isotropic distribution⁸.

2.3 Quantum Measurement

So far we have made a critical assumption in analysing the information gained from measurements, namely that measurements have well defined outcomes, and that we have a clear understanding of when and how a measurement has occurred. This is, of course, a deeply controversial aspect of the interpretation of quantum theory. Information theory has, occasionally, been applied to the problem [DG73, Chapter III, for example], but usually this is only in the context of a predefined theory of measurement (thus, in [DG73] the use of information theory is justified within the context of the Many-World Interpretation).

⁷The Bloch sphere represents a pure state in a Hilbert space of dimension 2 by a point on a unit sphere.

⁸Recent work [BZ99, BZ00a, Hal00, BZ00b] by Bruckner and Zeilinger criticises the use of Shannon-Schumacher information measures in quantum theory, on similar grounds. While their suggested replacement of *total information* has some interesting properties, it appears to be concerned exclusively with the density matrix itself, rather than the states that are combined to construct the density matrix.

In [AC97], Cerf and Adami argue that the properties of the quantum information relationships in Equation 2.5 can, in themselves, be used to resolve the measurement problem. We will now examine the problems in their argument.

Let us start by considering a measurement of a quantum system in a statistical mixture of orthogonal states $|\psi_n\rangle \langle\psi_n|$ with statistical weights w_n , so that

$$\rho = \sum_n w_n |\psi_n\rangle \langle\psi_n|$$

In this case, the density matrix is actually constructed from the $|\psi_n\rangle$ states, rather than some other mixture leading to the same statistical state. We now introduce a measuring device, initially in the state $|\phi_0\rangle$ and an interaction between system and device

$$|\psi_n\phi_0\rangle \rightarrow |\psi_n\phi_n\rangle \tag{2.6}$$

This interaction leads the joint density matrix to evolve from

$$\rho_n \otimes |\phi_0\rangle \langle\phi_0|$$

to

$$\rho^\theta = \sum_n w_n |\psi_n\phi_n\rangle \langle\psi_n\phi_n| \tag{2.7}$$

We can now consistently interpret the density matrix ρ^θ as a statistical mixture of the states $|\psi_n\phi_n\rangle$ occurring with probability w_n . In particular, when the measuring device is in the particular state $|\psi_n\rangle$ then the observed system is in the state $|\phi_n\rangle$. The interaction in 2.6 above is the correct one to measure the quantity defined by the $|\psi_n\rangle$ states.

Unfortunately, the linearity of quantum evolution now leads us to the measurement problem when the initial state of the system is not initial in a mixture of eigenstates of the observable. Supposing the initial state is

$$|\Psi\rangle = \sum_n \alpha_n |\psi_n\rangle$$

(where, for later convenience, we choose $|\alpha_n|^2 = w_n$), then the measurement interaction leads to a state

$$|\Psi\Phi\rangle = \sum_n \alpha_n |\psi_n\phi_n\rangle \tag{2.8}$$

This is a pure state, not a statistical mixture. Such an entangled superposition of states cannot be interpreted as being in a mixture of states, as there are observable consequences of interference between the states in the superposition.

To complete the measurement it is necessary that some form of non-unitary projection takes place, where the state $|\Psi\Phi\rangle$ is replaced by a statistical mixture of the $|\psi_n\phi_n\rangle$ states, each occurring randomly with probability $|\alpha_n|^2 = w_n$.

Information From the point of view of information theory, the density matrix in Equation 2.7 has a information content of

$$\begin{aligned} S_1[\phi] = S_1[\psi] = S_1[\phi, \psi] &= -\sum_n w_n \log_2 w_n = S_0 \\ S_1[\phi|\psi] = S_1[\psi|\phi] &= 0 \\ S_1[\phi : \psi] &= -S_0 \end{aligned}$$

The conditional information being zero indicates that, given the knowledge of the state of the measuring apparatus we have perfect knowledge of the state of the measured system, and the mutual information indicates a maximum level of correlation between the two systems.

For the superposition in Equation 2.8, the information content is

$$\begin{aligned} S_2[\phi, \psi] &= 0 \\ S_2[\phi] = S_2[\psi] &= S_0 \\ S_2[\phi|\psi] = S_2[\psi|\phi] &= -S_0 \\ S_2[\phi : \psi] &= -2S_0 \end{aligned}$$

We now have situation where the knowledge of the state of the combined system is perfect, while, apparently, the knowledge of the individual systems is completely unknown. This leads to a negative conditional information - which has no classical meaning, and a correlation that is twice the maximum that can be achieved with classical systems.

[AC95] do not attempt to interpret these terms. Instead they now introduce a third system, that 'observes' the measuring device. If we represent this by $|\xi\rangle$, this leads to the state

$$|\Psi\Phi\xi\rangle = \sum_n \alpha_n |\psi_n \phi_n \xi_n\rangle \quad (2.9)$$

Now, it would appear we have simply added to the problem as our third system is part of the superposition. However, by generalising the quantum information terms to three systems, [AC95] derive the quantities

$$\begin{aligned} S_3[\xi] = S_3[\phi] = S_3[\xi, \phi] &= -\sum_n w_n \log_2 w_n = S_0 \\ S_3[\xi|\phi] = S_3[\phi|\xi] &= 0 \\ S_3[\xi : \phi] &= -S_0 \end{aligned}$$

This shows the same relationships between the second 'observer' and the measuring device as we saw initially between the measuring device and the observed system *when the system was in a statistical state*. This essentially leads [AC95] to believe they can interpret the situation described after the second interaction as a classical correlation between the observer and the measuring device.

[AC95] do not claim that they have introduced a non-unitary wavefunction collapse, nor do they believe they are using a 'Many-Worlds' interpretation. What has happened is that, by considering

only two, out of three, subsystems in the superposition, they have traced over the third system (the original, 'observed' system), and produced a density matrix

$$\text{Tr}_\psi [|\Psi\Phi\xi\rangle \langle\Psi\Phi\xi|] = \sum_n w_n |\phi_n\xi_n\rangle \langle\phi_n\xi_n| \quad (2.10)$$

which has the same form as the classically correlated density matrix. They argue that the original, fundamentally quantum systems $|\Psi\rangle$ are always unobservable, and it is only the correlations between ourselves (systems $|\Xi\rangle$) and our measuring devices (systems $|\Phi\rangle$) that are accessible to us.

They argue that there is no need for a wavefunction collapse to occur to introduce a probabilistic uncertainty into the unitary evolution of the Schrödinger equation. It is the occurrence of the negative conditional information

$$S_3[\psi|\phi, \xi] = -S_0$$

that introduces the randomness to quantum measurements. This negative conditional information allows the Φ, Ξ system to have an uncertainty (non-zero information), even while the overall state has no uncertainty

$$S_3[\psi, \phi, \xi] = S_3[\psi|\phi, \xi] + S_3[\phi, \xi] = 0$$

The basic problem with this argument is the assumption that when we have an apparently classically correlated density matrix, such as in Equation 2.7 above, we can automatically interpret it as actually *being* a classical correlation. In fact, we can only do this if we know that it is actually constructed from a statistical ensemble of correlated states. As we have seen above, the quantum density matrix does not have a unique decomposition and so could have been constructed out of many different ensembles. These ensembles may be constructed with superpositions, entangled states, or even, as with the density matrix in Equation 2.10, without involving ensembles at all.

What [AC95] have shown is the practical difficulty of finding any observable consequences of the entangled superposition, as the results of a measurement upon the density matrix in Equation 2.10 are identical to those that would occur from measurements upon a statistical mixture of classically correlated states. However, to even make this statement, we have to have assumed that we know when a measurement has occurred in a quantum system, and this is precisely the point at issue⁹.

When applying this to Schrödinger's cat, treating Φ as the cat and Ξ as the human observer, they say

The observer notices that the cat is either dead or alive and thus the observer's own state becomes classically correlated with that of the cat, although in reality, the entire system (including atom . . . the cat and the observer) is in a *pure entangled state*. It is *practically* impossible, although not in principle, to undo this observation i.e. to resuscitate the cat

⁹Their argument is essentially a minimum version of the decoherence approach to the measurement problem[Zur91]. For a particularly sharp criticism of why this approach does not even begin to address the problem, see [Alb92, Chapter 4, footnote 16]

Unfortunately this does not work. The statement that the observer notices that the cat is either alive or dead must *presume* that it is actually the case that the cat is either alive or dead. That is, in each experimental realisation of the situation there is a matter of fact about whether the cat is alive or dead. However, if this was the case, that the cat is, in fact, either alive or dead, then the system would not be described by the superposition at all. It is *because* a superposition cannot readily be interpreted as a mixture of states that the measurement problem arises in the first place.

[AC97]'s resolution depends upon their being able to make the assumption that a superposition does, in fact, represent a statistical mixture of the cat being in alive and dead states, with it being a matter of fact, in each experimental realisation, which state the cat is in. Only then can we interpret the reduced density matrix (2.10) as a statistical correlation.

There are, in principle, observable consequences of the system actually being in the superposition, that depend upon the co-existence of all branches of the superposition¹⁰. Although these consequences are, in practice, very difficult to observe, we cannot simply trace over part of the system, and assume we have a classical correlation in the remainder. Indeed, the 'resuscitation' of the cat alluded to requires the use of all branches of the superposition. This includes the branch in which the observer sees the cat alive as well as the branch in which the observer sees the cat as dead. If both branches of the superposition contribute to the resuscitation of the cat, then both must be equally 'real'.

To understand the density matrix (2.10) as a classical correlation, we must interpret it as meaning that, in each experiment, the observer actually sees a cat as being alive or actually sees the cat as being dead. How are we then to understand the status of the unobserved outcome, the other branch of the superposition, that enables us to resuscitate the cat, without using the Many-Worlds interpretation? To make the situation even more difficult, we need only note that, not only can we resuscitate the Φ cat, we can also, in principle at least, restore the Ψ system to a reference state, leaving the system in the state

$$\psi_0\phi_0 \sum_n \alpha_n \xi_n$$

The observer is now effectively in a superposition of having observed the cat alive and observed the cat dead (while the cat itself is alive and well)! Now the superposition of the states of the observer is quite different from a statistical mixture. We cannot assume the observer either remembers the cat being alive or remembers the cat being, nor can we assume that the observer must have 'forgotten' whether the cat was alive or dead. The future behaviour of the observer will be influenced by elements of the superposition that depend upon his having remembered both. [AC95] must allow states like this, in principle, but offer no means of understanding what such a state could possibly mean.

¹⁰We will be examining some of these in more detail in Chapter 3.

2.4 Summary

The Shannon information plays several different roles in a classical system. It derives its primary operational significance as a measure of the capacity, in bits, a communication channel must have to faithfully transmit an ensemble of different messages. Having been so defined, it becomes possible to extend the definition to joint, conditional and mutual information. These terms can be used to describe the information shared between two different systems - such as a message sender and message receiver - or can be used to describe the changes in information an observer has on making measurements upon a classical system. In all cases, however, the concept essentially presupposes that the system is in a definite state that is revealed upon measurement.

For quantum systems the interpretation of information is more complex. Within the context of communication, Schumacher generalises Shannon's theorem to derive the capacity of a quantum communication channel and the Holevo bound demonstrates that this is the most information the receiver can acquire about the message sent.

However, when considering the information of unknown quantum states the situation is less clear. Unlike the classical case there is no unique decomposition of the statistical state (density matrix) into a probability distribution over individual states. A measurement is no longer necessarily revealing a pre-existing state. In this context, finally, we note that the very application of information to a quantum system presupposes that we have a well-defined measuring process.

Chapter 3

Active Information and Interference

In Chapter 2 we reviewed the status of information gain from a quantum measurement. This assumed that measurements have outcomes, a distinct problem in quantum theory.

We now look at the concept of 'active information' as a means of addressing the measurement problem within the Bohm approach to quantum theory. This approach has been recently criticised as part of a series of thought experiments attempting to explore the relationship between information and interference. These thought experiments rely upon the use of 'one-bit detectors' or 'Welcher-weg' detectors, in the two slit interference experiment. In this Chapter we will show why these criticisms are invalid, and use the thought experiment to illustrate the nature of active information. This will also clarify the relationship between information and interference.

Section 3.1 will introduce the Bohm interpretation and highlight its key features. This will introduce the concept of active information. The role of active information in resolving the measurement problem will be briefly treated.

Section 3.2 analyses the which-path interferometer. It has been argued that there is a complementary relationship between the information obtained from a measurement of the path taken by an atom travelling through the interferometer, and the interference fringes that may be observed when the atom emerges from the interferometer. As part of the development of this argument, a quantum optical cavity has been proposed as a form of which path, or 'welcher-weg' measuring device. The use of this device plays a key role in 'quantum eraser' experiments and in the criticism of the Bohm trajectories. We will therefore examine carefully how the 'welcher-weg' devices affect the interferometer.

Finally, in Section 3.3 we will argue that the manner in which the term 'information' has been used in the which path interferometers is ambiguous. It is not information in the sense of Chapter 2. Rather, it appears to be assuming that a quantum measurement reveals deeper properties of a system than are contained in the quantum description, and this is the information revealed by the

measurement.

We will show that this assumption is essential to the interpretation of the 'welcher-weg' devices as reliable which path detectors. However, it will be shown that the manner in which this interpretation is applied to the 'welcher-weg' devices is not tenable, and this is the reason they are supposed to disagree with the trajectories of the Bohm approach. By contrast, the concept of active information, in the Bohm interpretation, does provide a consistent interpretation of the interferometer, and this can clarify the relationship between which path measurements and interference.

3.1 The Quantum Potential as an Information Potential

The Bohm interpretation of quantum mechanics[Boh52a, Boh52b, BH87, BHK87, BH93, Hol93, Bel87] can be derived from the polar decomposition of the wave function of the system, $\Psi = Re^{iS}$, which is inserted into the Schrödinger equation¹

$$i\frac{\partial\Psi}{\partial t} = \left(-\frac{\nabla^2}{2m} + V\right)\Psi$$

yielding two equations, one that corresponds to the conservation of probability, and the other, a modified Hamilton-Jacobi equation:

$$-\frac{\partial S}{\partial t} = \frac{(\nabla S)^2}{2m} + V - \frac{\nabla^2 R}{2mR} \tag{3.1}$$

This equation can be interpreted in the same manner as a classical Hamilton- Jacobi, describing an ensemble of particle trajectories, with momentum $p = \nabla S$, subject to the classical potential V and a new quantum potential $Q = -\frac{\nabla^2 R}{2mR}$. The quantum potential, Q , is responsible for all the non-classical features of the particle motion. It can be shown that, provided the particle trajectories are distributed with weight R^2 over a set of initial conditions, the weighted distribution of these trajectories as the system evolves will match the statistical results obtained from the usual quantum formalism. It should be noted that although the quantum Hamilton-Jacobi equation can be regarded as a return to a classical deterministic theory, the quantum potential has a number of the non-classical features that make the theory very different from any classical theory. We should regard Q as being a new quality of global energy that augments the kinetic and classical potential energy to ensure the conservation of energy at the quantum level. Of particular importance are the properties of non-locality and form-dependence.

3.1.1 Non-locality

Perhaps the most surprising feature of the Bohm approach is the appearance of non-locality. This feature can be clearly seen when the above equations are generalised to describe more than one particle. In this case the polar decomposition of $\Psi(x_1, x_2, \dots, x_N) = R(x_1, x_2, \dots, x_N)e^{iS(x_1, x_2, \dots, x_N)}$ produces a quantum potential, Q_i , for each particle given by:

¹We set $\hbar = 1$

$$Q_i = -\frac{\nabla_i^2 R(x_1, x_2, \dots, x_N)}{2mR(x_1, x_2, \dots, x_N)}$$

This means that the quantum potential on a given particle i will, in general, depend on the instantaneous positions of all the other particles in the system. Thus an external interaction with one particle may have a non-local effect upon the trajectories of all the other particles in the system. In other words groups of particles in an entangled state are, in this sense, non-separable. In separable states, the overall wave function is a product of individual wave functions.

For example, when one of the particles, say particle 1, is separable from the rest, we can write $\Psi(x_1, x_2, \dots, x_N) = \phi(x_1)\xi(x_2, \dots, x_N)$. In this case $R(x_1, x_2, \dots, x_N) = R_1(x_1)R_{2\dots N}(x_2, \dots, x_N)$, and therefore:

$$Q_1 = -\frac{\nabla_1^2 R_1(x_1)R_{2\dots N}(x_2, \dots, x_N)}{2mR_1(x_1)R_{2\dots N}(x_2, \dots, x_N)} = -\frac{\nabla_1^2 R_1(x_1)}{2mR_1(x_1)}$$

In a separable state, the quantum potential does not depend on the position of the other particles in the system. Thus the quantum potential only has non-local effects for entangled states.

3.1.2 Form dependence

We now want to focus on one feature that led Bohm & Hiley [BH93] to propose that the quantum potential can be interpreted as an ‘information potential’. As we have seen above the quantum potential is derived from the R-field of the solution to the appropriate Schrödinger equation. The R-field is essentially the amplitude of the quantum field Ψ . However, the quantum potential is not dependant upon the amplitude of this field (i.e., the intensity of the R-field), but only upon its *form*. This means that multiplication of R by a constant has no effect upon the value of Q. Thus the quantum potential may have a significant effect upon the motion of a particle even where the value of R is close to zero. One implication of this is that the quantum potential can produce strong effects even for particles separated by a large distance. It is this feature that accounts for the long- range EPRB-type correlation upon which teleportation relies.

It is this form-dependence (amongst others things) that led Bohm & Hiley [BH84, BH93] to suggest that the quantum potential should be interpreted as an information potential. Here the word ‘information’ signifies the *action* of forming or bringing order into something. Thus the proposal is that the quantum potential captures a dynamic, self-organising feature that is at the heart of a quantum process.

For many-body systems, this organisation involves a non-local correlation of the motion of all the bodies in the entangled state, which are all being simultaneously organised by the collective R-field. In this situation they can be said to be drawing upon a common pool of information encoded in the entangled wave function. The informational, rather than mechanical, nature of this potential begins to explain why the quantum potential is not definable in the 3-dimensional

physical space of classical potentials but needs a $3N$ -dimensional configuration space. When one of the particles is in a separable state, that particle will no longer have access to this common pool of information, and will therefore act independently of all the other particles in the group (and vice versa). In this case, the configuration space of the independent particle will be isomorphic to physical space, and its activity will be localised in space-time.

3.1.3 Active, Passive and Inactive Information

In order to discuss how and what information is playing a role in the system, we must distinguish between the notions of active, passive and inactive information. All three play a central role in our discussion of teleportation. Where a system is described by a superposition $\Psi(x) = \Psi_a(x) + \Psi_b(x)$, and $\Psi_a(x)$ and $\Psi_b(x)$ are non-overlapping wavepackets, then

$$\Psi_a(x)\Psi_b(x) \approx 0$$

for all values of x . We will refer to this as *superorthogonality*. The actual particle position will be located within either one or the other of the wavepackets. The effect of the quantum potential upon the particle trajectory will then depend only upon the form of the wavepacket that contains the particle. We say that the information associated with this wavepacket is active, while it is passive for the other packet. If we bring these wavepackets together, so that they overlap, the previously passive information will become active again, and the recombination will induce complex interference effects on the particle trajectory.

Now let us see how the notion of information accounts for measurement in the Bohm interpretation. Consider a two-body entangled state, such as $\Psi(x_1, x_2) = \phi_a(x_1)\xi_a(x_2) + \phi_b(x_1)\xi_b(x_2)$, where the active information depends upon the simultaneous position of both particle 1 and particle 2. If the ϕ_a and ϕ_b are overlapping wave functions, but the ξ_a and ξ_b are non-overlapping, and the actual position of particle 2 is contained in just one wavepacket, say ξ_a , the active information will be contained only in $\phi_a(x_1)\xi_a(x_2)$, the information in the other branch will be passive. Therefore only the $\phi_a(x_1)$ wavepacket will have an active effect upon the trajectory of particle 1. In other words although ϕ_a and ϕ_b are both non-zero in the vicinity of particle 1, the fact that particle 2 is in $\xi_a(x_2)$ will mean that only $\phi_a(x_1)\xi_a(x_2)$ is active, and thus particle 1 will only be affected by $\phi_a(x_1)$.

If $\phi_a(x_1)$ and $\phi_b(x_1)$ are separated, particle 1 will always be found within the location of $\phi_a(x_1)$. The position of particle 2 may therefore be regarded as providing an accurate measurement of the position of particle 1. Should the ϕ_a and ϕ_b now be brought back to overlap each other, the separation of the wavepackets of particle 2 will continue to ensure that only the information described by $\phi_a(x_1)\xi_a(x_2)$ will be active. To restore activity to the passive branches of the superposition requires that both $\phi_a(x_1)$ and $\phi_b(x_1)$ and $\xi_a(x_2)$ and $\xi_b(x_2)$ be simultaneously brought back into overlapping positions. If the $\xi(x_2)$ represents a thermodynamic, macroscopic device, with many degrees of freedom, and/or interactions with the environment, this will not be realistically possible.

If it is never possible to reverse all the processes then the information in the other branch may be said to be inactive (or perhaps better still ‘deactivated’), as there is no feasible mechanism by which it may become active again. This process replaces the collapse of the wave function in the usual approach. For the application of these ideas to the problem of teleportation in quantum information, see Appendix A and [HM99].

Rather than see the trajectory as a particle, one may regard it as the ‘center of activity’ of the information in the wavefunction. This avoids the tendency to see the particle as a wholly distinct object to the wavefunction. As the two feature can never be separated from each other, it is better to see them as two different aspects of a single process.

In some respects the ‘center of activity’ behaves in a similar manner to the ‘point of execution’ in a computer program. The ‘point of execution’ determines which portion of the computer code is being read and acted upon. As the information in that code is activated, the ‘point of execution’ moves on to the next portion of the program. However, the information read in the program will determine where in the program the point of execution moves to. In the quantum process, it is the center of activity that determines which portion of the information in the wavefunction is active. Conversely, the activity of the information directs the movement of the ‘center’.

The activity of information, however, differs from the computer in two ways. Firstly, the wavefunction itself is evolving, whereas a computer program is unlikely to change it’s own coding (although this is possible). Secondly, when two quantum systems interact, this is quite unlike any interaction between two computer programs. The sharing of information in entangled systems means that the ‘center of activity’ is in the joint configuration space of both systems. The movement of the center of activity through one system depends instantaneously upon the information that is active in the other system, and vice versa. This is considerably more powerful than classical parallel processing and may well be related to the increased power of quantum computers[Joz96, Joz97].

3.2 Information and interference

In a series of papers[ESSW92, ESSW93, Scu98], the Bohm interpretation has been criticised as ‘metaphysical’, ‘surrealistic’ and even ‘dangerous’, on the basis of a thought experiment exploiting ‘one-bit’ welcher-weg, or which-way, detectors in the two slit interference experiment². Although these criticisms have been partially discussed elsewhere[DHS93, DFGZ93, AV96, Cun98, CHM00], there are a number of features to this that have not been discussed. The role of information, and active information has certainly not been discussed in this context. The thought experiment itself arises in the context of a number of similar experiments in quantum optics [SZ97, Chapter 20] which attempt to apply complementarity to information and interference fringes[WZ79] and the ‘delayed choice’ effect[Whe82] in the two-slit interference experiment. It is therefore useful to

²Similar criticisms were raised by [Gri99] in the context of the Consistent Histories interpretation of quantum theory. A full examination of Consistent Histories lies outside the scope of this thesis. However, an analysis of Gri’s argument, from[HM00] is reproduced in Appendix B.

examine how the problems of measurement, information and active information are applied to this situation.

To properly consider the issues raised by this thought-experiment, it will be necessary to re-examine the basis of the two-slit experiment. This will be considered in Subsection 3.2.1. The role of information in destroying the interference effects will be reviewed in Subsection 3.2.2. The analysis of this is traditionally based upon the exchange of momentum with a detector destroying the interference. We will find that the quantum optics welcher-weg devices, which we will discuss in Subsection 3.2.3 do not exhibit such an exchange of momentum, but still destroy the interference. Subsection 3.2.4 then examines the Bohm trajectories for this experiment, and shows why [ESSW92] regard them as 'surreal'.

3.2.1 The basic interferometer

We will now describe the basic interferometer arrangement in Figure 3.1. An atom, of position

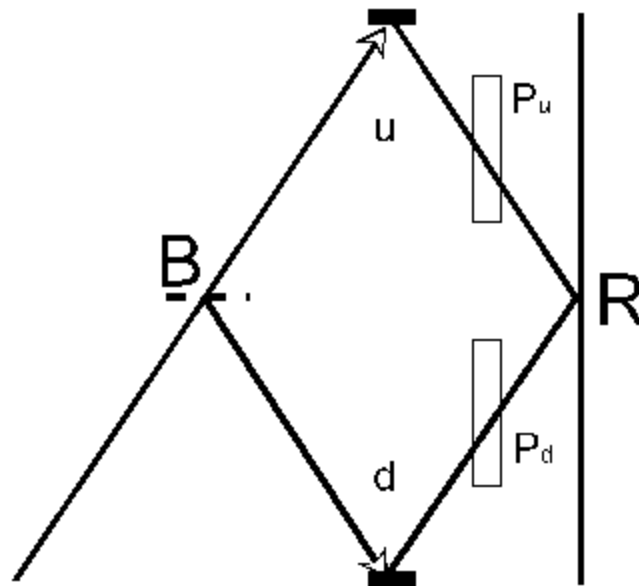


Figure 3.1: Basic Interferometer

co-ordinate x , is described by the narrow wavepacket

$$\psi(x, t)$$

. At time $t = t_0$, it is in the initial state

$$\psi(x, t_0)$$

and passes through a beam splitter at B, and at $t = t_1$ has divided into the states

$$\psi(x, t_1) = \frac{1}{\sqrt{2}} (\psi_u(x, t_1) + \psi_d(x, t_1))$$

where $\psi_u(x)$ is the wavepacket travelling in the upper branch of the interferometer, and $\psi_d(x)$ is the wavepacket in the lower branch.

After $t = t_1$, the wavepackets are reflected so that at $t = t_2$ they are moving back towards each other

$$\psi(x, t_2) = \frac{1}{\sqrt{2}} (\psi_u(x, t_2) + \psi_d(x, t_2))$$

They recombine at $t = t_3$, in the region R, where the atoms location is recorded on a screen. The probability distribution across the screen is then

$$|\psi(x, t_3)|^2 = \frac{1}{2} \left(|\psi_u(x, t_3)|^2 + |\psi_d(x, t_3)|^2 + \psi_u(x, t_3)^\alpha \psi_d(x, t_3) + \psi_u(x, t_3) \psi_u(x, t_3)^\alpha \right)$$

In Figure 3.1 we have also included phase shifters at locations P_u and P_d , in the two arms of the interferometer. These may be controlled to create a variable phase shift of ϕ_u or ϕ_d in the respective wavepacket. The settings of these phase shifters will play an important role in the later discussion, but for the moment, they will both be assumed to be set to a phase shift of zero, and thus have no effect upon the experiment.

If we apply the polar decomposition $\psi = Re^{iS}$ to this, we obtain

$$|\psi(x, t_3)|^2 = \frac{1}{2} (R_u(x, t_3)^2 + R_d(x, t_3)^2 + 2R_u(x, t_3)R_d(x, t_3) \cos(S_u(x, t_3) - S_d(x, t_3)))$$

We can simplify this by assuming the beam splitter divides the wavepackets equally, so that in the center of the interference region

$$R_u(x, t_3) = R_d(x, t_3) = R(x, t_3)$$

and

$$|\psi(x, t_3)|^2 = R(x, t_3)^2 (1 + \cos(\Delta S(x, t_3)))$$

where $\Delta S(x, t_3) = S_u(x, t_3) - S_d(x, t_3)$.

The cosine of the phase produces the characteristic interference fringes. Had we blocked one of the paths (u , for example) we would have found the probability distribution was $R(x, t_3)^2$. The probability distribution is not simply the sum of the probability distributions from each path. The superposition of states given by $\psi(x, t_3)$ cannot be simply interpreted as half the time the atom goes down the u path, and half the time going down the d path.

Now let us consider the addition to the interferometer of the phase shifters in each of the paths. These could be implemented by simply fine tuning the length of each arm. The u path is shifted by a phase ϕ_u and the d path by ϕ_d . The effect on the interference pattern is simply to modify the cosine term to

$$\cos(\Delta S(x, t_3) + (\phi_u - \phi_d))$$

Now we have

$$|\psi(x, t_3)|^2 = R(x, t_3)^2 (1 + \cos(\Delta S(x, t_3) + (\phi_u - \phi_d)))$$

At the points x_n , where

$$\Delta S(x_n, t_3) + (\phi_u - \phi_d) = \frac{\pi}{2} + n\pi$$

then the value of $|\psi(x_n, t_3)|^2 = 0$ ie. there is no possibility of the atom being located at that point. The important point to note is that the values of x_n are determined by the values of both ϕ_u and ϕ_d , that is by the setting of the phase shifters in *both* arms of the interferometer.

This emphasises the point that we are unable to regard the superposition of states in $\psi(x, t_1)$ as simply representing a situation where, in half the cases the atom travels the d-path, and in half the cases the u-path. Not only is the interference pattern not simply the sum of the probability distribution from each of the two paths, but critically, the location of the nodes in the interference pattern depends upon the settings of instruments in *both* paths.

A simplistic way of stating this is in terms of what the atom 'knows' it should do when reaching the screen. If the atom proceeds down one path, and the other path is blocked, it can arrive at locations that are forbidden if the other path is not blocked. How does the atom 'know' whether the other path is blocked or not? The phase shifters demonstrate that, not only must the atom 'know' whether or not the paths are blocked, but even if they are not blocked, the very locations which are forbidden to it depend upon the atom 'knowing' the values of the phase shifts in *both* arms. If the atom only travels down one path or the other, how is it to 'know' the phase shift in the other path?

This is a generic property of superpositions. We cannot interpret these as a statistical mixture as this implies that in each experiment either one or the other possibility is realized while we can always exhibit interference effects which depend upon both of the elements of the superposition.

3.2.2 Which way information

We now turn to the attempts to measure which way the atom went. The interference pattern builds up from the ensemble of individual atoms reaching particular locations of the screen. If we could know which path the atom takes, we could separate the ensemble of all the atoms that travelled down the u-branch from the atoms travelling down the d-branch, and this might shed light upon the questions raised by the introduction of the phase shifters.

As is well known, however, the attempt to measure the path taken by the atom destroys the interference pattern recorded on the screen. The paradigm explanation[Fey63, Chapter 37], originally due to Heisenberg, involves scattering a photon from the atom, to show it's location. To be able to determine which path the atom takes, the wavelength of the photon must be less than the separation of the paths. However, this scattering changes the momentum of the atom, according to the uncertainty relationship $\Delta x \Delta p \geq \hbar$. This random addition to the wavefunction of the atom destroys the phase coherence of the two branches of the superposition and so destroys

the interference. The measurement of the atoms location changes the quantum system from the pure state $\psi(x, t_1)$ to the statistical density matrix

$$\rho = \frac{1}{2} (|\psi_u(x, t_1)\rangle \langle \psi_u(x, t_1)| + |\psi_d(x, t_1)\rangle \langle \psi_d(x, t_1)|)$$

where $|\psi_u(x, t_1)\rangle \langle \psi_u(x, t_1)|$ is correlated to the measurement outcome locating the atom in the u-path, and $|\psi_d(x, t_1)\rangle \langle \psi_d(x, t_1)|$ is correlated to the atom located in the d-path. The values of the phase shifters is now irrelevant, and no interference occurs in the region R . We will not now find any inconsistency in treating the system as a statistical mixture.

Quantity of information The information obtained from the position measurement above is 'all or nothing'. We either do not measure the path, and get an interference pattern, or we measure it, and lose the interference pattern. This often leads to a tendency to adopt the language where the quantum object is said to behave in a 'particlelike' manner, when the which path information is measured, and in a 'wavelike' manner when the interference is observed.

In [WZ79] the experiment is refined by varying the certainty one has about the path taken by the atom. There are several different methods proposed for this, but the most efficient suggested is equivalent to changing the beam splitter in Figure 3.1, such that the atomic beam emerges with state

$$\psi^\theta(x, t_2) = \alpha\psi_u(x, t_2) + \beta\psi_d(x, t_2)$$

where $|\alpha|^2 + |\beta|^2 = 1$. Wootters and Zurek deem the information 'lacking' about the path of the atom to be

$$I_{WZ} = -p_u \log_2 p_u - p_d \log_2 p_d \tag{3.2}$$

where $p_u = |\alpha|^2$ and $p_d = |\beta|^2$.

The resulting interference pattern on the screen is given by

$$|\psi^\theta(x, t_3)|^2 = R(x, t_3)^2 (1 + 2\sqrt{p_u p_d} \cos(\Delta S(x, t_3) + (\phi_u - \phi_d) + \theta))$$

where θ is the relative phase between the complex numbers α and β . If the value of p_u approaches zero or one, then the atom will always go down one arm or the other. I_{WZ} goes to zero, so there is no information lacking about the path of the atom, but the interference term disappears. The largest interference term occurs when $p_u = p_d = \frac{1}{2}$, for which $I_{WZ} = -\log_2 2$ represents a maximum lack of information. It is noticeable that this experiment does not actually involve a measurement at all. However, Wootters and Zurek show that, for a given size of the interference term, the information that can be obtained from any measurement is no more than I_{WZ} . In this respect, the complementarity between the interference and I_{WZ} is equivalent to the equality in the uncertainty relationship $\Delta x \Delta p \geq \hbar$. What is significant here is that in Wootters and Zurek's view it is not the momentum transfer that destroys the interference effects, rather it is the information we have about the path of the atom.

Finally we can consider Wheeler's delayed choice experiment [Whe82] where the screen may be removed from Figure 3.1 and detectors are placed at D_1 and D_2 , as in Figure 3.2. Now the wavepackets continue through the interference region, and become separate again at $t = t_4$

$$\psi(x, t_4) = (\psi_u(x, t_4) + \psi_d(x, t_4))$$

A detection at D_1 of the wavepacket $\psi_d(x, t_4)$ is interpreted as detecting that the atom went through the d-path in the interferometer. Now, the choice of whether to insert the screen can

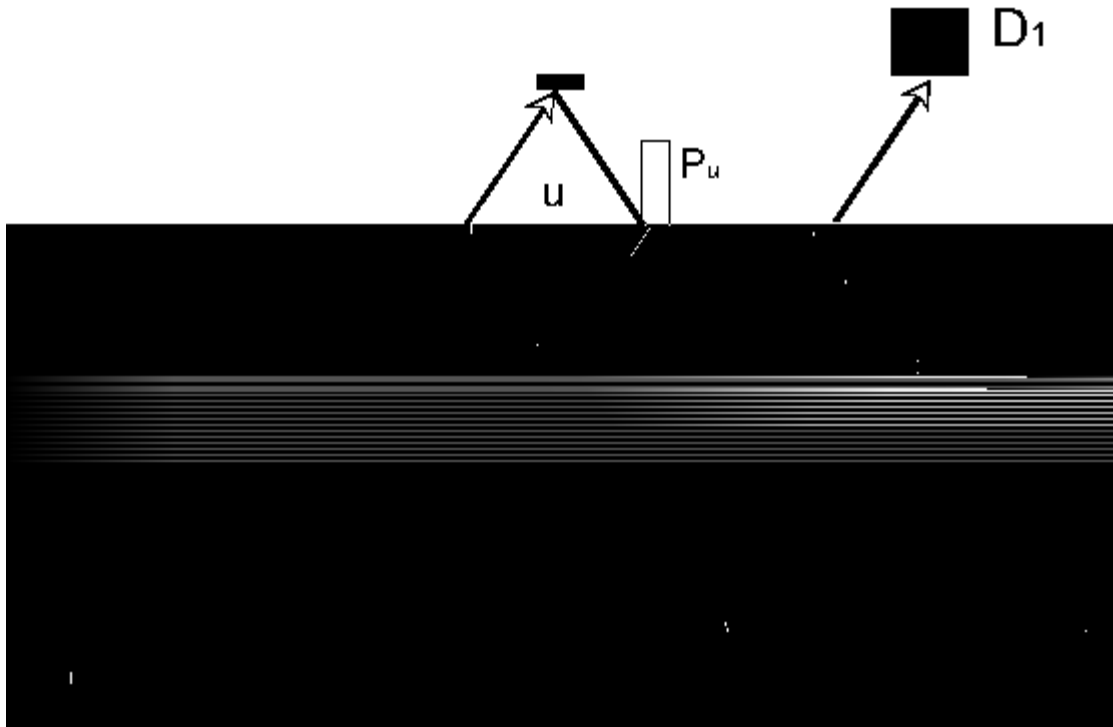


Figure 3.2: Which-path delayed choice

be made after the wavepackets have entered the interferometer arms (and even passed the phase shifters). The choice as to whether we obtain interference (the atom is a wave in both arms of the interferometer) or information about which path the atom took (the atom is a particle in one branch of the interferometer) is delayed until after the quantum system has actually entered the interferometer.

3.2.3 Welcher-weg devices

In a series of articles [ESW91, ESSW92, SZ97, and references within], it has been suggested that the which-path information can be measured by using certain quantum optical devices, which we will follow the authors of these papers in referring to as 'welcher-weg' (German for 'which way') devices. These devices do not make a random momentum transfer to the atom and so it is argued they represent an advance in the understanding of the which path interferometer. It is the use of

these devices that is essential to understanding the 'quantum eraser' experiments and the criticism of the Bohm interpretation.

There are three key physical processes that are involved in these experiments, all involving a two-level circular Rydberg atom. This is an atom whose outer shell contains only a single electron, the state of which can be treated effectively as in a hydrogen atom. The two levels refers to the ground ($|g\rangle$) and first excited ($|e\rangle$) state of the outer shell electron, which differ by the energy ΔE_R . The processes to which this atom is subjected are:

- Timed laser pulses producing Rabi oscillations.
- Interaction with a single mode micromaser cavity.
- Selective ionization

Full details of these processes can be found in[AE74, MW95, SZ97]. We will describe only their essential features here.

Rabi oscillations The atom rapidly passes through an intense electromagnetic field, oscillating at a single frequency. This can be achieved using a pulsed laser, and the intensity of the electromagnetic field allows it to be treated as a semiclassical perturbation on the atomic states.

The frequency ω_R of the laser is tuned to the energy gap between the ground and first excited state of the atom $\Delta E_R = \hbar\omega_R$. The effect upon the atomic state is to produce a superposition of ground and excited states

$$\alpha(t) |g\rangle + \beta(t) |e\rangle \tag{3.3}$$

whose equation of motion is

$$\begin{aligned} \frac{d\alpha(t)}{dt} &= \imath \frac{R}{2} \beta(t) \\ \frac{d\beta(t)}{dt} &= \imath \frac{R}{2} \alpha(t) \end{aligned}$$

where R is the Rabi oscillation term. This factor is a constant, whose exact value is a function of the overlap integral between the $|g\rangle$ and $|e\rangle$ states under the influence of perturbation field of the laser.

The solutions to these coupled equations are

$$\begin{aligned} \alpha(t) &= \alpha(0) \cos\left(\frac{Rt}{2}\right) + \imath\beta(0) \sin\left(\frac{Rt}{2}\right) \\ \beta(t) &= \beta(0) \cos\left(\frac{Rt}{2}\right) + \imath\alpha(0) \sin\left(\frac{Rt}{2}\right) \end{aligned}$$

If we time the length of the pulse carefully, we can manipulate the excitation of the atom. Of particular importance is the π pulse, where $Rt = \pi$, as this has the effect of flipping the atomic state so that $|e\rangle \rightarrow \imath|g\rangle$ and $|g\rangle \rightarrow \imath|e\rangle$.

Single Mode Cavity The Rabi oscillations are produced from an intense, semiclassical electromagnetic field. The single mode cavity involves the interaction of the atom with a field with very few photon states excited. The operation is essentially based upon the Jaynes-Cummings model[CJ63].

Instead of using a laser pulse, the circular Rydberg atom is sent through a high quality microwave cavity, which is tuned to have the same fundamental resonant frequency ω_R as the atom. We will describe the state of the electromagnetic field in the cavity using the Fock state basis, giving the number of photons excited in the cavity at the fundamental frequency. Where there are n photons in the cavity, it's quantum state is described as $|n\rangle$.

If the length of time the atom spends in the cavity is carefully controlled, there are only three interactions we need to consider for the purposes of the experiments involved:

$$\begin{aligned} |g0\rangle &\rightarrow |g0\rangle \\ |g1\rangle &\rightarrow |e0\rangle \\ |e0\rangle &\rightarrow |g1\rangle \end{aligned} \tag{3.4}$$

If an excited atom goes through an unexcited cavity, it decays to the ground state, and the $\hbar\omega_R$ energy excites the first photon state of the cavity. If the atom in the ground state goes through a cavity with a single photon excitation, the energy is absorbed, exciting the atom and de-exciting the cavity. If neither atom nor cavity are excited, then no changes can take place.

The most important property of these devices is that, if an excited atom passes through the cavity, it deposits its energy into the photon field with certainty. As we shall see, it is this that leads [ESSW92] to describe them as 'welcher-weg' devices ³.

Selective Ionization State selective field ionization passes the atom through a electric field that is sufficiently strong to ionize the atom when the electron in the excited state, but insufficiently strong to ionize the atom with the electron in the ground state. The ionized atom and electron are then detected by some amplification process. For completeness, the ionization of the excited state may be followed by a second selective ionization and detection, capable of ionizing the ground state. As long as the first ionization is very efficient, a reliable measurement of the ground or first excited state will have taken place.

[ESSW92] now proposed the experiment where a welcher-weg cavity is placed in each arm of the delayed choice interferometer, as shown in Figure 3.3. The atomic wavepackets, initially in the ground state, are given a π pulse just before entering the interferometer. The electron excitation is passed on to the cavity field mode, leaving the cavity excited. With the screen missing, the atomic wavepacket is then detected at either D_1 or D_2 . The location of the photon, in the upper or lower cavity, is detected by sending another ('probe') atom, initially in the ground state, through the cavity and performing a state selective ionization upon it.

³A second property of interest is that the interaction of the atom and cavity has negligible effect upon the momentum of the atomic wavepacket.

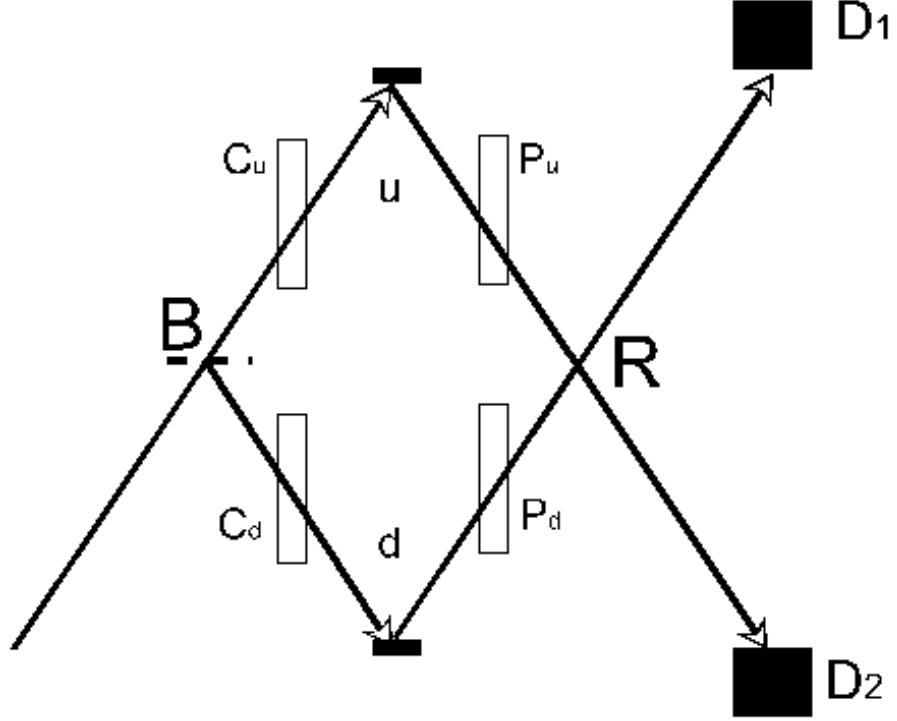


Figure 3.3: Welcher-weg cavities

If we follow the quantum evolution of this system, we have:

1. At $t = t_0$, the atom has not yet encountered the beam splitter, but is π pulsed into the excited state $|e\rangle$, while the u-path and d-path cavities are in the ground state ($n = 0$).

$$|\Psi(t_0)\rangle = |\psi(t_0), e, 0_u, 0_d\rangle$$

2. The atom passes into the interferometer and the wavepacket is split into the two arms:

$$|\Psi(t_1)\rangle = \frac{1}{\sqrt{2}} (|\psi_u(t_1), e, 0_u, 0_d\rangle + |\psi_d(t_1), e, 0_u, 0_d\rangle)$$

3. The wavepackets encounter the welcher-weg cavities. The excited electron energy is deposited in the photon field of the relevant cavity

$$|\Psi(t_2)\rangle = \frac{1}{\sqrt{2}} (|\psi_u(t_2), g, 1_u, 0_d\rangle + |\psi_d(t_2), g, 0_u, 1_d\rangle)$$

4. The wavepackets pass through the interference region. The triggering of the measuring device D_1 collapses the state to

$$|\psi_d(t_4), g, 0_u, 1_d\rangle$$

while triggering D_2 produces

$$|\psi_u(t_4), g, 1_u, 0_d\rangle$$

5. Probe atoms are sent through the welcher-weg cavities. If D_1 was triggered, then the d-path probe atom will absorb a photon and be detected by the selective ionization, while a D_2 detector triggering will be accompanied by the u-path probe atom absorbing a photon and being ionized.

This certainly appears to confirm Wheeler's interpretation of the delayed choice path measurement. If the atom travels down the d-path, it deposits the energy in the d-cavity, passes through the interference region and is detected by D_1 . Conversely, if the atom travels down the u-path, it deposits the energy in the u-cavity, passes through the interference region and is detected by D_2 .

If we place the screen back in the interference region, what pattern do we see? The answer is now

$$|\langle x | \Psi(t_3) \rangle|^2 = R(x, t_3)^2$$

There is no interference term. The reason the interference disappears is due to the orthogonality of the

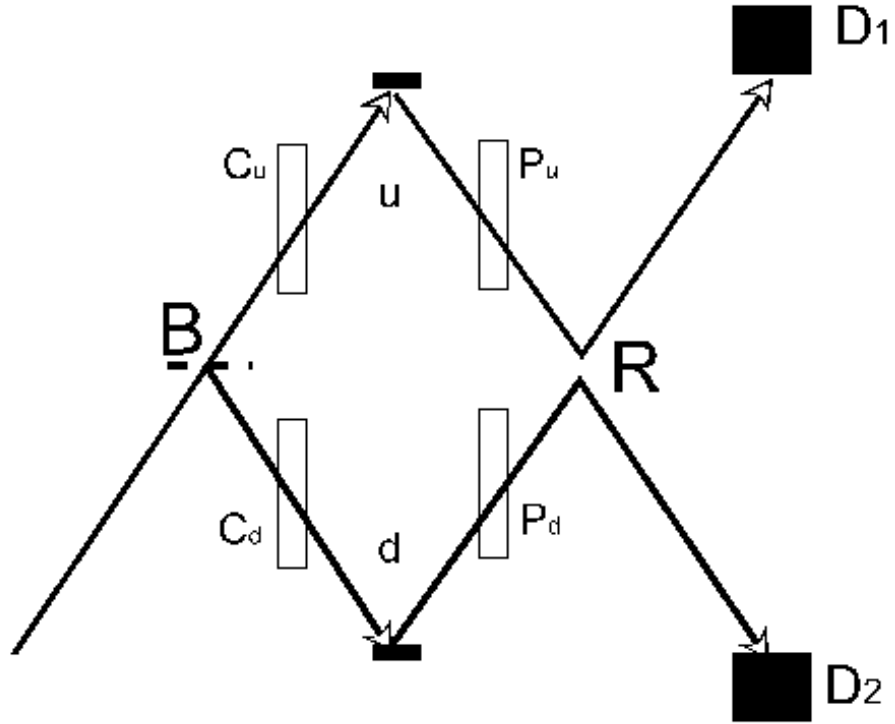


Figure 3.4: Surrealistic Trajectories

Delayed choice trajectories

Let us first note that trajectories of the kind shown in Figure 3.4 have long been known in the Bohm interpretation, and discussed in the context of the Wheeler delayed choice experiment [DHP79, Bel87]. However, these discussions of the delayed choice experiment suggested that the effect occurs only when the path of the atom is not measured in the arm of the interferometer. If detectors are placed in the interferometer arms, then the result should be the trajectories shown in Figure 3.3. It is then argued that the detection of an atom at D_1 in the arrangement of Figure 3.2 cannot be taken to imply the atom actually travelled down the d-path, except through the application of a 'naive classical picture' [Bel87, Chapter 14] and the possibility of observing the interference fringes in the region R undermine any such picture.

By adding their welcher-weg devices [ESSW92] appear to destroy this position. Two properties emerge. Firstly, the location of the atom in the detectors coincides with the location of the photon in the cavity, in the manner shown in Figure 3.3. This is taken to confirm Wheeler's assumption that atom did indeed pass down the d-path when detected in the D_1 detector, and the u-path when detected in the D_2 detector. Secondly, the Bohm trajectories still are able to behave in the manner shown in Figure 3.4 despite the measurement of the atom's path by the welcher-weg devices. [ESSW92] conclude that "the Bohm trajectory goes through one [path], but the atom [goes] through the other", the Bohm trajectories are "at variance with the observed track of the particle" and are therefore "surrealistic". In [ESSW93] they say

If the trajectories ... have no relation to the phenomena, in particular to the detected path of the particle, then their reality remains metaphysical, just like the reality of the ether of Maxwellian electrodynamics

and emphasise

this trajectory can be macroscopically at variance with the detected, actual way through the interferometer

We will consider the basis of [ESSW92]'s arguments in detail in the next Section. Before we do this, however, we will need to examine in more detail how the Bohm trajectories behave in the interferometer, and how the ionization of the probe atoms become correlated to the detectors.

The cavity field

The treatment of the field theory in the Bohm interpretation is developed in [BHK87, BH93, Hol93, Kal94]. In essence, while the particle theory given in Section 3.1 has a particle position co-ordinate x , guided by the wavefunction, the field theory supposes that there is an actual field, whose evolution is guided by a wavefunctional. This wavefunctional is the same as the probability amplitude for a particular field configuration in the standard approach to quantum field theory.

For a single mode cavity, such as the welcher-weg devices, this takes a particularly simple form and has been examined in great detail in [DL94a, DL94b]. The Bohm field configuration can be represented by a single co-ordinate (the field mode co-ordinate for the resonant cavity mode) and the wavefunctional reduces to a wavepacket representing the probability amplitude for the field mode co-ordinate. As long as one remembers that the 'beable' is field mode co-ordinate representing a distribution of an actual field, rather than a localised position co-ordinate, the single mode cavity may be treated in much the same manner as the particle theory in Section 3.1.

For the cavity C_u , therefore, we need only introduce a mode co-ordinate q_u , the wavefunctional for the cavity mode ground state $|0_u\rangle$ and for the first excited state $|1_u\rangle$. Similarly, for the cavity C_d we introduce q_d , $|0_d\rangle$ and $|1_d\rangle$. It is important to note that, although the states $|0\rangle$ and $|1\rangle$ are orthogonal, they are *not* superorthogonal.

Basic interferometer

We now review the evolution of the Bohm trajectories in the experimental arrangements in Figures 3.1 and 3.2

As in Subsection 3.2.1, the atomic wavefunction, in state $\psi(x, t_1)$ divides at the beam splitter. The trajectory of the atom will move into one or the other of the wavepackets $\psi_u(x, t_2)$ or $\psi_d(x, t_2)$. As the wavepackets move through the interferometer arms, the information in only one wavepacket is active and the other is passive. However, when the interference region is reached, the two wavepackets begin to overlap and the previously passive information becomes active once more. Now the information from both arms of the interferometer is active upon the particle trajectory.

This allows the phase shift information ϕ_u and ϕ_d from both phase shifters to guide the path of the trajectory, and the interference pattern can show nodes at locations dependant upon the setting of both devices.

If the screen is not present, the wavepackets separate again. As both wavepackets were active in the interference region, there is no guarantee that the trajectory emerges in the same wavepacket in which it entered. In fact, for the simplest situations, the trajectory will never be in the same wavepacket! The trajectories follow the type of paths in Figure 3.4[DHP79, Bel80].

Which way measurement

We now add conventional measuring devices to the arms of the interferometer. These will be described by a co-ordinate (y_u or y_d) and a wavefunction, initially in state $\xi_0(y)$. When the wavepacket of the atom moves through the arm of the interferometer, it interacts with the measuring device to change it's state to $\xi_1(y)$:

$$\begin{aligned} |\psi_u(t_2)\xi_0(y_u)\xi_0(y_d)\rangle &\rightarrow |\psi_u(t_2)\xi_1(y_u)\xi_0(y_d)\rangle \\ |\psi_d(t_2)\xi_0(y_u)\xi_0(y_d)\rangle &\rightarrow |\psi_d(t_2)\xi_0(y_u)\xi_1(y_d)\rangle \end{aligned}$$

The states ξ_0 and ξ_1 are superorthogonal and represent macroscopically distinct outcomes of the measurement (such as pointer readings). We will assume further that the measuring device has large number of constituents and interacts with the environment, in such a manner as to destroy any phase coherence between the ξ_0 and ξ_1 states.

Now, the state of the atom and measuring devices after the interaction is

$$\frac{1}{\sqrt{2}} (|\psi_u(t_2)\xi_1(y_u)\xi_0(y_d)\rangle + |\psi_d(t_2)\xi_0(y_u)\xi_1(y_d)\rangle)$$

As described in Section 3.1, if the atom trajectory is located in the u-path of the interferometer, then only the information in $\psi_u(x, t_2)$ is active. The y_u co-ordinate moves into the ξ_1 wavepacket and the y_d co-ordinate remains in the ξ_0 wavepacket. We describe the information in the other half of the superposition as passive. Had the atom trajectory initially entered the d-path, y_d would have entered the ξ_1 wavepacket.

When the atomic wavepackets encounter the interference region, the $\psi_u(x, t_3)$ and $\psi_d(x, t_3)$ begin to overlap. However the measuring device states are still superorthogonal. The information in the other branch of the superposition does not become active again. Consequently, the atom trajectory continues to be acted upon only by the wavepacket it entered at the start of the interferometer. No interference effects occur in the R region, and, if the screen is not present, the u-path trajectory passes through the interference region to encounter the detector at D_2 while the d-path trajectory goes through to the detector at D_1 . The superorthogonality of the measuring devices ensures that the trajectories do not reflect in the interference region, and the results of the measuring devices in the arms of the interferometer agree with the detectors at D_1 and D_2 that the atom has followed the paths indicated in Figure 3.3.

Although it is the superorthogonality that plays the key role in producing the measurement outcome, we will now say a few words about the role of the loss of phase coherence. As the macroscopic ξ states interact with the environment, further entangled correlations build up with large numbers of environmental particles. This leads to habitual decoherence in the macroscopic states. From the point of view of active information, however, what is most significant is that if even a *single* one of the environmental particles is correlated to the measuring device states in superorthogonal states, then the passive information in the measuring device states cannot be made active again. As an example, if the measuring device at ξ_1 leads to the scattering of an atom in the air to a different place than if the device had been at ξ_0 , then the passive information in ξ_0 cannot be made active unless the atom in the air is also brought back into overlapping states. As, for all practical purposes, the interaction with the environment makes this impossible, we can describe the information in the 'empty' wavepacket as inactive, or deactivated.

Welcher weg devices

We are now in a position to examine the *experimentum crucis* of [ESSW92]. In place of the measuring devices above, we have optical cavities in the paths of the interferometer. At $t = t_2$ the wavefunction is

$$|\Psi(t_2)\rangle = \frac{1}{\sqrt{2}} (|\psi_u(t_2), g, 1_u, 0_d\rangle + |\psi_d(t_2), g, 0_u, 1_d\rangle)$$

Now if the atom trajectory is in the u-path, then in cavity C_u the information in $|1_u\rangle$ is active, and the field mode co-ordinate q_u will behave as a single photon state. In cavity C_d , it is $|0_d\rangle$ that is active, so q_d behaves as a ground state. Had the atom trajectory been in the d-path, the situation would be reversed.

Now, unlike the measurement above, the welcher-weg states are not superorthogonal, and undergo no loss of phase coherence. When the atomic wavepackets enter the overlap region R , all the wavepackets in the state

$$|\Psi(t_3)\rangle = \frac{1}{\sqrt{2}} (|\psi_u(t_3), g, 1_u, 0_d\rangle + |\psi_d(t_3), g, 0_u, 1_d\rangle)$$

are overlapping. The trajectory co-ordinates for x , q_u and q_d are in non-zero portions of the wavefunction for both branches of the superposition. The previously passive information becomes active again. It is this that allows the atomic trajectories to become reflected in R and emerge from this region in the opposite wavepacket to the one they entered, as in Figure 3.4.

If the atom trajectory emerges from R in the wavepacket $\psi_u(x, t_4)$, then the information in the d-path wavepacket becomes passive again. This includes the activity of the q_u and q_d field mode co-ordinates, so only the $|1_u\rangle$ information is active for q_u and the $|0_d\rangle$ information is active for q_d . The C_u cavity therefore appears to hold the photon, while the C_d cavity appears empty. *This will be the case even if the atom trajectory originally passed through the C_d cavity.*

Finally, the atom trajectory encounters the detector either at D_1 or D_2 and the probe atoms are sent through the cavities. The probe atom that is sent through the cavity for which the $|1\rangle$

information is active will be excited, and ionized, and the correlation between the excited state ionization and the atom detectors will appear to be that of Figure 3.3. This shows how, despite having trajectories of the form in Figure 3.4, the Bohm approach produces exactly the same experimentally verifiable predictions as quantum theory.

3.2.5 Conclusion

The Bohm interpretation clearly provides an internally consistent means for describing the interference experiments, and produces all the same observable predictions as 'standard' quantum mechanics. Nevertheless, [ESSW92, ESSW93, Scu98] argue that the trajectories followed by the atom in the Bohm interpretation are

macroscopically at variance with the detected, actual way through the interferometer

The claim is that the location of the photon in the welcher-weg device, after the atomic wavepackets have left the region R tell us the way the atom actually went. If this claim is true the Bohm trajectories cannot be an accurate representation of what actually happened. As we have established the internal consistency of the Bohm interpretation, we must now examine the internal consistency of [ESSW92]'s interpretation of their welcher-weg devices. This examination should not be from the point of view of the Bohm interpretation, but rather from the point of view of 'standard' quantum mechanics.

It should be clear from the discussion above that the essential difference between the standard measuring device, for which the Bohm trajectories behave as in Figure 3.3, and the welcher-weg devices, is that in the cavities there is a coherent overlap between the excited and ground states throughout the experiment. This is the property of the welcher-weg devices that allows the Bohm trajectories to reverse in the region R and produce the effect that [ESSW92] call 'surrealistic'. If, for example, the probe atoms were sent through the cavities and ionized *before* the interference region was encountered, then the ionization and detection process would lead to a loss of phase coherence, or in the Bohm approach a deactivation of information in the passive wavepacket. In this case the Bohm trajectories could not reverse, and the trajectories would follow the paths in 3.3. We must therefore investigate the consequences of the persistence of phase coherence in standard quantum theory, to see how this affects our understanding of the welcher-weg devices.

3.3 Information and which path measurements

First we will examine the nature of the which-path 'information' obtained in the conventional measurement. This, it turns out, is not information in the sense we encountered it in Chapter 2, although it is related to the Shannon information from a measurement. The information can be interpreted in two ways: as a strictly operational term, referring to the observable consequences

of a conventional measurement, or as revealing a pre-existing situation or property of the object being measured. The second interpretation implicitly assumes that there is a deeper level of reality than that provided by the quantum mechanical description of a system.

We will then consider the quantum cavity "welcher-weg" devices. These do not fulfil the criteria of a conventional measuring device and there are observable consequences of this. The interpretation [ESSW92] place upon the information derived from their "welcher-weg" devices is that of revealing pre-existing properties of the atom, namely it's location. To make this interpretation, they must implicitly make two assumptions - that quantum objects, such as atoms or photons, possess an actual location, beyond the quantum description, and that the atom can only interact with the welcher-weg devices if the actual location of the atom is within the device.

However, we will demonstrate that the continued existence of phase coherence between the welcher-weg states does allow the observation of interference effects, and these make the combination of these two assumptions untenable. The welcher-weg devices cannot be interpreted as providing a reliable measurement of the location of the atom. This conclusion will be from the perspective of 'standard' quantum mechanics. We will therefore find that [ESSW92]'s argument that the location of the ionized electron reveals the actual path taken by the atom (and contradicting the Bohm trajectories) is not supported by standard quantum mechanics, and cannot be consistently sustained. Finally, we will show how the interference effects observed can be naturally explained within the context of active information.

3.3.1 Which path information

In [WZ79] it is suggested that it is not the momentum transfer of a scattered photon that destroys interference fringes, but rather the gathering of information about the path taken by the atom. This would appear to be supported by the welcher-weg devices, as these do not significantly affect the momentum of the atom. However, we need to consider what we mean by the information gathered. We will assume the beam splitter can be adjusted, as in Subsection 3.2.2, to produce the state

$$\psi^\theta(x, t_2) = \alpha\psi_u(x, t_2) + \beta\psi_d(x, t_2)$$

The information term I_{WZ} in Equation 3.2, although expressed as a Shannon information, does not correspond to the quantum information terms in Chapter 2. The atom is initially in the pure state $\psi(x, t_0)$. It continues to be in a pure state after it has split into two separate beams in the interferometer. The Schumacher information of the atomic state is zero. This represents a complete knowledge of the system. If we calculate the information gain from a conventional measurement of the path taken by the atom, we find that it is always zero. The initial state is $\psi(x, t_0)$ with probability one. The measurement of the location of the particle has outcomes u and d with probabilities $|\alpha|^2$ and $|\beta|^2$, so Bayes's rule (Equation 2.4) produces the trivial result

$$p(\psi|u) = \frac{j\alpha j^2 1}{j\alpha j^2} = 1$$

$$p(\psi|d) = \frac{j\beta j^2 1}{j\beta j^2} = 1$$

We saw this in Subsection 2.2.4. The information gain from a measurement relates to the selection of particular state from a statistical mixture of states. As this particular situation is not described by a mixture⁵ but by a pure state, there is no uncertainty. Information revealed by the measurement is *not* a gain of information about the *quantum* properties of the system.

From the perspective of information gain, only if the wavepacket

$$\psi^\theta(x, t_1) = \alpha\psi_u(x, t_1) + \beta\psi_d(x, t_1)$$

was replaced by the statistical mixture

$$\rho^\theta = |\alpha|^2 |\psi_u(x, t_1)\rangle \langle\psi_u(x, t_1)| + |\beta|^2 |\psi_d(x, t_1)\rangle \langle\psi_d(x, t_1)|$$

of $|\psi_u(t_1)\rangle$ and $|\psi_d(t_1)\rangle$ states, would there be an information gain I_{WZ} from a measurement, but in this case there would be no interference.

Information about the measurement How can we understand I_{WZ} when the initial state is a pure state? There are two possible ways of doing this. The first method is to note that I_{WZ} does represent the Shannon uncertainty about the outcome of the measurement. Let us be very careful what we mean here. We are proposing that the measuring device is a conventionally defined, macroscopic object, with an observable degree of freedom, such as the pointer on a meter. I_{WZ} represents our prior ignorance of the state the pointer will be in when the measurement is concluded. Naturally, this assumes the measurement problem is solved so that it is meaningful to talk about the pointer being in a state, and the measurement being concluded.

This remains a controversial topic in the interpretation of quantum theory. However, it is generally accepted, and is certainly part of the 'standard' approach to quantum theory, that such a measurement involves an amplification of the quantum state to macroscopic levels that is, for all practical purposes, irreversible, and is accompanied by an irretrievable loss of phase information between the different measurement outcomes. At the end of such a process, the entangled state between the measuring device and the measured object can be replaced by a statistical mixture *without in any way affecting the future evolution of the experiment*. It more or less follows that it can only be applied to the kind of macroscopically large objects for which a classical description is valid.

At the end of the measurement, we would know what state the quantum object was in, as a result of the correlation to the measuring device. However, we could not infer from this that the quantum object was in that state *prior* to making the measurement. If we had considered making a complementary measurement before our path measurement, we could have observed the kind of interference effects that preclude the assumption that the measured object was in one or the other state, but that the state was unknown to us.

⁵Or, equivalently, is described by the trivial mixture, for which $p(\psi) = 1$

In this respect we would be viewing the experiment in the manner Bohr[Boh58] appears to recommend:

all unambiguous use of space-time concepts in the description of atomic phenomena is confined to the recording of observations which refer to marks on a photographic plate or to similar practically irreversible amplification effects

From this point of view, the quantity I_{WZ} refers to the properties of the macroscopically observable measuring device outcomes in the particular experimental arrangement. It does *not* represent a statement of the ignorance of the properties of the atom itself. Our knowledge of the state of the atom, as a quantum object, is already complete (it is in a pure state). It is only the future states of the measuring device of which we are uncertain.

Information about the atom The second way of viewing I_{WZ} is to suppose that the measuring device does precisely what it was intended to do - that is, measure the actual location of the atom. This must assume that the atom does indeed have an actual location, and the measurement reveals that location. This involves the attribution to the atom of a property (well defined location) which goes beyond the *quantum* description of the object.

When we have only the either/or options of designing an interference experiment to test the wave nature of the quantum object, or a which path experiment to test the particle nature of the quantum object, the tendency is to talk loosely of the quantum object as being a particle or a wave depending upon the experimental arrangement. However, the intermediate cases introduced by [WZ79] make this more difficult, as the object is supposedly manifesting both particlelike and wavelike properties in the one arrangement:

The sharpness of the interference pattern can be regarded as a measure of how wavelike the [object] is, and the amount of information we have obtained about the [object]'s trajectories can be regarded as a measure of how particlelike it is

The problem here is the talk of our possessing information about the trajectory taken. The normal meaning of this sentence would be clear: it would mean that the object had a well-defined trajectory, and we had some probabilistic estimate of which path was taken in any given experiment. This meaning applies even when the ignorance of the path is maximal. This would be the case where $I_{WZ} = 1$. In this case, the consistent use of the word *information* must be taken to mean that the atom follows the u-path half the time and the d-path the other half the time.

Unfortunately, this is exactly the situation considered in the basic interferometer (Subsection 3.2.1). The proponents of an information-interference complementarity would argue the interference fringes appear because we lack information about which path was taken. To consistently understand the meaning of the word information here, we must assume that the atom does, in fact follow a particular path, it is just that we ourselves are ignorant of which one. However, the settings of the phase shifters demonstrates that the ultimate location of the atom in the interference

region depends upon the phase shift in *both* arms of the interferometer. This leads to the exact situation Bohr[Boh58] warns against, where

we would, thus, meet with the difficulty: to be obliged to say, on the one hand, that the [atom] always chooses *one* of the two ways and, on the other hand, that it behaves as if it had passed *both* ways.

3.3.2 Welcher-weg information

We have seen that the interpretation of which-path information in the context of a conventional quantum measurement is not without its problems. We will now consider the welcher-weg devices.

As we have seen, these devices maintain phase coherence between the u- and d-branches of the superposition, and this phase coherence is essential to produce the 'surrealistic' behaviour of the Bohm trajectories. Such phase coherence is a property that a conventional measuring device must not possess. It is only when the state selective ionization takes place that a conventional measurement can be said to have taken place. This must be after the atoms have traversed the interference region R .

When considering the 'which-path' measurement above, the destruction of phase coherence in the measurement prevented the occurrence of interference fringes in the region R . With the welcher-weg devices in place, we similarly lose interference fringes. If we add the phase shifters to the welcher-weg experiment, this leads to the state at $t = t_3$

$$|\Psi(t_3)^{\text{th}}\rangle = \frac{1}{\sqrt{2}} (e^{i\phi_u} |\psi_u(t_3), g, 1_u, 0_d\rangle + e^{i\phi_d} |\psi_d(t_3), g, 0_u, 1_d\rangle)$$

The probability distribution in the interference region turns out to be

$$|\langle x | \Psi(t_3)^{\text{th}} \rangle|^2 = R(x, t_3)^2$$

The values of ϕ_u and ϕ_d have no effect upon the pattern that emerges if a screen is placed in the region R .

The reason for this is that the atom is not, in itself, in a pure state. It is in an entangled superposition with the photon states of the fields in the two micromaser cavities. If one traces over the entangled degrees of freedom, one obtains the density matrix

$$\frac{1}{2} (|\psi_u(t_3)\rangle \langle \psi_u(t_3)| + |\psi_d(t_3)\rangle \langle \psi_d(t_3)|)$$

which is the same result one would have obtained if there had been a statistical mixture of atomic wavepackets travelling down one path or the other. As all the observable properties of a system are derivable from the density matrix there is no way, *from measurements performed upon the atom alone*, to distinguish between the state $|\Psi(t_3)\rangle$ and the statistical mixture.

It might therefore seem unproblematical to argue, as [ESSW93] do, that, although the welcher-weg devices are not *conventional* measurement devices, they are still reliable

Perhaps it is true that it is "generally conceded that ... [a measurement] ... requires a ... device which is more or less macroscopic" but our paper disproves this notion because it clearly shows that one degree of freedom per detector is quite sufficient. That is the progress represented by the quantum optical which-way detectors.

To [ESSW92, SZ97] the absence of the interference terms demonstrates information *has* been gathered, and that correspondingly a measurement must have taken place

As long as no information is available about which alternative has been realized, interference may be observed. On the other hand, if which-path information is stored in the cavities, then complementarity does not allow for interference [SZ97, pg574]

However, the tracing over the cavity states does not mean we can simply replace the entangled superposition with the density matrix, nor does it mean that we can interpret the entangled superposition as a statistical mixture. Although interference properties can no longer be observed from operations performed upon a single subsystem, we *can* observe interference effects from correlated measurements upon the entire system because, *unlike in a conventional measurement*, phase coherence still exists.

Interference We will now demonstrate how to observe interference effects, by operations performed upon the probe atom, *after* the atomic wavepacket has reached the region R and *after* the probe has left the cavity. The location of the photon excitation energy is determined by the selective ionization of a probe atom sent through the cavity. The probe atom is initially in the ground state $|g_P\rangle$. The evolution is

$$\begin{aligned} |g_P0\rangle &\rightarrow |g_P0\rangle \\ |g_P1\rangle &\rightarrow |e_P0\rangle \end{aligned}$$

The state of the system becomes

$$|\Psi(t_4)\rangle = \frac{1}{\sqrt{2}} (e^{i\phi_u} |\psi_u(t_3), g, e_{P_u}, g_{P_d}\rangle + e^{i\phi_d} |\psi_d(t_3), g, g_{P_u}, e_{P_d}\rangle) |0_u, 0_d\rangle$$

where $|g_{P_u}\rangle$ represents the ground state of the u-cavity probe atom etc. The ionization measurement of the probe atoms leads to the states:

$$\begin{aligned} |e_{P_u}, g_{P_d}\rangle &\Rightarrow |\psi_u(x, t_4)\rangle \\ |g_{P_u}, e_{P_d}\rangle &\Rightarrow |\psi_d(x, t_4)\rangle \end{aligned}$$

which appears to give us a measurement of the atomic position.

We should remember that this is a measurement of the atomic position *after* the atomic wavepackets have left the interference region R , and for which there is no disagreement between the Bohm trajectories and [ESSW92]'s interpretation of the location of the atom.

Let us consider what happens if the screen had been placed in the interference region R . Each experiment would lead to a scintillation at some point on the screen. By correlating the detected

position of the atom in the interference region with the outcomes of the probe atom ionizations, we would select two subensembles, which would each have a distribution of $R(x, t_3)^2$. No interference would be visible.

Now we consider the modification necessary to observe interference. Before ionizing the probe atoms, let us pass them each through a pulsed laser beam, producing Rabi oscillations, as in Equation 3.3. The size of the pulse should now be $Rt = \frac{1}{2}\pi$. This produces the rotation

$$\begin{aligned} |g\rangle &\rightarrow \frac{1}{\sqrt{2}} (|g\rangle + \iota |e\rangle) \\ |e\rangle &\rightarrow \frac{1}{\sqrt{2}} (\iota |g\rangle + |e\rangle) \end{aligned}$$

and the state of the system (ignoring the now irrelevant cavity modes) is

$$\begin{aligned} |\Psi(t_3)\rangle &= \frac{1}{2} (e^{i\phi_u} (|\psi_u(t_3), e_{P_u}, g_{P_d}\rangle + \iota |\psi_u(t_3), g_{P_u}, g_{P_d}\rangle \\ &\quad + \iota |\psi_u(t_3), e_{P_u}, e_{P_d}\rangle - |\psi_u(t_3), g_{P_u}, e_{P_d}\rangle) \\ &\quad + e^{i\phi_d} (|\psi_d(t_3), g_{P_u}, e_{P_d}\rangle + \iota |\psi_d(t_3), e_{P_u}, e_{P_d}\rangle \\ &\quad + \iota |\psi_d(t_3), g_{P_u}, g_{P_d}\rangle - |\psi_d(t_3), e_{P_u}, g_{P_d}\rangle)) \end{aligned}$$

which can be rewritten as

$$\begin{aligned} |\Psi(t_3)\rangle &= (e^{i\phi_u} |\psi_u(t_3)\rangle - e^{i\phi_d} |\psi_d(t_3)\rangle) \frac{|e_{P_u}, g_{P_d}\rangle - |g_{P_u}, e_{P_d}\rangle}{2} \\ &\quad + \iota (e^{i\phi_u} |\psi_u(t_3)\rangle + e^{i\phi_d} |\psi_d(t_3)\rangle) \frac{|g_{P_u}, g_{P_d}\rangle + |e_{P_u}, e_{P_d}\rangle}{2} \end{aligned}$$

Now when the probe atoms are ionized the atomic wavefunction is either

$$|\Psi_a(t_3)\rangle = \frac{1}{\sqrt{2}} (e^{i\phi_u} |\psi_u(t_4)\rangle - e^{i\phi_d} |\psi_d(t_4)\rangle)$$

or

$$|\Psi_b(t_3)\rangle = \frac{1}{\sqrt{2}} (e^{i\phi_u} |\psi_u(t_4)\rangle + e^{i\phi_d} |\psi_d(t_4)\rangle)$$

The probability distribution in the interference region is now either

$$|\langle x | \Psi_a(t_3) \rangle|^2 = \frac{R(x, t_3)^2}{2} (1 + \cos(\Delta S(x, t_3) + (\phi_u - \phi_d)))$$

or

$$|\langle x | \Psi_b(t_3) \rangle|^2 = \frac{R(x, t_3)^2}{2} (1 - \cos(\Delta S(x, t_3) + (\phi_u - \phi_d)))$$

Both of these exhibit interference patterns in the region R and, critically for our understanding of the situation, the location of the nodes of this interference pattern will be dependant upon the phase shifts ϕ_u and ϕ_d in *both* arms of the interferometer. Had the cavities been conventional measuring devices, no such interference patterns could have been observed. The mixture of the two distributions loses the interference pattern. It is only when the results of the probe atom measurements are correlated to the ensemble of atomic locations that the interference effects can

be observed. This is characteristic of entangled systems, where the interference can only ever be seen using correlated or joint measurements⁶.

It is important to note that the choice of whether or not to pulse the probe atoms with the $\frac{1}{2}\pi$ pulse can be made *after* the atomic wavepacket has entered into the region R and had its location recorded on a screen. The information about the phase shift settings must somehow be present in the atom position measurements *before* we choose whether to pulse the probe atoms or not.

Quantum erasers The arrangement considered here is similar to the quantum eraser experiments [ESW91, SZ97]. It may be argued that, by pulsing the probe atom, we are 'erasing' the which path information and so restoring the interference. The problem is that this implicitly assumes that there is a matter of fact about which path the atom took, and that the interference appears only because the information as to which path the atom took is not stored anywhere.

Thus we read in [SZ97]

As long as no information is available about which alternative has been realized, interference may be observed

This ignores the fact that it is not simply the existence of interference that is the problem. It is also a problem that the location of the nodes in the interference pattern so clearly depend upon the settings of the phase shifters in both arms of the interferometer. If there is a matter of fact about which path the atom took ("which alternative has been realized"), that is if we understand the term 'information' in its normal usage, then we cannot account for the fact that the atom is able to avoid locations that depend upon the configuration of both phase shifters. There is a fundamental ambiguity in [SZ97]'s description of the quantum 'eraser': is it only the *information* about which path the atom took that is erased, or is it the very fact that the atom *did* take one or the other path? We are forced, as Bohr warned, to say the atom travels down one path, but behaves as if it has travelled down both.

3.3.3 Locality and teleportation

We have established that the welcher-weg devices are not conventional measuring devices and that there are observable consequences of this. We will now examine what affect this has upon [ESSW92, ESSW93, Scu98]'s criticism of the Bohm interpretation.

The essence of the argument is that when the photon is found in the cavity the atom must have travelled down that arm of the interferometer

we do have a framework to talk about path detection: it is based upon the local interaction of the atom with the ... resonator, described by standard quantum theory with its short range interactions only [ESSW93]

⁶If interference effects could be seen without such correlations, they could be used to violate the no-signalling theorem, and send signals faster than light.

The local interaction between the atom and photon, in terms of the Hamiltonian interaction in the Schrödinger equation, is here being taken to mean that the atom can deposit a photon in the cavity only if it actually passed through the cavity.

We can identify two key assumptions that are necessary for the interpretation of the welcher-weg devices as reliable indicators of the *actual* path of the atom:

1. This storage of information is a valid measurement, even though it is not a conventional quantum measurement. The atom can only interact with the welcher-weg device, and deposit a photon in it, if the actual path of the atom passes through the device.
2. The reason the interference pattern initially disappears is because the cavity stores information about the path of the atom. The storage of information implies that there is a matter of fact, which may be unknown, about which path the atom took, in all realizations of the experiment.

Local interactions Let us consider why these two assumptions are necessary. The first assumption is based upon the local interaction Hamiltonian between the atom and the cavity field. However, when the atom is in a superposition, as in the interferometer, the effect of this Hamiltonian is to produce an entangled correlation between the atom and the cavity mode wavefunctions. Part of the atomic *wavefunction* interacts with *each* cavity wavefunction. If we took the wavefunction to be a physically real entity, we could not say that the atom in the interferometer interacts with only one cavity, we would have to say that the atom interacts with both cavities, in all experiments. If this were the case, then could draw no conclusions about the path taken by the atom from the location of the photon. To reach [ESSW92]’s conclusion we must argue, as is standard, that the wavefunction is not physically real but

a tool used by theoreticians to arrive at probabilistic predictions

If one is consistently to take this view, however, one must also apply it to the Hamiltonian interaction, which acts upon the wavefunctions. Consequently, the first assumption is not based upon the

local interaction of the atom with the ... resonator, described by standard quantum theory with its short range interactions only

In [Scu98], it is stated that

the photon emission process is always (physically and calculationally) driven locally by the action of the cavity field on the atom

While the emission process can be said to be *calculationally* driven by the local Hamiltonian acting upon the wavefunction, to say that it is also *physically* local is to attribute reality to something deeper than the quantum level of description. The assumption that finding the photon in one

cavity implies the atom actually passed through that cavity is an addition to 'standard' quantum theory.

In [Scu98], this is made particularly clear. To defend his interpretation of the experiment, Scully wishes to rule out the transfer of the photon from one cavity to the other, as the atom traverses the interference region. He argues that the transfer of the photon from one micromaser cavity to the other, in the Bohm approach, represents a teleportation of energy. This teleportation of energy is 'qualitatively different' and a 'stronger type' of non-locality to that found in EPR correlations⁷.

However, the non-locality of entangled photon states in micromaser cavities has been studied and has even been suggested to be used in quantum teleportation experiments [BDH⁺93, BDH⁺94, CP94]. In Appendix A and [HM99] we can see that the welcher-weg interferometer involves exactly the same processes as in EPR entanglement and quantum teleportation, whether one uses the Bohm interpretation or 'standard' quantum mechanics. Consequently, Scully's argument that finding the photon in the cavity after the interference region has been passed implies that the photon *must* have been in the cavity before the interference region was encountered is, again, an argument that is not part of standard quantum mechanics, and rests upon the assumptions above.

Actual paths of atoms The second assumption is necessary to understand the use of the term 'information'. If the welcher-weg device stores information about the actual path of atom, this implies that there is a matter of fact about which path the atom actually takes. The erasure of such information would simply affect our, real or potential, knowledge of which path the atom took, but would not affect the actual reality of which path the atom took.

Can we deny this point without losing the interpretation of the welcher-weg devices as reliable measuring devices? It would seem not, as if we do deny this we find ourselves contradicting the first assumption. Suppose we interpret the atom having a path only in the experiments where the probe atoms are not pulsed, but not having a path when the probe atoms are pulsed (and interference is observed). The problem lies in the fact that the cavities are themselves simply two level quantum systems. The location of the photon in the cavity, which is taken to represent the information about the path the atom travelled, is a quantum state of the optical field. If there is no matter of fact about whether the atom is taking one path or the other, before the measurement is performed, there is equally no matter of fact about which cavity contains the photon. The interaction of the atom with the cavity does not create a matter of fact about whether the atom took one path or the other, so cannot be said to represent a measurement of the atoms location.

So when would the measurement take place that determines whether there is a matter of fact about the path of the atom? The answer is only when the probe atom is ionized. In other words, when a *conventional* quantum measurement takes place. It is not the welcher-weg devices that are

⁷[SZ97, Scu98] appears to state that EPR correlations can be attributed to 'common cause' and there is 'nothing really shockingly non-local here'. It is precisely because EPR correlations violate the Bell inequalities that this point of view encounters considerable difficulties [Red87, Bel87].

measuring the path of the atom at all. There is no matter of fact about whether the atom travelled down one path or the other, or any matter of fact about which cavity contains the photon, until the probe atom is ionized, which cannot take place until *after* the interference region has been traversed.

It is in the interference region that the atom changes wavepackets and the excitation of the cavity modes switches from one cavity to the other in the Bohm interpretation. In other words, if we deny the second assumption, the 'surrealistic' behaviour of the Bohm trajectories will take place only if there is no matter of fact about which path the atom took and which cavity contains the photon. In which case we cannot conclude that the Bohm trajectories are at variance with the actual path taken by the atom, as it is not meaningful to talk about the actual path of the atom. Without the second assumption the addition of the welcher-weg devices to Wheeler's delayed choice experiment has had no effect on its interpretation.

This demonstrates that these two assumptions are essential to the interpretation [ESSW92] wish to place upon the welcher-weg devices, and further that neither assumption can be considered part of 'standard' quantum theory.

Phase coherence As we have seen, to contradict the Bohm trajectories it is essential that the welcher-weg devices maintain phase coherence in the entangled superposition. However, this allows us to display interference effects in the location of the atom that depend upon the settings of phase shifters in both arms of the interferometer. Such a result seems to undermine both of these assumptions necessary for [ESSW92]'s interpretation of the welcher-weg devices.

We can emphasise this by removing the phase shifter from one arm and the cavity from the other. Firstly, let us consider the results of ionizing an unpulsed probe atom. If the unpulsed probe atom is measured to be in the excited state, we would assume that the atom passed down the arm of the interferometer containing the cavity, while if the probe atom is measured in the unexcited state, we would assume that the atom passed down the other arm. These would each occur with a 50% probability. In other words, half of the atoms could not have interacted with the phase shifter, and the other half could not have interacted with the cavity.

Now let us consider what happens if we pulse the probe atom. We separate the pattern the atom makes upon the screen in the interference region R into subensembles based upon the outcome of the ionized probe atom measurement. These subensembles each display the full interference pattern, the location of whose maxima and minima are determined by the phase shifter. Now, if we are to assume that the atom did, in fact, travel down only one path or the other, and could only interact with the device in the path it travelled through we cannot consistently interpret these results.

Consider the atom that hypothetically travelled down the arm with the cavity. This deposited a photon in the cavity, and encountered the screen. Neither cavity nor atom interact locally with the phase shifter. However if we pulse the probe atom, before ionization, the location of the atom

in the interference region shows fringes which depend upon the setting of the phase shifter, which neither atom nor cavity interacted with.

If we consider the atom that hypothetically travels down the arm with the phase shifter, we find the situation even worse. Now the cavity does not interact with the atom and is left empty. If we send the probe atom through this empty cavity, then pulse and ionize it, the result of this ionization is to produce interference patterns, with minima at different locations. If the cavity never interacted with the atom, how can the result of measuring the probe atom possibly be correlated to the location of the forbidden zones in the interference patterns?

3.3.4 Conclusion

It seems to consistently interpret these results we must either abandon the notion that there is a matter of fact about which path the atom takes or abandon the idea that the atom can only interact with the cavity (or phase shifter) if it actually passes down the same arm of the interferometer. If either of these concepts are abandoned, however, the interpretation [ESSW92] place upon the welcher-weg devices is untenable. We are therefore forced to conclude that the welcher-weg devices do not have the properties necessary to be interpreted as detectors.

If we abandon the second assumption, and we apply the information term (3.2) strictly to the outcomes of experiments, we can make no inference at all about the actual path taken by the atom. This takes us to the interpretation urged by Bohr[Boh58] and to 'standard' quantum theory. Here only the outcomes of macroscopic measurements can be meaningfully discussed. The macroscopic phenomena emerges, but cannot be interpreted in terms of microscopic processes. In the case of the experiments above, the interference effects are predicted by the quantum algorithm, but no explanation is offered, nor can be expected, as to how they arise. In particular, the single mode cavities are normal quantum devices, and so cannot be interpreted as reliable measuring devices.

If we abandon the first assumption, how do we understand an atom travelling down one path, but acting as if it travels down both? We can interpret this in terms of the active information in the Bohm approach. A trajectory travels down one path, but a wavepacket travels down both paths. The wavepackets interact with the cavity or phase shifter, according to the local Hamiltonian, regardless of which path the atomic trajectory actually takes.

Now the entangled state means that the information on the setting of the phase shifter is part of the common pool of information that guides both the atomic trajectory and the cavity field mode. When the atom enters the interference region, all the branches of the superposition become active. The behaviour of the atom is now being guided by the information from both wavepackets and so can be influenced by the phase information from both arms of the interferometer. However, the field modes are also being guided by this common pool of information.

If the atom encounters the screen at some location x in the interference region, this is amplified in some, practically irreversible process, that renders all the other information in the entangled quantum state inactive. The non-local quantum potential connects the motion of the atomic

trajectory to the motion of the cavity field mode, so now the excitation of the cavity field is correlated to the position at which the atom was detected. If the atom is detected at the specific location X , the active wavefunction for the cavity field modes is now proportional to

$$\psi_u(X) |1_u, 0_d\rangle + \psi_d(X) |0_u, 1_d\rangle$$

where $\psi_u(X)$ and $\psi_d(X)$ are just the complex numbers corresponding to the probability amplitudes for the actually detected location of the atom at X . This demonstrates how the information active upon the cavity field modes is correlated to the measured location of the atom through the non-locality of the quantum potential.

When the probe atom is sent through the cavity, and pulsed, this can be rewritten as

$$\begin{aligned} & (e^{i\phi_u}\psi_u(X, t_3) - e^{i\phi_d}\psi_d(X, t_3)) \frac{|e_{P_u}, g_{P_d}\rangle - |g_{P_u}, e_{P_d}\rangle}{2} \\ & + i (e^{i\phi_u}\psi_u(X, t_3) + e^{i\phi_d}\psi_d(X, t_3)) \frac{|g_{P_u}, g_{P_d}\rangle + |e_{P_u}, e_{P_d}\rangle}{2} \end{aligned}$$

The probabilities of detection of the states of the probe atoms are therefore

$$\begin{aligned} |e_{P_u}, g_{P_d}\rangle, |g_{P_u}, e_{P_d}\rangle & \Rightarrow \frac{|e^{i\phi_u}\psi_u(X, t_3) - e^{i\phi_d}\psi_d(X, t_3)|^2}{R(X, t_3)^2} \\ |g_{P_u}, g_{P_d}\rangle, |e_{P_u}, e_{P_d}\rangle & \Rightarrow \frac{|e^{i\phi_u}\psi_u(X, t_3) + e^{i\phi_d}\psi_d(X, t_3)|^2}{R(X, t_3)^2} \end{aligned}$$

We can express this as the conditional probabilities

$$\begin{aligned} P(ee, gg|X) &= \frac{1}{2} (1 + \cos(\Delta S(X, t_3) + (\phi_u - \phi_d))) \\ P(eg, ge|X) &= \frac{1}{2} (1 - \cos(\Delta S(X, t_3) + (\phi_u - \phi_d))) \end{aligned}$$

Correlating the ionisation state back to the location of the atom, using Bayes's rule, reveals the interference fringes

$$\begin{aligned} P(X|ee, gg) &= R(X, t_3)^2 (1 + \cos(\Delta S(X, t_3) + (\phi_u - \phi_d))) \\ P(X|eg, ge) &= R(X, t_3)^2 (1 - \cos(\Delta S(X, t_3) + (\phi_u - \phi_d))) \end{aligned}$$

The interference exists as a correlation between the entangled systems. It is usual to regard this as the probe atom ionization leading to the selection of subensembles of the atomic position which display interference. As we can see here, we may equally well have regarded the location of the atom on the screen as selecting interference subensembles in the ionization of the probe atom. The phase shifts, ϕ_u and ϕ_d , do not act upon a single subsystem, rather they form part of the common pool of information which guides the joint behaviour of both systems.

Information We can modify this to produce a POVM measure of the which-path information suggested by Wootters and Zurek. Suppose that the resonance between the atomic beam and the cavities are adjusted, by speeding up the atoms. The transition is no longer

$$|e0\rangle \rightarrow |g1\rangle$$

but becomes

$$|e0\rangle \rightarrow \alpha |g1\rangle + \beta |e0\rangle$$

We then send the probe atoms through the cavities, and ionise them *while the atomic wavepacket is still in the interferometer*. The ionisation of the probe atom can now represent a measurement of the atom's location. The POVM is

$$\begin{aligned} A_u &= \frac{1}{2} |\alpha|^2 |\phi_u\rangle \langle \phi_u| \\ A_d &= \frac{1}{2} |\alpha|^2 |\phi_d\rangle \langle \phi_d| \\ A_0 &= |\beta|^2 \mathbf{I} \end{aligned}$$

If we represent the location of the Bohm trajectory in the u-branch by X_u and in the d-branch by X_d , then the initial probabilities are

$$\begin{aligned} P(X_u) &= \frac{1}{2} \\ P(X_d) &= \frac{1}{2} \end{aligned}$$

giving an initial information of $I(X) = 1$. The probability of the measurement outcomes are

$$\begin{aligned} P(u) &= \frac{1}{2} |\alpha|^2 \\ P(d) &= \frac{1}{2} |\alpha|^2 \\ P(0) &= |\beta|^2 \end{aligned}$$

where $P(u)$ is the probability of the u-probe atom ionising, $P(d)$ the d-probe atom ionising, and $P(0)$ neither ionising.

If either probe atom ionises, the wavepacket in the other branch is deactivated and the correlated ensemble of atoms in the region R displays no interference. If neither ionises, both wavepackets become active again and a full interference pattern occurs. The total pattern is

$$R(X, t_3)^2 \left(1 + |\beta|^2 \cos(\Delta S(X, t_3) + (\phi_u - \phi_d)) \right)$$

The conditional probabilities after the measurement are

$$\begin{aligned} P(X_u|u) &= 1 \\ P(X_d|d) &= 1 \\ P(X_u|0) &= \frac{1}{2} \\ P(X_d|0) &= \frac{1}{2} \end{aligned}$$

so the conditional information on the path (X) taken by the atom after the measurement (M) is

$$I(X|M) = |\beta|^2$$

which represents the remaining ignorance of the path taken. The gain in information is

$$I(X : M) = |\alpha|^2$$

The size of the interference fringes are given by $|\beta|^2 = 1 - |\alpha|^2$. As we gain more information about the path, we reduce the size of the interference pattern.

The concept of active information, in the Bohm interpretation, thus provides a natural way to understand the interference effects in the experiments considered.

3.4 Conclusion

We have considered in detail the relationship between information and interference proposed in a series of thought experiments. We have found that the concept of 'information' being used, although quantified by a Shannon information term (3.2) is not the same as information used in the sense of Chapter 2. Shannon information represents a state of ignorance about an actual state of affairs. The measurement in a quantum system cannot, in standard quantum theory, be interpreted as revealing a pre-existing state of affairs. If we can interpret the term I_{WZ} at all, in standard quantum theory, it is as our ignorance of the outcome of a particular measurement. It cannot be used to make inference about the existence of actual properties of quantum objects.

The measurements that must be used, in standard quantum theory, involve macroscopic devices, for which the phase coherence between the different measurement outcomes is, for all practical purposes, destroyed. This allows us to replace the entangled pure state with a statistical density matrix, without in any way affecting the future behaviour of the system. The welcher-weg devices suggested by [ESSW92, SZ97] do not have this essential feature. It is entirely because they do not have this feature that they produce the effects in the quantum eraser experiments [ESW91] and that appear to contradict the Bohm trajectories. However, the interpretation [ESW91, ESSW92, SZ97] placed upon the welcher-weg devices is not consistent with standard quantum theory, precisely because they lack this feature, and it seems difficult how this interpretation can be sustained.

The concept of active information, by contrast, provides a natural way of interpreting these results. If we measure the path taken by the trajectory, we render the information in the other wavepacket inactive, because of the superorthogonality of the measuring device states. When the atom encounters the interference region it is guided only by the information in the one wavepacket, and so cannot display interference effects that depend upon phase differences between both branches of the superposition. If we do not measure the path taken, then both wavepackets are active when the interference region is encountered, and the atomic trajectory is guided by information from both arms of the interferometer.

Active information is clearly different from that given by I_{WZ} . Here we are not talking about our ignorance of a particular state of affairs ('information-for-us'), but rather a dynamic principle of how the experimental configuration acts upon the constituent parts of the quantum system ('informing the behaviour of the object'). Nevertheless, it connects to our measurements as, when we gather information-for-us from a measurement, the dynamic information in the other

wavepackets becomes inactive. This explains why, in the interference experiments, as we increase our 'information-for-us' about the path measurements, we increase the *deactivation* of the information about the phase shifts in the arms of the interferometer, and this leads to the attenuation of the interference fringes. The Bohm interpretation provides a coherent means of understanding the information-interference complementarity in experiments such as [WZ79], while *welcher-weg* devices do not.

Chapter 4

Entropy and Szilard's Engine

In this part of the thesis we will examine the role of information in thermodynamics. We will be particularly interested in the quantitative connections suggested between the Shannon/Schumacher measure of information and the thermodynamic entropy. This will require us to analyse in detail the quantum mechanical version of Szilard's thought experiment [Szi29] relating entropy to the information gained by a measurement. This thought experiment has been made the paradigm argument to demonstrate the information theoretic explanation of entropy [LR90, for example] but it continues to be strongly criticised [BS95, EN98, EN99, She99].

The structure of this is as follows:

- Chapter 4 will review the attempts that have been made to make a quantitative link between information and entropy, based upon Maxwell's Demon and the Szilard Engine. This will be in some detail, in order to clarify the points that are at issue, and to motivate the analysis in subsequent Chapters. This will allow us to construct a modified, and quantum mechanical, form of the "demonless" Szilard Engine, which will be used to examine the validity of the various 'resolutions'.
- In Chapter 5 we will make a careful and detailed description of the quantum mechanical operation of all stages of the Szilard Engine. The only physical restriction we place upon this Engine is that it must be consistent with a unitary time evolution.
- Chapter 6 adds statistical mechanics to the microscopic motion, by introducing canonical heat baths and ensembles. No other thermodynamic concepts (such as entropy or free energy) will be used at this stage. The behaviour of the Engine will then be shown to quite consistent with the statistical mechanical second law of thermodynamics.
- Thermodynamic concepts are introduced and justified in Chapter 7. It will be shown that the entropy of the Szilard Engine never decreases. In Chapter 8 the behaviour of the Engine is generalised to give a complete explanation of why Maxwell's Demon cannot produce anti-entropic behaviour. We then show how the other resolutions suggested, where they are

correct, are contained within our analysis.

Our analysis will show that both the information theoretic resolution, and its criticisms, are incomplete, each concentrating on only part of the problem. When we complete this analysis, we will show that, despite the formal similarity between Shannon/Schumacher information and Gibbs/Von Neumann entropy, information theory is both unnecessary and insufficient to give a complete resolution of the issues raised by the Szilard Engine.

We will now consider the general arguments for a relationship between entropy and information. Section 4.1 will review one of the issues raised by statistical mechanics, and why this may be taken to identify entropy with information. Section 4.2 then considers the Szilard Engine version of Maxwell's demon. This has been used as the paradigm thought experiment to demonstrate the relationship between the entropy of a system and the information gained from performing measurements on the system. The final Subsection will consider a 'demonless' version of the thought experiment, used to deny the role of information in understanding the problem. Finally, in Section 4.3 we review what we believe are the key points of contention in Section 4.2, and how we propose to address them in Chapters 5 to 8.

4.1 Statistical Entropy

The attempts to derive the phenomenological laws of thermodynamics from classical mechanics lead to the identification of entropy with a statistical property of a system, rather than an intrinsic property. Unlike other intensive thermodynamic variables (such as mass or energy) the statistical entropy is not expressed as the average over some property of the microstates, but is a property of the averaging process itself. The unfortunate consequence of this is that there may not appear to be a well-defined entropy of an individual system. So, the Boltzmann entropy of a microstate $S_B = k \ln W$ depends upon a particular (and possibly arbitrary) partitioning of phase space, while the Gibbs entropy $S_G = -k \int p \ln p$ depends upon the inclusion of the microstate in a 'representative' (and possibly arbitrary) ensemble. If we were to choose to describe the partition of phase space differently, or include the same microstate in a different ensemble, we would ascribe a different entropy to it.

Attempting to understand how something as fundamental as entropy could be so apparently arbitrary has lead many to suggest that entropy, and its increase, represents a measure of our ignorance about the exact microstate of the individual system:

the idea of dissipation of energy depends on the extent of our knowledge ... [it] is not a property of things in themselves, but only in relation to the mind which perceives them [DD85, pg 3, quoting Maxwell]

irreversibility is a consequence of the explicit introduction of ignorance into the fundamental laws [Bor49]

The entropy of a thermodynamic system is a measure of the degree of ignorance of a person whose sole knowledge about its microstate consists of the values of the macroscopic quantities . . . which define its thermodynamic state [Jay79]

What has happened, and this is very subtle, is that my knowledge of the possible locations of the molecule has changed . . . the less information we have about a state, the higher the entropy [Fey99]

How this ignorance arises, whether it is a subjective or objective property, and why or how it increases with time have been argued in many ways. For example, it is often suggested that the ignorance arises because of the large number of microstates available to macroscopic bodies, and the difficulty of physically determining exactly which microstate the body is in. Similarly, the growth of entropy with time is then identified with the difficulty of following the exact trajectories of a large number of interacting bodies.

A frequent criticism that is raised against this interpretation is that it seems to be implying that the large number of irreversible processes that surround us (gas diffuses, ice melts, the Sun shines) are illusory and occur only because of our lack of detailed knowledge of the exact microstate of the gas, ice cube, or star:

it is clearly absurd to believe that pennies fall or molecules collide in a random fashion *because we do not know* the initial conditions, and that they would do otherwise if some demon were to give their secrets away to us [Pop56]

The discussions and criticisms of this point of view is too large to fully review here [Pop57, Pop74, LT79, DD85, LR90, Red95, Bri96]. Nor will we be dealing with the problem of the origin of irreversibility [HPMZ94, Alb94, Uff01]. Instead we will concentrate on a quantitative link between knowledge (information) and entropy. In particular we will be considering the issues raised by the following problem:

If entropy is a measure of ignorance, and information is a measure of lack of ignorance, how is it that entropy increases with time, while our information, or knowledge, also increases with time?

If we cannot follow the exact microstates of a system, it may appear that our information about the system is decreasing. The knowledge we have about a system, at some given point in time, *when defined in terms of coarse-grained 'observational states'* [Pen70], will provide less and less information about the system as time progresses, due to coarse-grained 'mixing'. This decrease in information will be identical (with a sign change) to the increase in the *coarse-grained* entropy of the system.

On the other hand, the problem arises as we are constantly increasing our knowledge, or information, by observing the world around us. Each observation we make provides us with new information that we did not possess at the earlier time. Does this process of acquiring *new*

information reduce the entropy of the world, and should this be regarded as an apparent violation of the second law of thermodynamics? This is the key paradox which needs to be investigated.

We will quantify our knowledge by using the Shannon-Schumacher measure of information obtained from measurements we perform. The Gibbs-von Neumann entropy is identical in form to this measure, and so will be used for the thermodynamic entropy (we will avoid using 'coarse-grained' entropy as we will be dealing with microscopic systems for which 'observational states' cannot be sensibly defined). We now need to consider how the gain in information from a measurement can be related to the change in entropy of the system that is measured.

4.2 Maxwell's Demon

When we measure a system, we only gain information about it if it was possible for the measurement to have had several different outcomes. In the case of a thermodynamic ensemble, the measurement amounts to the selection of subensembles. The potentially anti-entropic nature of such a selection was first suggested by Maxwell[LR90, and references therein] when he proposed a sorting demon that would, by opening and closing a shutter at appropriate times, allow a temperature difference to develop between two boxes containing gases initially at the same temperature. Once such a temperature difference develops heat can be allowed to flow back from the hotter to the colder, via a Carnot cycle, turning some of it into work in the process. As energy is extracted from the system, in the form of work, the two gases will cool down. The result would be in violation of the Kelvin statement of the second law of thermodynamics:

No process is possible whose sole result is the complete conversion of heat into work.

There have been many variations upon this theme, and attempts to resolve the apparent 'paradox'. 'Demonless' versions like Smoluchowski's trapdoor, or Feynman's ratchet [Fey63] emphasise the manner in which thermal fluctuations develop in the physical mechanism designed to effect the sorting, and prevent the mechanism from operating. A quite different approach was started by Szilard[Szi29] which will concern us here.

The Szilard Engine (Figure 4.1) consists of a single atom (G) confined within a tube of volume V . The tube is in constant contact with a heat bath at temperature T_G , providing a source of energy for the random, thermal kinetic motion of the atom. At some point a piston (P) is inserted in the center of the tube, trapping the atom upon one side or the other, or confining it to a volume $V/2$. If we now attach a pulley and weight (W) to the piston, we may use the collision of the atom against the piston to assist us in moving the piston and lifting the weight. If we consider this as the expansion of a gas from a volume $V/2$ to V then the isothermal work which may be extracted in this manner is $kT_G \ln 2$. At the end of the procedure the atom again occupies the full volume of the tube V and the piston may be reinserted into the center. It appears we have extracted work from heat, in violation of the second law of thermodynamics. This is the essence of the Szilard Paradox.

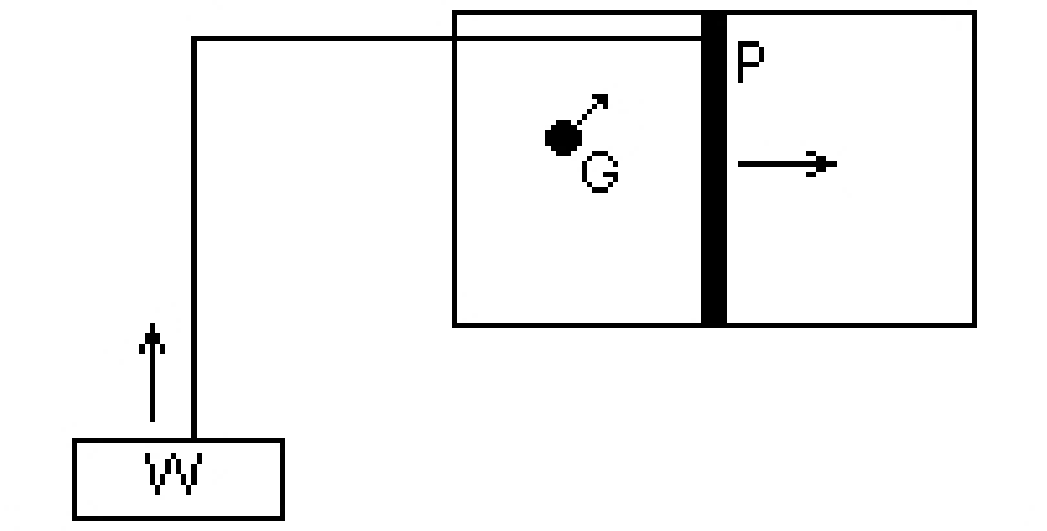


Figure 4.1: The Szilard Engine

Szilard argued that the problem lay in determining upon which side of the piston the atom was located. Without this information, the pulley and weight cannot be connected up to the piston in the correct manner. Having eliminated all other sources of a compensating entropy increase, he concluded that the act of making a measurement must be responsible for an increase in entropy. Thus a 'demon' cannot decrease the entropy of a system by acquiring information about it, without creating at least as much entropy when performing the measurement necessary to acquire the information.

We will now examine the developments of Szilard's idea, and their criticisms.

4.2.1 Information Acquisition

The next major development of Szilard's argument [Bri51, Gab64, Bri56] (referred to as [GB]) tried to quantify the link between the information gained from a measurement and the entropy decrease implied by that measurement. The essence of their development was to demonstrate situations in which the process of acquiring information required a dissipation of energy. The amount of this dissipation more than offset any gain in energy that could be achieved by decreasing the entropy of the system.

Although [GB]'s arguments are no longer supported by the main proponents of an information-entropy link, their physical models are (rather ironically) often still supported by opponents of that link [DD85, EN99, for example] so we will need to give consideration to them here.

[GB] were able to make a quantitative statement of the information gained from a measurement based upon Shannon's work. They then went on to produce models to show that at least as much entropy was created by the physical process by which the information was acquired. Their analysis

was based upon the need for the 'demon' to *see* the location of the atom, and that this required the atom to scatter at least one photon of light. The tube containing the atom at temperature T_G would, in thermal equilibrium, already be filled with photons with a blackbody spectrum. In order to locate the atom accurately, the scattered photon must be reliably distinguishable from a photon whose source was the blackbody radiation. This requires the photon to be of a frequency $\hbar\omega \gg kT_G$. Brillouin later refined this to argue that the minimum frequency for a 50% reliable observation was given by $\hbar\omega = kT_G \ln 2$. This photon would be absorbed by a photo-detector, and the energy in the photon would be lost. This would represent an increase in entropy of the environment of $\frac{\hbar\omega}{T_G} \geq k \ln 2$ which compensates for the entropy decrease in the state of the one atom gas.

Both Gabor and Brillouin generalised from this basic result to claim that any measurement that yielded information would require a dissipation of energy, with an entropy increase at least as large as the information gained. Brillouin, in particular developed a theory of information as negentropy [Bri56], essentially based upon the equivalence of the Shannon and Gibbs formula.

However, it is easy to argue that this equivalence can be ignored, and with it the information link, and instead concentrate upon the physical process involved. We note there are two steps in the above argument: firstly that an information increase occurs when an entropy decrease occurs; and secondly that this information increase requires an entropy expenditure. Given the identical form of the Shannon and Gibbs formulas, this first step may be regarded as an almost trivial relabelling exercise. If we dispense with this relabelling as superfluous, we are still left with the second step, now as an argument that the entropy reducing measurement must involve entropy increasing dissipation, without reference to information at all. This approach is essentially that advocated by [DD85, Section 5.4] and [EN99, Appendix 1].

There are other criticisms of this resolution, however, that rest upon the question of how universal the measurement procedure used by [GB] is. We will examine these next, and will return to the arguments of [GB] in Section 8.3

4.2.2 Information Erasure

The current principal advocates of the Szilard Engine as the paradigm of a quantitative information-entropy link no longer accept the arguments of [GB] [Ben82, Zur84, Zur89a, Zur90a, Cav90, LR90, Cav93, LR94, Sch94, Lef95, Fey99]. Instead they focus upon the need to restore the Engine, and demon, to their initial states to make a cyclic operation. This, they argue, requires the demon's memory to be 'erased' of the information gained from the measurement, and that this erasure requires the dissipation of energy.

The origin of the information erasure argument comes from work on the thermodynamics of computation. The work of Gabor and Brillouin was rapidly developed into an assumption that, for each logical operation, such as the physical measurement or transmission of 1 bit of information, there was a minimum dissipation of $kT \ln 2$ (bit)⁻¹ (and) of

analysing the physical basis of computation, argued that most logical operations can be performed reversibly and have no minimal thermodynamic cost. The only operation which requires the dissipation of energy is the *erasure* of a bit of information, which loses $kT \ln 2$ energy. This has become known as Landauer's Principle. Given the importance attached to this principle, we shall now present a simplified version of Landauer's argument (see also [Lan92]) We shall assume

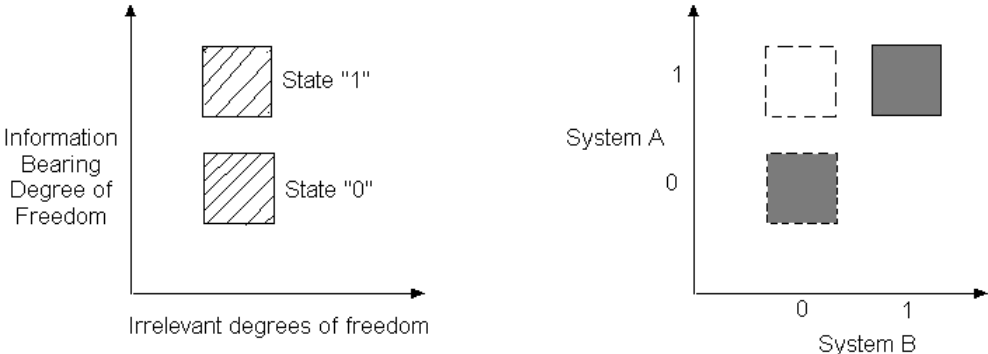


Figure 4.2: Landauer Bit and Logical Measurement

that each logical state of a system has one relevant (information bearing) degree of freedom, and possibly many irrelevant (internal or environmental) degrees of freedom. We will represent this by a diagram such as Figure 4.2(a) where the marked areas represent the area of phase space occupied by the physical representation of the logical state.

A measurement can be represented, in logical terms, by a Controlled-Not (CNOT) gate (Table 4.1), where some System B is required to measure the state of some System A. System A is in one of two possible states, 0 or 1, while System B is initially in the definite state 0 (represented by the areas bounded by dotted lines in Figure 4.2(b) - the 'irrelevant' degrees of freedom now occupying a third axis). After System B interacts with System A, through a CNOT interaction, it moves into the same state as A (the states of the two systems are now represented by the shaded areas). System B has 'measured' System A. The operation is completely reversible. If we allow the systems to interact by the CNOT operation again, they return to their initial states.

The essential point argued by Landauer is that both before and after there are only two possible logical states of the combined system, and the area of phase space occupied by the combined system has not changed. As the entropy is a function of the accessible area of phase space, then the entropy has not increased. The operation is both logically *and* thermodynamically reversible.

The development of [GB]'s work, to argue that each logical operation required a minimal dissipation of energy, is shown to be invalid. A measurement may be performed, and reversed, without any dissipation. Landauer did identify a logical procedure which is inherently dissipative. This was called RESTORE TO ZERO. This operation requires the logical bit, initially in one of the two states as in Figure 4.2(a), to be set to the state zero, regardless of it's initial state, leading

Input		Output	
A	B	A	B
0	0	0	0
0	1	0	1
1	0	1	1
1	1	1	0

Table 4.1: The Controlled Not Gate

to Figure 4.3. The triangles represent the location of the original microstate in Figure 4.2. The "width" of phase space occupied by the information bearing degree of freedom has been reduced from the width of the 0 and 1 states to the width of the 0 state. To satisfy Liouville's theorem, the "width" occupied by the *non-information* bearing degrees of freedom must be doubled. This amounts to the increase of entropy of the environment by a factor of $k \ln 2$. If the environment is a heat bath at temperature T , then we must dissipate at least $kT \ln 2$ energy into the heat bath.

Landauer was not principally concerned with issues such as the Szilard Engine, and it was left to Bennett[Ben82] to re-examine the exorcism of Maxwell's demon. Bennett's analysis accepted that the Demon did not have to dissipate energy to measure the location of the atom. Instead, he argues the demon has acquired one bit of information, and that bit of information must be stored somewhere in the demon's memory. After the demon has extracted $kT_G \ln 2$ energy from the expansion of the one atom gas, the demon is left with a memory register containing a record of the operation. In order to complete the cycle, the demon's memory must be restored to its initial, clear, state. This requires a RESTORE TO ZERO operation, which, by the Landauer Principle, will dissipate $kT_G \ln 2$ energy. This exactly compensates for the energy gained from the expansion of the gas. A similar conclusion was reached by [Pen70, Chapter VI].

This then forms the basis of the argument forging a quantitative link between entropy and information theory. We will summarise it as follows:

- Entropy represents a state of ignorance about the actual state system;
- When an observer makes a measurement upon a system, she gains information about that system, and so reduces her ignorance;
- This does indeed reduce the entropy of the observed system, by an amount equal to the gain in Shannon information from the measurement;
- However, she must store this information in her memory;
- To perform this operation cyclically the memory must be erased;
- By Landauer's Principle, the erasure must dissipate energy equal to the temperature times the Shannon information erased, compensating for the entropy gain due to the measurement.

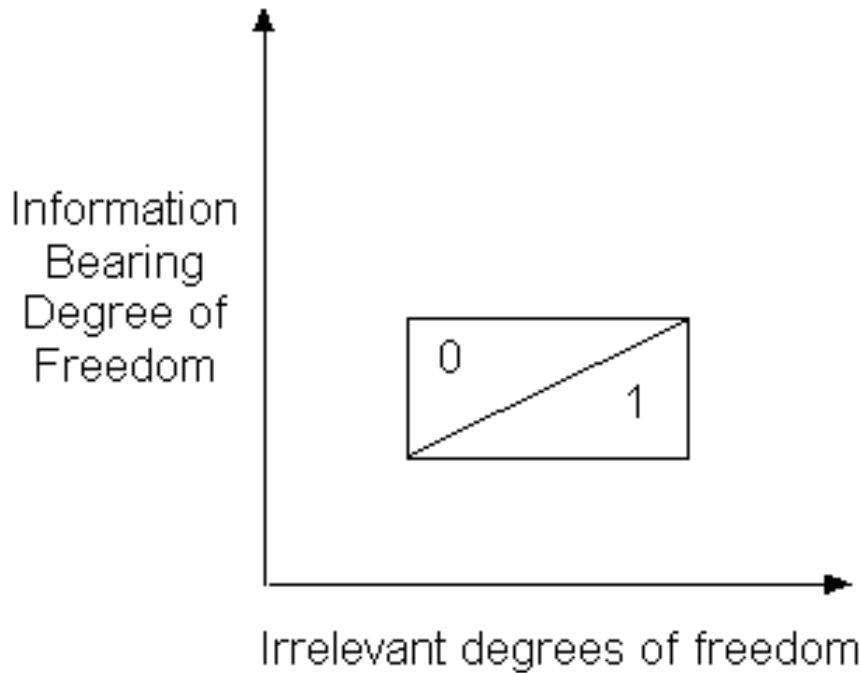


Figure 4.3: Bit Erasure

Perhaps the clearest problem in this 'resolution' of Maxwell's Demon is the circularity of the argument. Landauer's Principle, that the 'erasure' of a bit of information costs $kT \ln 2$ energy, was derived by Landauer *on the assumption that the second law is true*. It's use by Bennett to prove that the second law is *not* violated is appealing to the truth of the very point which is in doubt. This is what Earman and Norton[EN98] refer to as the "sound vs. profound" dilemma of the information theoretic resolution, and undermines confidence in its universality.

We will now review the main counter-example to the information-entropy link using Szilard's Engine.

4.2.3 "Demonless" Szilard Engine

In this Subsection we will examine the question, first raised by Popper, of whether it is possible to construct a "demonless" version of Szilard's Engine. The issues raised by this will form the basis of the analysis of Szilard's Engine in the subsequent Chapters.

The "demonless" Engine has been suggested many times by critics of the information-entropy link[Pop57, Fey66, JB72, Cha73, Pop74], to demonstrate that a measurement is unnecessary to understand the operation of the Engine. Unfortunately, both the consequence of these modifications, and their criticism, have been poorly thought out, and leave the question of a violation of

the second law of thermodynamics unanswered.

We will present a simple modification of the "demonless" Engine to answer criticisms that have been made of this approach, and which appears to lead to a systematic entropy reduction. The detailed analysis of this version of the Engine, and showing where and how it fails, will occupy the following three Chapters, and will be used to critically examine the resolution of the Maxwell's Demon problem. The simplest version of the "demonless" engine is described by

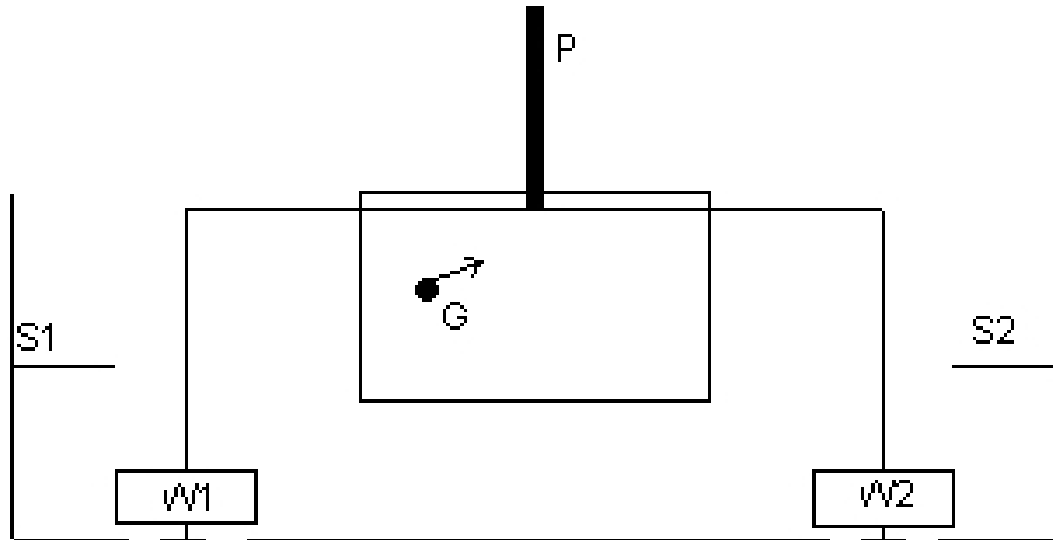


Figure 4.4: The Popper version of Szilard's Engine

Feyerabend[Fey66] (Figure 4.4). The essence of this is that weights are attached on each side of the partition, and rest upon a floor. If the atom, G, is located on the left when the piston, P, is inserted, then the piston will move to the right, raising the left weight, W1, and leaving the right weight, W2, on the floor. If G is located to the right, then W2 will be raised and W1 will remain upon the floor. The height that a weight of mass M can be raised through is $\frac{kT_G}{Mg} \ln 2$. The result is that heat has apparently been used to lift a weight against gravity, without the need for a demon to perform a measurement, dissipative or not.

It is very unclear whether this version should be taken as a violation of the second law. Feyerabend certainly takes the situation at face value and claims this is a perpetual motion machine. Popper [Pop74] argues that the machine works only because it contains only a single atom, and that the atom only occupies a small fraction of the volume of the cylinder at any one time, so its entropy is not increasing. Only if the gas were composed of many atoms would it make sense to describe it as expanding. Similarly, Chambadal[Cha73] argues that thermodynamic concepts are only applicable to many-body systems, so that the Szilard Engine has nothing to do with entropy, and Jauch and Baron[JB72] claim the example is invalid because inserting the partition violates the ideal gas laws ¹.

¹Jauch and Baron earlier state that a demon is unable to operate a Szilard Engine because of thermal fluctuations,

The logic of these arguments is hard to follow. They seem to accept that heat can be used to lift a weight, and may continue to do so, without any compensating dissipation. If this is the case, the fact that a single atom gas has been used is irrelevant: the Kelvin statement of the second law of thermodynamics has been violated. The fact that the amount of energy obtained in this way is small is also irrelevant. Advances in nanotechnology and quantum computing develop technologies that allow the manipulation of the states of individual atoms. It is conceivable that, in the not-too-distant future, it would be possible to construct an engine consisting of a macroscopically large number of microscopic Popper-Szilard Engines. As long as each engine could reliably transfer a small amount of heat to work per cycle, we would be able to extract significant amounts of work directly from the temperature of the environment.

Unfortunately many objections to the Popper-Szilard Engine are equally obscure. [dBT74, Rot79] appear to argue that it is the design of the engine that now embodies the 'information' that balances the entropy reduction. However, this can hardly be supported, as such 'structural negentropy' is a one-off cost, while the engine, once built, could extract unlimited energy. Others [Bri96][SB98, page74] appear to confuse the Engine with Feyerabend and Popper's opinions on Brownian motion[Pop57, Pop74, Fey93].

However, there are two objections to the Popper-Szilard Engine which do require consideration. These are due to Leff and Rex[LR90, pages 25-28] and to Zurek[Zur84] and Biedenharn and Solem[BS95].

Leff and Rex offer an argument based upon Landauer's Principle. They argue that, at the end of the cycle, when one of the weights has been raised, the location of the piston and pulleys serves as a memory of the location of the atom. In order to commence the new cycle, the piston must be removed from either end of the container, and reinserted in the center. This constitutes an 'erasure' of the memory and must be accompanied by a $kT_G \ln 2$ dissipation.

It is certainly the case that the analysis of the Popper-Szilard Engine leaves out how this restoration is to take place without having to perform a measurement of the position of the piston. In order to see if Leff and Rex's criticism is justified, we will now suggest a method by which the restoration may take place.

In Figure 4.4 there are two shelves, S1 and S2, on the left and right of the Engine, at a height $\frac{kT_G}{Mg} \ln 2$ above the floor. When the gas has expanded, these shelves emerge on both sides of the Engine. This will support whichever weight has been raised. There is now a correlation between the location of the weights and the position of the piston. By means of the reversible CNOT interaction (Table 4.1 and Figure 4.2(b)) we can use the location of the raised weights as System A and the piston as System B. The correlation of the logical states "0" and "1" is equivalent to that between the states of the piston and weights. If W1 is raised the piston is to the right while if W2 is raised, the piston is to the left. This should allow us to conditionally remove the piston from whichever end of cylinder it is in and move it to the central position outside the cylinder. This but give no explanation of how these thermal fluctuations enter into their actual analysis of the Engine later

would appear to be in complete agreement with Landauer's Principle, without having to perform an external measurement, or dissipate energy.

Of course, it may be argued that now we have the weight to restore to its unraised position before we have truly 'completed' a cycle². An obvious way of doing this is to pull the shelves back and allow the raised weight to fall inelastically to the floor, dissipating the $kT_G \ln 2$ energy required to raise it. This appears to confirm the resolution based upon Landauer's Principle. However, this is deceptive.

To dissipate the raised energy, the weights must be in contact with an environment at some temperature (we will assume a heat bath located below the floor). Nothing so far has required that the heat bath of the weight need be the same as the heat bath of the one atom gas (we will also assume that the partition and pulleys are perfect insulators). Consider what happens if the heat bath into which the weight dissipates its energy is at a *higher* temperature than T_G . Now we appear to have completed the cycle, to the satisfaction of everyone, and have apparently satisfied the Landauer Principle. Unfortunately, we have also reliably transferred energy from a colder heat bath to a hotter one, and can continue to do so. Such a state of affairs would still constitute a violation of the second law of thermodynamics, according to the Clausius version:

No process is possible whose sole result is the transfer of heat from a colder to a hotter body

We could now attach a small Carnot engine between the two heat baths and allow the same small amount of energy to flow back by conventional means, extracting some of it as work in the process. It is far from clear that information theory is of any use in identifying where the argument above must fail.

The second objection, due to Zurek³, is more subtle. Zurek argues that quantum measurement plays a role in preventing the demonless Engine from operating. A classical atom is trapped on one side or other of the piston, when it is inserted. The demonless Engine seeks to exploit this without making a measurement, to prove that the "'potential to do work' [is] present even before ... a measurement is performed" [Zur84].

For a quantum object, the situation is more complex:

The classical gas molecule, considered by Szilard, as well as by Jauch and Baron, may be on the unknown side of the piston, but cannot be on 'both' sides of the piston. Therefore intuitive arguments concerning the potential to do useful work could not be unambiguously settled in the context of classical dynamics and thermodynamics. Quantum molecule, on the other hand, can be on 'both' sides of the potential barrier,

²It could be objected that raising the weight is precisely the 'work' that we were trying to achieve. To demand that all weights be restored to their initial conditions appears a vacuous way of ensuring that 'work' cannot be extracted. This shows that even the concept of 'work' needs to be clarified.

³This objection was endorsed by [BS95] although they disagree with the information interpretation of entropy

even if its energy is far below the energy of the barrier top, and it will 'collapse' to one of the two potential wells only if [it] is 'measured' [Zur84]

This is non-intuitive . . . but quantum mechanics is unequivocal on this point . . . the objections of Popper and Jauch and Baron - that the Szilard engine could extract energy without requiring any observation - is clearly wrong. Even with the shutter closed, the single-molecule gas has both sides available for its thermal wave function. Observation is require to isolate it on one side or the other. [BS95]

If true, this would certainly invalidate the arguments of Jauch and Baron, Popper and Feyrabend, and would make the act of quantum measurement a fundamental part of reducing the entropy of an ensemble by gaining information about it's microstate. The attempt to connect 'wavefunction collapse' with entropy changes is widespread[Neu55, WZ83, Lub87, Par89a, Par89b, Alb94], although it is usually associated with an entropy *increase*. If Zurek's argument here holds good, this calls into question how 'no-collapse' versions of quantum theory, such as Bohm's or the Many-Worlds Interpretation could explain the Szilard Engine. Unfortunately, neither Zurek nor Biedenbarn and Solem actually demonstrate that the piston does not move.

Zurek calculates the Free Energies, based upon the quantum partition function, to justify the argument that the gas can only lift a weight if it is completely confined to one side or the other. This requires us to assume that the statistical Free Energy is a valid measure of the 'potential to do work'. A little thought should show that this will *only* be the case if the second law of thermodynamics is known to be valid, and this is precisely the point which is under contention.

Biedenbarn and Solem simply state that "the pressure on both sides of the shutter is the same, the piston remains stationary" without showing their calculations. They proceed to argue that the act of observation must perform work *upon* the gas, and it is this work which is extracted in the subsequent expansion. Again, however, they do not provide a convincing demonstration of how this work is performed.

This leaves the quantum superposition argument an intriguing possibility to block the operation of the modified Popper-Szilard Engine, but essentially incomplete. We will address this by constructing an explicitly quantum mechanical version of the Popper-Szilard Engine in the next Chapter.

4.3 Conclusion

The thorough analysis of the points of contention regarding the Szilard Engine has lead us to construct a modified version of it which, aside from the question of quantum superposition, appears to be capable of producing anti-entropic behaviour. The operation of this Engine is summarised in Figure 4.5 In Stage (a), the piston is inserted into the box, which contains a single atom in contact with a heat bath. Stage (b) shows how the pressure of the atom on the piston, from the left, causes the lefthand weight to be lifted. The righthand weight remains at rest upon the floor. In Stage (c),

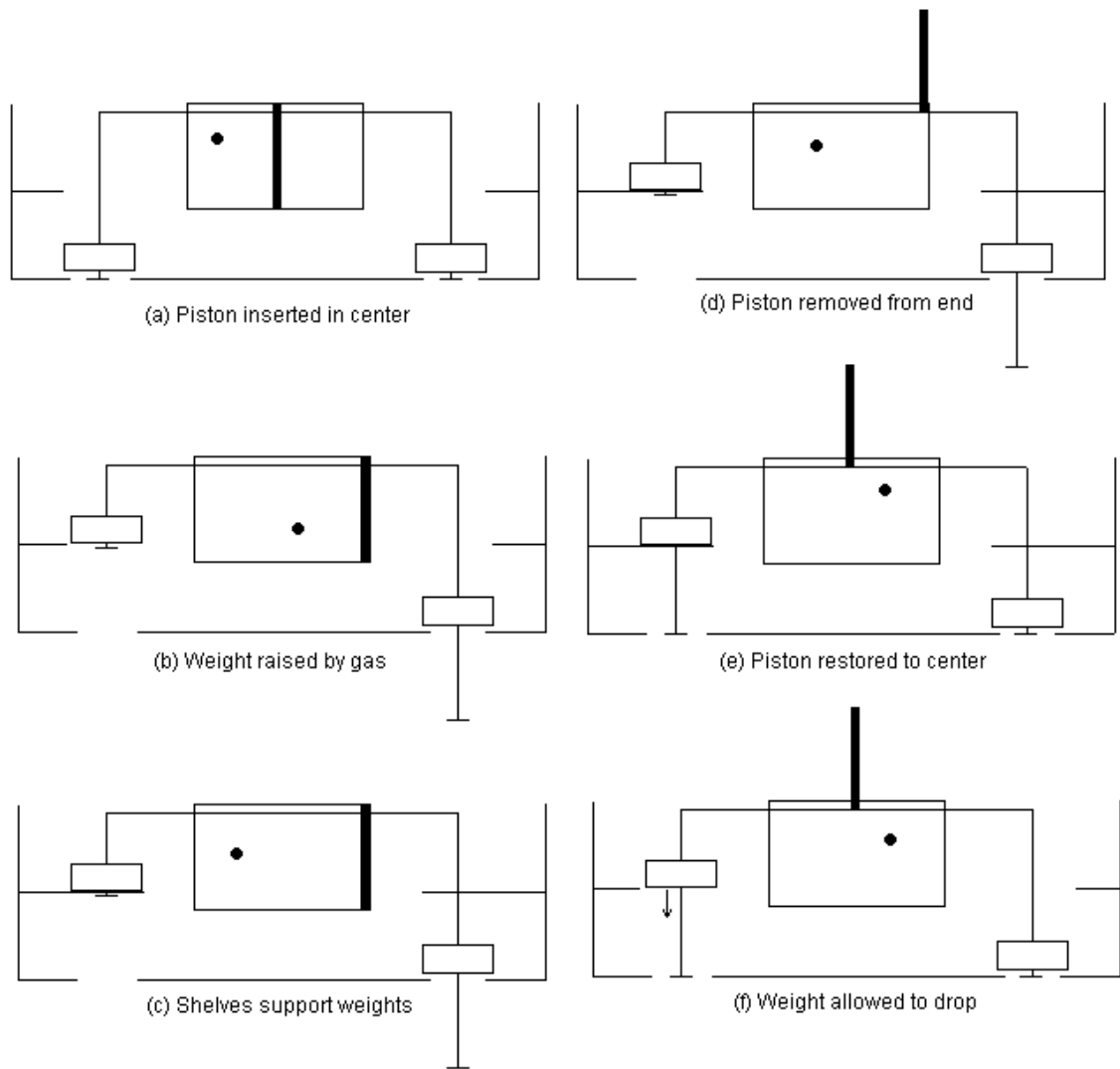


Figure 4.5: The Cycle of the Popper-Szilard Engine

moveable shelves come out on both sides, and support whichever weight has been raised. Stage (d) removes the piston from the box. In this case it is on the righthand side. It's position outside the box is correlated to the position of the raised weight. Stage (e) uses this correlation to reset the piston, by means of a Controlled-NOT type interaction. The 'information' as to which side of the box originally contained the atom is now recorded in the location of the raised weight. If we now remove both shelves, whichever weight is raised will fall to the floor. This dissipates the energy used to raise it, and restores the machine to it's initial state. However, if the weight is in contact with a *higher* temperature heat bath than the atom, then heat has been transferred from a colder to a hotter heat bath, in apparent violation of the second law of thermodynamics.

A detailed analysis of the physics of this cycle will be pursued in Chapters 5 and 6. We will not assume any thermodynamic relationships which depend upon the second law for their validity. We will start by examining the interactions between the microscopic states of the Engine. When

we have thoroughly analysed the time evolution of the system at the level of individual quantum states, we will introduce a statistical ensemble of these states, by means of density matrices. This will enable us to calculate the mean, and long term, behaviour of the Engine, and show that, in the long term, it is not capable of producing heat flows which violate the Clausius statement.

The central issues that must be addressed, when constructing the quantum mechanical Popper-Szilard Engine, are:

1. What is involved in the process of 'confining' the particle to one side of the box? Does this require only the inserting of a potential barrier in the center of the box or must there also be a 'measurement' upon the position of the particle?
2. Does this 'confining' require an input of energy to the system? This input of energy may come through perturbing existing eigenvalues, or by a transition between eigenstates. The effect on energy expectation values of both of these processes must be calculated.
3. Can a piston in the center of the box move, when the gas is still in a superposition of being on both sides of the box?
4. Can this movement be coupled to a pulley, to lift a weight? Two weights may be involved.
5. Can the partition be restored to the center of the box without making an external measurement?

Only after we have done this will we introduce the concepts of entropy and free energy, in Chapter 7. Our introduction of these concepts will be justified on the basis of the analysis of the previous chapters, rather than the reverse. We will show that these concepts are valid, even for single atom systems, and that the entropy of the Engine is always increasing.

Finally, in Chapter 8 we will use the thermodynamic concepts to generalise the resolution beyond the specific case of the Popper-Szilard Engine. We will show that this generalisation resolves the problems found in our discussion of the Szilard Engine and Maxwell's Demon above, and provides a complete answer to the Szilard Paradox. This will show that the information theoretic resolutions are both unnecessary and insufficient. The Szilard Engine is unsuccessful as a paradigm of the information-entropy link.

Chapter 5

The Quantum Mechanics of Szilard's Engine

In Chapter 4 we reviewed the historical analysis of the Maxwell's Demon, and Szilard Engine thought experiments. In particular the question was raised of whether information processing or quantum measurement was an essential part of understanding these problems.

In this Chapter we will analyse the quantum mechanics of the operation of the Szilard Engine. We are particularly interested in whether the arguments of [Zur84] or [BS95] regarding the role of quantum measurements are valid. To complete the analysis of the Szilard Engine, the machine must be connected up to statistical mechanical heat reservoirs. The effects of the resulting statistical considerations will be examined in Chapter 6.

We can summarise the two issues that need to be assessed in each stage of the operation of the quantum Szilard Engine as:

1. Can the operation proceed without an external agent ('demon') needing to acquire and make conditional use of knowledge of the systems microstate?
2. Can the transformation be achieved without making a significant alteration in the internal energy of the Engine? In other words, does it require work upon the system in order to drive its operation?

This Chapter will be primarily concerned with the first question, although it will also calculate changes in internal energy of specific microstates. The complete answer to the second question will need consideration of the statistics of thermal ensembles in Chapter 6.

In order to analyse the questions above, it will, of course, be necessary to make a number of abstractions and idealisations. All motion is, as usual, considered to be frictionless. In the absence of thermal heat baths, the systems are not decoherent so pure states will evolve into pure states, not density matrices. In Appendix C we argue that the requirement that no measurements are performed upon the system by external agents ('Demons' and the like), is equivalent to the

requirement that a single unitary operator is capable of describing the evolution of the system. Rather than attempt to construct explicit Hamiltonians for the interaction between parts of the Szilard Engine, we will focus upon the question of how to describe the evolution of the engine in terms of unitary operators. If the required evolution is unitary, then there is *some* Hamiltonian that, in principle, could be used to construct a suitable Engine. This approach will enable us to make more general conclusions than if we were to attempt to solve a particular Hamiltonian. We nevertheless will show that the essential properties of our idealised unitary evolution operators are the same as those that would result from a more realistically constructed Hamiltonian.

The evolution of the quantum states of the Szilard Engine will be studied in six sections. We will avoid introducing any external measuring devices, and will concentrate upon the constraints that unitarity imposes upon the evolution of the system. The sections are:

1. The unperturbed eigenstates of the particle in a box of width $2L$. This is a standard quantum mechanical problem. Hereafter, the particle in the box will be referred to as a 'gas';
2. The perturbation of these eigenstates as a potential barrier of width $2d$ ($d \ll L$) is raised in the center of the box, up to an infinite height. This must be considered in detail as [JB72] have pointed out the gas laws cannot be relied upon for a single atom. The adiabatic transition was analysed essentially correctly by [Zur84, BS95], but more detail is presented here. Further, an error in the asymptotic form of the energy eigenvalues given by Zurek is examined and corrected;
3. The barrier is replaced by a moveable piston, also treated as a quantum system. The effect of the interaction pressure from the gas is analysed on both sides of the piston, and then combined into a single time evolution operator;
4. The quantum state of the weight to be lifted against gravity is analysed. Again, this is a standard problem, with solutions given by Airy functions. An evolution operator is constructed to connect the weight, piston and gas;
5. The problem of restoring the piston to the center of the box is analysed in terms of unitary operators, which will be shown to require correlating the movement of the piston to the final state of the raised weights. However, it is found that the quantum state of the weight leads to an uncertainty in the operation of the resetting mechanism. This uncertainty leads to the possibility of the Engine going into reverse. The effects of this reversal will be evaluated in Chapter 6;
6. The conclusion of Sections 5.3 and 5.4 is that, if the gas is capable of raising a weight when the gas is confined to one side of the piston (which is generally accepted), then it can still raise a weight when the single-atom gas is in a superposition on both sides of the piston. This is contrary to the analysis of [Zur84, BS95] and calls into question the role that the demon is alleged to play in either of their analysis. Some of the objections of

[Pop74, Pop56, Fey66, JB72, Cha73] are therefore shown to be valid in the quantum domain. This constitutes the main result of this Chapter. However, the problem of restoring the system, including piston, to its initial state has only been partially resolved and can only be fully evaluated in the next Chapter.

5.1 Particle in a box

We start by analysing the eigenstates of the one atom gas in the engine, before any potential barrier or piston is inserted. The one atom gas occupies the entire length of the Szilard Box, as in Figure 4.1. The Hamiltonian for the atom in the box is then

$$H_{CO}\Psi_n = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi_n \quad (5.1)$$

with

$$V(x) = \left\{ \begin{array}{ll} \infty & (x < -L) \\ 0 & (-L < x < L) \\ \infty & (x > L) \end{array} \right\}$$

This is the standard particle in an infinite square well potential, with integer n solutions of energy

$$E_n = \frac{\hbar^2 \pi^2}{8mL^2} n^2$$

It will be easier to divide these into odd ($n = 2l$) and even ($n = (2l - 1)$) symmetry ¹ solutions and make the substitutions

$$\begin{aligned} K_n &= L \frac{\sqrt{2mE_n}}{\hbar} \\ X &= \frac{x}{L} \\ \epsilon &= \frac{\hbar^2 \pi^2}{8mL^2} \end{aligned}$$

Odd symmetry solutions

$$\begin{aligned} \psi_l &= \frac{1}{\sqrt{L}} \sin(K_l X) \\ E_l &= 4\epsilon l^2 \end{aligned} \quad (5.2)$$

Even symmetry solutions

$$\begin{aligned} \psi_l &= \frac{1}{\sqrt{L}} \cos(K_l X) \\ E_l &= 4\epsilon \left(\frac{2l - 1}{2} \right)^2 \end{aligned} \quad (5.3)$$

¹Unfortunately odd symmetry solutions have even values of n and vice-versa. Odd and even will exclusively be used to refer to the *symmetry* properties.

5.2 Box with Central Barrier

We now need to consider the effect of inserting the partition into the Szilard Engine (Figure 4.5(a)). It will be simplest to follow Zurek, and treat this as a potential barrier of width $2d$ ($d \ll L$), and variable height V , in the center of the box:

$$V(x) = \left\{ \begin{array}{ll} \infty & (x < -L) \\ 0 & (-L < x < -d) \\ V & (-d < x < d) \\ 0 & (d < x < L) \\ \infty & (L < x) \end{array} \right\}$$

Initially the barrier is absent, $V = 0$. As the partition is inserted, the barrier rises, until, when the partition is fully inserted, dividing the box in two, the barrier has become infinitely large, $V = \infty$. This is a time dependant perturbation problem as the barrier height V is a function of time. The instantaneous Hamiltonian, for a barrier height V , can be written in terms of the instantaneous eigenstates and eigenvalues as:

$$H_{G1}(V) = \sum_l \{ E_l^{odd}(V) |\Psi_l^{odd}(V)\rangle \langle \Psi_l^{odd}(V)| + E_l^{even}(V) |\Psi_l^{even}(V)\rangle \langle \Psi_l^{even}(V)| \}$$

The adiabatic theorem (see [Mes62, chapter 17] and Appendix C) shows that if the barrier is raised sufficiently slowly, the n 'th eigenstate will be continuously deformed without undergoing transitions between non-degenerate eigenstates. The unitary evolution operator for the rising barrier is then approximated by

$$U_G(t) \approx \sum_l \left\{ \begin{array}{l} e^{\frac{i}{\hbar} \int^t E_l^{odd}(\tau) d\tau} |\Psi_l^{odd}(V)\rangle \langle \Psi_l^{odd}(0)| \\ + e^{\frac{i}{\hbar} \int^t E_l^{even}(\tau) d\tau} |\Psi_l^{even}(V)\rangle \langle \Psi_l^{even}(0)| \end{array} \right\} \quad (5.4)$$

As this is from a time dependant Hamiltonian, it is not energy conserving. In agreement with Zurek, and Biedenharn and Solem, we will not regard this as a problem, as long as the change in energy caused by inserting the potential barrier can be shown to be negligible when compared to the energy extracted by the engine (this will be shown in Chapter 6).

The problem of raising the potential barrier is now that of solving the stationary Schrödinger equation for an arbitrary barrier height V . This is analysed in detail in Appendix D. It is shown (see Figure D.1) that the energy eigenvalues and eigenstates change continuously from the zero potential barrier to the infinitely high barrier.

The main results of Appendix D are now summarised, for the limit of a high potential barrier, $V \gg E$ and $p = d/L \ll 1$.

Odd Symmetry

$$\Psi \approx \left\{ \begin{array}{ll} \frac{1}{\sqrt{L(1-p)}} \sin(K_{al}(1+X)) & (-1 < X < -p) \\ \frac{1}{L} \left(\frac{K_{al}}{K_{cl}} \right) \frac{e^{-K_{cl}(p-X)}_l e^{-K_{cl}(p+X)}}{\sqrt{(1-p)}} & (-p < X < p) \\ -\frac{1}{\sqrt{L(1-p)}} \sin(K_{al}(1-X)) & (p < X < 1) \end{array} \right. \quad (5.5)$$

$$\begin{aligned}
K_{al} &\approx \frac{l\pi}{(1-p)} \left(1 - \frac{(1-2e^{i2K_{cl}p})}{K_{cl}(1-p)} \right) \\
E_l &\approx \epsilon \left(\frac{2l}{(1-p)} \right)^2 \left(1 - 2 \frac{(1-2e^{i2K_{cl}p})}{K_{cl}(1-p)} \right) \\
K_{cl}p &\approx \frac{d\sqrt{2mV}}{\hbar} \gg 1
\end{aligned}$$

Even Symmetry

$$\begin{aligned}
\Psi &\approx \begin{cases} \frac{1}{\sqrt{L(1-p)}} \sin(K_{al}(1+X)) & (-1 < X < -p) \\ \left(\frac{p}{L}\right)^l \left(\frac{K_{al}}{K_{cl}}\right) \frac{e^{-K_{cl}(p-X)} + e^{-K_{cl}(p+X)}}{\sqrt{(1-p)}} & (-p < X < p) \\ \frac{1}{\sqrt{L(1-p)}} \sin(K_{al}(1-X)) & (p < X < 1) \end{cases} \quad (5.6) \\
K_{al} &\approx \frac{l\pi}{(1-p)} \left(1 - \frac{(1+2e^{i2K_{cl}p})}{K_{cl}(1-p)} \right) \\
E_l &\approx \epsilon \left(\frac{2l}{(1-p)} \right)^2 \left(1 - 2 \frac{(1+2e^{i2K_{cl}p})}{K_{cl}(1-p)} \right) \\
K_{cl}p &\approx \frac{d\sqrt{2mV}}{\hbar} \gg 1
\end{aligned}$$

The l^{th} odd and even eigenstates become degenerate² in the limit, with energy levels $E_l = \epsilon \left(\frac{2l}{1-p} \right)^2$.

As the adiabatic theorem shows we can insert the barrier without inducing transitions between states, the only energy entering into the system when inserting the partition is the shift in eigenvalues. From the above results the energy level changes are

$$\begin{array}{ccc}
V = 0 & V = E & V = \infty \\
\text{Odd} & \epsilon (2l)^2 & \epsilon (2l)^2 & \epsilon \left(\frac{2l}{1-p} \right)^2 \\
\text{Even} & \epsilon (2l-1)^2 & \epsilon \left(\frac{2l-1}{1-p} \right)^2 & \epsilon \left(\frac{2l}{1-p} \right)^2
\end{array}$$

The fractional changes in odd and even symmetry energies, respectively, are

$$\frac{E(\infty) - E(0)}{E(0)} = \begin{cases} \frac{p(2l-p)}{(1-p)^2} & \approx 2p \\ \frac{p(2l-p)}{(1-p)^2} + \frac{4l-1}{(1-p)^2(2l-1)^2} & \approx 2p + \frac{1+2p}{l} \end{cases}$$

where the approximations assume $p \ll 1$ and $l \gg 1$. In both cases it can be seen that the energy added is a small fraction of the initial energy. However, for low energy even states, where $l \gg 1$ is not valid, relatively large amounts of energy must be added even when $p \ll 1$. For example $l = 1$ leads to $\Delta E \approx 3E(0)$. Some work must be done upon the gas to insert the partition. The size of this work required will be evaluated in Section 6.2 as part of the statistical mechanics of the system.

These results can be best understood in terms of the wavelength of the eigenstate in the region where the potential barrier is zero

$$\lambda_l = 2\pi K_{al}L$$

²The question of whether the asymptotic degeneracy of the odd and even solutions represents a problem for the application of the adiabatic theorem can be answered by noting that, as the perturbing potential is symmetric, then the probability of transition between odd and even solutions is always zero.

The number of nodes within the box is $2L/\lambda_l$, as the box is of width $2L$. The energy of the eigenstate is directly related to the *density of nodes* within the box.

The odd symmetry wavefunctions are simply expelled from the region of the barrier, without changing the number of nodes. The same number of nodes are therefore now confined in a volume reduced by a factor $1 - p$. The wavelength must decrease by this factor, leading to an increase in energy levels.

Even symmetry wavefunctions must, in addition, become zero in the center of the box, as the barrier becomes high. This requires an additional node, increasing their number to the same as the next odd symmetry wavefunction. The wavelength must decrease sufficiently so that the original number of nodes, plus one, is now confined to the reduced volume. This is a higher increase in density of nodes than the corresponding odd symmetry, but as the original number of nodes increases, the effect of the additional node becomes negligible.

In the limit of very high barriers, the wavefunctions become

$$\begin{aligned}\Psi_l^{even} &\approx \Psi_l^{odd} \approx \frac{1}{\sqrt{L(1-p)}} \sin\left(l\pi \frac{1+X}{1-p}\right) & (-1 < X < -p) \\ \Psi_l^{even} &\approx \Psi_l^{odd} \approx 0 & (-p < X < p) \\ \Psi_l^{even} &\approx -\Psi_l^{odd} \approx \frac{1}{\sqrt{L(1-p)}} \sin\left(l\pi \frac{1-X}{1-p}\right) & (p < X < 1)\end{aligned}$$

As these are degenerate, we may form energy eigenstates from any superposition of these states

$$\Psi_i(r, \alpha) = r e^{i\alpha} \Psi_i^{even} + \sqrt{1-r^2} e^{i\alpha} \Psi_i^{odd}$$

Figure 5.1 shows the probability density $|\Psi_1(\frac{1}{2}, \alpha)|^2$ as α varies between $-\pi/4$ and $3\pi/4$. Of particular interest are the pair of orthogonal states that occur when $\alpha = 0$ and $\alpha = \pi/2$

$$\begin{aligned}\Psi_l^\lambda &= \frac{1}{\sqrt{2}} (\Psi_l^{even} - \Psi_l^{odd}) \\ &= \begin{cases} \sqrt{\frac{2}{L(1-p)}} \sin\left(l\pi \frac{1+X}{1-p}\right) & (-1 < X < -p) \\ 0 & (-p < X < 1) \end{cases} \\ \Psi_l^\rho &= \frac{1}{\sqrt{2}} (\Psi_l^{even} + \Psi_l^{odd}) \\ &= \begin{cases} 0 & (-1 < X < p) \\ \sqrt{\frac{2}{L(1-p)}} \sin\left(l\pi \frac{1-X}{1-p}\right) & (p < X < 1) \end{cases}\end{aligned}$$

These represent situations where the one atom gas is located entirely on the left or the right of the partition, respectively. When we consider the system with the partition fully inserted, the natural inclination is to describe the Hilbert space by a basis in which the one-atom gas is confined to one side or the other. The Ψ_l^λ and Ψ_l^ρ provide this basis and allow us to write the final Hamiltonian in the form:

$$H_{G1} = \frac{4\epsilon}{(1-p)^2} \sum_l l^2 (|\Psi_l^\lambda\rangle \langle \Psi_l^\lambda| + |\Psi_l^\rho\rangle \langle \Psi_l^\rho|) \quad (5.7)$$

We can now start to consider Zurek's argument that the one-atom gas must be measured to be confined to one side or the other of the Szilard Engine. Suppose the gas is initially in an even

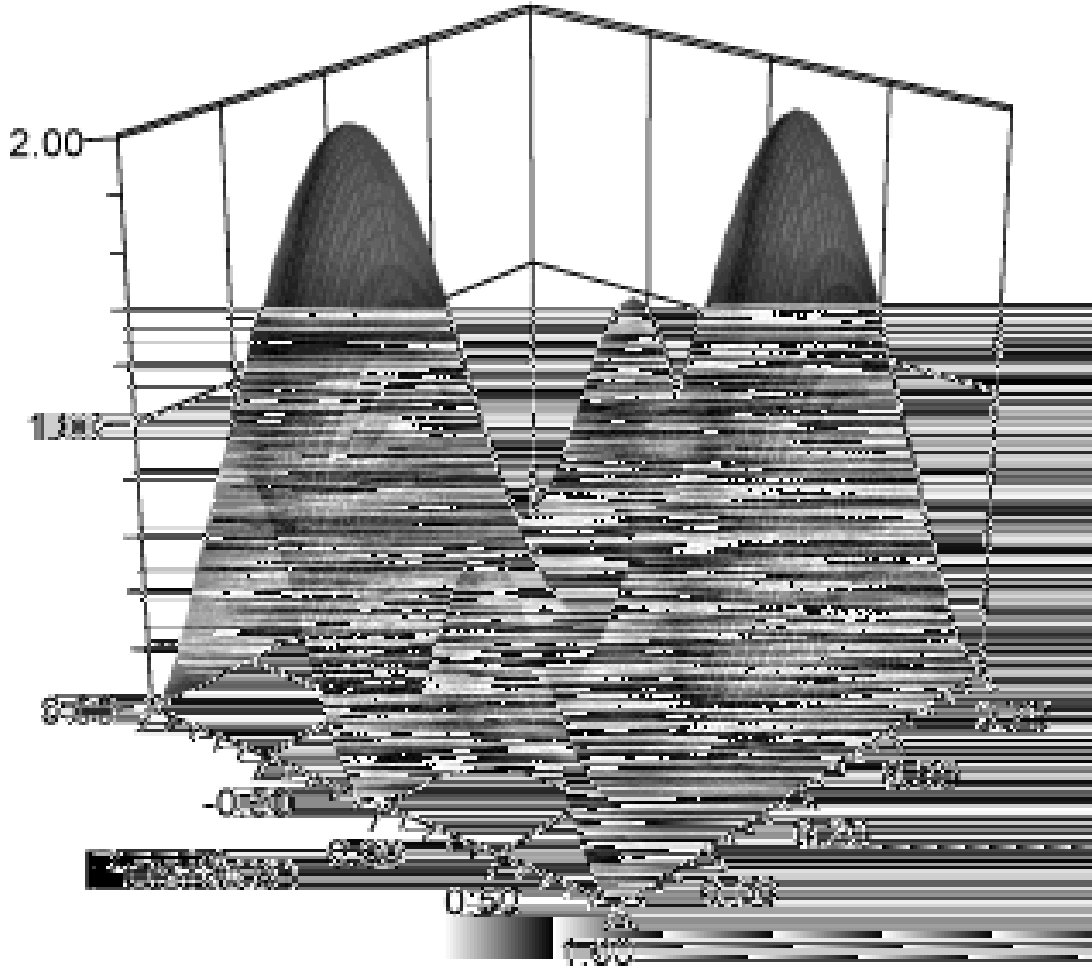


Figure 5.1: Superpositions of odd and even symmetry states

symmetry eigenstate $\Psi_l^{even}(0)$, with no barrier. As the barrier is gradually inserted this eigenstate is deformed continuously through $\Psi_l^{even}(V)$ until in the limit it reaches $\frac{1}{\sqrt{2}} (\Psi_l^\lambda + \Psi_l^\rho)$. The single atom is not confined, or in a mixture of states, but is in a superposition of being on both sides of the barrier. The same will be true if we had started with an odd symmetry eigenstate.

It is worth noting, though, that if we had started with a superposition of energy eigenstates³

$$\Psi = \frac{1}{\sqrt{2}} (\Psi_l^{even}(0) - \Psi_l^{odd}(0))$$

the adiabatic insertion of the potential barrier leads to the state Ψ_l^λ . This *is* confined entirely to the left of the barrier. A similarly constructed initial state leads to the one-atom gas being confined entirely to the right of the barrier. In order to draw a conclusion about the effect of the quantum superposition upon the Szilard Engine we will need to explicitly construct the full

³Ignoring a trivial, time dependant phase factor that arises between the odd and even symmetry states as their energy levels change by different quantities

interaction between the one-atom gas and the piston itself. This will be performed in Section 5.3, below.

5.2.1 Asymptotic solutions for the HBA, $V \gg E$

In this subsection we will briefly investigate a discrepancy between Zurek's results, and those given above. The expressions derived for energy eigenvalues in Appendix D differ from those presented in [Zur84]. We will compare these two expressions with the numerical solutions to the eigenvalue equations, and show that the HBA solutions are a closer match to the numerical results.

In the High Barrier Approximation (HBA), the eigenvalues differ only by an energy splitting:

$$\begin{aligned} E_l^{even} &\approx 4\epsilon \left(\frac{l}{1-p} \right)^2 \left(1 - 2 \frac{1 + 2e^{i 2K_{cl}p}}{K_{cl}(1-p)} \right) = E_l - \Delta_l \\ E_l^{odd} &\approx 4\epsilon \left(\frac{l}{1-p} \right)^2 \left(1 - 2 \frac{1 - 2e^{i 2K_{cl}p}}{K_{cl}(1-p)} \right) = E_l + \Delta_l \end{aligned}$$

where

$$\begin{aligned} E_l &= \epsilon \left(\frac{2l}{1-p} \right)^2 \left(1 - \frac{2}{K_{cl}(1-p)} \right) \\ \Delta_l &= \epsilon \left(\frac{4l}{1-p} \right)^2 \frac{e^{i 2K_{cl}p}}{K_{cl}(1-p)} \end{aligned}$$

For comparison, in [Zur84] Zurek appears to be suggesting the following results (after adjusting for different length scales):

$$\begin{aligned} E_{Zl} &= \epsilon \left(\frac{2l}{1-p} \right)^2 \\ \Delta_{Zl} &= \frac{\epsilon}{\pi} \left(\frac{4}{1-p} \right)^2 e^{i 2K_{cl}p} \end{aligned}$$

Notice, that this would imply that the odd symmetry energy levels are *falling* slightly for very high barrier heights, despite initially being *lower* than the limiting value. Numerical analysis of the eigenvalue equations (Appendix D.3) leads to Figure 5.2. This shows the results for the first and third pairs of eigenstates. The dotted lines are Zurek's solution, while the dashed lines are the HBA approximations. Finally the unbroken lines give the numerical solution, for which the energy splitting becomes less than the difference between the limiting energy and the mean energy. The odd and even numerical solutions approach degeneracy faster than they approach the limiting value and the odd symmetry eigenvalues are always less than the limit.

The HBA results closely match the numerical solution while Zurek's results are too high, and his splitting is too large. The reason for this is unclear, as Zurek gives no explanation for his approximation. However, it is very similar to the central potential barrier problem considered by Landau and Lifshitz [LL77, chapter 5]. Landau and Lifshitz give a formula for the energy splitting, which matches Zurek's Δ_{Zl} , but no formula for the mean energy - which Zurek appears to assume to be equal to the limiting value. This assumption, that the mean energy approaches the limiting value much faster than the energy levels become degenerate, is clearly incorrect in this instance.

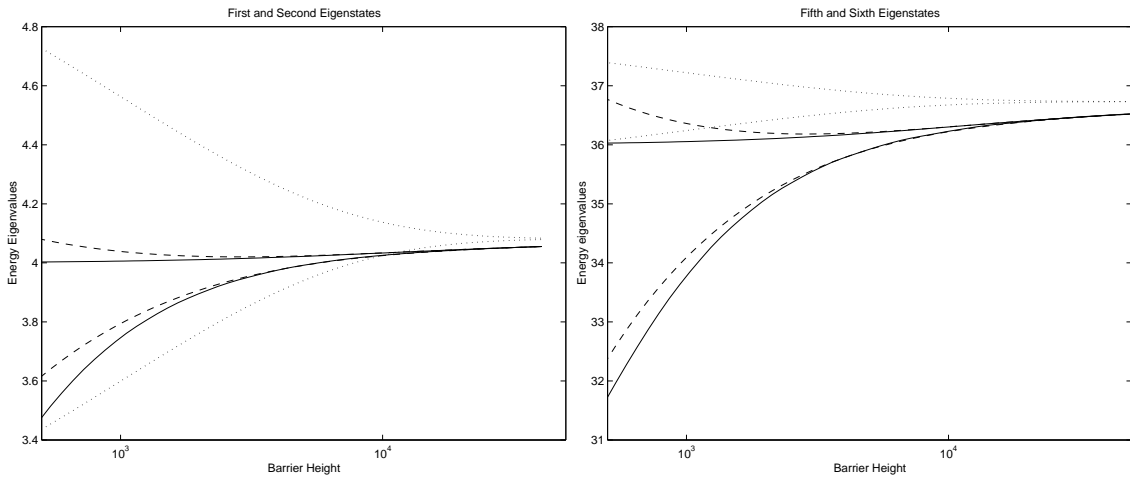


Figure 5.2: Asymptotic Values of Energy Levels

As the energy splitting formula of Landau and Lifshitz does not agree with either the asymptotic approximation calculated here, or the numerical solutions to the equations, it is also unclear that the semi-classical approximation they use is applicable to this situation.

5.3 Moveable Partition

In Section 4.2 one of the key arguments against the operation of the Popper-Szilard Engine was that of Zurek[Zur84], and Biedenharn and Solem[BS95], that in the quantum case the partition does not move when the particle is in a superposition of being on both sides of the partition.

However, neither actually provide a description of the interaction between the one atom gas and the piston. Instead, both refer to thermodynamic concepts to justify their arguments. Zurek, somewhat confusingly, goes on to concede that

..one can almost equally well maintain that this ... describes a molecule which is on an 'unknown but definite' side of the partition

There is as much reliance upon 'intuitive' arguments as the classical analysis they criticise. To improve on this situation it is necessary to analyse the actual interaction between the piston and the one-atom gas, in terms of unitary evolution operators. Only when this has been completed can the effect on a statistical ensemble be calculated, and the validity of thermodynamic concepts evaluated.

There are two main issues that need to be considered:

- The description of the moveable partition (piston). We will need to treat the piston as a quantum object. To do this rigorously would require dealing with some very subtle difficulties regarding Hilbert spaces with continuous parameters and localised states (e.g. see [Per93, Chapter 4]). However, these difficulties are not relevant to the problem considered here.

Instead we will construct a fairly simple Hilbert space, with a basis that corresponds to the minimum properties a piston is required to possess.

- The interaction between the piston and the one atom gas. Before dealing with the problem of the gas in a superposition, we shall analyse the situation where the gas is already confined to one side of the piston. In this situation it is generally agreed that the gas is capable of expanding, and pushing the piston in doing so. If it were not the case, then it would be impossible to extract any energy from an expanding one atom gas even when a demon had knowledge of its location, and the entire debate over Szilard's Engine would be redundant.

We will therefore assume only those properties of the piston state that are necessary to be able to describe the expansion of the gas when it is known to be confined to one side or another. We will then use these properties, and the description of the expansion of the gas, to examine the situation when the gas is in a superposition of both sides of the piston. We will not attach a weight to the piston until Section 5.4.

5.3.1 Free Piston

The first problem we need to solve is to find a suitable description of a piston as a quantum system. We will start by defining a simple Hilbert space, without taking the gas into account, with an appropriate unitary evolution operator for a frictionless piston.

We will consider the piston to be an object, centered at some point $-(1-p) > Y > (1-p)$, with a width $2p \ll 1$. The quantum state for a piston located at Y will be $|\Phi(Y)\rangle$. The width p represents the width of the 'hard sphere repulsion' potential that the piston will have for the gas. This corresponds to an effective potential for the gas of

$$V(X, Y) = \begin{cases} \infty & (X < -1) \\ 0 & (-1 < X < Y - p) \\ \infty & (Y - p < X < Y + p) \\ 0 & (Y + p < X < 1) \\ \infty & (X > 1) \end{cases}$$

It is important to note that p is not the spread (or quantum uncertainty) in the position co-ordinate Y . If the piston is a composite object, Y would be a collective co-ordinate describing the center of the object. For a reasonably well localised object, the spread in the co-ordinate Y , denoted by δ , is expected to be much smaller than the extent of the object, represented by p . Now consider the behaviour required of the frictionless piston in the absence of the gas. If the piston is initially in state $|\Phi(Y)\rangle$, and is moving to the right, then after some short period

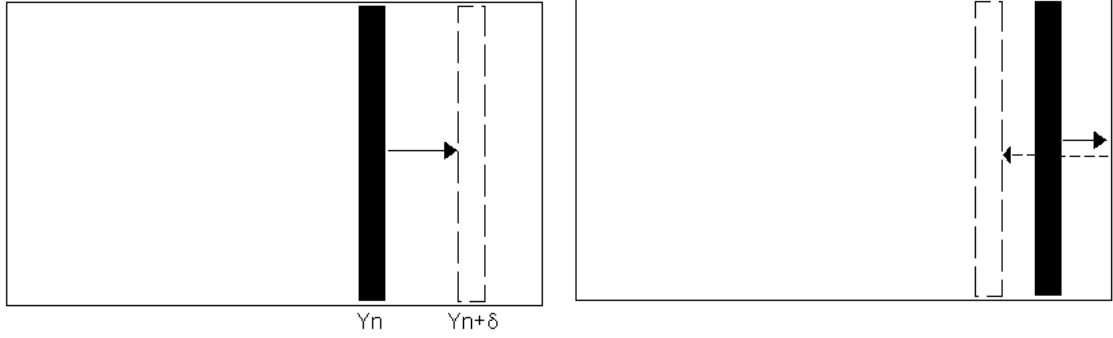


Figure 5.3: Motion of Piston

The motion to the right must be described by a unitary operation

$$U(\tau) |\Phi(Y)\rangle = |\Phi(Y + \delta)\rangle$$

When the piston reaches the end of the Szilard Box ($|\Phi(1)\rangle$) it cannot come to a complete halt as this would require an evolution operator of

$$\begin{aligned} U(\tau) |\Phi(1 - \delta)\rangle &= |\Phi(1)\rangle \\ U(\tau) |\Phi(1)\rangle &= |\Phi(1)\rangle \end{aligned}$$

and a mapping of orthogonal onto non-orthogonal states is not unitary. Instead the piston must collide elastically with the edge of the box and start moving uniformly to the left (Figure 5.3(b)).

We now have to distinguish left from right moving piston states, so that

$$\begin{aligned} U(\tau) |\Phi_L(Y)\rangle &= |\Phi_L(Y - \delta)\rangle \\ U(\tau) |\Phi_R(Y)\rangle &= |\Phi_R(Y + \delta)\rangle \end{aligned}$$

Without this distinction we would need a left moving evolution

$$U(\tau) |\Phi(Y)\rangle = |\Phi(Y - \delta)\rangle$$

and a right moving evolution

$$U(\tau) |\Phi(Y)\rangle = |\Phi(Y + \delta)\rangle$$

and again, this would not be unitary, as the same state $|\Phi(Y)\rangle$ is mapped to different states.

Left and right moving states are automatically required to be orthogonal, even if they are spatially overlapping, owing to the fact that inner products are invariant under unitary evolution, so that

$$\begin{aligned} \langle \Phi_L(Y) | U^y(\tau) U(\tau) |\Phi_R(Y)\rangle &= \langle \Phi_L(Y - \delta) | \Phi_R(Y + \delta)\rangle \\ \langle \Phi_L(Y) | \Phi_R(Y)\rangle &= 0 \end{aligned}$$

From this, we can now construct a Hilbert space spanned by a set of $N = 2(2j + 1)$ states, each centered on $Y_n = n\delta$, $n = -j, \dots, j$ where $j = \frac{1_i p}{\delta}$. The required evolution operator is:

$$\begin{aligned}
 U_{P1}(\tau) = & \sum_{n=i}^{j-1} |\Phi_R(Y_{n+1})\rangle \langle \Phi_R(Y_n)| + |\Phi_L(Y_j)\rangle \langle \Phi_R(Y_j)| \\
 & + \sum_{n=i}^j |\Phi_L(Y_{n+1})\rangle \langle \Phi_L(Y_n)| + |\Phi_R(Y_{-j})\rangle \langle \Phi_L(Y_{-j})| \quad (5.8)
 \end{aligned}$$

The first line represents a piston moving to the right, and reversing direction at $n = j$, while the second line is the piston moving to the left, and reversing at $n = -j$. Movement is with a fixed speed $\omega = \frac{\delta}{\tau}$, so that over the characteristic period of time τ it has moved exactly one 'step' to the left or right.

This operator will be unitary, providing

$$\langle \Phi_A(Y_n) | \Phi_B(Y_m) \rangle = \delta_{AB} \delta_{nm} \quad (5.9)$$

It is possible to construct a Hilbert space and unitary evolution satisfying these conditions, by adapting the quantum clock system [Per80]. It is important to note that the moving piston states above are *not* eigenstates of the Hamiltonian associated with $U_{P1}(\tau)$, and so do not have well defined energies. This is necessary to ensure that they are *moving* states. States with well defined energies would necessarily be stationary.

5.3.2 Piston and Gas on one side

Having defined our piston states, we can now start to consider the interaction between the piston and the single atom gas. This requires us to define a unitary evolution operator that acts upon the joint space of the piston and gas states. The key question that has been raised is whether the piston will move when the gas is in a superposition of being on both sides of the Szilard Box. We must not prejudice this question by *assuming*

and $-1 < X < Y_n - p$. We will use the superscript λ to represent a gas state on the left of the piston, and ρ for states of the gas on the right of the piston.

The left gas states and the piston states are combined to define a joint basis:

$$|\Psi_l^\lambda(Y_n)\Phi_B(Y_n)\rangle$$

First we will define the internal energy of the gas subsystem, then we will construct an evolution operator for the joint system, including the interaction between the gas and piston.

The internal energy of the gas state $|\Psi_l^\lambda(Y_n)\rangle$ is $4\epsilon\left(\frac{l}{Y_n+1-p}\right)^2$ so the Hamiltonian for the one-atom gas subsystem's internal energy is given by

$$\begin{aligned} H_{G2}^\lambda &= \sum_{n=0}^j \rho(Y_n) H_{G2}^\lambda(Y_n) \\ H_{G2}^\lambda(Y_n) &= \sum_l 4\epsilon \left(\frac{l}{Y_n+1-p}\right)^2 |\Psi_l^\lambda(Y_n)\rangle \langle \Psi_l^\lambda(Y_n)| \end{aligned} \quad (5.11)$$

It is important to be clear about the role played by the operators $\rho(Y_n) = |\Phi_L(Y_n)\rangle \langle \Phi_L(Y_n)| + |\Phi_R(Y_n)\rangle \langle \Phi_R(Y_n)|$. This does not imply that the piston is part of the gas subsystem, or that this particular Hamiltonian includes an interaction energy between the gas and piston. The $H_{G2}^\lambda(Y_n)$ represent the internal energy states of the gas, given a particular position of the piston. The combined Hamiltonian H_{G2}^λ includes $\rho(Y_n)$ to project out the position of the piston. The parameter Y is an external parameter of the gas, describing an external configuration, or boundary condition, upon the gas, as opposed to X which is an internal parameter. It is the motion associated with X that generates the internal energy in H_{G2} , not Y .

Details of the internal energy of the piston would depend upon it's construction as a composite system, so we will simply include a term H_P to represent this, and assume that there is no interaction between the internal piston states and it's external position, or the gas states.

Neither H_{G2} nor H_P represent the interaction between the gas and piston properly, as they give only internal energies for each subsystem. A Hamiltonian consisting of $H = H_{G2} + H_P$ would not lead to a moving piston at all. Instead we must construct an idealised evolution operator to describe the expansion of the gas, pushing the piston. When the piston reaches the end of the box, it will collide elastically, as before, and as it's direction reverses it will compress the gas. For simplicity we assume that when the piston reaches the center of the box, it is not capable of compressing the gas any further, and will reverse back to it's original direction⁴. This motion can be described by the unitary operator:

$$\begin{aligned} U_{P2}^\lambda(\tau) &= \sum_l \left\{ \sum_{n=1}^{j_i-2} |\Psi_l^\lambda(Y_{n+1})\Phi_R(Y_{n+1})\rangle \langle \Psi_l^\lambda(Y_n)\Phi_R(Y_n)| \right. \\ &\quad + \sum_{n=2}^{j_i-1} |\Psi_l^\lambda(Y_{n-1})\Phi_L(Y_{n-1})\rangle \langle \Psi_l^\lambda(Y_n)\Phi_L(Y_n)| \\ &\quad \left. + |\Psi_l^\lambda(1-p)\Phi(1-p)\rangle \langle \Psi_l^\lambda(Y_{j_i-1})\Phi_R(Y_{j_i-1})| \right\} \end{aligned}$$

⁴This assumption will be more realistic when the attached weight is included in the system, in the next Section.

$$\begin{aligned}
& + |\Psi_l^\lambda(Y_{j_i-1})\Phi_L(Y_{j_i-1})\rangle \langle \Psi_l^\lambda(1-p)\Phi(1-p) | \\
& + |\Psi_l^\lambda(0)\Phi(0)\rangle \langle \Psi_l^\lambda(Y_1)\Phi_L(Y_1) | \\
& + |\Psi_l^\lambda(Y_1)\Phi_R(Y_1)\rangle \langle \Psi_l^\lambda(0)\Phi(0) | \}
\end{aligned} \tag{5.12}$$

The first and second lines represent the piston moving to the right (gas expanding) and the left (gas compressing) respectively. The third and fourth lines represent the right moving piston reaching the end of the box, coming to an instantaneous halt in the state $|\Phi(1-p)\rangle$, and reflecting to the left, starting to recompress the gas. The fifth and sixth lines, similarly, represents the piston, reaching the maximum compression of the gas in the center of the box, coming to a halt in $|\Phi(0)\rangle$, before starting to move back to the right under pressure from the gas⁵.

The eigenstates of $U_{P_2}^\lambda(\tau)$ are superposition of all the Y_n states:

$$\begin{aligned}
|\Lambda_{al}\rangle & = \sum_{n=1}^{j_i-1} \{ e^{ina} |\Psi_l^\lambda(Y_n)\Phi_R(Y_n)\rangle + e^{i ina} |\Psi_l^\lambda(Y_n)\Phi_L(Y_n)\rangle \} \\
& + |\Psi_l^\lambda(0)\Phi(0)\rangle + e^{ija} |\Psi_l^\lambda(1-p)\Phi(1-p)\rangle \\
U_{P_2}^\lambda(\tau) |\Lambda_{al}\rangle & = e^{ia} |\Lambda_{al}\rangle
\end{aligned}$$

Continuity at $|\Psi_l^\lambda(1-p)\Phi(1-p)\rangle$ requires that $e^{i ja} = e^{ija}$. This imposes a periodic boundary condition upon the system, and gives a discrete set of eigenstates $|\Lambda_{al}\rangle$ that satisfy $ja = \pi m$, $m = -j+1, \dots, j$

The Hamiltonian that drives the unitary evolution $U_{P_2}^\lambda(\tau)$ is

$$H_{\tau_2}^\lambda = \frac{1}{\tau} \sum_{a,l} a |\Lambda_{al}\rangle \langle \Lambda_{al}|$$

This does not offer any simple interpretation in terms of an internal energy H_{G_2} of the gas plus an interaction term representing the pressure of the gas upon the piston. The simplest way to take into account the internal energy of the gas, and also any internal states of the piston system, is with a total Hamiltonian:

$$H_{T_2}^\lambda = (1-h(t))H_{G_2}^\lambda + h(t)H_{\tau_2}^\lambda + H_P$$

The time dependant function $h(t)$ allows the 'switching on' and 'switching off' of the pressure interaction between the piston and the gas. It is equal to one when the piston is present in the box, and zero when the piston is absent⁶. While $h(t)$ is one, the interaction of gas and piston drives the system through the evolution $U_{P_2}^\lambda(t) = e^{iH_{\tau_2}^\lambda t}$, causing the gas to expand, with the piston moving to the right, or to compress, with the piston moving to the left, in a cyclic motion.

⁵This operator assumes the expansion does not cause transitions between internal states of the gas. As long as the expansion period τ is sufficiently long, this will be consistent with the adiabatic theorem (Appendix C).

⁶It may be objected that H_{T_2} is unrealistic as it appears to requires the internal energy of the gas to be 'switched off' during the expansion phase. An obvious, if woefully contrived, way to correct this is to have H_{G_2} at all times, but to 'switch on' an interaction Hamiltonian $H_{I_2} = (H_{T_2} - H_{G_2})$. That more realistic Hamiltonians will ultimately produce the same result is argued later.

If the interaction is 'switched on' for just long enough to expand the gas to it's full extent, and then 'switched off', the final states will be at a lower energy than they were before the expansion⁷. The excess energy will have been stored in the interaction between the gas and piston, and the combination of 'switching on' and 'switching off' of the interaction requires energy to be deposited in, or drawn from, a work reservoir.

We have now constructed a suitable Hamiltonian, and a unitary evolution operator, that encapsulates the expected behaviour of the gas and piston system, when the gas is confined to one side of the piston. We now turn to the case where the gas can be in a superposition.

5.3.3 Piston with Gas on both sides

This subsection will demonstrate one of the main results of this Chapter, that the superposition of gas states does not lead to a stationary piston.

We will extend the results of the previous subsection to include the situation where the gas is confined entirely to the right. The combination of the left and right unitary evolution operators will then be shown to produce a unitary evolution operator that acts upon the entire space of the gas and piston system, including situations where the gas is in a superposition of being on the left and right side of the piston. Applying this unitary operator to the superposition of gas states and shows that, rather than staying in the center, the piston moves into an entangled superposition of states, contrary to the arguments of Zurek and of Biedenharn and Solem. We will then show how this result generalises beyond the specific unitary evolution operator constructed here. Finally we will examine how this evolution affects the internal energy of the one atom gas.

It is evident that had we considered the situation where the gas was confined entirely to the right of the piston, we would have obtained the Hamiltonians:

$$H_{\tau 2}^{\rho} = \sum_l \frac{1}{\tau} \sum_{a,l} a |R_{al}\rangle \langle R_{al}|$$

$$H_{G2}^{\rho} = \sum_{n=i}^0 \sum_j \rho(Y_n) H_{G2}^{\rho}(Y_n)$$

with

$$H_{G2}^{\rho}(Y_n) = \sum_l 4\epsilon \left(\frac{l}{1-p-Y_n} \right)^2 |\Psi_l^{\rho}(Y_n)\rangle \langle \Psi_l^{\rho}(Y_n)|$$

$$|R_{al}\rangle = \sum_{n=i}^{j+1} \{ e^{ina} |\Psi_l^{\rho}(Y_n)\Phi_R(Y_n)\rangle + e^{i ina} |\Psi_l^{\rho}(Y_n)\Phi_L(Y_n)\rangle \}$$

$$+ |\Psi_l^{\rho}(0)\Phi(0)\rangle + e^{ija} |\Psi_l^{\rho}(-1+p)\Phi(-1+p)\rangle$$

and the gas state $|\Psi_l^{\rho}(Y_n)\rangle$ represents the gas confined entirely to the right of the piston ($Y_n + p < X < 1$), with wavefunction

$$\Psi_l^{\rho}(Y_n, X) = \langle X | \Psi_l^{\rho}(Y_n) \rangle = \sqrt{\frac{2}{L(1-p-Y_n)}} \sin \left(l\pi \frac{1-X}{1-p-Y_n} \right)$$

⁷The Hamiltonian H_{T2} is time dependant

During an interaction period, in which $H_{\tau_2}^\rho$ is 'switched on', the unitary evolution operator is

$$\begin{aligned}
U_{P_2}^\rho(\tau) = & \sum_l \left\{ \sum_{n=j+1}^{j+2} |\Psi_l^\rho(Y_{n+1})\Phi_R(Y_{n+1})\rangle \langle \Psi_l^\rho(Y_n)\Phi_R(Y_n)| \right. \\
& + \sum_{n=j+2}^{j+1} |\Psi_l^\rho(Y_{n+1})\Phi_L(Y_{n+1})\rangle \langle \Psi_l^\rho(Y_n)\Phi_L(Y_n)| \\
& + |\Psi_l^\rho(0)\Phi(0)\rangle \langle \Psi_l^\rho(Y_{j+1})\Phi_R(Y_{j+1})| \\
& + |\Psi_l^\rho(Y_{j+1})\Phi_L(Y_{j+1})\rangle \langle \Psi_l^\rho(0)\Phi(0)| \\
& + |\Psi_l^\rho(-1+p)\Phi(-1+p)\rangle \langle \Psi_l^\rho(Y_{j+1})\Phi_L(Y_{j+1})| \\
& \left. + |\Psi_l^\rho(Y_{j+1})\Phi_R(Y_{j+1})\rangle \langle \Psi_l^\rho(-1+p)\Phi(-1+p)| \right\} \quad (5.13)
\end{aligned}$$

We now need to construct a Hamiltonian and corresponding unitary time evolution operator that acts upon the Hilbert space for the gas particle on either (or both) sides of the piston. The natural assumption would be to use:

$$H_{T_2} = h(t) [H_{\tau_2}^\lambda + H_{\tau_2}^\rho] + (1 - h(t)) [H_{G_2}^\lambda + H_{G_2}^\rho] + H_P$$

where $h(t)$ is again a time dependant function, zero when the pressure interaction between the piston and gas is 'switched off' and one otherwise. The question is whether the left and right Hamiltonians can be added without changing the resultant unitary evolution. We will be able to answer this affirmatively from the fact that left and right Hamiltonians, and their respective unitary evolution operators, act upon disjoint subspaces of the joint gas-piston Hilbert space.

Firstly, we must prove that the addition of the Hamiltonians leads to an operator that acts upon the whole of the joint system Hilbert space. This will be the case if the states $|\Psi_l^\alpha(Y_n)\Phi_B(Y_n)\rangle$ form an orthonormal basis for the joint Hilbert space.

Consider the inner product:

$$\langle \Psi_k^\alpha(Y_m)\Phi_A(Y_m) | \Psi_l^\beta(Y_n)\Phi_B(Y_n) \rangle = \delta_{nm}\delta_{\alpha\beta}\delta_{kl}\delta_{AB} \quad (5.14)$$

- δ_{nm} and δ_{AB} come from the orthonormality of the different piston states (Equation 5.9).
- $\delta_{\alpha\beta}$ clearly holds if the wavefunctions of the α and β gas states have no overlap. A right gas wavefunction is non-zero only to the right of the piston position. Similarly a left gas wavefunction is non-zero only to the left of the piston position. The right and left gas wavefunctions can therefore only be overlapping if their respective piston states are to the left and right of the other. If this is the case, then $Y_n \neq Y_m$ and then δ_{nm} guarantees orthogonality, so the joint states are orthogonal.
- δ_{kl} is certainly true for wavefunctions where α and β are the same. The $\delta_{\alpha\beta}$ term then automatically prevents interference between these states in the combined Hilbert space.

For any given piston position, the combination of left and right gas states will span the subspace of the gas states, and the piston states span the piston subspace, so the above states form an

orthonormal basis for the joint space. This basis splits into two disjoint subspaces, corresponding to the gas on the left or right of the piston.

Now let us consider a general property of unitary operators acting upon subspaces. If U_a acts entirely upon the subspace S_a and U_b acts upon S_b , each unitary operator can be extended to act upon the entire space $S^T = S_a \oplus S_b$ by means of:

$$\begin{aligned} U_a^T &= U_a \oplus I_b \\ U_b^T &= I_a \oplus U_b \end{aligned}$$

where I_a and I_b are the identity operators upon S_a and S_b respectively. It is therefore possible to form the joint operator

$$U^T = U_a \oplus U_b = U_a^T U_b^T = U_b^T U_a^T$$

The commutativity implies that, with a unitary operator written in the form $U = e^{iK}$, where K is a Hermitian operator

$$U^T = e^{iK^T} = e^{iK_a} e^{iK_b} = e^{i(K_a \oplus K_b)}$$

Applying this back to the equation of motion,

$$i\hbar \frac{\partial U}{\partial t} = HU$$

it is deducible that if H_a and H_b are Hamiltonians defined upon disjoint subspaces, and U_a and U_b are their associated evolution operators, then the joint Hamiltonian $H^T = H_a + H_b$ has an associated evolution operator given by U^T . This proves that the solutions for the separate cases of the gas confined to the left and right side of the piston can be combined into a single unitary evolution operator for the combined Hilbert space.

Combined Evolution Operator

We have now shown that the complete unitary evolution operator for the combined gas piston system, with the interaction 'switched on', is

$$U_{T2}(\tau) = U_{P2}^\rho(\tau) \oplus U_{P2}^\lambda(\tau)$$

To study the properties of this evolution we will simplify the operator in two ways. Firstly, we will allow the interaction to run for exactly the time necessary for the gas wavefunction to completely expand or compress. This will take $j = \frac{1_j p}{\delta}$ steps, and will result in a unitary evolution $U_{T2}(j\tau) = (U_{T2}(\tau))^j$.

Secondly, we will start with only those states for which the piston is in the central position and only look at those states that occur from $U_{T2}(j\tau)$ acting upon this initial subspace.

With these two simplifications, the evolution operator becomes

$$U_{T2} = \sum_l |\Psi_l^\rho(-1+p)\Phi(-1+p)\rangle \langle \Psi_l^\rho(0)\Phi(0)|$$

$$\begin{aligned}
& + |\Psi_l^p(0)\Phi(0)\rangle \langle \Psi_l^p(-1+p)\Phi(-1+p)| \\
& + |\Psi_l^\lambda(1-p)\Phi(1-p)\rangle \langle \Psi_l^\lambda(0)\Phi(0)| \\
& + |\Psi_l^\lambda(0)\Phi(0)\rangle \langle \Psi_l^\lambda(1-p)\Phi(1-p)|
\end{aligned}$$

If we apply this evolution operator to an initial state, where the gas is in a superposition of being on both sides of the piston:

$$|\chi_{initial}\rangle = (\alpha |\Psi_l^p(0)\rangle + \beta |\Psi_m^\lambda(0)\rangle) |\Phi(0)\rangle$$

this state will evolve into

$$|\chi_{final}\rangle = \alpha |\Psi_l^p(-1+p)\Phi(-1+p)\rangle + \beta |\Psi_m^\lambda(1-p)\Phi(1-p)\rangle$$

This demonstrates the central result of this Section. Guided only by the argument that the *confined* one-atom gas is capable of pushing the piston, we have shown that the condition of unitarity leads to an evolution operator which does *not* leave the piston stationary when the gas is initially in a superposition. This is contrary to the arguments of Zurek and of Biedenharn and Solem. However, it is also the case that the piston is now in an entangled quantum superposition, so the situation is still quite different from the classical case.

We have examined the piston gas interaction in considerable detail, in order to carefully demonstrate that the evolution operator U_{T2} can be derived from a continuous expansion of the gas states and is consistent with the agreed behaviour of the one atom gas when it is confined. The unitary operator, however, was not derived from a particularly realistic interaction Hamiltonian. We will now present a simple argument that a less idealised Hamiltonian would produce the same result.

The key property is that the confined one atom gas can expand adiabatically against the piston. If the gas is initially on the right of the piston, this expansion is given by some unitary operation U

$$U |\Psi_l^p(0)\rangle |\Phi(0)\rangle = |\Psi_l^p(-1+p)\rangle |\Phi(-1+p)\rangle$$

while if the gas is initially to the left, the expansion is

$$U |\Psi_l^\lambda(0)\rangle |\Phi(0)\rangle = |\Psi_l^\lambda(1-p)\rangle |\Phi(1-p)\rangle$$

These equations⁸ must be derivable from *any* interaction Hamiltonian H that, over a sufficiently long period, allows the adiabatic expansion of a one atom gas. Provided the two expansions can be combined into a single unitary operator, and we have shown that they can, it follows from the linearity of U that a superposition of gas states leads to the same entangled superposition of piston and gas states as we reached with U_{T2} above. The piston state will not be stationary, even with a more realistically derived Hamiltonian.

⁸up to a phase factor

Expansion of the Gas States

We will now examine the effect of the expansion upon the internal energy states of the one atom gas. It is assumed that, as long as τ is sufficiently large, or equivalently, that the expansion takes place sufficiently slowly, the adiabatic theorem will apply, and there will be no transitions between eigenstates. However, the internal energy eigenstates and eigenvalues continuously change as the piston position Y_n changes. This forms the basis of the 'work' that will be extracted from the expansion of the gas.

For an initial, odd symmetry state, $|\Psi_l^{odd}\rangle$ the insertion of the piston makes negligible change upon the energy, but splits the wavefunction into a superposition of left and right wavefunctions $\Psi_l^\lambda(0)$ and $\Psi_l^\rho(0)$. The energy of this state is approximately $4\epsilon l^2$. As the piston moves into a superposition, the energies of the left and right states go down, until at the end of the expansion, the internal energy of the gas state is approximately ϵl^2 .

The reason for this can be seen from the wavelength, and node density of the gas wavefunction. The wavefunction for a left gas state is

$$\Psi_l^\lambda(Y_n, X) = \sqrt{\frac{2}{L(Y_n + 1 - p)}} \sin\left(l\pi \frac{1 + X}{Y_n + 1 - p}\right)$$

The number of nodes in this wavefunction is constant, and equal to half the number of nodes in the initial odd symmetry wavefunction. When the expansion has finished, these nodes are spread over twice the volume, so the density of nodes has decreased by a factor of two, and the energy decreased by a factor of four.

The same is true for the right gas wavefunctions. In fact, at the end of the expansion stages, the wavefunctions are

$$\begin{aligned} \Psi_l^\lambda(1 - p, X) &= \frac{1}{\sqrt{L(1 - p)}} \sin\left(\frac{\pi l}{2} \left(\frac{1 + X}{1 - p}\right)\right); (-1 < X < 1 - 2p) \\ \Psi_l^\rho(-1 + p, X) &= \frac{1}{\sqrt{L(1 - p)}} \sin\left(\frac{\pi l}{2} \left(\frac{1 - X}{1 - p}\right)\right); (-1 + 2p < X < 1) \end{aligned}$$

These differ by, at most, a sign change and a shift in position of order $2p \ll 1$:

$$\Psi_l^\lambda(1 - p, X) \approx \Psi_l^\rho(-1 + p, X) \approx \begin{cases} \psi_{l/2} & l \text{ even} \\ \psi_{(l+1)/2} & l \text{ odd} \end{cases} \quad (5.15)$$

where ψ_l are the unperturbed wavefunctions given in Section 5.1. The value of l is approximately halved during the expansion.

For an initial even symmetry wavefunction, the same analysis applies, only now a single node is inserted in the center of the wavefunction, as the piston is inserted, requiring some work. This corresponds, neglecting terms of order p , to an energy input and output of:

Symmetry	Input	Output	Net
Odd	0	$3\epsilon l^2$	$3\epsilon l^2$
Even	$\epsilon(4l - 1)$	$3\epsilon l^2$	$\epsilon(l - 1)(3l - 1)$

The net energy extracted is always positive, with the single exception of the ground state, which is the even symmetry $l = 1$ state. In this case one node is added, when the barrier is inserted, and one node is removed, when the wavefunction expands, so the energy input exactly matches the energy output. So on each cycle of the Szilard Engine, some energy is extracted, as the number of the eigenstate is approximately halved, and the gas is left in a lower energy state than it started. This continues until the ground state is reached, at which point no more energy can be extracted, and the work output during the expansion phase is the work done upon the system when the barrier is inserted.

There are two points that can be drawn from this. Firstly, this shows that energy could be extracted from the operation of the Szilard Engine, if all the other stages of the Engine operate as required. This energy is not energy that is inserted into the system by performing a measurement.

Secondly, the state of the one atom gas will fall to the ground state, at which point no further energy can be extracted. In Chapter 6 the gas will be brought into contact with a heat bath. This will allow energy to flow back into the gas, restoring the energy extracted by the expansion.

5.4 Lifting a weight against gravity

In the previous Section it was shown that the single atom gas can be made to expand against a piston, and that this expansion is associated with a reduction in the internal energy of the gas. We now need to incorporate the manner in which that internal energy is converted into work. The paradigm of work being performed is taken to be the raising of a weight.

In the Popper version of the Szilard engine, it is the connection of a weight on either side of the engine that is supposed to allow work to be extracted without a measurement of the position of the gas particle (Figure 4.5(b)). However, when the one atom gas is initially in a superposition of left and right gas states, the quantum Popper-Szilard Engine becomes a superposition of left moving and right moving piston states. To include the piston raising a weight, we must include the weights themselves in the quantum mechanical description of the system.

A quantum weight, of mass M_w , resting upon a floor at height h , in a gravitational field g is described by the Schrödinger equation

$$H_W(h)A_n(z, h) = \left(-\frac{\hbar}{2M_w} \frac{\partial^2}{\partial z^2} + V(z, h) \right) A_n(z, h) \quad (5.16)$$

with

$$V(z, h) = \left\{ \begin{array}{ll} \infty & (z \leq h) \\ M_w g(z - h) & (z > h) \end{array} \right\}$$

The solution to this equation is derived from the Airy function $A(z)$ (see [AS70, NIS]) by applying the requirements that the wavefunction $A_n(z, h)$ be normalised, and the boundary condition $A_n(h, h) = 0$. This leads to wavefunction solutions

$$A_n(z, h) = \begin{cases} \frac{A\left(\frac{z-h}{L} + a_n\right)}{H A'(a_n)} & (z > h) \\ 0 & (z \leq h) \end{cases} \quad (5.17)$$

with a characteristic height, depending upon the strength of the gravitational field and the mass of the weight

$$H = \left(\frac{\hbar^2}{2M_w^2 g} \right)^{\frac{1}{3}}$$

and an energy eigenvalue

$$E_n = (h - a_n H) M_w g$$

The values a_n correspond to the values of z for which the Airy function $A(z) = 0$. These values are always negative, and become increasingly negative as n increases. For large n they have the asymptotic form $a_n = -\left(\frac{3\pi n}{2}\right)^{\frac{2}{3}}$. $A'(z)$ is the first derivative of the Airy function. Note that $A_n(z, h) = A_n(z - h, 0)$. The first, fifth and tenth eigenstates are shown in Figure 5.4(a). We will

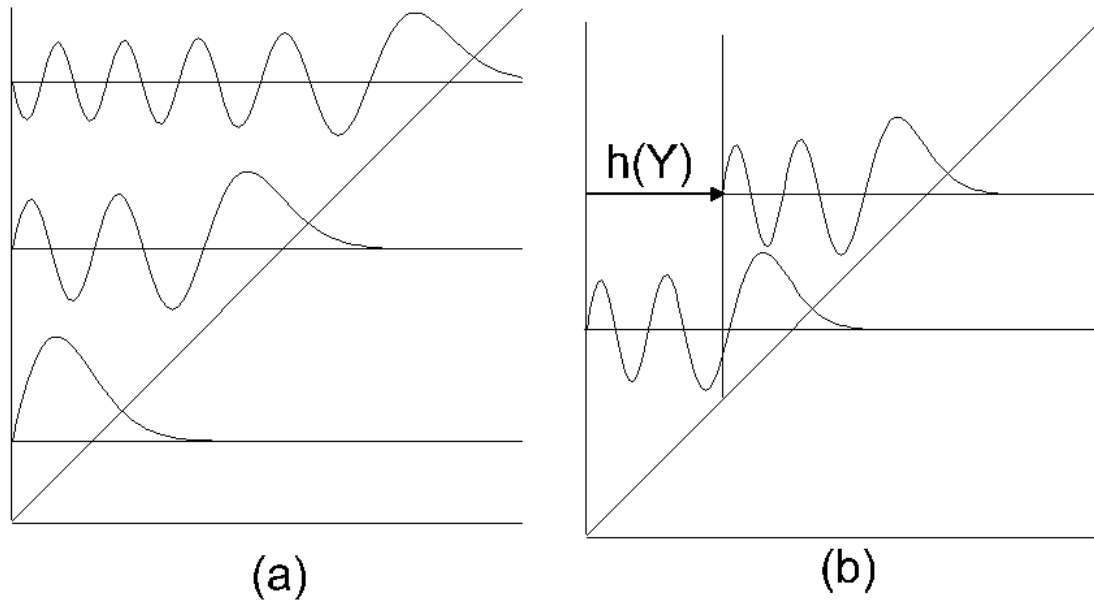


Figure 5.4: Airy Functions for a Mass in Gravitational Field

proceed as before, by considering the gas on one side of the piston (the left), and lifting a weight attached to that side, by raising the floor below it. From now on, when referring to the piston, or it's position, we will be referring to the entire system of piston, pulleys, and 'pan' supporting the weight.

If the floor is raised through a distance δh the change in energy will be $\delta E = M_w g \delta h$ (which is independent of the eigenstate⁹). By contrast, when the piston expands through a distance δY ,

⁹The old set of eigenstates $A_n(x)$ will transform into new eigenstates $A_n(x - \delta h)$. If the floor is raised sufficiently slowly, then by the adiabatic theorem, there will be no transitions between states.

the change in internal energy of the n 'th eigenstate of the gas will be $\delta E_n = -\frac{8\epsilon n^2}{(1-p+Y)^3}\delta Y$. If the expansion of the gas is to exactly supply the energy to lift the weight, a gearing mechanism that raises the weight through a different distance than that moved by the piston is required, so that $h = h(Y)$ and

$$\frac{\partial h}{\partial Y} = \frac{8\epsilon n^2}{M_w g (1-p+Y)^3}$$

However, the height raised should not be dependant upon the specific eigenstate of the gas as there will be a statistical ensemble of gas states. We cannot arrange for pulley connecting the piston to the weight to have a different gearing ratio for different states of the gas. Instead a mean gearing ratio must be used, such as

$$\frac{\partial h}{\partial Y} = \frac{\alpha}{(1-p+Y)^3}$$

The exact form of the function $h(Y)$ can only be determined when we know the statistical ensemble, in Section 6.4¹⁰. For now we will simply represent the gearing by the function $h(Y)$. The final height of the floor of the raised weight is $h_T = h(1-p)$ and we will assume $h(0) = 0$. We will simplify the Dirac notation by dropping the h , so that the wavefunction $A_n(z, h(Y)) = \langle z | A_n(Y) \rangle$. Figure 5.4(b) shows the effect upon the fifth eigenstate $A_5(z, h)$ as the floor height is raised.

Following the same procedure as in Section 5.3 above, the subsystem internal energy for the lefthand weight is given by the Hamiltonian

$$H_{W2}^\lambda = \sum_n \rho(Y_n) H_W(h(Y_n)) \quad (5.18)$$

where $\rho(Y_n) = |\Phi_R(Y_n)\rangle \langle \Phi_R(Y_n)| + |\Phi_L(Y_n)\rangle \langle \Phi_L(Y_n)|$ and we can write

$$H_W(h(Y_n)) = \sum_m (h(Y_n) - a_m H) M_w g |A_m^\lambda(Y_n)\rangle \langle A_m^\lambda(Y_n)|$$

We now need to construct a 'raising weight' unitary operator $U_{W3}(t)$ to describe the joint motion of the combined gas, piston and weights. If we look at the situation where the gas is located on the left, and only include the description of the lefthand weight, the appropriate unitary operator is

$$\begin{aligned} U_{W3}^\lambda(\tau) = & \sum_{l,m} \left\{ \sum_{n=1}^{j_l-2} |A_m^\lambda(Y_{n+1})\Psi_l^\lambda(Y_{n+1})\Phi_R(Y_{n+1})\rangle \langle A_m^\lambda(Y_n)\Psi_l^\lambda(Y_n)\Phi_R(Y_n)| \right. \\ & + \sum_{n=2}^{j_l-1} |A_m^\lambda(Y_{n_j-1})\Psi_l^\lambda(Y_{n_j-1})\Phi_L(Y_{n_j-1})\rangle \langle A_m^\lambda(Y_n)\Psi_l^\lambda(Y_n)\Phi_L(Y_n)| \\ & \left. + |A_m^\lambda(1-p)\Psi_l^\lambda(1-p)\Phi(1-p)\rangle \langle A_m^\lambda(Y_{j_l-1})\Psi_l^\lambda(Y_{j_l-1})\Phi_R(Y_{j_l-1})| \right\} \end{aligned}$$

¹⁰The insensitivity of $h(Y)$ to n means that there will be a difference between the energy extracted from the expanding gas and the energy put into raising the weight. This will have to be drawn from a work reservoir. Fortunately it will be shown, in Section 6.4, that the energy drawn from the work reservoir can be made negligible.

$$\begin{aligned}
& + |A_m^\lambda(Y_{j-1})\Psi_l^\lambda(Y_{j-1})\Phi_L(Y_{j-1})\rangle \langle A_m^\lambda(1-p)\Psi_l^\lambda(1-p)\Phi(1-p) | \\
& + |A_m^\lambda(0)\Psi_l^\lambda(0)\Phi(0)\rangle \langle A_m^\lambda(Y_1)\Psi_l^\lambda(Y_1)\Phi_L(Y_1) | \\
& + |A_m^\lambda(Y_1)\Psi_l^\lambda(Y_1)\Phi_R(Y_1)\rangle \langle A_m^\lambda(0)\Psi_l^\lambda(0)\Phi(0) | \}
\end{aligned}$$

This operator expresses the same behaviour as the operator $U_{P_2}^\lambda(\tau)$, in Equation 5.12, but now includes the lifting of the weight. The first line represents the piston moving to the right, the gas state on the left of the piston expanding slightly, and the lefthand weight rising from $h(Y_n)$ to $h(Y_{n+1})$. The second line gives the corresponding motion of the piston moving to the left, the gas on the left compressing, and the lefthand weight being lowered slightly. Third and fourth lines show the piston reaching the right end of the Szilard box, and the weight reaching it's maximum height, before the piston is reflected and starts to compress the gas while lowering the weight. Finally the fifth and sixth lines represent the left moving piston reaching maximum compression of the gas, on the left of the piston, in the center of the box, with the weight coming to a rest on the floor, before the piston reverses direction under pressure from the gas, and starts to move to the right again, with the expanding gas lifting the weight.

As Figure 5.4(b) shows, raising the weight can leave substantial overlap between states, so that $\langle A_m^\lambda(Y_i) | A_m^\lambda(Y_j) \rangle \neq \delta_{ij}$ in general. However, as in Equation 5.14, the orthogonality of the piston states ensures that the operator is a permutation of orthonormal states. Furthermore, for any given position Y of piston, and so by $h(Y)$ a given position of the pan under the weight, the $|A_m^\lambda(Y)\rangle$ form a complete basis for the subspace of the weight. The set of joint (l, m, n, A) states $|A_m^\lambda(Y_n)\Psi_l^\lambda(Y_n)\Phi_A(Y_n)\rangle$ therefore spans the accessible space of the joint system, and the operator is unitary.

We now, by symmetry, construct a similar operator for the one atom gas located entirely to the right of the piston. Now we temporarily ignore the lefthand weights, and obtain from Equation 5.13

$$\begin{aligned}
U_{W_3}^\rho(\tau) &= \sum_{l,m} \{ \sum_{n=i}^{j-2} |A_m^\rho(Y_{n+1})\Psi_l^\rho(Y_{n+1})\Phi_R(Y_{n+1})\rangle \langle A_m^\rho(Y_n)\Psi_l^\rho(Y_n)\Phi_R(Y_n) | \\
& + \sum_{n=i}^{j-1} |A_m^\rho(Y_{n+1})\Psi_l^\rho(Y_{n+1})\Phi_L(Y_{n+1})\rangle \langle A_m^\rho(Y_n)\Psi_l^\rho(Y_n)\Phi_L(Y_n) | \\
& + |A_m^\rho(0)\Psi_l^\rho(0)\Phi(0)\rangle \langle A_m^\rho(Y_{j-1})\Psi_l^\rho(Y_{j-1})\Phi_R(Y_{j-1}) | \\
& + |A_m^\rho(Y_{j-1})\Psi_l^\rho(Y_{j-1})\Phi_L(Y_{j-1})\rangle \langle A_m^\rho(0)\Psi_l^\rho(0)\Phi(0) | \\
& + |A_m^\rho(-1+p)\Psi_l^\rho(-1+p)\Phi(-1+p)\rangle \langle A_m^\rho(Y_{j+1})\Psi_l^\rho(Y_{j+1})\Phi_L(Y_{j+1}) | \\
& + |A_m^\rho(Y_{j+1})\Psi_l^\rho(Y_{j+1})\Phi_R(Y_{j+1})\rangle \langle A_m^\rho(-1+p)\Psi_l^\rho(-1+p)\Phi(-1+p) | \}
\end{aligned}$$

We now need to combine this into a single unitary operator. Denoting the identity operator upon the unraised lefthand weight space by

$$I_W^\lambda = \sum_m |A_m^\lambda(0)\rangle \langle A_m^\lambda(0)|$$

and that on the unraised righthand weight by

$$I_W^\rho = \sum_m |A_m^\rho(0)\rangle \langle A_m^\rho(0)|$$

we have a combined operator

$$U_{W4}(\tau) = [U_{W3}^\lambda(\tau) \otimes I_W^\rho] \oplus [I_W^\lambda \otimes U_{W3}^\rho(\tau)] \quad (5.19)$$

This unitary operator may be associated with a Hamiltonian H_{W4} , constructed from the subsystem interaction Hamiltonians, in the same manner as discussed above in Section 5.3, and the complete expansion of the system of gas, piston and weights has the Hamiltonian

$$H_{T4} = (1 - h(t)) [H_{G2}^\lambda + H_{W2}^\lambda + H_{G2}^\rho + H_{W2}^\rho] + h(t)H_{W4} + H_P$$

We now simplify Equation 5.19, by allowing the interaction to run for exactly the time necessary for a complete expansion, or compression, of the one atom gas, and include only those states which can be obtained from an initial subspace in which the piston is located in the center of the box ($Y = 0$). This gives us the unitary operation

$$\begin{aligned} U_{W4} = & \sum_{l,m,n} |A_m^\lambda(0)A_n^\rho(h(-1+p))\Psi_l^\rho(-1+p)\Phi(-1+p)\rangle \langle A_m^\lambda(0)A_n^\rho(0)\Psi_l^\rho(0)\Phi(0)| \\ & + |A_m^\lambda(0)A_n^\rho(0)\Psi_l^\rho(0)\Phi(0)\rangle \langle A_m^\lambda(0)A_n^\rho(h(-1+p))\Psi_l^\rho(-1+p)\Phi(-1+p)| \\ & + |A_m^\lambda(h(1-p))A_n^\rho(0)\Psi_l^\lambda(1-p)\Phi(1-p)\rangle \langle A_m^\lambda(0)A_n^\rho(0)\Psi_l^\lambda(0)\Phi(0)| \\ & + |A_m^\lambda(0)A_n^\rho(0)\Psi_l^\lambda(0)\Phi(0)\rangle \langle A_m^\lambda(h(1-p))A_n^\rho(0)\Psi_l^\lambda(1-p)\Phi(1-p)| \end{aligned} \quad (5.20)$$

This operator simply generalises the conclusions of Section 5.3, to include the two weights in the quantum description of the Popper-Szilard Engine. With the initial state

$$|\chi_{\text{initial}}\rangle = (\alpha |A_l^\lambda(0)A_m^\rho(0)\Psi_n^\rho(0)\rangle + \beta |A_l^\lambda(0)A_m^\rho(0)\Psi_n^\lambda(0)\rangle) |\Phi(0)\rangle$$

the system will evolve into

$$\begin{aligned} |\chi_{\text{final}}\rangle = & \alpha |A_l^\lambda(0)A_m^\rho(-1+p)\Psi_n^\rho(-1+p)\Phi(-1+p)\rangle \\ & + \beta |A_l^\lambda(1-p)A_m^\rho(0)\Psi_n^\lambda(1-p)\Phi(1-p)\rangle \end{aligned}$$

The internal energy of the one atom gas can apparently be converted into the energy required to lift a quantum weight, although it may leave the system of piston and weights in an entangled superposition. This completes the analysis of the stage of the Popper-Szilard Engine shown in Figure 4.5(b).

5.5 Resetting the Engine

The previous two Sections have analysed the interaction of the one atom gas, moveable piston and weights, using quantum mechanics. We have seen that, contrary to the assertions of [Zur84, BS95],

the piston is not stationary when the one atom gas is in a superposition. Instead, the joint system evolves into an entangled superposition. This has significance for the final problem that must be addressed in this Chapter: the issue of restoring the Popper-Szilard Engine to its initial state before commencing a second cycle. As we recall, it is this, according to [LR90, pages 25-28] that requires work to be performed upon the system. The three stages identified in Section 4.3 associated with resetting the piston position are shown in Figure 4.5(c-e) and are dealt with in this Section.

First, for Stage (c), we must see what the effect of inserting a shelf at height $h_T = h(1-p)$ has upon the weights. This stage is significant as the weights are quantum systems and this leads to a wavefunction where there is a probability of finding an unraised weight *above* the shelf.

For Stage (d) we construct states to describe the piston when it is outside the box, and a unitary operator that incorporates the effect upon the gas of inserting and removing the piston.

In Stage (e) we will attempt to construct a unitary operator that restores the piston to the center, ready for re-insertion. We will find that correlating the position of the piston to the position of the weights is necessary to attempt to return the piston to the center, but even so, cannot be achieved without some error, due to the quantum nature of the weights shown in Stage (c).

The effects of this error will be shown to lead to a possibility of the Popper-Szilard Engine going into reverse. The consequences of this will be evaluated in later Chapters.

5.5.1 Inserting Shelves

The insertion of the shelves on each side can be considered as the raising of an infinitely high potential barrier at height $h_T = h(1-p)$ in the Hamiltonians of *both* weights. For the raised weight, this will have no effect upon the wavefunction, as the quantum weight wavefunction $A_n(z, h(1-p))$ is non-zero only above the height h_T .

For the unraised weight, however, the wavefunction $A_n(z, 0)$ has a 'tail' that, for large values of z , has the form $\frac{e^{-\frac{2}{3}z^{2/3}}}{z^{1/4}}$. While this is small, it is non-zero and so there is always some possibility of finding a quantum weight above the height h_T . While we could attempt to treat this by an adiabatic raising of the potential barrier, as we did for the one atom gas, the form of the wavefunction below the shelf does not have a simple solution. Instead we will proceed by a rapid insertion of the potential barrier, and project out the portions of the wavefunctions above and below the shelf height.

For a given state, $|A_n(0)\rangle$, the projected state on finding the weight above the shelf height is given by:

$$\begin{aligned} |RA_n(h_T)\rangle &= \frac{1}{\alpha_n(h_T)} \int_{h_T}^1 |z\rangle \langle z | A_n(0)\rangle dz \\ |\alpha_n(h_T)|^2 &= \int_{h_T}^1 |A_n(z, 0)|^2 dz \end{aligned}$$

while the 'unraised' state (below the shelf height) is

$$|UN_n(h_T)\rangle = \frac{1}{\beta_n(h_T)} \int_0^{h_T} |z\rangle \langle z| A_n(0)\rangle dz$$

$$|\beta_n(h_T)|^2 = \int_0^{h_T} |A_n(z,0)|^2 dz$$

so that

$$|A_n(0)\rangle = \alpha_n(h_T) |RA_n(h_T)\rangle + \beta_n(h_T) |UN_n(h_T)\rangle$$

$|\alpha_n(h)|^2$ is the probability of finding an unraised weight above the height h . Unfortunately, the values of $\alpha_n(h_T)$ and $\beta_n(h_T)$ do not generally have simple expressions¹¹. However, using the properties of Airy functions we are able to calculate approximate values of these for large values of n . The wavefunction $A_n(z,0)$ has n nodes above the floor at $z = 0$, which occur at heights

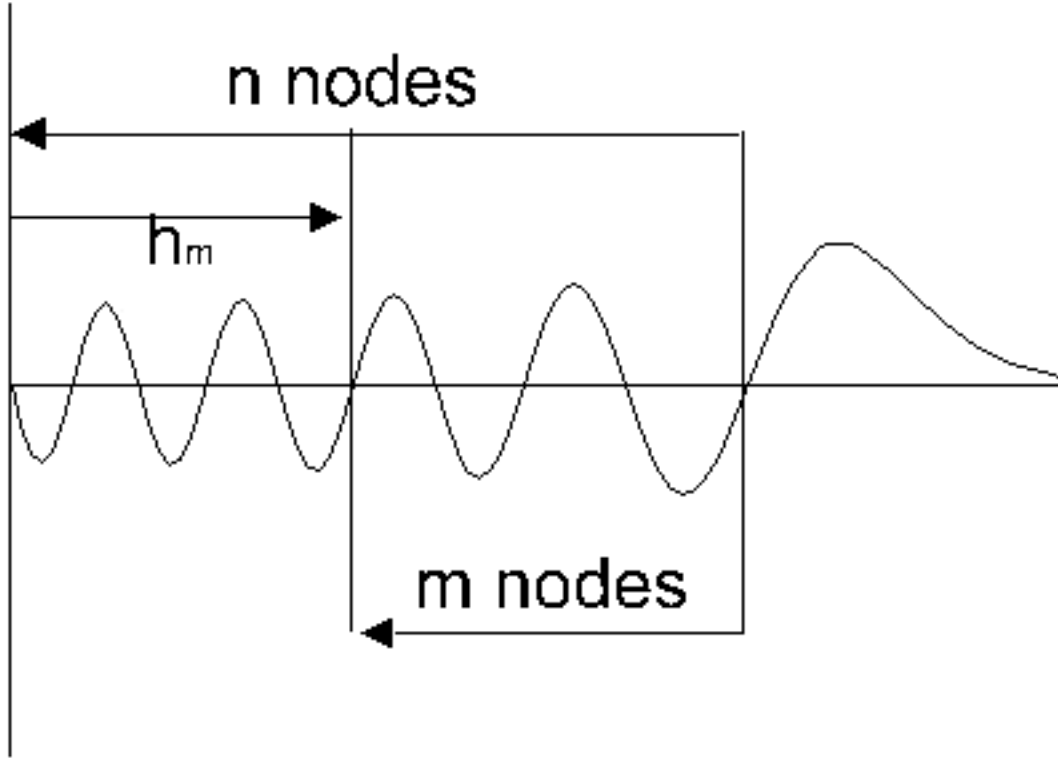


Figure 5.5: Splitting Airy Function at Height h

$h_m = (a_m - a_n)H$, where $m < n$ (remembering that the values $a_n, a_m < 0$). This is shown in Figure 5.5. When the shelf is inserted at the height of a node a_m , we can calculate the value of $\alpha_n(h_m)$ from Equation 5.17, and the properties of integrals of Airy functions $A(z)$

$$\int_{h_m}^1 |A_n(z,0)|^2 dz = \frac{1}{A^0(a_n)^2 H} \int_{(a_n i a_m)H}^1 A\left(\frac{z}{H} - a_n\right)^2 dz$$

¹¹Although as $A_n(z,0)$ is a real function, $\alpha_n(h_T)$ and $\beta_n(h_T)$ will always be real numbers.

$$\begin{aligned}
&= \frac{1}{A^\theta(a_n)^2} \int_{a_m}^1 A(z)^2 dz \\
&= \frac{1}{A^\theta(a_n)^2} [-A^\theta(z)^2 + zA(z)^2]_{a_m}^1 \\
&= \left(\frac{A^\theta(a_m)}{A^\theta(a_n)} \right)^2
\end{aligned}$$

If $m \gg 1$ the asymptotic value $A^\theta(a_m) \approx \frac{(i)^\pi}{\pi} \left(\frac{3\pi m}{2} \right)^{\frac{1}{6}}$ leads to the result

$$\alpha_n(h_m) = \left(\frac{m}{n} \right)^{\frac{1}{6}}$$

If the shelf is not inserted at the position of a node, we must interpolate between the nearest two nodes. As $\alpha_n(h_m)$ varies slowly for large m , this will be a reasonable approximation. Using the asymptotic value $a_l = -\left(\frac{3\pi l}{2}\right)^{\frac{2}{3}}$ and $h_m = (a_n - a_m)H$ to estimate an interpolated (non-integer) value of m , we can approximate $\alpha_n(h)$ for any shelf height from:

$$\begin{aligned}
h &= \left(\left(\frac{3\pi n}{2} \right)^{\frac{2}{3}} - \left(\frac{3\pi m}{2} \right)^{\frac{2}{3}} \right) H \\
m &= n \left(1 - \left(\frac{2}{3\pi n} \right)^{\frac{2}{3}} \frac{h}{H} \right)^{\frac{3}{2}} \\
\alpha_n(h) &\approx \left(1 - \left(\frac{2}{3\pi n} \right)^{\frac{2}{3}} \frac{h}{H} \right)^{\frac{1}{4}} \tag{5.21}
\end{aligned}$$

This is valid whenever the height is lower than the final node ($h < -a_n H$). If $h > -a_n H$ the shelf is inserted into the 'tail' of the wavefunction. To estimate the value of $\alpha_n(h)$ in this case, we will evaluate the probability that the weight is located anywhere above the height $-a_n H$, which must be larger than the probability of the weight located above h

$$\begin{aligned}
\alpha_n(-a_n H)^2 &= \frac{1}{A^\theta(a_n)^2} \int_{a_n}^1 A(z)^2 dz \\
&= \left(\frac{A^\theta(0)}{A^\theta(a_n)} \right)^2
\end{aligned}$$

Using $A^\theta(0) \approx -0.25$ and $n \gg 1$ as before, this gives

$$\alpha_n(h)^2 < \frac{\pi}{16} \left(\frac{2}{3\pi n} \right)^{\frac{1}{3}}$$

which may be treated as negligible. In effect, we have shown that if $h > \left(\frac{3\pi n}{2}\right)^{\frac{2}{3}} H$, or, equivalently,

$$n < \frac{2}{3\pi} \left(\frac{h}{H} \right)^{\frac{3}{2}}$$

then we can approximate

$$\begin{aligned}
\alpha_n(h) &= 0 \\
\beta_n(h) &= 1 \tag{5.22}
\end{aligned}$$

When

$$n \geq \frac{2}{3\pi} \left(\frac{h}{H} \right)^{\frac{3}{2}}$$

we calculate $\alpha_n(h)$ from Equation 5.21 above, and $\beta_n(h)$ from

$$\beta_n(h) = \sqrt{1 - \alpha_n(h)^2} \quad (5.23)$$

This completes the calculation of the effect of inserting the shelves at height h in Stage (c) of the Popper-Szilard cycle.

5.5.2 Removing the Piston

We will now consider Stage (d) of the cycle. The piston state is removed from the ends of the box, effectively 'switching off' the interaction between the gas and the piston.

Firstly, we need to introduce quantum states to describe the piston outside the box. These will be the orthonormal states, with $|\phi_L\rangle, |\phi_R\rangle$ and $|\phi_0\rangle$ describing the piston outside the box, but in the lefthand, righthand and central positions, respectively. These states also include the pulley and pan, and so the state $|\phi_L\rangle$ implies that the righthand weight is raised, and so on.

We now need a general unitary operator to account for the insertion and removal of the piston from the box. This will have an effect upon the internal states of the gas. As noted in Equation 5.15, when the piston is at one or the other end of the box, the gas will be approximately in an unperturbed energy eigenstate¹² and so will be unaffected by the piston's removal. If the piston was in the center of the box when it was removed, however, its removal can have a significant effect upon the state of the gas. This effect is the adjoint operation to inserting the piston into the center of the box, in Section 5.2. The complete insertion and removal operator is therefore

$$\begin{aligned} U_{IR} = & I_G \otimes \{ |\phi_L\rangle \langle \Phi(-1+p)| + |\Phi(-1+p)\rangle \langle \phi_L| \\ & + |\phi_R\rangle \langle \Phi(1-p)| + |\Phi(1-p)\rangle \langle \phi_R| \} \\ & + U_G \otimes |\Phi(0)\rangle \langle \phi_0| + U_G^\dagger \otimes |\phi_0\rangle \langle \Phi(0)| \end{aligned} \quad (5.24)$$

where I_G is the identity operator upon the gas states, and U_G is from Equation 5.4 in the limit of the infinitely high barrier.

5.5.3 Resetting the Piston

We now need to consider Stage (e). This is the critical stage to the argument of Leff and Rex. They argue that Landauer's Principle implies an expenditure of $kT_G \ln 2$ energy to reset the piston states. However, we have suggested that the piston may be returned to $|\phi_0\rangle$ without such an expenditure, by correlating it to the weights. We will now show that the piston may indeed be returned in this way, but, due to the quantum nature of the weights, there is always some possibility of error in the resetting mechanism.

¹²There will be a slight expansion of the gas states, of order $2p$ as the piston is removed. Technically this could be used to perform work upon the piston during its removal. However, we shall ignore this effect as negligible.

First, it will be useful to consider if we can reset the piston without correlating to the weights. The ideal operation would include

$$\begin{aligned} U_{R1} |\phi_L\rangle &= |\phi_0\rangle \\ U_{R1} |\phi_R\rangle &= |\phi_0\rangle \end{aligned}$$

but this is clearly non-unitary as orthogonal states are being mapped to non-orthogonal states. The most general operation acting only upon the piston states is

$$\begin{aligned} U_{R2} |\phi_0\rangle &= a_1 |\phi_0\rangle + b_1 |\phi_L\rangle + c_1 |\phi_R\rangle \\ U_{R2} |\phi_L\rangle &= a_2 |\phi_0\rangle + b_2 |\phi_L\rangle + c_3 |\phi_R\rangle \\ U_{R2} |\phi_R\rangle &= a_3 |\phi_0\rangle + b_3 |\phi_L\rangle + c_3 |\phi_R\rangle \end{aligned}$$

Unitarity requires that the vectors a_i, b_i and c_i (with $i = 1, 2, 3$) are orthonormal (or, equivalently, the vectors α_1, α_2 and α_3 with $\alpha = a, b, c$).

To maximise the probability of the piston being returned to the center, we need to maximise $|a_2|^2 + |a_3|^2$. This would imply setting $a_1 = 0$. However, if we are not going to change the state of the weights, the piston initially in the state $|\phi_0\rangle$ cannot be moved to either $|\phi_L\rangle$ or $|\phi_R\rangle$ as these states both imply one of the pans is raised. We are therefore constrained to have $a_1 = 1$ and so there is no possibility of resetting the piston. We must, therefore, include the states of the weights.

After the piston is removed from the box, we will have combined piston and weight states of:

$$\begin{aligned} &|A_m^\lambda(0)A_n^\rho(1-p)\phi_L\rangle \\ &|A_m^\lambda(1-p)A_n^\rho(0)\phi_R\rangle \end{aligned}$$

If we simply attempt to correlate the action on the piston with the raised and unraised states, $|A_m(1-p)\rangle, |A_m(0)\rangle$ we would construct a resetting operator along the lines of

$$\begin{aligned} U_{R3} |A_m^\lambda(0)A_n^\rho(1-p)\phi_L\rangle &= |A_m^\lambda(0)A_n^\rho(1-p)\phi_0\rangle \\ U_{R3} |A_m^\lambda(1-p)A_n^\rho(0)\phi_R\rangle &= |A_m^\lambda(1-p)A_n^\rho(0)\phi_0\rangle \end{aligned}$$

However, the inner product of these input states is given by

$$\begin{aligned} \langle A_m^\lambda(0)A_n^\rho(1-p)\phi_L | A_m^\lambda(1-p)A_n^\rho(0)\phi_R \rangle &= \langle A_m^\lambda(0) | A_m^\lambda(1-p) \rangle \langle A_n^\rho(1-p) | A_n^\rho(0) \rangle \langle \phi_L | \phi_R \rangle \\ &= 0 \end{aligned}$$

while the inner product of the output states is

$$\begin{aligned} \langle A_m^\lambda(0)A_n^\rho(1-p)\phi_0 | A_m^\lambda(1-p)A_n^\rho(0)\phi_0 \rangle &= \langle A_m^\lambda(0) | A_m^\lambda(1-p) \rangle \langle A_n^\rho(1-p) | A_n^\rho(0) \rangle \langle \phi_0 | \phi_0 \rangle \\ &= \langle A_m^\lambda(0) | A_m^\lambda(1-p) \rangle \langle A_n^\rho(1-p) | A_n^\rho(0) \rangle \\ &\neq 0 \end{aligned}$$

The output states are not orthogonal as the Airy functions of the raised and unraised weight states overlap, as shown in Figure 5.4. U_{R3} is still not a unitary operator.

To construct a proper unitary operator we need to correlate the movement of the piston to the projection of the weights above or below the shelf. The relevant projection operators are

$$\begin{aligned} P(RA) &= \int_{h_T}^1 |z\rangle \langle z| dz \\ P(UN) &= \int_0^{h_T} |z\rangle \langle z| dz \end{aligned}$$

However it is more useful to construct them from the raised eigenstates:

$$P(RA) = \sum_n |A_n(1-p)\rangle \langle A_n(1-p)|$$

or from the projections of the unraised eigenstates:

$$\begin{aligned} P(RA) &= \sum_n \alpha_n (h_T)^2 |RA_n\rangle \langle RA_n| \\ &= \int_{h_T}^1 \int_{h_T}^1 |z\rangle \langle z| \sum_n |A_n\rangle \langle A_n| z^\theta \rangle \langle z^\theta| dz dz^\theta \\ &= \int_{h_T}^1 |z\rangle \langle z| dz \\ P(UN) &= \sum_n \beta_n (h_T)^2 |UN_n\rangle \langle UN_n| \\ &= \int_0^{h_T} \int_0^{h_T} |z\rangle \langle z| \sum_n |A_n\rangle \langle A_n| z^\theta \rangle \langle z^\theta| dz dz^\theta \\ &= \int_0^{h_T} |z\rangle \langle z| dz \end{aligned}$$

From these it follows that:

$$\begin{aligned} P(RA) |A_n(0)\rangle &= \alpha_n |RA_n\rangle \\ P(UN) |A_n(0)\rangle &= \beta_n |UN_n\rangle \\ P(RA) |A_n(1-p)\rangle &= |A_n(1-p)\rangle \\ P(UN) |A_n(1-p)\rangle &= 0 \end{aligned}$$

We will now examine the correlation between the state of the weights and the piston position. There are eight orthonormal sets of states that are accessible for the combined system. These are shown in Figure 5.6.

- (a) Both weights are resting upon the floor, below the shelf. The piston must be located in the center of the Engine. The allowed state is:

$$|UN^\lambda(h_T)UN^\rho(h_T)\phi_0\rangle$$

- (b) The left weight on the shelf and the right weight on the floor. The piston can be in the center, or at the right of the engine. Allowed states are:

$$\begin{aligned} &|RA^\lambda(h_T)UN^\rho(h_T)\phi_0\rangle \\ &|A^\lambda(1-p)UN^\rho(h_T)\phi_R\rangle \end{aligned}$$

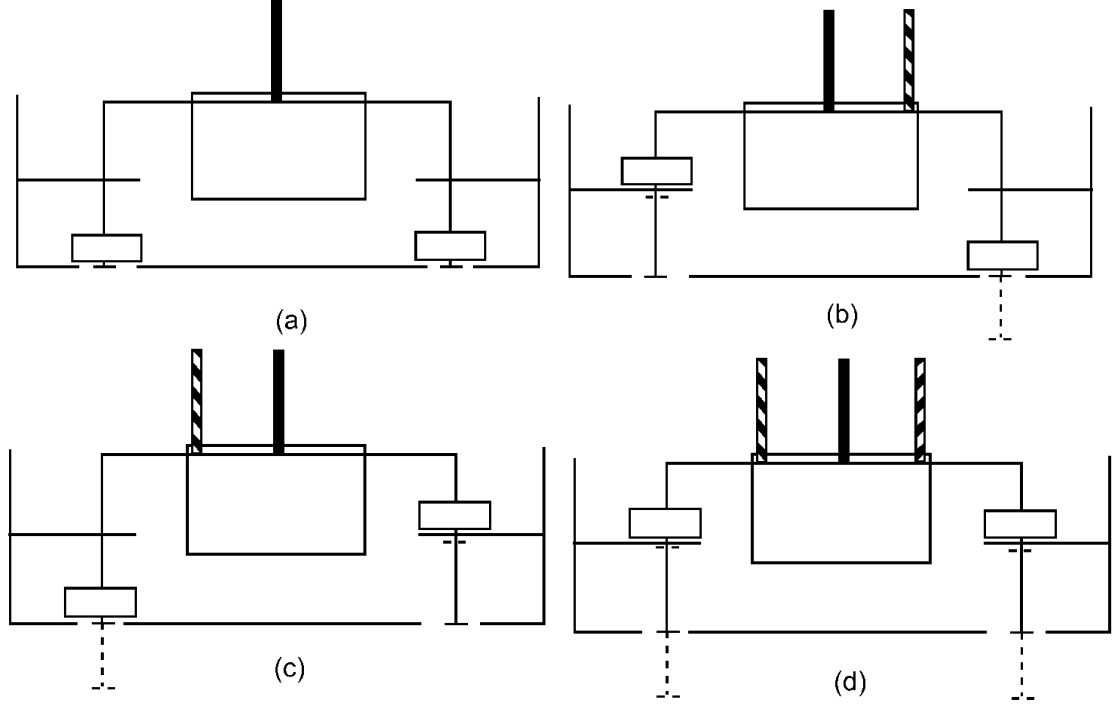


Figure 5.6: Correlation of Weights and Piston Position

- (c) The left weight on the floor and the right weight on the shelf. The piston may now be found either in the center, or at the left of the engine. Allowed states are:

$$|UN^\lambda(h_T)RA^\rho(h_T)\phi_0\rangle$$

$$|UN^\lambda(h_T)A^\rho(1-p)\phi_L\rangle$$

- (d) Both weights are upon the shelves. The piston may be located at any of the three locations:

$$|RA^\lambda(h_T)RA^\rho(h_T)\phi_0\rangle$$

$$|RA^\lambda(h_T)A^\rho(1-p)\phi_L\rangle$$

$$|A^\lambda(1-p)RA^\rho(h_T)\phi_R\rangle$$

If the resetting interaction is not to change the location of the weights, these must form four separate subspace under the operation.

We can now state the most general form of the resetting operation, consistent with the requirements of unitarity.

$$U_{RES} = |\phi_0\rangle \langle\phi_0| P^\lambda(UN)P^\rho(UN)$$

$$+ [|\phi_R\rangle \langle\phi_0| + |\phi_0\rangle \langle\phi_R|] P^\lambda(RA)P^\rho(UN)$$

$$+ [|\phi_L\rangle \langle\phi_0| + |\phi_0\rangle \langle\phi_L|] P^\lambda(UN)P^\rho(RA)$$

$$+ [|\phi_1\rangle \langle\phi_0| + |\phi_2\rangle \langle\phi_L| + |\phi_3\rangle \langle\phi_R|] P^\lambda(RA) P^\rho(RA) \quad (5.25)$$

The first line represents the subspace where both weights are located beneath the shelf height. The only possible location of the piston is in the center.

The second and third lines represent one weight above and one weight below the shelf. When the piston is located in the corresponding left or right position, we want to reset the piston by moving it to the center. To preserve unitarity with this, the reset operator must also include a term moving the piston initially located in the center to the appropriate left or right position.

Finally, when both weights are located above the shelf height, in line four, the weights do not correlate to the location of the piston. The most general transformation possible is given, where the $|\phi_j\rangle$ states are superpositions of the $|\phi_0\rangle$, $|\phi_L\rangle$ and $|\phi_R\rangle$ states:

$$\begin{aligned} |\phi_1\rangle &= a_1 |\phi_0\rangle + b_1 |\phi_L\rangle + c_1 |\phi_R\rangle \\ |\phi_2\rangle &= a_2 |\phi_0\rangle + b_2 |\phi_L\rangle + c_2 |\phi_R\rangle \\ |\phi_3\rangle &= a_3 |\phi_0\rangle + b_3 |\phi_L\rangle + c_3 |\phi_R\rangle \end{aligned}$$

For the operation to be unitary, orthonormal states must transform into orthonormal states, so $\langle\phi_i|\phi_j\rangle = \delta_{ij}$. This leads to the conditions

$$\begin{aligned} a_1^2 a_2 + b_1^2 b_2 + c_1^2 c_2 &= 0 \\ a_1^2 a_3 + b_1^2 b_3 + c_1^2 c_3 &= 0 \\ a_2^2 a_3 + b_2^2 b_3 + c_2^2 c_3 &= 0 \\ a_1^2 a_1 + b_1^2 b_1 + c_1^2 c_1 &= 1 \\ a_2^2 a_2 + b_2^2 b_2 + c_2^2 c_2 &= 1 \\ a_3^2 a_3 + b_3^2 b_3 + c_3^2 c_3 &= 1 \end{aligned} \quad (5.26)$$

Rearranging the expression

$$\begin{aligned} & [|\phi_1\rangle \langle\phi_0| + |\phi_2\rangle \langle\phi_L| + |\phi_3\rangle \langle\phi_R|] \\ = & |\phi_0\rangle \{a_1 \langle\phi_0| + a_2 \langle\phi_L| + a_3 \langle\phi_R|\} \\ & + |\phi_L\rangle \{b_1 \langle\phi_0| + b_2 \langle\phi_L| + b_3 \langle\phi_R|\} \\ & + |\phi_R\rangle \{c_1 \langle\phi_0| + c_2 \langle\phi_L| + c_3 \langle\phi_R|\} \end{aligned}$$

$$\begin{aligned}
a_1^{\bar{a}}b_1 + a_2^{\bar{a}}b_2 + a_3^{\bar{a}}b_3 &= 0 \\
a_1^{\bar{a}}c_1 + a_2^{\bar{a}}c_2 + a_3^{\bar{a}}c_3 &= 0 \\
b_1^{\bar{a}}c_1 + b_2^{\bar{a}}c_2 + b_3^{\bar{a}}c_3 &= 0
\end{aligned}$$

We can examine the effect of this operator by considering the effect upon the state where the piston is to the left, before the shelves are inserted

$$|A_m^\lambda(0)A_n^\rho(1-p)\phi_L\rangle$$

When the shelves are inserted this becomes separated into raised and unraised portions of the lefthand weight

$$\alpha_m(h_T) |RA_m^\lambda(h_T)A_n^\rho(1-p)\phi_L\rangle + \beta_m(h_T) |UN_m^\lambda(h_T)A_n^\rho(1-p)\phi_L\rangle$$

. The operation of U_{RES} on the unraised portion of the wavefunction moves the piston to the center. The effect of U_{RES} on the raised portion is to set the piston state to $|\phi_2\rangle$. This makes the state

$$\begin{aligned}
&\alpha_m(h_T) |RA_m^\lambda(h_T)A_n^\rho(1-p)\phi_2\rangle + \beta_m(h_T) |UN_m^\lambda(h_T)A_n^\rho(1-p)\phi_0\rangle \\
&= \alpha_m(h_T)b_2 |RA_m^\lambda(h_T)A_n^\rho(1-p)\phi_L\rangle \\
&+ \alpha_m(h_T)c_2 |RA_m^\lambda(h_T)A_n^\rho(1-p)\phi_R\rangle \\
&+ (\alpha_m(h_T)a_2 |RA_m^\lambda(h_T)\rangle + \beta_m(h_T) |UN_m^\lambda(h_T)\rangle) |A_n^\rho(1-p)\phi_0\rangle
\end{aligned}$$

Although the resetting operation has partially succeeded, there is still some probability of finding the piston to the left or right of the Engine, whatever choice we make for the values of a_i etc. Selection of the optimum values of the a_i 's can only be made once we include the full statistical mechanics in Chapter 6.

This completes the analysis of Stage (e) of the Popper-Szilard Engine in this chapter. We have found that the quantum state of the weight leads to the possibility of an unraised weight being spontaneously located above the height h_T through which the raised weight has been lifted. This possibility, combined with the requirement that the resetting operation be unitary, leads to an imperfect resetting. This is clearly not sufficient to show that the Popper-Szilard Engine does not work. The error in the resetting is only partial, and it is not yet certain that an optimal choice of resetting operation could not violate the second law of thermodynamics.

5.6 Conclusions

We have examined the operation of the quantum Popper-Szilard Engine given in Figure 4.5 in detail, explicitly constructing unitary operations for all relevant stages of the cycle. We will now summarise this cycle, and consider the effects of the errors in the resetting operation.

There is a final unitary operation we need to add to the ones constructed. This is the act of inserting and removing the shelves at height h_T , at Stages (c) and (f). This can be treated by

assuming a narrow potential barrier is inserted in the Hamiltonian in Equation 5.16. The result is a time dependant perturbation of the Hamiltonian, exactly equivalent to the raising or lowering of the potential barrier in the one atom gas, in Section 5.2. The unitary operator for this can be constructed in the same manner as the operator U_G in Equation 5.4. We will not explicitly do this, but will simply describe the unitary operator corresponding to the insertion of the shelves by U_S and their removal by U_S^Y . The complete cycle of the Popper-Szilard Engine is now given by the unitary operation:

$$U_T = U_S^Y U_{RES} U_{RI} U_S U_{W4} U_{RI} \quad (5.27)$$

Moving from right to left through U_T , the successive stages are:

- U_{RI} Stage (a) Equation 5.24
- U_{W4} Stage (b) Equation 5.20
- U_S Stage (c) above
- U_{RI} Stage (d) Equation 5.24
- U_{RES} Stage (e) Equation 5.25
- U_S^Y Stage (f) above

We will now review the effect of U_T on the system.

5.6.1 Raising Cycle

If we start from the state where the piston is in the center, outside the box, and both weights are at rest upon the floor, the state is

$$|A_m^\lambda(0)A_n^\rho(0)\phi_0\rangle$$

We can now see how the operation of U_T attempts to reproduce the cycle in Figure 4.5.

- U_{RI} The insertion of the piston in the center of the box (Section 5.2)
- U_{W4} The expansion of the one atom gas against the piston, lifting one of the weights. This may leave the system in an entangled superposition (Sections 5.3, 5.4).
- U_S Inserting shelves on both sides at height h_T .
- U_{RI} Removing the piston from the box (Section 5.5)
- U_{RES} Resetting the piston by correlating it's state to the location of the raised or unraised weights (Section 5.5)
- U_S^Y Removing the shelves and allowing any raised weights to fall to the floor

This will be described as a 'raising cycle'.

We saw in Section 5.5 above, that this leaves the Engine in a superposition of states. To complete the cycle, we want the Engine to be in state

$$|A_m^\lambda(0)A_n^\rho(0)\phi_0\rangle$$

at the end of Stage (f). However, due to the imperfect nature of the resetting, the Engine is in a superposition with states such as

$$\begin{aligned} &|A_m^\lambda(0)A_n^\rho(1-p)\phi_L\rangle \\ &|A_m^\lambda(1-p)A_n^\rho(0)\phi_R\rangle \end{aligned}$$

We must now consider the effect of starting a new cycle with these states.

5.6.2 Lowering Cycle

If the Engine starts with a raised weight on the righthand side, and the piston to the left side of the Engine, the state will be

$$|A_m^\lambda(0)A_n^\rho(1-p)\phi_L\rangle$$

We must now consider the effect of U_T on this state.

- U_{RI} The piston is inserted into the box on the lefthand side. Negligible compression of the gas takes place. The state is now

$$|A_m^\lambda(0)A_n^\rho(1-p)\Psi_l^\rho(-1+p)\Phi(-1+p)\rangle$$

- U_{W4} The combined gas, piston and weight system now runs through a *compression* phase. The righthand weight is lowered, and the piston moves from the left to the center of the box, compressing the gas to the right. The energy of the weight is reduced and the internal energy of the gas is raised. The system is left in state

$$|A_m^\lambda(0)A_n^\rho(0)\Psi_l^\rho(0)\Phi(0)\rangle$$

- U_S At the end of Stage (b) both weights are in the unraised state. When the shelves emerge there is a possibility that either, or both, could be trapped above the shelf height h_T . This involves rewriting

$$\begin{aligned} |A_m^\lambda(0)A_n^\rho(0)\Psi_l^\rho(0)\Phi(0)\rangle &= (\alpha_m(h_T)\alpha_n(h_T) |RA_m^\lambda(h_T)RA_n^\rho(h_T)\rangle \\ &\quad + \alpha_m(h_T)\beta_n(h_T) |RA_m^\lambda(h_T)UN_n^\rho(h_T)\rangle \\ &\quad + \beta_m(h_T)\alpha_n(h_T) |UN_m^\lambda(h_T)RA_n^\rho(h_T)\rangle \\ &\quad + \beta_m(h_T)\beta_n(h_T) |UN_m^\lambda(h_T)UN_n^\rho(h_T)\rangle) |\Psi_l^\rho(0)\Phi(0)\rangle \end{aligned}$$

- U_{RI} The piston is removed from the *center* of the box. As the one atom gas was confined to the right of the piston, this will have a significant effect upon the gas state, as it is allowed to expand to occupy the entire box. This involves replacing $|\Psi_l^\rho(0)\rangle$ with $\frac{1}{\sqrt{2}}(|\Psi_l^{\text{even}}\rangle - |\Psi_l^{\text{odd}}\rangle)$ and $|\Phi(0)\rangle$ with $|\phi_0\rangle$.
- U_{RES} The resetting operation moves the piston according to the location of the weights. As noted in Stage (c), all four combinations of weight states occur with some probability. After this operation the piston may therefore be found in the left, right or central position

$$\begin{aligned}
& (\alpha_m(h_T)\alpha_n(h_T) |RA_m^\lambda(h_T)RA_n^\rho(h_T)\phi_1\rangle \\
& + \alpha_m(h_T)\beta_n(h_T) |RA_m^\lambda(h_T)UN_n^\rho(h_T)\phi_R\rangle \\
& + \beta_m(h_T)\alpha_n(h_T) |UN_m^\lambda(h_T)RA_n^\rho(h_T)\phi_L\rangle \\
& + \beta_m(h_T)\beta_n(h_T) |UN_m^\lambda(h_T)UN_n^\rho(h_T)\phi_0\rangle) \frac{1}{\sqrt{2}} (|\Psi_l^{\text{even}}\rangle - |\Psi_l^{\text{odd}}\rangle)
\end{aligned}$$

- U_S The shelves are removed, allowing unsupported weights to fall to the floor. If the piston state is in the $|\phi_L\rangle$ or $|\phi_R\rangle$, then the corresponding right or lefthand weight will be supported at height h_T . However, if the piston state is $|\phi_0\rangle$ then both weights will fall to the floor.

We will describe this as the 'lowering cycle' and it is shown in Figure 5.7. The key point to this cycle is that energy is transferred from the *weight* to the *gas* during Stage (b) . This is in the opposite direction to the 'raising cycle'. At the end of the 'lowering cycle' the piston may again be found, outside the box, in the lefthand, righthand or central positions. If the piston is in the center, then the next cycle of U_T will result in a 'raising cycle'. If the piston is instead in the left or right states, then a weight is trapped at the height h_T and the system will continue with another 'lowering cycle'.

5.6.3 Summary

This completes the analysis of the quantum mechanics of the Popper-Szilard Engine. We have demonstrated how the Engine proceeds without the need for external measurements or interventions from 'demons'. The arguments of [Zur84, BS95] do not appear to be sustained with respect to the quantum state of the one atom gas.

With respect to the arguments of [LR90] we have shown that an imperfect resetting does appear to be possible, without the need to perform work upon the system. However, the imperfect resetting leads to the possibility of the cycle of the Popper-Szilard Engine reversing from a 'raising cycle' to a 'lowering cycle'. However, at the end of a lowering cycle, there is a possibility of reversing back onto a raising cycle. The Engine therefore switches between the two cycles.

On raising cycles, energy is transferred from the one atom gas to the weight. On lowering cycles, the energy is pumped in the opposite direction. To avoid violating the second law of thermodynamics, the energy flow must go from the hotter to the colder system. This requires

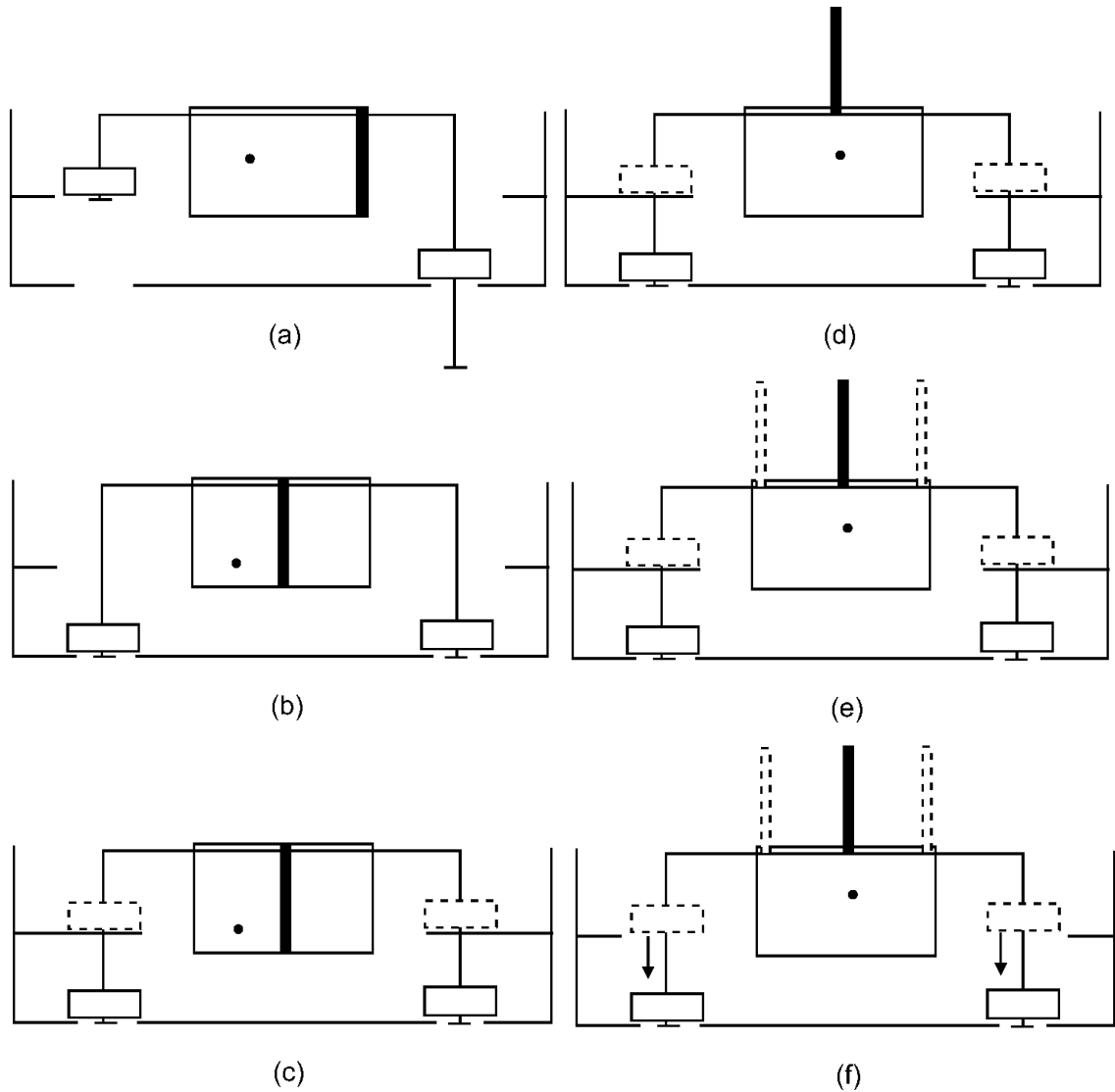


Figure 5.7: The Lowering Cycle of the Popper-Szilard Engine

a delicate balance of probabilities. If the temperature of the gas heat bath is lower than the temperature of the weight heat bath, then the Engine must spend more time transferring heat from the weights to the gas, and so must spend most of its time on the lowering cycle. Conversely, if the one atom gas is hotter than the weights, the Engine must spend most of its time on the raising cycle. This must continue to hold true for *all possible* choices of the parameters for U_{RES} given in Equation 5.26. To verify that this is the case, we must introduce the statistical mechanical properties of the Engine. We will do this in the next Chapter.

Chapter 6

The Statistical Mechanics of Szilard's Engine

In Chapter 5 we examined the physical limitations imposed by quantum theory upon the interactions of the microstates of the Popper-Szilard Engine. This would be sufficient if we wished to analyse the Engine as a closed system, initially in a definite quantum state. However, this is not the problem for which the thought experiment was designed. The purpose of the analysis is to decide whether the Engine is capable of transferring energy between heat baths in an anti-entropic manner. For this we need to introduce statistical mechanical concepts. These concepts will be introduced and applied in this Chapter, and will demonstrate that such anti-entropic behaviour is *not* possible.

Section 1 summarises the statistical mechanical concepts which will be used. This includes ensembles, heat baths and generalised pressure. With the exception of the temperature of the heat baths, we will avoid making use of any explicitly thermodynamic quantities, such as entropy or free energy.

Sections 2 and 3 will apply these concepts to the gas and the weight subsystems, respectively, paying particularly close attention to the changes in pressure and internal energies of these systems, for different piston positions. In Section 4 we will use the results of the previous two sections to calculate the optimum gearing ratio $h(Y)$ for the piston and pulley system (see Section 5.4).

In Sections 5 and 6 we will put together these results to describe the behaviour of the Popper-Szilard Engine for the raising and lowering cycles, respectively. Section 7 will finally analyse the mean flow of energy between the gas and weight heat baths. It will now be possible to show that, for any choice of temperatures of the two heat baths, and for any choice of resetting operation U_{RES} , the long term behaviour of the Engine is to produce a flow of energy from the hotter to the colder heat bath. The Popper-Szilard Engine is therefore unable to produce anti-entropic heat flows.

6.1 Statistical Mechanics

Statistical Ensemble

Many textbooks ([Pen70, Wal85], for example) introduce statistical mechanics as the study of systems which have a large number of constituents. It has been argued [Pop74, Cha73] that this is part of the explanation of the Szilard Paradox. However, it is not necessary that a system be large for statistical mechanics to be used. Statistical mechanical concepts can be applied whenever the preparation of a system, however large or small, does not uniquely specify the initial state of the system. Instead we must specify the probabilities p_i of the different possible initial states $|\Gamma_i\rangle$.

We will describe such a system using the Gibbs ensemble, where we conceive of an infinite number of equivalently prepared systems, with the initial states $|\Gamma_i\rangle$ occurring with relative frequencies p_i . The ensemble is represented by the density matrix $\rho = \sum_i p_i |\Gamma_i\rangle \langle \Gamma_i|$ ([Tol79, BH96a], for example). Obviously such an ensemble does not actually exist. However, if we use the preparation method to prepare a finite number of systems, with no special ordering, then the statistics of the outcomes of the real systems will approach the statistics of the ensemble¹ as the number of systems becomes large. The ensemble is a representation of the mean behaviour when the same experiment is repeated a large number of times, and applies even when each experiment is performed upon a system which consists of only a few constituents.

In our case we are therefore supposing an infinite number of Popper-Szilard Engines, each connected to their own heat baths and each containing only a single atom. We will describe the behaviour of this 'representative ensemble' of Engines as the mean behaviour of the Popper-Szilard Engine.

Generalised Pressure

The mean energy of a system is given by $E = \text{Tr}[\rho H]$, where H is the Hamiltonian. If the $|\Gamma_i\rangle$ are energy eigenstates, with eigenvalues E_i , then this leads to $E = \sum_i p_i E_i$, as we would expect. Typically, these E_i depend upon both internal co-ordinates (such as the location of the atoms in a gas) and external co-ordinates (such as the location of the walls surrounding the gas). The energy is a property of the internal co-ordinate (such as the kinetic energy of the motion of the atoms in the gas), while the external parameters define the boundary conditions upon the eigenstates.

If the system is in state $|\Gamma_i\rangle$ and an external parameter (X for example) is changed, this affects the eigenstate, and through it the energy of the state. The force that is required to change the parameter is given by $\frac{\partial E_i}{\partial X}$. For the ensemble the mean force, or generalised pressure, on co-ordinate X is

$$P(X) = \sum_i p_i(X) \frac{\partial E_i}{\partial X}$$

¹In [Per93] the large finite number of systems is referred to as an 'assembly'. If instead the systems can be considered as occurring in a particular order, it may be more accurate to describe them as a 'string'[Zur89a].

The work done, or mean energy required, to change the co-ordinate from X_1 to X_2 is therefore

$$W = \int_{X_1}^{X_2} \sum_i p_i(X) \frac{\partial E_i}{\partial X} dX$$

Heat Baths

An infinitesimal change in the Energy of a system is given by $dE = \sum_i p_i dE_i + \sum_i E_i dp_i$. As $dE_i = \frac{\partial E_i}{\partial X} dX$ we can see the first term corresponds to the work, dW , done upon the system. The second term corresponds to the change in heat, $dQ = \sum_i E_i dp_i$, and requires the system to be in contact with an environment (in an isolated system, occupation probabilities do not change). The 'environment' system we will use will be the canonical heat bath.

The canonical heat bath consists of a large assembly of weakly interacting systems, parameterised by the temperature T . Each system has an internal Hamiltonian H_B . The density matrix of individual system n , removed from the assembly, is given by the canonical ensemble:

$$\rho_n = \frac{e^{i H_B(n)/kT}}{\text{Tr} [e^{i H_B(n)/kT}]}$$

The ensemble of the heat bath is

$$\rho_B = \prod_n \frac{e^{i H_B(n)/kT}}{\text{Tr} [e^{i H_B(n)/kT}]}$$

This is the *most likely* distribution consistent with a given mean energy.

The most significant property of the canonical heat bath is the effect of bringing another system into temporary contact² with one of the heat bath subsystems. It can be shown that if a system which is *not* initially described by canonical distribution, is brought into successive contact with many systems, which are each in a canonical distribution with temperature T , the first system will approach a canonical distribution, also with temperature T [Tol79, Par89a, Par89b, Per93].

When a system is brought into contact with a heat bath, we assume that it is in effect brought sequentially into contact with randomly selected subsystems of the heat bath. This will gradually bring the system into a canonical distribution with the same temperature as the heat bath, so the density matrix of the system itself becomes

$$\rho = \frac{e^{i H/kT}}{\text{Tr} [e^{i H/kT}]}$$

where H is the systems internal Hamiltonian. As the heat bath subsystems are weakly interacting, and there is a large number of them, we will assume that any energy transferred to or from the heat bath does not significantly affect the state of the heat bath, and that any correlations that develop between heat bath and system states are rapidly lost. This process of *thermalisation*, by which the system is brought into equilibrium with the heat bath at temperature T , occurs with a characteristic time τ , the thermal relaxation time.

²By 'temporary contact' we mean that for a short period there is a non-zero interaction Hamiltonian affecting the two systems

This property needs qualifying with regard to *accessible* states. It may be the case that the Hamiltonian H can be subdivided into separate Hamiltonians $H = H_1 + H_2 + \dots$ where H_1, H_2 correspond to disjoint subspaces, between which there are no transitions, or transitions can only take place at a very slow rate.

An example of this would be locating a particle in one of several large boxes, with the separate Hamiltonians corresponding to the states within each box. In this case, placing the boxes in contact with the heat bath over a time period of order τ will cause a particle to be thermalised with a given box but would not cause transitions between boxes. The resulting thermalised density matrix ρ^θ will be

$$\rho^\theta = \text{Tr}[P_1\rho] \frac{e^{i H_1/kT}}{\text{Tr}[e^{i H_1/kT}]} + \text{Tr}[P_2\rho] \frac{e^{i H_2/kT}}{\text{Tr}[e^{i H_2/kT}]} + \dots \quad (6.1)$$

where ρ is the initial, unthermalised, density matrix and P_1 is the projection operator onto the subspace of H_1 and so forth. If the contact is maintained for a much longer period of time $\tau^{\theta\theta}$, so that significant numbers of transitions between the H_i states can take place, the complete thermalisation will occur and

$$\rho^{\theta\theta} = \frac{e^{i H/kT}}{\text{Tr}[e^{i H/kT}]}$$

It should be noted that this implies there can be more than one thermal relaxation time associated with a given system.

Developing this further, we must consider *conditional* Hamiltonians

$$H = \Pi_1 H_1 + \Pi_2 H_2 + \dots$$

where the Π_i 's are orthogonal projection operators on states of a *second* quantum system, or Hilbert space. An example of this might be a situation where a system has *spin*, but the interaction between the system and the heat bath does not allow transitions between spin states (or these transitions are suppressed) and the H_i do not explicitly include the spin states. In this case the thermalisation will take place separately within the separate spin subspaces.

In this case the effect of contact with the heat bath will be to thermalise the density matrix to

$$\rho^{\theta\theta\theta} = \text{Tr}_1[\Pi_1\rho] \frac{e^{i H_1/kT}}{\text{Tr}[e^{i H_1/kT}]} + \text{Tr}_1[\Pi_2\rho] \frac{e^{i H_2/kT}}{\text{Tr}[e^{i H_2/kT}]} + \dots \quad (6.2)$$

where the trace is taken only over the Hilbert space of the first system. This produces a density matrix for the *joint* system, which has the property of no interference terms between the subspaces of the *second* system. However, we should be clear that there has been no interaction between the heat bath and the second Hilbert space. Again, if there is a process by which transitions take place between the states of the second Hilbert space, then the complete thermalisation of the joint system may take place, with a second, longer thermal relaxation time.

Within the context of the Popper-Szilard Engine, Equation 6.1 will apply to situations where a single Hilbert space is divided into a tensor sum of subspaces. This includes the one atom gas, when the partition is raised in the center of the box, or the unraised weight when the shelf is inserted. The Hamiltonian in Equation 5.7 shows how the gas Hilbert space divides into the two

disjoint subspaces. Equation 6.2 applies when there is a joint Hilbert space composed of a tensor product of two (or more) Hilbert spaces, only one of which is in thermal contact with a heat bath. This will apply to the joint systems of the gas and piston located in the box, and to the joint system of a raised weight and the pan located beneath it. Equations 5.11 and 5.18 give the relevant conditional Hamiltonians for these cases.

In general there may be many relaxation times associated with the thermalisation of a system, depending upon the different subspaces and interactions with the heat bath. We will assume all relaxation times are either very short (or effectively instantaneous), or very long (or effectively infinite), with respect to the time period over which the Popper-Szilard Engine operates.

The following transitions will be assumed to have short thermal relaxation times:

- Transitions between one atom gas states when the partition is not inserted in the box.
- Transitions between one atom gas states on the same side of the piston or partition.
- Transitions between quantum weight states when the shelves are not present.
- Transitions between quantum weight states on the same side of the shelf.

Transitions with long thermal relaxation times are assumed to be:

- Transitions of the one atom gas states across the partition or piston.
- Transitions of the quantum weight states across the shelf.
- All transitions of the piston states.

We will also always assume that temperatures T are high enough for us to approximate summations over energy eigenstates by integrations of the form

$$\sum_{n=1, \uparrow} e^{i \frac{E_n}{kT}} f(E_n) \approx \int_0^{\uparrow} e^{i \frac{E(n)}{kT}} f(E(n)) dn$$

where the eigenvalue relations for integer n are replaced by the corresponding functions of a continuous parameter n , so that $E_n = E(n)$. This approximation is valid if kT is much greater than the spacing of the energy levels.

6.2 Thermal state of gas

In this Section we will analyse the effect on the one atom gas of bringing it into contact with a heat bath at temperature T_G . It is assumed that the thermal relaxation time is very short.

We will start by analysing the energy levels, and mean internal energy of the one-atom gas, in equilibrium, before and after the partition is inserted. Proceeding in a similar manner to Chapter 5 we will then consider the situation where the one atom gas is confined entirely to the left of the partition, at some variable position Y . Finally we will consider the situation where there is a moving piston in the box.

6.2.1 No partition

The initial Hamiltonian in Equation 5.1, can be written as

$$H_{G0} = \sum_n \epsilon n^2 |\psi_n\rangle \langle \psi_n|$$

In contact with a heat bath at T_G , the gas will be in an initial equilibrium ensemble of³

$$\begin{aligned} \rho_{G0} &= \frac{1}{Z_{G0}} \sum_n e^{i \frac{\epsilon n^2}{kT_G}} |\psi_n\rangle \langle \psi_n| \\ Z_{G0} &= \sum_n e^{i \frac{\epsilon n^2}{kT_G}} \\ &\approx \int e^{i \frac{\epsilon n^2}{kT_G}} dn = \frac{1}{2} \sqrt{\frac{\pi kT_G}{\epsilon}} \end{aligned} \quad (6.3)$$

The mean internal energy of the gas states is given by

$$\langle E_{G0} \rangle \approx \frac{1}{Z_{G0}} \int \epsilon n^2 e^{i \frac{\epsilon n^2}{kT_G}} dn = \frac{1}{2} kT_G$$

which confirms the usual formula for the internal energy of a gas with a single degree of freedom.

6.2.2 Partition raised

Raising of the partition in the center of the box is equivalent to applying the operator U_G , in Equation 5.4. The final Hamiltonian in Equation 5.7 from Section 5.2 is

$$H_{G1} = \frac{4\epsilon}{(1-p)^2} \sum_l l^2 \{ |\Psi_l^\lambda\rangle \langle \Psi_l^\lambda| + |\Psi_l^\rho\rangle \langle \Psi_l^\rho| \}$$

which, taking account a degeneracy factor of 2, leads to

$$\begin{aligned} \rho_{G1} &= \frac{1}{Z_{G1}} \sum_l e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} \{ |\Psi_l^\lambda\rangle \langle \Psi_l^\lambda| + |\Psi_l^\rho\rangle \langle \Psi_l^\rho| \} \\ Z_{G1} &= \sum_n 2e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} \approx \frac{1-p}{2} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ \langle E_{G1} \rangle &\approx \frac{1}{Z_{G1}} \int 2\epsilon \left(\frac{2l}{1-p}\right)^2 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} dl = \frac{1}{2} kT_G \end{aligned} \quad (6.4)$$

The fact that the internal energy has not changed does not mean that no work has been performed upon the system, only that any energy that enters the gas while inserting the partition has been transferred to the heat bath. We will now prove that the insertion of the partition requires negligible work.

As the partition is inserted, the odd and even wavefunctions are perturbed, leading to shifts in energy. There will also be a shift in occupation probabilities, if the gas is kept in contact with a heat bath. As the size of the energy change is small compared with the initial energy, for all but the lowest eigenstates, we can assume that the change in occupation probabilities is negligible.

³In some situations the normalisation constant Z will coincide with the thermodynamic partition function. However, this will *not* necessarily be the case, so we will not make use of this fact in this Chapter.

For odd symmetry states, the change in energies is given by

$$\begin{aligned} W_l^{(odd)} &= \epsilon \left(\frac{2l}{1-p} \right)^2 f(p) \\ f(p) &= p(2-p) \end{aligned}$$

so the work done is

$$\begin{aligned} W^{(odd)} &= \frac{\epsilon}{Z^{(odd)}} \sum_l \left(\frac{2l}{1-p} \right)^2 f(p) e^{i \frac{\epsilon}{kT_G} (2l)^2} \\ Z^{(odd)} &= \sum_l e^{i \frac{\epsilon}{kT_G} (2l)^2} \approx \frac{1}{4} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ W^{(odd)} &\approx \frac{\epsilon}{Z^{(odd)}} \left(\frac{2}{1-p} \right)^2 f(p) \frac{2Z_{odd}^3}{\pi} = \frac{\frac{1}{2} kT_G}{(1-p)^2} f(p) \end{aligned}$$

For even symmetry states, the energy shift is more complicated

$$\begin{aligned} W_l^{(even)} &= \epsilon \left(\frac{1}{1-p} \right)^2 [f(p)4l^2 - (4l-1)(1-p)^2] \\ W^{(even)} &= \frac{\epsilon}{Z^{(even)}} \sum_l \left(\frac{1}{1-p} \right)^2 [f(p)4l^2 - (4l-1)(1-p)^2] e^{i \frac{\epsilon}{kT_G} (2l-1)^2} \\ Z^{(even)} &= \sum_l e^{i \frac{\epsilon}{kT_G} (2l-1)^2} \end{aligned}$$

This requires a substitution $2y = 2l - 1$ to give

$$\begin{aligned} W^{(even)} &= \frac{\epsilon}{Z^{(even)}} \sum_y \left(\frac{1}{1-p} \right)^2 [f(p)4y^2 + 4y + 1] e^{i \frac{\epsilon}{kT_G} (2y)^2} \\ Z^{(even)} &\approx \frac{1}{4} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ W^{(even)} &\approx \frac{\epsilon}{Z^{(even)}} \left(\frac{2}{1-p} \right)^2 \left[f(p) \frac{2(Z^{(even)})^3}{\pi} + \frac{2(Z^{(even)})^2}{\pi} + \frac{Z^{(even)}}{4} \right] \\ &\approx \frac{\frac{1}{2} kT_G}{(1-p)^2} \left[f(p) + 4 \sqrt{\frac{\epsilon}{kT_G}} + 2 \left(\frac{\epsilon}{kT_G} \right) \right] \end{aligned}$$

The mean work done is approximately $W = \frac{1}{2} W^{(odd)} + \frac{1}{2} W^{(even)}$. As can be seen, when $p \ll 1$ and ground state energy $\epsilon \ll kT_G$, then $W \ll \frac{1}{2} kT_G$. This confirms that the insertion of the barrier does not require a significant amount of work, when the barrier is narrow and the internal energy is high with respect to the ground state.

6.2.3 Confined Gas

If we restrict the gas to be located on the lefthand side of the partition, the density matrix only includes half the states

$$\begin{aligned} \rho_{G2}^\lambda &= \frac{1}{Z_{G2}} \sum_l e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} |\Psi_l^\lambda\rangle \langle \Psi_l^\lambda| \\ Z_{G2} &= \sum_n e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} \approx \frac{1-p}{4} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ \langle E_{G2}^\lambda \rangle &\approx \frac{1}{Z_{G2}} \int \epsilon \left(\frac{2l}{1-p} \right)^2 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} dl = \frac{1}{2} kT_G \end{aligned} \tag{6.5}$$

Similar expressions can be calculated from ρ_{G2}^ρ , Z_{G2}^ρ and $\langle E_{G2}^\rho \rangle$, where the gas is confined entirely to the right of the partition.

6.2.4 Moving partition

We will now proceed with the gas located entirely on the left of the piston, and consider the mean internal energy of the gas states, and the pressure upon the piston, as the piston moves.

For the piston located at a position Y we use the Hamiltonian H_{G2}^λ given in Equation 5.11 for the internal energy of the gas states. The energy and pressure of the individual gas states are

$$\begin{aligned} E_l^\lambda(Y) &= \frac{4\epsilon l^2}{(Y+1-p)^2} \\ \frac{\partial E_l(Y)}{\partial Y} &= \frac{-8\epsilon l^2}{(Y+1-p)^3} \end{aligned}$$

The evaluation of the effect of the moving partition depends upon how the probabilities of each state changes as the piston moves. We will consider three cases: perfectly isolated, essentially isolated and isothermal. The definition of these follows that given in [Tol79, Chapter 12 B]⁴.

Perfect Isolation

For this condition, we assume the gas is completely isolated, and the expansion takes place sufficiently slowly, that the probabilities are unchanged from their initial values, proportional to $e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2}$

$$\begin{aligned} \rho_{G3}^\lambda(Y) &= \frac{1}{Z_{G3}} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \\ Z_{G3} &= \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} \approx \frac{1-p}{4} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ \langle E_{G3}^\lambda(Y) \rangle &= \frac{1}{Z_{G3}} \int \epsilon \left(\frac{2l}{Y+1-p}\right)^2 e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} dl = \frac{1}{2} kT_G \left(\frac{1-p}{Y+1-p}\right)^2 \\ P_{G3}^\lambda(Y) &= \frac{1}{Z_{G3}} \int \frac{-8\epsilon l^2}{(Y+1-p)^3} e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} dl = -kT_G \frac{(1-p)^2}{(Y+1-p)^3} \end{aligned}$$

The pressure term is derived from the change in internal energies of the gas, when the piston position Y changes. Note, the piston position is an *external* co-ordinate for the gas. The work performed upon the piston by the gas, when the piston is initially in the center of the box ($Y=0$) is

$$W_{G3}^\lambda(Y) = \int_0^Y kT_G \frac{(1-p)^2}{(Y^\theta+1-p)^3} dY^\theta = \frac{1}{2} kT_G \frac{Y(Y+2(1-p))}{(Y+1-p)^2}$$

As the system is completely isolated, the change in internal energy must exactly equals work performed so that $\langle E_{G3}(Y) \rangle + W_{G3}(Y) = \frac{1}{2} kT_G$.

⁴It will be seen that essential isolation broadly corresponds to those processes that are traditionally referred to as 'adiabatic' in thermodynamics. We have not used this term to avoid confusion with the 'adiabatic theorem' in quantum mechanics, which will be applicable to all three of the above processes

After the expansion has ended at $Y = (1 - p)$, the gas has internal energy $\frac{1}{8}kT_G$, and the work extracted is $\frac{3}{8}kT_G$. If the system is allowed to continue in perfect isolation, the piston will now reverse direction and start to compress the gas. This requires work to be performed by the piston upon the gas

$$W_{G3}^\lambda(Y) = \int_{1-p}^Y kT_G \frac{(1-p)^2}{(Y^\theta + 1 - p)^3} dY^\theta$$

Again the total energy is constant, and when the piston has reached the center, the gas has internal energy $\frac{1}{2}kT_G$ and the work performed upon the gas is $\frac{3}{8}kT_G$. As the work extracted during the expansion is the same as that performed during the compression, the cycle is reversible.

If, when the piston was at $Y = 1 - p$, instead of allowing the piston to immediately return to the center, we brought the gas into contact with the heat bath, it would return to the state ρ_{G0} above, absorbing $\frac{3}{8}kT_G$ heat from the bath in the process. When the piston starts to compress the gas from this state, different results occur, as the initial probabilities are now proportional to $e^{j \frac{\epsilon}{kT_G} (\frac{l}{1-p})^2}$

$$\begin{aligned} \rho_{G4}^\lambda(Y) &= \frac{1}{Z_{G4}} \sum_l e^{j \frac{\epsilon}{kT_G} (\frac{l}{1-p})^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \\ Z_{G4} &= \sum_l e^{j \frac{\epsilon}{kT_G} (\frac{l}{1-p})^2} \approx \frac{1-p}{2} \sqrt{\frac{\pi kT_G}{\epsilon}} \\ \langle E_{G4}^\lambda(Y) \rangle &= \frac{1}{Z_{G4}} \int \epsilon \left(\frac{2l}{Y+1-p} \right)^2 e^{j \frac{\epsilon}{kT_G} (\frac{l}{1-p})^2} dl = 2kT_G \left(\frac{1-p}{Y+1-p} \right)^2 \\ P_{G4}^\lambda(Y) &= \frac{1}{Z_{G4}} \int \frac{-8\epsilon l^2}{(Y+1-p)^3} e^{j \frac{\epsilon}{kT_G} (\frac{l}{1-p})^2} dl = -4kT_G \frac{(1-p)^2}{(Y+1-p)^3} \\ W_{G4}^\lambda(Y) &= \int_{1-p}^Y -P_{G4}(Y^\theta) dY^\theta = -2kT_G \left(\left(\frac{1-p}{Y+1-p} \right)^2 - \frac{1}{4} \right) \end{aligned}$$

Again, $\langle E_{G4}^\lambda(Y) \rangle + W_{G4}^\lambda(Y) = \frac{1}{2}kT_G$, but after compression to $Y = 0$, the gas has internal energy $2kT_G$. The work performed upon the gas during the compression was $\frac{3}{2}kT_G$. If we now bring the gas back into contact with heat bath, it will be restored to the original state ρ_{G2}^λ with energy $\frac{1}{2}kT_G$, transferring the $\frac{3}{2}kT_G$ to the heat bath. During the course of the complete cycle, a total amount of work equal to $\frac{3}{2}kT_G - \frac{3}{8}kT_G = \frac{9}{8}kT_G$ has been dissipated.

Essential Isolation

The perfect isolation assumed above is not achievable in practice. The interactions with the surrounding environment will cause transitions between eigenstates. As the energy levels change, the system moves out of Boltzmann equilibrium, but the interactions with the environment will cause the system to return to Boltzmann equilibrium over a characteristic time τ_{G5} . An essentially isolated system is one for which this contact with the environment takes place, but involves no net transfer of energy.

This can be considered as dividing the changes into a series of infinitesimal changes in energy $dE = \sum_n p_n dE_n + \sum_n E_n dp_n$. First, the system is in perfect isolation, so that $dp_n = 0$, and

eigenstates are allowed to change. The work performed upon the system is $dE = \sum_n p_n dE_n$. The next stage holds the eigenstates constant, but brings the system into contact with a heat bath, for a time τ_{G5} . This will bring the system into a new Boltzmann equilibrium. The key element to essential isolation is that, at each point that the system is brought into contact with a heat bath, the temperature of the heat bath is chosen so that there is no net change in internal energy of the system ($\sum_n E_n dp_n = 0$) even though there is a change in occupation probabilities ($dp_n \neq 0$).

A system which is essentially isolated is, therefore, always in equilibrium with some notional heat bath at temperature T , but this temperature is variable, and depends upon the external parameters. Changes in internal energy of the system can only come about through work extracted from, or performed upon the system.

For the Popper-Szilard Engine, the temperature of the gas is now a function of the piston position $T = T(Y)$

$$\begin{aligned}\rho_{G5}^\lambda(Y) &= \frac{1}{Z_{G5}^\lambda(Y)} \sum_l e^{j \frac{\epsilon}{kT} \left(\frac{2l}{Y+1-p}\right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \\ Z_{G5}^\lambda(Y) &= \sum_l e^{j \frac{\epsilon}{kT} \left(\frac{2l}{Y+1-p}\right)^2} \approx \frac{Y+1-p}{4} \sqrt{\frac{\pi kT}{\epsilon}} \\ \langle E_{G5}^\lambda(Y) \rangle &= \frac{1}{Z_{G5}^\lambda(Y)} \int \epsilon \left(\frac{2l}{Y+1-p}\right)^2 e^{j \frac{\epsilon}{kT} \left(\frac{2l}{Y+1-p}\right)^2} dl = \frac{1}{2} kT \\ P_{G5}^\lambda(Y) &= \frac{1}{Z_{G5}^\lambda(Y)} \int \frac{-8\epsilon l^2}{(Y+1-p)^3} e^{j \frac{\epsilon}{kT} \left(\frac{2l}{Y+1-p}\right)^2} dl = \frac{-kT}{Y+1-p}\end{aligned}$$

We cannot immediately evaluate $W = \int P_{G5}^\lambda(Y) dY$ as we do not know the variation of T with Y . We can solve this by noting the essential isolation requires

$$P(Y)dY = dW = dE = \frac{1}{2}k dT$$

so

$$\frac{k}{2} \frac{dT}{dY} = P(Y) = \frac{-kT}{Y+1-p}$$

which has the solution (given the initial temperature is T_G)

$$T = T_G \left(\frac{Y_0 + 1 - p}{Y + 1 - p} \right)^2$$

For an expansion phase, $Y_0 = 0$, while for a compression phase $Y_0 = 1 - p$. It can be readily verified that this gives the same results as for perfect isolation above⁵.

Isothermal

The third method we use is to keep the system in constant contact with a heat bath at the initial temperature T_G . As the values of the energy eigenvalues $E_n(Y)$ changes depending upon the

⁵This equivalence between essential and perfect isolation occurs whenever the energy eigenstates have the form $E_n = \alpha(V)n^\beta$, where $\alpha(V)$ depends upon the varying external parameters, but β is a constant. This applies only to mean pressure. The effect of fluctuations will still be different.

	Expansion	Compression
Isolated	$\frac{3}{8}kT_G$	$-\frac{3}{2}kT_G$
Isothermal	$kT_G \ln 2$	$-kT_G \ln 2$

Table 6.1: Work extracted from gas

external parameters, the occupation probabilities continuously adjust to be proportional to $e^{j \frac{E_n}{kT_G}}$. As this means the infinitesimal change $\sum_n E_n dp_n \neq 0$ heat will be drawn from or deposited in the heat bath.

$$\begin{aligned}
\rho_{G6}^\lambda(Y) &= \frac{1}{Z_{G6}^\lambda(Y)} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \quad (6.6) \\
Z_{G6}^\lambda(Y) &= \sum_n e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} \approx \frac{Y+1-p}{4} \sqrt{\frac{\pi kT_G}{\epsilon}} \\
\langle E_{G6}^\lambda(Y) \rangle &= \frac{1}{Z_{G6}^\lambda(Y)} \int \epsilon \left(\frac{2l}{Y+1-p}\right)^2 e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} dl = \frac{1}{2}kT_G \\
P_{G6}^\lambda(Y) &= \frac{1}{Z_{G6}^\lambda(Y)} \int \frac{-8\epsilon l^2}{(Y+1-p)^3} e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} dl = -\frac{kT_G}{(Y+1-p)}
\end{aligned}$$

Unlike in the isolated cases, the internal energy remains constant, and the sum of internal energy and work is not constant, as heat is drawn from, or deposited in the heat bath, to compensate for work extracted or added by the moving piston. For expansion we have

$$W = \int_0^Y -\frac{kT_G}{Y^\theta + 1 - p} dY^\theta = kT_G \ln \left(\frac{1-p}{Y+1-p} \right)$$

and compression gives

$$W = \int_{1-p}^Y -\frac{kT_G}{Y^\theta + 1 - p} dY = kT_G \ln \left(\frac{2(1-p)}{Y+1-p} \right)$$

The work extracted from expansion is $kT_G \ln 2$ which equals the work required for compression. The complete cycle therefore requires no net work to be dissipated into the heat bath.

If we summarise the results of the three types of expansion in Table 6.2.4, we can see that the maximum energy extracted from the expansion phase is under isothermal expansion, while the minimum energy required during compression is also for isothermal expansion. We will therefore assume that the gas is in isothermal contact with a heat bath at temperature T_G from now on.

Fluctuations

The mean values derived above are valid as an average over an ensemble. However, that is no guarantee that the value for any individual case will be close to the average. The usual formula for 'fluctuations' about the mean is given by

$$\frac{\langle A^2 \rangle - \langle A \rangle^2}{\langle A \rangle^2} \approx \frac{1}{m}$$

where m is a large number of degrees of freedom in the system. However, in this situation there is only one degree of freedom, and this suggests that fluctuations in the pressure, and hence work done, may be very large.

Evaluation of the size of $\langle E^2 \rangle$ and $\langle P^2 \rangle$ for perfect isolation gives

$$\begin{aligned}\langle E_{G3}^2 \rangle &= \frac{1}{Z_{G3}} \int \frac{16\epsilon^2}{(Y+1-p)^4} l^4 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} dl = \frac{3}{4} (kT_G)^2 \left(\frac{1-p}{Y+1-p} \right)^4 \\ &= 3 \langle E_{G3} \rangle^2 \\ \langle P_{G3}^2 \rangle &= \frac{1}{Z_{G3}} \int \frac{64\epsilon^2}{(Y+1-p)^6} l^4 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p}\right)^2} dl = 3(kT_G)^2 \left(\frac{(1-p)^2}{(Y+1-p)^3} \right)^2 \\ &= 3 \langle P_{G3} \rangle^2\end{aligned}$$

This gives substantial fractional deviations from the mean energy and pressure. In the case of perfect isolation, the actual gas state will not change during the course of the expansion, and the net energy transferred is $\Delta W_n = \int \frac{\partial E_n}{\partial X} dX = \Delta E_n$, which will imply that over the ensemble we will have

$$\frac{\langle W^2 \rangle - \langle W \rangle^2}{\langle W \rangle^2} = 2$$

which corresponds to large fluctuations in the amount of energy drawn from, or deposited in the work reservoir over each cycle.

Clearly the size of the fluctuation at any given time will be the same for the essentially isolated expansion. For the isothermal expansion, we have

$$\begin{aligned}\langle E_{G6}^2 \rangle &= \frac{1}{Z_{G6}} \int \frac{16\epsilon^2}{(Y+1-p)^4} l^4 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} dl = \frac{3}{4} (kT_G)^2 \\ &= 3 \langle E_{G6} \rangle^2 \\ \langle P_{G6}^2 \rangle &= \frac{1}{Z_{G6}} \int \frac{64\epsilon^2}{(Y+1-p)^6} l^4 e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p}\right)^2} dl = 3(kT_G)^2 \frac{1}{(Y+1-p)^2} \\ &= 3 \langle P_{G6} \rangle^2\end{aligned}$$

so the fractional variation is still 2.

For the cases of essential isolation, or isothermal expansion, however, we are assuming that, after each small expansion step, the system is allowed to interact with an environment, so that it is restored to a Boltzmann equilibrium. This contact, over a characteristic thermal relaxation period τ_θ effectively randomises the state of the system, in accord with the probabilities of the Boltzmann distribution, from one expansion step to the next. If we suppose the expansion takes place over a time $t = n\tau_\theta$ there will be n such randomisations. From this it can be shown (see Appendix F), that, although the fractional fluctuation in the energy transferred is of order 2 on each small step, the fractional fluctuation in energy transferred over the course of an entire expansion or compression phase is of order $1/n = \tau_\theta/t$. For essentially isolated and isothermal expansions, as the expansion takes place over a large time with respect to the thermal relaxation time, the deviation from the mean work extracted from, or deposited within, the work reservoir is negligible.

Conclusion

We have now examined the thermal state of the one atom gas, when it is confined to the left side of the piston. The isothermal expansion of this gas, as the piston moves from the center, to the right end of the box, extracts $kT_G \ln 2$ energy from the gas. Evidently, had we started with the gas confined to the right side of the piston, we would have equally well extracted $kT_G \ln 2$ work.

Now, if we start with the gas occupying the entire box, and insert the partition in the center, we would have the state

$$\rho_{G1} = \frac{1}{2} (\rho_{G2}^\lambda + \rho_{G2}^\rho)$$

Inserting the piston into the center, $|\Phi_0\rangle \langle \Phi_0|$, and applying the expansion operators U_{W4} leads to the state

$$\frac{1}{2} (\rho_{G6}^\lambda(1-p) |\Phi(1-p)\rangle \langle \Phi(1-p)| + \rho_{G6}^\rho(-1+p) |\Phi(-1+p)\rangle \langle \Phi(-1+p)|)$$

In both cases the energy $kT_G \ln 2$ is extracted from the gas. This confirms that the Szilard Paradox is still valid for quantum systems, and the question of superposition of the wavefunction, raised by Zurek, is irrelevant.

6.3 Thermal State of Weights

We now wish to describe the thermal states of the weights as they are raised and lowered by the pulleys, and when a shelf is inserted into an unraised weight at height h . The probability of finding an unraised weight above the shelf height h is also the probability of an imperfect correlation between the location of the weights and the piston states. This governs the tendency of the Popper-Szilard Engine to switch between raising and lowering cycles, and plays a critical role in the long term behaviour of the Engine.

We will bring the weights into contact with a heat bath at temperature T_W . It will be shown that, due to properties of the quantum states, described by Airy functions, that there is no difference between perfect isolation, essential isolation or isothermal expansion, when raising or lowering a weight. We will assume, for simplicity, that the weight is always in contact with the heat bath. The initial density matrix, with the weights resting upon the floor, is given by

$$\begin{aligned} \rho_{W0} &= \frac{1}{Z_{W0}} \sum_n e^{\frac{a_n M_w g H}{k T_W}} |A_n(0)\rangle \langle A_n(0)| \\ Z_{W0} &= \sum_n e^{\frac{a_n M_w g H}{k T_W}} \end{aligned} \quad (6.7)$$

(recall $a_n < 0$)

6.3.1 Raising and Lowering Weight

We will consider the case of raising a weight, and then show that the resulting density matrix describes a lowered weight as well. If we start with the system in perfect isolation and the floor

beneath the weight is raised slowly from 0 to a height $h(Y)$ then, by the adiabatic theorem, the new density matrix will be⁶

$$\rho_{W1}^{\circ}(h) = \frac{1}{Z_{W0}} \sum_n e^{\frac{a_n M_w g H}{k T_W}} |A_n(Y)\rangle \langle A_n(Y)|$$

while the equilibrium density matrix, that results from bringing $\rho_{W1}^{\circ}(h)$ into contact with the heat bath, will be

$$\begin{aligned} \rho_{W1}(h) &= \frac{1}{Z_{W1}} \sum_n e^{\frac{(H a_n - h) M_w g}{k T_W}} |A_n(Y)\rangle \langle A_n(Y)| \\ Z_{W1}(h) &= \sum_n e^{\frac{(H a_n - h) M_w g}{k T_W}} \end{aligned} \quad (6.8)$$

Comparing these, it can be seen that the probability of a given state $|A_n(Y)\rangle$ is the same in both cases

$$p_n(h) = \frac{e^{\frac{(H a_n - h) M_w g}{k T_W}}}{\sum_n e^{\frac{(H a_n - h) M_w g}{k T_W}}} = \frac{e^{-\frac{h M_w g}{k T_W}} e^{\frac{a_n M_w g H}{k T_W}}}{e^{-\frac{h M_w g}{k T_W}} \sum_n e^{\frac{a_n M_w g H}{k T_W}}} = p_n^{\circ}(h)$$

In other words, as

$$\rho_{W1}^{\circ}(h) = \rho_{W1}(h)$$

the density matrix resulting from perfect isolation is already in equilibrium at T_W . By definition this will also apply to essential isolation. As this holds for any height h , the three processes are identical. It also follows that the density matrix that arises from *starting* with a raising floor, and then *lowering* it to a height h will be the same.

One implication of this equivalence is that net exchange of heat between the weight and the heat bath while it is being raised or lowered isothermally will be zero. Any change in the internal energy of the weight comes about through the work done upon the weight. To examine this, we will now look at the generalised pressure exerted upon the co-ordinate $h(Y)$.

The energy and pressure of the state $|A_n(Y)\rangle$ is given by

$$\begin{aligned} E_n &= (h - a_n H) M_w g \\ \frac{\partial E_n}{\partial h} &= M_w g \end{aligned}$$

The pressure $P_n(h) = \frac{\partial E_n}{\partial h}$ is independent of both n and h . This means we can evaluate the average pressure for *any* ensemble as it is clearly simply $\langle P(h) \rangle = M_w g$. It should also be clear that $\langle P(h)^2 \rangle = \langle P(h) \rangle^2$ so there is zero fluctuation in the pressure! From this it will also follow there is zero fluctuation in the work required to raise the weight. This constancy of the pressure gives the very pleasing result that if the weight is raised slowly through a height of h the work performed upon the weight is always exactly $M_w g h$. This makes a raised weight a particularly useful system to use as a work reservoir.

⁶We have continued to use the notation developed in Chapter 5 where the quantum wavefunction $A_n(z, h(Y))$ is represented by the Dirac ket $|A_n(Y)\rangle$.

As we know that no net flow of heat has entered or left the system we can immediately state that the internal energy of the weight must be of the form

$$\langle E(h, T_W) \rangle = M_W gh + f(T_W)$$

We now use the asymptotic approximation

$$a_n \approx - \left(\frac{3\pi n}{2} \right)^{\frac{2}{3}}$$

valid for large n , to complete this equation.

$$\begin{aligned} Z_{W1}(h) &= \sum_n e^{\frac{M_w g(H a_n - h)}{kT_W}} \approx e^{i \frac{M_W g h}{kT_W}} \int_0^1 e^{i \left(\frac{3\pi n}{2} \right)^{\frac{2}{3}} \frac{M_W g H}{kT_W}} dn \\ &\approx \frac{e^{i \frac{h M_W g}{kT_W}}}{2\sqrt{\pi}} \left(\frac{kT_W}{M_W g H} \right)^{\frac{3}{2}} \\ \langle E(h, T_W) \rangle &= \frac{1}{Z_{W1}(h)} \sum_n M_w g(h - H a_n) e^{\frac{(H a_n - h) M_w g}{kT_W}} \\ &= M_W gh - \frac{M_W g H}{Z_{W1}} e^{i \frac{M_W g h}{kT_W}} \sum_n a_n e^{\frac{M_w g H a_n}{kT_W}} \\ &\approx M_W gh + 2\sqrt{\pi} M_W g H \left(\frac{M_w g H}{kT_W} \right)^{\frac{3}{2}} \int_0^1 \left(\frac{3\pi n}{2} \right)^{\frac{2}{3}} e^{i \left(\frac{3\pi n}{2} \right)^{\frac{2}{3}} \frac{M_W g H}{kT_W}} dn \\ &\approx M_W gh + \frac{3}{2} kT_W \end{aligned}$$

Further analysis of the energy fluctuations gives

$$\begin{aligned} \langle E^2 \rangle &= (M_W gh)^2 + \frac{15}{4} (kT_W)^2 + 3M_W gh kT_W \\ \langle E^2 \rangle - \langle E \rangle^2 &= \frac{3}{2} (kT_W)^2 \end{aligned}$$

although, as noted above, there is no fluctuation in the pressure.

With regard to the internal energy term $\frac{3}{2}kT_W$, we can break the Hamiltonian H_W into two terms

$$\begin{aligned} H_{KE} &= -\frac{\hbar}{2M_W} \frac{\partial^2}{\partial z^2} \\ H_{PE} &= M_W g z \end{aligned}$$

representing kinetic and potential energies, and find they have expectation values

$$\begin{aligned} \langle H_{KE} \rangle &= \frac{1}{2} kT_W \\ \langle H_{PE} \rangle &= kT_W \end{aligned}$$

The internal energy dividing in this ratio between kinetic and potential energy is an example of the virial theorem.

6.3.2 Inserting Shelf

We now consider the effect of inserting a shelf at height h into an unraised thermal state ρ_{W0} . This projects out raised and unraised portions of the wavefunction. The statistical weight of these two portions gives the probability of locating the unraised weight above or below the shelf height, and so determines the reliability of the resetting mechanism at the end of a cycle of the Popper-Szilard Engine.

For simplicity we will deal only with the projection of ρ_{W0} into raised and unraised density matrices. Although there will, in general, be interference terms between the two subspaces when the shelf is inserted using U_S , in the situations we will be considering the contact with the T_W heat bath will destroy these coherence terms.

The projections of the unraised density matrix to below and above the height h , respectively, are given by:

$$\begin{aligned}\rho_{W0}(0)^\theta &= P(UN)\rho_{W0}P(UN) \\ &= \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \beta_m^2(h) |UN_m(h)\rangle \langle UN_m(h)| \\ \rho_{W0}(h)^\theta &= P(RA)\rho_{W0}P(RA) \\ &= \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \alpha_m^2(h) |RA_m(h)\rangle \langle RA_m(h)|\end{aligned}$$

These have not been normalised. We must be careful when doing this, as the $|RA_m(h)\rangle$ and $|UN_m(h)\rangle$ do not form an orthonormal basis.

$$\begin{aligned}\text{Tr}[\rho_{W0}(0)^\theta] &= \sum_n \langle A_n(Y) | \left\{ \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \beta_m^2(h) |UN_m(h)\rangle \langle UN_m(h)| \right\} |A_n(Y)\rangle \\ &= \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \beta_m^2(h) \sum_n \beta_n^2(h) \langle UN_n(h) |UN_m(h)\rangle \langle UN_m(h) |UN_n(h)\rangle \\ &= \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \beta_m^2(h)\end{aligned}$$

In the last step we have used the fact that $\sum_n \beta_n^2(h) |UN_n(h)\rangle \langle UN_n(h)|$ is the identity operator for the unraised subspace to substitute⁷

$$\langle UN_m(h) | \left\{ \sum_n \beta_n^2(h) |UN_n(h)\rangle \langle UN_n(h)| \right\} |UN_m(h)\rangle = \langle UN_m(h) |UN_m(h)\rangle = 1$$

We may similarly obtain the result

$$\text{Tr}[\rho_{W0}(h)^\theta] = \frac{1}{Z_{W0}} \sum_m e^{a_m \frac{M_W g H}{k T_W}} \alpha_m^2(h)$$

Using the asymptotic approximations for a_m we get the high temperature values

$$Z_{W0} = \sum_m e^{a_m \frac{M_W g H}{k T_W}} \approx \int_0^1 e^{i \left(\frac{3\pi n}{2}\right)^{\frac{2}{3}} \frac{M_W g H}{k T_W}}$$

⁷This can be generalised to the produce useful result $\text{Tr} \left[\sum_n c_n |UN_n(h)\rangle \langle UN_n(h)| \right] = \sum_n c_n$ despite the non-orthogonality of the $|UN_n(h)\rangle$

$$\begin{aligned}
&= \frac{\sum_m e^{\frac{M_W g H}{k T_W} a_m} E_m \alpha_m^2(h) \langle R A_m(h) | R A_m(h) \rangle}{\sum_m e^{\frac{M_W g H}{k T_W} a_m} \alpha_m^2(h) \langle R A_m(h) | R A_m(h) \rangle} \\
&\approx \frac{1}{P_1(h, T_W) Z_{W0}} \int_{\frac{2}{3\pi} \left(\frac{h}{H}\right)^{3/2}}^1 e^{\frac{M_W g H}{k T_W} a_m} (-a_m M_W g H) \left(1 - \left(\frac{2}{3\pi m}\right)^{\frac{2}{3}} \frac{h}{H}\right)^{\frac{1}{2}} dm \\
&\approx \frac{3}{2} k T_W + M_W g h
\end{aligned}$$

using the asymptotic value of a_m . This is the same energy as for the equilibrium density matrix $\rho_{W1}(h)$.

We can likewise calculate for the weight trapped below the shelf:

$$\begin{aligned}
E_W(z < h) &= \frac{1}{(1 - P_1(h, T_W)) Z_{W0}} \sum_m e^{\frac{M_W g H}{k T_W} a_m} E_m \beta_m^2(h) \\
&\approx \frac{3}{2} k T_W - M_W g h \left(\frac{e^{i \frac{M_W g h}{k T_W}}}{1 - e^{i \frac{M_W g h}{k T_W}}} \right)
\end{aligned}$$

If we now calculate the mean height of the weight, conditional upon it being above the shelf

$$\begin{aligned}
\langle z > h \rangle &= \frac{\int_h^1 \langle z | z \rho_{W0} | z \rangle dz}{\int_h^1 \langle z | \rho_{W0} | z \rangle dz} \\
&\approx \frac{k T_W}{M_W g} + h
\end{aligned}$$

giving a mean potential energy

$$\begin{aligned}
PE_W(z > h) &\approx k T_W + M_W g h \\
&= E_W(z > h) - \frac{1}{2} k T_W
\end{aligned}$$

and for below the shelf

$$\begin{aligned}
\langle z < h \rangle &= \frac{\int_0^h \langle z | z \rho_{W0} | z \rangle dz}{\int_0^h \langle z | \rho_{W0} | z \rangle dz} \\
&\approx \frac{k T_W}{M_W g} - h \left(\frac{e^{i \frac{M_W g h}{k T_W}}}{1 - e^{i \frac{M_W g h}{k T_W}}} \right)
\end{aligned}$$

$$\begin{aligned}
PE_W(z < h) &\approx k T_W - M_W g h \left(\frac{e^{i \frac{M_W g h}{k T_W}}}{1 - e^{i \frac{M_W g h}{k T_W}}} \right) \\
&= E_W(z < h) - \frac{1}{2} k T_W
\end{aligned}$$

so the mean kinetic energy is still $\frac{1}{2} k T_W$. This is an important result, as it demonstrates that the mean kinetic energy of a particle, in thermal equilibrium in a gravitational field, is the same at any height.

It will be useful to note that

$$\begin{aligned}
\langle E(T_W) \rangle &= P_1(h, T_W) E_W(z > h) + P_2(h, T_W) E_W(z < h) \\
\langle PE(T_W) \rangle &= P_1(h, T_W) PE_W(z > h) + P_2(h, T_W) PE_W(z < h)
\end{aligned}$$

If the height of the shelf is large ($h \gg \frac{kT_W}{M_W g}$) then the mean energy of the weight below the shelf approaches $\frac{3}{2}kT_W$ - the same energy as without the shelf. This corresponds to the case where there is little probability of the weight being above the shelf, so inserting it has no effect. If the shelf is low ($h \ll \frac{kT_W}{M_W g}$) then the mean height below the shelf is simply $\frac{1}{2}h$. In this case the mean kinetic energy of the particle is much higher than the gravitational potential below the shelf and the probability distribution of the height is almost flat. The mean energy becomes negligibly different from the mean kinetic energy $\frac{1}{2}kT_W$. These are consistent with the approximations for the perturbed Airy function eigenvalues derived in Appendix E.

When the potential barrier is raised in the center of the one-atom gas, it was possible to show how the wavefunction deforms continuously, and so we could demonstrate in Section 6.2 that, for kT_G much higher than the ground state energy, negligible work is done by raising the potential. We would like to show a similar result for the Airy functions, as the shelf is inserted. Unfortunately, there is no simple solution for the intermediate stages, or even for the weight confined between the floor and the shelf. However, in Appendix E it is argued that, for high quantum numbers ($m \gg 1$) it is reasonable to assume that there is negligible perturbation of the energy eigenvalues as the shelf is inserted. For situations where the weight's internal energy kT_W is large in comparison to the ground state energy of the weight, $-a_1 M_W g H$, then the work done inserting the shelves can be disregarded.

6.4 Gearing Ratio of Piston to Pulley

We now need to calculate the height h_T at which the shelves are inserted, to complete the calculation of the probability that an unraised weight is trapped above the shelf. In Section 5.4 it was noted that the height h through which the weight is raised is not necessarily proportional to the position of the piston Y . Some frictionless gearing system is required to provide a gearing ratio $h(Y)$. In this Section we calculate the optimal gearing ratio, and use this to calculate the maximum height h_T through which the weight can be raised by the expansion of the gas. This will be the height at which the shelves must be inserted into the Popper-Szilard Engine.

We wish the mean energy given up by the expansion of the gas to exactly match the energy gained by the raising of the weight, or

$$\begin{aligned} \int_0^{h(1-p)} P_W(h) dh &= - \int_0^{1-p} P_G(Y) dY \\ \int_0^{1-p} P_W(h(Y)) \frac{\partial h}{\partial Y} dY &= - \int_0^{1-p} P_G(Y) dY \\ \frac{\partial h}{\partial Y} &= - \frac{P_G(Y)}{P_W(h(Y))} \end{aligned}$$

For essential isolation of the gas, this would give

$$\frac{\partial h(Y)}{\partial Y} = \frac{kT_G(1-p)^2}{M_W g(Y+1-p)^3}$$

$$h^0(Y) = \frac{kT_G}{2M_W g} \left(1 - \left(\frac{1-p}{Y+1-p} \right)^2 \right)$$

giving a maximum $h^0(1-p) = \frac{3kT_G}{8M_W g}$

However, we can extract more energy from the gas per cycle if we use an isothermal expansion, which requires a different gearing ratio

$$\begin{aligned} \frac{\partial h(Y)}{\partial Y} &= \frac{kT_G}{M_W g(Y+1-p)} \\ h(Y) &= \frac{kT_G}{M_W g} \ln \left(1 + \frac{Y}{1-p} \right) \end{aligned}$$

giving $h_T = h(1-p) = \frac{kT_G}{M_W g} \ln 2$.

This is the optimum gearing, based upon the mean energy transfer. On average, the work extracted from the gas is equal to the work done upon the weight, and vice versa. As noted in Sections 6.2 and 6.3 above, there are fluctuations in the pressure exerted upon the piston by the gas, but none in the pressure exerted by the weight upon the floor. However, as demonstrated in Appendix F, the fluctuation about the mean energy extracted from the gas becomes negligible, so we have now justified our statement in Section 5.4 that the amount of energy drawn from or deposited in the external work reservoir is negligible.

6.4.1 Location of Unraised Weight

We now know the height at which the shelves are inserted, so we can calculate the probability of locating the weight above or below the shelf, as a function only of the temperatures of the gas and the weight.

Substituting $h_T = \frac{kT_G}{M_W g} \ln 2$ into Equations 6.9 and 6.10 we obtain:

Above Shelf at h_T

$$P_1 = \left(\frac{1}{2} \right)^{\frac{T_G}{T_W}} \tag{6.12}$$

Below Shelf at h_T

$$P_2 = 1 - \left(\frac{1}{2} \right)^{\frac{T_G}{T_W}} \tag{6.13}$$

The form of these results will be shown to play a critical role in the failure of the Popper-Szilard Engine to produce anti-entropic behaviour. We will be examining the origin of this relationship in detail in Chapter 8.

6.5 The Raising Cycle

We can now use the unitary operators in Equation 5.27 to describe the complete operation of the engine. In this section we will move through each step of the 'raising cycle' given in Section 5.6.

We will confirm that the fully quantum mechanical description of the Popper-Szilard Engine does not lead to the conclusions of [Zur84, BS95], that the piston does not move as the one atom gas is in a superposition. With regard to the arguments of [LR90], we will show that the operation U_{RES} is capable of achieving a partial resetting of the engine, without the requirement for external work. However, as noted in Section 5.5, there are inevitable errors in the resetting operation. We will now be able to evaluate the effect of these errors upon the state of the Engine at the end of the cycle.

Extracting Energy from the T_G Heat Bath

For the 'raising cycle' (Figure 4.5) the initial density matrix is given by

$$\rho_{T0} = \rho_{G0} \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\phi_0\rangle \langle \phi_0|$$

The internal energy of this state is

$$E_{T0} = \frac{1}{2}kT_G + 3kT_W$$

During Stage (a), the operator U_{RI} is applied. As the piston is initially in state $|\phi_0\rangle$ this corresponds to the raising of a potential barrier in the center of the gas and the insertion of the piston. The state of the system is now

$$\begin{aligned} \rho_{T1}(0) &= \rho_{G1} \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\Phi(0)\rangle \langle \Phi(0)| \\ &= \frac{1}{2} (\rho_{G6}^\lambda(0) + \rho_{G6}^\rho(0)) \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\Phi(0)\rangle \langle \Phi(0)| \end{aligned}$$

and the internal energy is unchanged. As the expansion and lifting (operator U_{W4}) takes place in Stage (b) this evolves through the Y states

$$\begin{aligned} \rho_{T1}(Y) &= \frac{1}{2} (\rho_{G6}^\lambda(Y) \otimes \rho_{W1}^\lambda(h(Y)) \otimes \rho_{W0}^\rho \otimes |\Phi(Y)\rangle \langle \Phi(Y)| \\ &\quad + \rho_{G6}^\rho(-Y) \otimes \rho_{W0}^\lambda \otimes \rho_{W1}^\rho(h(Y)) \otimes |\Phi(-Y)\rangle \langle \Phi(-Y)|) \end{aligned} \quad (6.14)$$

until the piston wavepackets reach the sides of the box at $Y = 1 - p$. It is important to note how the parameter Y has been applied in this equation. For those states where the gas is to the left of the piston, the value Y represents the distance the piston has moved to the right, from the center of the box. This varies from 0 to $1 - p$ as the piston moves to the righthand side of the box.

However, for the states where the gas is to the right of the piston, the piston moves to the left. This would be represented by a negative value of Y . To simplify the expression of this, we have substituted $-Y$. The value of Y goes from 0 to $1 - p$ again, but now represents the piston moving from position 0 to the lefthand side of the box, at position $-1 + p$.

When $Y = 1 - p$, the state of the system is

$$\begin{aligned} \rho_{T1}(1-p) &= \frac{1}{2} (\rho_{G6}^\lambda(1-p) \otimes \rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho \otimes |\Phi(1-p)\rangle \langle \Phi(1-p)| \\ &\quad + \rho_{G6}^\rho(-1+p) \otimes \rho_{W0}^\lambda \otimes \rho_{W1}^\rho(h_T) \otimes |\Phi(-1+p)\rangle \langle \Phi(-1+p)|) \end{aligned}$$

The internal energy is now

$$E_{T1}(1-p) = \frac{1}{2}kT_G + 3kT_W + M_Wgh_T$$

This refutes the arguments of [Zur84, BS95], that the piston cannot move because the quantum gas exerts an even pressure upon it until an external measurement is performed. Clearly the piston is not left in the center of the box. The gas expands, exerting pressure upon the piston, and lifts one of the weights. This extracts energy from the gas, but the isothermal contact with the T_G heat bath replaces this. At the end of the expansion, one of the weights has been raised through the distance h_T . The energy has increased by $M_Wgh_T = kT_G \ln 2$, which has been drawn from the T_G heat bath during the isothermal expansion. At this point we appear to have proved the contention of Popper et al. that an 'information gathering measurement' is not necessary to extract energy from the Szilard Engine.

The M_Wgh_T energy is stored in the internal energy of the raised weight. If we remove the support for the weight it will start to fall to the floor. Contact with the T_W heat bath will then return it to the thermal equilibrium state ρ_{W0} . This will have reduced it's energy by M_Wgh_T . The extra energy is dissipated into the T_W heat bath. As we argued in Section 4.2.3, we have encountered no reason, so far, that prevents us from setting $T_W > T_G$. If we can reliably transfer M_Wgh_T energy per cycle from the T_G to the T_W heat baths, we will then have violated the second law of thermodynamics. However, we still have to address the problem of resetting the Engine for the next cycle. Before we can allow the weight to fall to the floor and dissipate the M_Wgh_T energy into the T_W heat bath we must correlate it's position to the location of the piston. As we found in Section 5.5, without this correlation in the resetting stage we will be unable to start a new cycle, or if we attempted to start a new cycle, the Engine would automatically reverse into a lowering cycle.

Resetting the Piston Position

At this point, Stage (c), the shelves are inserted at a height h_T , by the operator U_S and then, Stage (d), the piston is removed from the box by U_{IR} .

The effect of U_S is to divide each of the unraised weight wavefunctions $|A_n(0)\rangle$ into raised ($|RA_n(h_T)\rangle$) and unraised ($|UN_n(h_T)\rangle$) portions. We will assume that contact with the T_W heat bath destroys interference terms between the raised and unraised wavefunctions⁸. In terms of the projected density matrices in Equation 6.11, the system is now:

$$\begin{aligned} \rho_{T2} = & \frac{1}{2} (\rho_{G6}^\lambda(1-p) \otimes \rho_{W1}^\lambda(h_T) \otimes \{P_1\rho_{W0}^\rho(h_T)^{00} + P_2\rho_{W0}^\rho(0)^{00}\} \otimes |\Phi(1-p)\rangle \langle\Phi(1-p)| \\ & + \rho_{G6}^\rho(-1+p) \otimes \{P_1\rho_{W0}^\lambda(h_T)^{00} + P_2\rho_{W0}^\lambda(0)^{00}\} \otimes \rho_{W1}^\rho(h_T) \otimes |\Phi(-1+p)\rangle \langle\Phi(-1+p)|) \end{aligned}$$

⁸Strictly, we can only be certain this will have happened when the system is allowed to thermalise, after the operation U_{RES} . However, it makes no difference to the calculation, while simplifying the description, if we also assume this happens after the shelves are inserted.

The operation of U_{RI} upon ρ_{T2} , during Stage (d), removes the piston states, and allows the gas state to return to ρ_{G0} :

$$\begin{aligned}\rho_{T3} &= \frac{1}{2}\rho_{G0} \otimes (\rho_{W1}^\lambda(h_T) \otimes \{P_1\rho_{W0}^\rho(h_T)^{\text{oo}} + P_2\rho_{W0}^\rho(0)^{\text{oo}}\}) \otimes |\phi_R\rangle \langle\phi_R| \\ &\quad + \{P_1\rho_{W0}^\lambda(h_T)^{\text{oo}} + P_2\rho_{W0}^\lambda(0)^{\text{oo}}\} \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle\phi_L|\end{aligned}$$

The density matrices $\rho_{W0}(h_T)^{\text{oo}}$ show the possibility that the unraised weights have been trapped above the shelf height h_T . This is a 'thermal fluctuation' in the internal energy of the weights. It was shown in Section 6.3 that the internal energy of the $\rho_{W0}(h_T)^{\text{oo}}$ states is M_Wgh_T higher than the equilibrium state ρ_{W0} . The source of this energy is the T_W heat bath. Trapping the unraised weight does *not* constitute energy drawn from the T_G heat bath, in contrast to the increase in internal energy of the raised weight $\rho_{W1}(h_T)$.

If we calculate the mean internal energy of ρ_{T3} , we find it is unchanged:

$$\begin{aligned}E_{T3} &= \frac{1}{2}kT_G + \frac{1}{2}P_2 \left(3kT_W + M_Wgh_T \left(1 - \frac{e^{j\frac{M_Wgh_T}{kT_W}}}{1 - e^{j\frac{M_Wgh_T}{kT_W}}} \right) \right) \\ &\quad + \frac{1}{2}P_2 \left(3kT_W + M_Wgh_T \left(1 - \frac{e^{j\frac{M_Wgh_T}{kT_W}}}{1 - e^{j\frac{M_Wgh_T}{kT_W}}} \right) \right) \\ &\quad + \frac{1}{2}P_1(3kT_W + 2M_Wgh_T) + \frac{1}{2}P_1(3kT_W + 2M_Wgh_T) \\ &= \frac{1}{2}kT_G + 3kT_W + M_Wgh_T \left(P_2 \left(1 - \frac{P_1}{P_2} \right) + 2P_1 \right) \\ &= E_{T1}(1 - p)\end{aligned}$$

Re-writing ρ_{T3} in a form more suitable for applying U_{RES} in Stage (e) we get

$$\begin{aligned}\rho_{T3} &= \rho_{G0} \otimes \left(\frac{1}{2}P_2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(0)^{\text{oo}} \otimes |\phi_R\rangle \langle\phi_R| + \frac{1}{2}P_2\rho_{W1}^\lambda(0)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \otimes |\phi_L\rangle \langle\phi_L| \right. \\ &\quad \left. + \frac{1}{2}P_1\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(h_T)^{\text{oo}} \otimes |\phi_R\rangle \langle\phi_R| + \frac{1}{2}P_1\rho_{W1}^\lambda(h_T)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \otimes |\phi_L\rangle \langle\phi_L| \right)\end{aligned}$$

The first line of this represents the unraised weight trapped below the shelf height. When this happens, the location of the weight is correlated to the location of the piston, and can be used to reset the piston. The second line corresponds to situations where the unraised weight has been trapped above the shelf height. It not possible to identify the location of the piston from the location of the weights in this portion of the density matrix.

Now applying U_{RES} to ρ_{T3} we are left with the state

$$\begin{aligned}\rho_{T4} &= \rho_{G0} \otimes \left(\frac{1}{2}P_2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(0)^{\text{oo}} \otimes |\phi_0\rangle \langle\phi_0| + \frac{1}{2}P_2\rho_{W1}^\lambda(0)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \otimes |\phi_0\rangle \langle\phi_0| \right. \\ &\quad \left. + \frac{1}{2}P_1\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(h_T)^{\text{oo}} \otimes |\phi_3\rangle \langle\phi_3| + \frac{1}{2}P_1\rho_{W1}^\lambda(h_T)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \otimes |\phi_2\rangle \langle\phi_2| \right)\end{aligned}$$

Where the unraised weight is found below the shelf, in the first line, the piston has been restored to the center. However, it is left in states $|\phi_2\rangle$ and $|\phi_3\rangle$ on the second line. These are in general superpositions of the piston states $|\phi_L\rangle$, $|\phi_R\rangle$ and $|\phi_0\rangle$. As both weights are above the shelf, the piston may be located anywhere. However, as the probabilities of the locations of the weights have not changed, the internal energy of the system is the same as E_{T3} .

Return to Equilibrium

We now remove the shelves, in Stage (f), by the operation of U_S^Y , and allow the weights to come to a thermal equilibrium at temperature T_W . The equilibrium states of the weights depends upon the location of the piston and pulley system. The piston states $|\phi_L\rangle$ and $|\phi_R\rangle$ will each support one of the weights at a height h_T , while state $|\phi_0\rangle$ allows both weights to fall to the floor. This corresponds to an conditional internal Hamiltonian for the weights of

$$\begin{aligned} H_{W3} &= H_W^\lambda(0)H_W^\rho(0)|\phi_0\rangle\langle\phi_0| \\ &\quad + H_W^\lambda(h_T)H_W^\rho(0)|\phi_R\rangle\langle\phi_R| + H_W^\lambda(0)H_W^\rho(h_T)|\phi_L\rangle\langle\phi_L| \end{aligned}$$

As shown in Section 6.1, thermalisation of a system with conditional Hamiltonian leads to a canonical distribution within each of the projected subspaces $|\phi_L\rangle$, $|\phi_R\rangle$ and $|\phi_0\rangle$. The probability of each subspace is given by the trace of the projection onto the subspaces in the original density matrix:

$$\begin{aligned} |\phi_L\rangle\langle\phi_L|\rho_{T3}|\phi_L\rangle\langle\phi_L| &= \rho_{G0} \otimes \left(\frac{1}{2}P_1|b_3|^2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(h_T)^{\text{oo}} \right. \\ &\quad \left. + \frac{1}{2}P_1|b_2|^2\rho_{W1}^\lambda(h_T)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \right) \otimes |\phi_L\rangle\langle\phi_L| \\ \text{Tr}[|\phi_L\rangle\langle\phi_L|\rho_{T3}|\phi_L\rangle\langle\phi_L|] &= \frac{1}{2}P_1(|b_2|^2 + |b_3|^2) \\ |\phi_R\rangle\langle\phi_R|\rho_{T3}|\phi_R\rangle\langle\phi_R| &= \rho_{G0} \otimes \left(\frac{1}{2}P_1|c_3|^2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(h_T)^{\text{oo}} \right. \\ &\quad \left. + \frac{1}{2}P_1|c_2|^2\rho_{W1}^\lambda(h_T)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \right) \otimes |\phi_R\rangle\langle\phi_R| \\ \text{Tr}[|\phi_R\rangle\langle\phi_R|\rho_{T3}|\phi_R\rangle\langle\phi_R|] &= \frac{1}{2}P_1(|c_2|^2 + |c_3|^2) \\ |\phi_0\rangle\langle\phi_0|\rho_{T3}|\phi_0\rangle\langle\phi_0| &= \rho_{G0} \otimes \left(\frac{1}{2}P_2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(0)^{\text{oo}} + \frac{1}{2}P_2\rho_{W1}^\lambda(0)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \right. \\ &\quad \left. + \frac{1}{2}P_1|a_3|^2\rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho(h_T)^{\text{oo}} \right. \\ &\quad \left. + \frac{1}{2}P_1|a_2|^2\rho_{W1}^\lambda(h_T)^{\text{oo}} \otimes \rho_{W0}^\rho(h_T) \right) \otimes |\phi_0\rangle\langle\phi_0| \\ \text{Tr}[|\phi_0\rangle\langle\phi_0|\rho_{T3}|\phi_0\rangle\langle\phi_0|] &= P_2 + \frac{1}{2}P_1(|a_2|^2 + |a_3|^2) \end{aligned}$$

The weights now come into equilibrium on with the heat bath at temperature T_W , with the final state of the weights conditional upon the projected state of the piston. The canonical distributions of the weights are:

$$\begin{aligned} |\phi_0\rangle\langle\phi_0| &\rightarrow \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \\ |\phi_R\rangle\langle\phi_R| &\rightarrow \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \\ |\phi_L\rangle\langle\phi_L| &\rightarrow \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \end{aligned}$$

When the piston is in the center, the equilibrium consists of the two weights in a thermal state on the floor. If the piston is in the righthand position, the equilibrium thermal state has a raised lefthand weight, with the righthand weight on the floor, and vice versa.

Conclusion

We have now completed the 'Raising Cycle' of the Popper-Szilard Engine. The final state of the density matrix of the system is:

$$\begin{aligned}\rho_{T5} &= \rho_{G0} \otimes (w_1 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \otimes |\phi_0\rangle \langle \phi_0| + w_2 \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| \\ &\quad + w_3 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L|)\end{aligned}\quad (6.15)$$

where the statistical weights w_1 , w_2 and w_3 are calculated from the projection onto the subspaces of $|\phi_0\rangle \langle \phi_0|$, $|\phi_R\rangle \langle \phi_R|$ and $|\phi_L\rangle \langle \phi_L|$ above.

$$\begin{aligned}w_1 &= P_2 + \frac{1}{2}P_1 (|a_2|^2 + |a_3|^2) \\ &= 1 - \frac{1}{2}P_1 (1 + |a_1|^2) \\ w_2 &= \frac{1}{2}P_1 (|b_2|^2 + |b_3|^2) \\ &= \frac{1}{2}P_1 (1 - |b_1|^2) \\ w_3 &= \frac{1}{2}P_1 (|c_2|^2 + |c_3|^2) \\ &= \frac{1}{2}P_1 (1 - |c_1|^2)\end{aligned}\quad (6.16)$$

and we have made use of the identities, from the unitarity of U_{RES} , in Equation 5.26.

The internal energy of ρ_{T5} is

$$\begin{aligned}E_{T5} &= \frac{1}{2}kT_G + 3kT_W + (w_2 + w_3)M_Wgh_T \\ &= E_{T1}(1 - p) - w_1M_Wgh_T\end{aligned}$$

In w_1 proportion of cycles, the piston is restored to the center of the Engine. In these cases, the raised weight has been allowed to fall back to the floor. This dissipates M_Wgh_T energy into the T_W heat bath. The system is then ready to perform another raising cycle of the Popper-Szilard Engine.

However, with probability $(w_2 + w_3)$, the piston will not be restored to the center. On these cycles, the energy extracted from the T_G heat bath has been transferred to the weights, but it has not been dissipated into the T_W heat bath⁹. Instead, one of the weights has been trapped by the imperfect resetting of the piston leaving it on the left or right of the Engine. The system will not be able to continue with a raising cycle, but will instead 'reverse direction' and use the trapped energy to start upon a lowering cycle.

⁹Strictly speaking, it is possible that the cycle has ended with the *unraised* weight trapped in a thermal fluctuation, while the raised weight *is* allowed to fall dissipatively. The result of this, however, is still no net transfer of energy to the T_W heat bath.

6.6 The Lowering Cycle

We will now repeat the analysis of Section 6.5, but this time we will consider the 'lowering cycle' described in Section 5.6. In this cycle, we start with the piston to one or the other side of the Engine, and with the corresponding weight trapped at the height h_T . We will then apply the stages of the operator U_T , exactly as we did for the raising cycle. This will be shown to take us through the steps in Figure 5.7.

Pumping Energy into the T_G Heat Bath

We start with the initial density matrix corresponding to the piston located on the right of the Engine:

$$\rho_{T6} = \rho_{G0} \otimes \rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho \otimes |\phi_R\rangle \langle \phi_R|$$

This has internal energy

$$E_{T6} = \frac{1}{2}kT_G + 3kT_W + M_W g h_T$$

Stage (a) consists of the operation U_{RI} , which in this case simply corresponds to inserting the piston in the right end of the box, at $Y = (1 - p)$. The gas will be entirely to the left of the piston, and will be subject to a negligible compression. The state is now

$$\rho_{T7}(1-p) = \rho_{G6}^\lambda(1-p) \otimes \rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho \otimes |\Phi(1-p)\rangle \langle \Phi(1-p)|$$

We now go through Stage (b), which involves the operation U_{W4} . This causes the gas to compress, while the lefthand weight is lowered. As the position of the piston moves from $Y = 1 - p$ to $Y = 0$, the system moves through

$$\rho_{T7}(Y) = \rho_{G6}^\lambda(Y) \otimes \rho_{W1}^\lambda(h(Y)) \otimes \rho_{W0}^\rho \otimes |\Phi(Y)\rangle \langle \Phi(Y)|$$

until it reaches

$$\rho_{T7}(0) = \rho_{G6}^\lambda(0) \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\Phi(0)\rangle \langle \Phi(0)|$$

at the end of Stage (b). This state has internal energy

$$E_{T7}(0) = \frac{1}{2}kT_G + 3kT_W$$

The compression of the gas is isothermal, so the internal energy of the gas remains constant throughout this stage at $\frac{1}{2}kT_G$. The work performed upon the gas is passed into the T_G heat bath. The system has transferred $M_W g h_T = kT_G \ln 2$ energy from the raised weight to the heat bath.

Resetting the Piston Position

Operation U_S , during Stage (c), inserts shelves at height h_T into the space of the weights. As both of these weights are in the unraised position, both of the weights will be projected out:

$$\begin{aligned} \rho_{T8} &= \rho_{G6}^\lambda(0) \otimes \{P_1 \rho_{W0}^\lambda(h_T)^{\circ\circ} + P_2 \rho_{W0}^\lambda(0)^{\circ\circ}\} \\ &\quad \otimes \{P_1 \rho_{W0}^\rho(h_T)^{\circ\circ} + P_2 \rho_{W0}^\rho(0)^{\circ\circ}\} \otimes |\Phi(0)\rangle \langle \Phi(0)| \end{aligned}$$

(again, for convenience we have assumed that thermal contact with the T_W heat bath destroys coherence between the raised and unraised density matrices). The mean energy is unaffected by this.

Stage (d) now removes the piston from the center of the box. Unlike the raising cycle, this has a significant effect upon the internal state of the one atom gas. In ρ_{T8} the gas is confined entirely to the left half of the box. When the piston is removed, the internal Hamiltonian for the gas becomes H_{G0} . With the full extent of the box accessible, the contact with the T_G heat bath allows the gas to expand to the equilibrium state ρ_{G0} , leaving the system in the state

$$\begin{aligned} \rho_{T9} = & \rho_{G0} \otimes ((P_1)^2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} + P_1 P_2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \\ & + P_1 P_2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(0)^{00} + (P_2)^2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(0)^{00}) \otimes |\phi_0\rangle \langle \phi_0| \end{aligned}$$

However, the internal energy of the gas is still $\frac{1}{2}kT_G$ so the energy of the system has not been affected by the free expansion of the one atom gas.

We can see all four of the possible configurations of the weights are present. The resetting of the piston, U_{RES} , in Stage(e) leads to the piston being in any of the possible locations, including the superposition $|\phi_1\rangle$

$$\begin{aligned} \rho_{T10} = & \rho_{G0} \otimes ((P_1)^2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \otimes |\phi_1\rangle \langle \phi_1| \\ & + P_1 P_2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \otimes |\phi_L\rangle \langle \phi_L| \\ & + P_1 P_2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(0)^{00} \otimes |\phi_R\rangle \langle \phi_R| \\ & + (P_2)^2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(0)^{00} \otimes |\phi_0\rangle \langle \phi_0|) \end{aligned}$$

The second and third lines represent the situation where one weight was trapped above the shelf, and one below. In this situation, the piston is moved to the corresponding side of the engine, to hold up the trapped weight. This allows the machine to continue with a lowering cycle.

The fourth line gives the situation where both weights are trapped below the shelf height. As neither weight is in a raised position, the piston cannot be moved without changing the location of a weight. U_{RES} therefore leaves the piston in the central position. This means that at the start of the next cycle, the piston will be in the central position, and a raising cycle will begin.

When both weights are trapped above the shelf height h_T , the effect of U_{RES} is to put the piston into the superposition of states given by $|\phi_1\rangle$. This superposition is constrained by the unitarity requirements on U_{RES} given in Equation 5.26.

Return to Equilibrium

As with the raising cycle, the shelves are removed by U_S^Y operation in Stage (f), and the weights come to a thermal equilibrium with the T_W heat bath.

The internal Hamiltonian for the weights is H_{W3} as in the raising cycle above. The process of thermalisation is therefore exactly the same as for the raising cycle, requiring us to project out each of the subspaces of the piston:

$$\begin{aligned}
|\phi_L\rangle \langle \phi_L| \rho_{T10} |\phi_L\rangle \langle \phi_L| &= \rho_{G0} \otimes \left((P_1)^2 |b_1|^2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \right. \\
&\quad \left. + P_1 P_2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \right) \otimes |\phi_L\rangle \langle \phi_L| \\
\text{Tr} [|\phi_L\rangle \langle \phi_L| \rho_{T10} |\phi_L\rangle \langle \phi_L|] &= (P_1)^2 |b_1|^2 + P_1 P_2 \\
|\phi_R\rangle \langle \phi_R| \rho_{T10} |\phi_R\rangle \langle \phi_R| &= \rho_{G0} \otimes \left((P_1)^2 |c_1|^2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \right. \\
&\quad \left. + P_1 P_2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(0)^{00} \right) \otimes |\phi_R\rangle \langle \phi_R| \\
\text{Tr} [|\phi_R\rangle \langle \phi_R| \rho_{T10} |\phi_R\rangle \langle \phi_R|] &= (P_1)^2 |c_1|^2 + P_1 P_2 \\
|\phi_0\rangle \langle \phi_0| \rho_{T10} |\phi_0\rangle \langle \phi_0| &= \rho_{G0} \otimes \left((P_1)^2 |a_1|^2 \rho_{W0}^\lambda(h_T)^{00} \otimes \rho_{W0}^\rho(h_T)^{00} \right. \\
&\quad \left. + (P_2)^2 \rho_{W0}^\lambda(0)^{00} \otimes \rho_{W0}^\rho(0)^{00} \right) \otimes |\phi_0\rangle \langle \phi_0| \\
\text{Tr} [|\phi_0\rangle \langle \phi_0| \rho_{T10} |\phi_0\rangle \langle \phi_0|] &= (P_1)^2 |a_1|^2 + (P_2)^2
\end{aligned}$$

Contact with the T_W heat bath will then bring the weights into canonical equilibrium distributions, conditional upon the location of the piston:

$$\begin{aligned}
|\phi_0\rangle \langle \phi_0| &\rightarrow \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \\
|\phi_R\rangle \langle \phi_R| &\rightarrow \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \\
|\phi_L\rangle \langle \phi_L| &\rightarrow \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T)
\end{aligned}$$

Conclusion

The density matrix that results from the thermalisation in Stage (f) is

$$\begin{aligned}
\rho_{T11} &= \rho_{G0} \otimes (w_4 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \otimes |\phi_0\rangle \langle \phi_0| + w_5 \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| \\
&\quad + w_6 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L|)
\end{aligned} \tag{6.17}$$

where the statistical weights w_4 , w_5 and w_6 are calculated from the projections onto the $|\phi_0\rangle \langle \phi_0|$, $|\phi_R\rangle \langle \phi_R|$ and $|\phi_L\rangle \langle \phi_L|$ subspaces, respectively. Making use of the identities in Equation 5.26 that come from the unitarity of U_{RES} , we have:

$$\begin{aligned}
w_4 &= (P_2)^2 + (P_1)^2 |a_1|^2 \\
&= (1 - 2P_1) + (P_1)^2 (1 + |a_1|^2) \\
w_5 &= P_1 (P_2 + P_1 |b_1|^2) \\
&= P_1 - (P_1)^2 (1 - |b_1|^2) \\
w_6 &= P_1 (P_2 + P_1 |c_1|^2) \\
&= P_1 - (P_1)^2 (1 - |c_1|^2)
\end{aligned}$$

After thermal equilibrium has been established, the mean energy is

$$E_{T11} = \frac{1}{2} kT_G + 3kT_W + (w_5 + w_6) M_W g h_T$$

In $(w_5 + w_6)$ proportion of the cases, the cycle will complete with one of the weights trapped at height h_T , gaining an energy $M_W g h_T$. This energy comes from thermal fluctuations of the weight, and therefore is drawn from the T_W heat bath. In these cases, the piston is located to one side, or the other, of the Engine, and when the next cycle starts it will be another lowering cycle. This shows that the lowering cycle proceeds by capturing thermal fluctuations from the T_W heat bath, and using them to compress the single atom gas. This transfers heat from the T_W to the T_G heat bath. We have confirmed that the flow of energy in the lowering cycle is in the opposite direction to the flow of energy in the raising cycle.

In w_4 proportion of the cases, however, both weights will be on the floor at the end of a lowering cycle, and the piston will be in the center. The next cycle of the Popper-Szilard Engine will therefore be a raising cycle.

6.7 Energy Flow in Popper-Szilard Engine

We have now reached the conclusion of our analysis of the behaviour of the quantum mechanical Popper-Szilard Engine. We shall briefly review the situation, before calculating the long term behaviour of the Engine. This will enable us to prove that, for any choice of U_{RES} , the energy flow will be from the hotter to the colder of T_W and T_G . Thus we will show that the Popper-Szilard Engine is incapable of producing anti-entropic heat flows.

In Chapter 5 we analysed the detailed interactions between the microstates of the Engine, restricting ourselves only by the requirement that the evolution of the system be expressed as a unitary operator. We found that it was possible to extract energy from the quantum mechanical one atom gas, and use it to lift a weight, without making a measurement upon the system. We also found that we could try to reset the piston position, without having to perform work upon it, albeit with some error. This error leads to some probability of the Engine going into a reverse lowering cycle. However, we found that there was also a corresponding tendency for the Engine on the lowering cycle to change back to a raising cycle.

An Engine which spends most of its time on raising cycles will transfer energy from the T_G to the T_W heat baths, while an Engine which spends more time on lowering cycles will transfer energy in the opposite direction. For the second law of thermodynamics to hold, these tendencies must be balanced so that the long term flow of energy is always in the direction of the hotter to the colder heat bath.

In this Chapter we have added statistical mechanics to the analysis. This allows us to optimise the energy transferred between the one atom gas and the weights per cycle, and calculate the probabilities that the Engine changes between the raising and lowering cycles. We can now use these results to calculate the long term energy flow between the two heat baths.

Energy Transfer per Cycle

On the raising cycle, the energy transfer is $kT_G \ln 2$ per cycle, from the T_G heat bath to the T_W heat bath. We will regard the energy of any raised weights at the end of the cycle as part of the energy of the T_W system, even though it has not been dissipatively transferred to the T_W heat bath itself.

$$\Delta E_r = kT_G \ln 2$$

On the lowering cycle, the energy transfer is from the raised weight to the T_G heat bath. Again, regarding the weights as part of the T_W system, this constitutes a transfer of $kT_G \ln 2$ energy, but now in the opposite direction

$$\Delta E_l = -kT_G \ln 2$$

Length of Cycles

If the probability of a cycle reversing is p , and of continuing is $(1-p)$, then mean number of cycles before a reversal takes place is $1/p$.

For raising cycle, the probability of the cycle continuing is given by

$$\begin{aligned} 1 - P_r &= w_1 \\ &= 1 - \frac{1}{2}P_1 (1 + |a_1|^2) \end{aligned}$$

and of reversing

$$\begin{aligned} P_r &= w_2 + w_3 \\ &= \frac{1}{2}P_1 (1 - |b_1|^2) + \frac{1}{2}P_1 (1 - |b_1|^2) \\ &= \frac{1}{2}P_1 (1 + |a_1|^2) \end{aligned}$$

The mean number of raising cycles that takes place is therefore

$$N_r = 1/P_r = \frac{2}{P_1 (1 + |a_1|^2)}$$

The lowering cycle has continuation and reversal probabilities of

$$\begin{aligned} 1 - P_l &= w_5 + w_6 \\ &= P_1 (2P_2 + P_1 (|b_1|^2 + |c_1|^2)) \\ &= 2P_1 - (P_1)^2 (1 + |a_1|^2) \\ &= 2P_1(1 - P_r) \\ P_l &= w_4 \\ &= (P_2)^2 + (P_1)^2 |a_1|^2 \\ &= (1 - 2P_1) + (P_1)^2 (1 + |a_1|^2) \\ &= 1 - 2P_1(1 - P_r) \end{aligned}$$

respectively. The mean number of lowering cycles is

$$N_l = 1/P_l = \frac{1}{(1 - 2P_1) + (P_1)^2 (1 + |a_1|^2)}$$

Mean Energy Flow

As the Popper-Szilard Engine will alternate between series of raising and lowering cycles, in the long term the net flow of energy from the T_G to the T_W heat baths, per cycle, is given by:

$$\Delta E = \frac{N_r \Delta E_r + N_l \Delta E_l}{N_r + N_l}$$

Substituting in the values and re-arranging leads to the final equation for the flow of energy in the Popper-Szilard Engine

$$\Delta E = kT_G \ln 2 \left(\frac{(1 - 2P_1) \left(1 - \frac{P_1}{2} (1 + |a_1|^2)\right)}{(1 - 2P_1) + (1 + 2P_1) \frac{P_1}{2} (1 + |a_1|^2)} \right) \quad (6.18)$$

It is interesting to note that, of all the possible values that could be chosen for the operation U_{RES} , in the long run it is only the value $|a_1|^2$ that has any effect. The value of $|a_1|^2$ is related to the probability of the lowering cycle reversing direction when both weights are trapped above the shelf height. The symmetry of the Popper-Szilard Engine between the righthand and lefthand states, and the existence of the unitarity constraints on U_{RES} , such as $\sum_i |a_i|^2 = 1$, lead to all relevant properties expressible in terms of $|a_1|^2$.

The function

$$f(P_1, |a_1|^2) = \frac{(1 - 2P_1) \left(1 - \frac{P_1}{2} (1 + |a_1|^2)\right)}{(1 - 2P_1) + (1 + 2P_1) \frac{P_1}{2} (1 + |a_1|^2)}$$

is plotted in Figure 6.1 as P_1 and $|a_1|^2$ vary between the values of 0 and 1. This shows that

$$\begin{aligned} P_1 < \frac{1}{2} &\Rightarrow f(P_1, |a_1|^2) > 0 \\ P_1 = \frac{1}{2} &\Rightarrow f(P_1, |a_1|^2) = 0 \\ P_1 > \frac{1}{2} &\Rightarrow f(P_1, |a_1|^2) < 0 \end{aligned}$$

regardless of the value of a_1

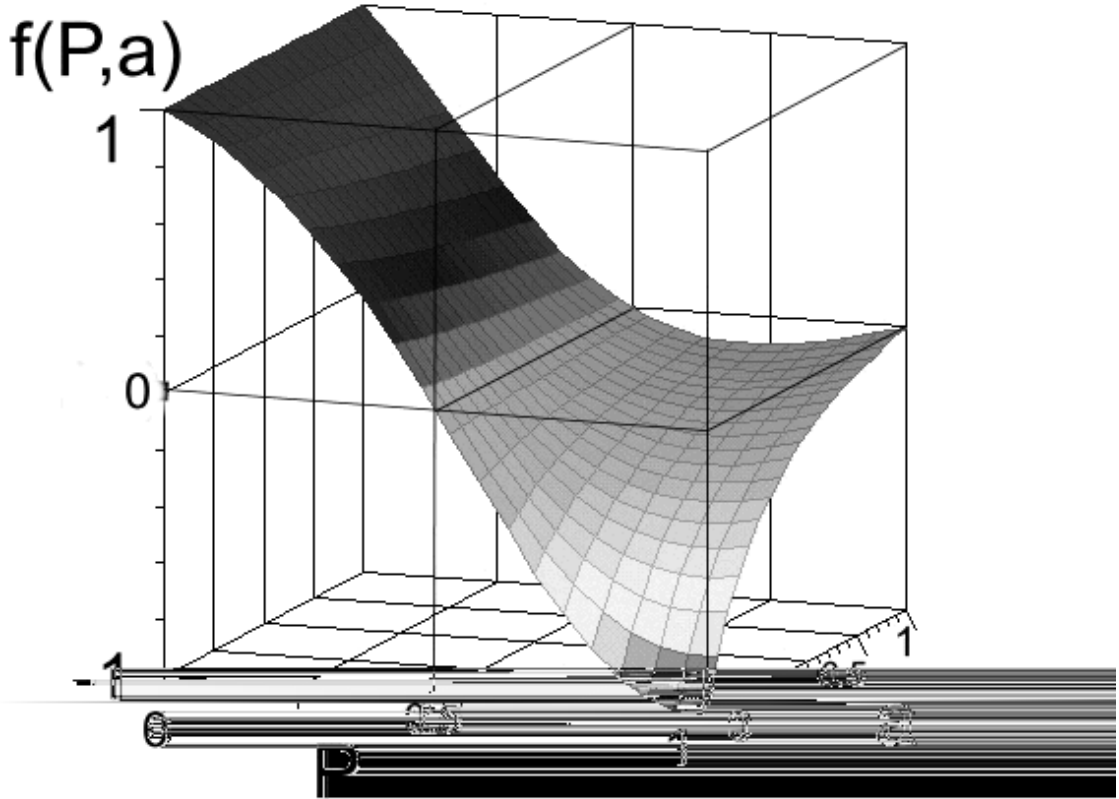


Figure 6.1: Mean Flow of Energy in Popper-Szilard Engine

Solution to Popper-Szilard Engine

$$T_G > T_W \Rightarrow P_1 < \frac{1}{2} \Rightarrow \Delta E > 0$$

$$T_G = T_W \Rightarrow P_1 = \frac{1}{2} \Rightarrow \Delta E = 0 \quad (6.19)$$

$$T_G < T_W \Rightarrow P_1 > \frac{1}{2} \Rightarrow \Delta E < 0$$

This proves that despite the arguments in Chapter 4, the Popper-Szilard Engine is not, in the long run, capable of violating the second law of thermodynamics, as defined by Clausius

No process is possible whose sole result is the transfer of heat from a colder to a hotter body

Although we have now achieved our primary goal, of providing a complete analysis of the quantum mechanical Popper-Szilard Engine, and demonstrating that it does not violate the second law of thermodynamics, it will be useful to examine how the function $f(P_1, |a_1|^2)$ varies with the choice of $|a_i|^2$, T_G and T_W .

$T_G \gg T_W$ When $T_G \gg T_W$, then $P_1 \approx 0$. In this situation, the gas is able to lift the weight through a very large distance, compared with the mean thermal height of the weight. There is correspondingly a vanishingly small probability that the unraised weights will be found above the shelf height.

On the raising cycle, this leads to an unambiguous correlation between the piston states and the location of the raised and unraised weights, and the piston will be reset with negligible error. The raising cycle will therefore continue almost indefinitely.

Should the Engine find itself in a lowering cycle, however, at the end of the cycle both weights will be found below the shelf height. The operation of U_{RES} will leave the piston in the center. Lowering cycles will therefore immediately reverse into raising cycles.

The result is that the Engine will switch to and reliably stay on a raising cycle, and will transfer $kT_G \ln 2$ energy from the hotter T_G to the colder T_W per cycle.

$T_G = T_W$ If $P_1 = \frac{1}{2}$, there is exactly 50% probability of finding an unraised weight above the shelf height. The probabilities of continuing and reversing become

$$P_r = P_l = \frac{1}{4} (1 + |a_1|^2)$$

This varies between 1/4 and 1/2. The mean number of cycles before a reversal takes place is between 2 and 4. As it is equal for raising and lowering cycles, in the long term there is no mean flow of energy between the two heat baths. However, the energy transfer will fluctuate about this mean.

$T_G \ll T_W$ When the gas temperature is much lower than the weight temperature the situation is more complex, and the value of $|a_i|^2$ becomes more significant. $P_1 \approx 1$ implies that unraised weights will always be located above the shelf height. The only part of U_{RES} that will be relevant will be the projection onto the $P^\lambda(RA)P^\rho(RA)$ subspace. This part of the operation puts the piston state into a superposition, which is dependant upon the values of the a_i etc. parameters in U_{RES} .

Let us first consider an operator for which $a_1 = 0$. On the lowering cycle, the piston is in the center of the Engine, and U_{RES} will always move it to one of the lefthand or righthand states. Lowering cycles will therefore continue indefinitely. For the raising cycle, the piston comes out of the box in the lefthand or righthand position, with equal probability, $\frac{1}{2}$. The unitarity requirements then lead to $|a_2|^2 + |a_3|^2 = 1$. These are the probabilities of the raising cycle continuing, from the lefthand and righthand piston positions, respectively. The overall probability of the raising cycle continuing is therefore $\frac{1}{2} (|a_2|^2 + |a_3|^2)$. This gives only a 50% chance that a raising cycle will continue. On average, a raising cycle will only perform two cycles before reversing into a lowering cycle. The long term behaviour of this is to stay on the lowering cycle, and transfer $kT_G \ln 2$ from the hotter T_W to the colder T_G heat baths.

If we increase a_1 , we start to introduce a possibility of the lowering cycle reversing into a raising cycle. However, as we do this, we simultaneously reduce $|a_2|^2 + |a_3|^2$, reducing the ability of the raising cycle to continue. If we reach $a_1 = 1$, we guarantee that the lowering cycle will reverse into a raising cycle. However, we have simultaneously removed all possibility of the raising cycle continuing. The machine simply switches between the two cycles, producing a net zero energy flow, despite the high temperature of T_W .

If the value of $P_1 < 1$, though, there is some possibility of an unraised weight being trapped below the shelf. This increases the possibility of the machine staying on a lowering cycle, and allows some flow of heat.

Density Matrix

We have derived these results in terms of the long term behaviour of the Popper-Szilard Engine, implicitly assuming that on each cycle of the Engine it is in either a raising or lowering cycle. We now wish to re-examine this in terms of the density matrix of the system. For simplicity, we will make use of the symmetry of the Engine, and set $|b_1|^2 = |c_1|^2$, and use the lowering cycle density matrix

$$\rho_{T12} = \frac{1}{2}\rho_{G0} \otimes (\rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| + \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L|)$$

If the Engine starts the cycle in a general state, with some probability w_r of being on a raising cycle, the density matrix is:

$$\rho_{T13} = w_r\rho_{T0} + (1 - w_r)\rho_{T12}$$

After one cycle, it will be left in the state

$$\rho_{T14} = (w_4 + w_r(w_1 - w_4))\rho_{T0} + 2(w_5 + w_r(w_2 - w_5))\rho_{T12}$$

The Engine rapidly converges¹⁰ to a value of w_r^θ for which $\rho_{T14} = \rho_{T13}$. This value is given by

$$w_r^\theta = \frac{w_4}{2w_2 + w_4}$$

for which the density matrix can be shown to be

$$\rho_{T15} = \frac{N_r}{N_r + N_l}\rho_{T0} + \frac{N_l}{N_r + N_l}\rho_{T12}$$

This demonstrates that, even if we do not wish to interpret the system as being in a determinate state, whose long run energy flow is given by Equation 6.18, the system will still rapidly settle into a density matrix for which the mean flow *on each cycle* is given by ΔE . Thus, for this system the statistical state at a particular time rapidly produces the same results as the average behaviour over a large number of cycles.

¹⁰Excluding the case where $P_1 = 1$, $a_1 = 0$, which oscillates between ρ_{T13} and $(1 - w_r)\rho_{T0} + w_r\rho_{T12}$

6.8 Conclusion

Let us step back from the detail by which the simple and expected result was achieved, and try to understand why the attempt to produce anti-entropic behaviour fails. As we saw, the essential property of the Engine's long term behaviour is that it must spend more time on the raising cycle when $T_G > T_W$, and more time on the lowering cycle when $T_G < T_W$. This turns on the value of P_1 , and it's dependency on the temperatures of the gas and weights, and critically takes the value of $\frac{1}{2}$ when $T_G = T_W$. It is the relationship

$$P_1 = \left(\frac{1}{2}\right)^{\frac{T_G}{T_W}}$$

which determines the direction of the mean flow of energy.

We must now examine how the various features that go into the derivation of P_1 produce this balance. The key relationship is between the thermal states of the weights and the gas. The thermal state of the weight gives it a height above the floor of the Engine. This leads to a probability of the weight being located above a given height. The thermal state of the gas, on the other hand, allows energy to be extracted and used to raise the floor beneath the weight, to some height (or the lowering of the floor beneath the weight, from some height, can be use to compress the gas).

The probability¹¹ of finding the weight above a height h is $e^{-i \frac{M_W g h}{k T_W}}$. The median height of the weight is $h_m = \frac{k T_W}{M_W g} \ln 2$, which gives the height above which it is 50% likely that the weight will spontaneously be found (the mean height $\langle h \rangle = \frac{k T_W}{M_W g}$, which confirms the expectation value of the potential energy $k T_W$ in Section 6.3) This height may be reduced by increasing the mass of the weight, or by reducing it's temperature.

However, the height through which the weight can be lifted, is set by it's weight, and by the temperature of the gas T_G . The maximum height that can be achieved is using isothermal expansion, which raises it by $h_T = \frac{k T_G}{M_W g} \ln 2$. This may be increased by reducing the mass, or increasing the temperature of the gas.

We want $h_m < h_T$ to be reliably transferring energy from T_G to T_W . If we decrease the likelihood that an unraised weight is found above the height h_T , we improve the probability that the machine is properly reset to start the next cycle. Changing the mass does not help, as any reduction in the median height of the weight is offset by a reduction in the height through which it is lifted. Instead, we are forced to reduce T_W or increase T_G .

However, clearly, for $h_m < h_T$, then $T_W < T_G$. If we wish to transfer energy from a cold to a hot heat bath we need $T_W > T_G$. In more than 50% of the cases, a shelf inserted at h_T will find the weight already lifted, without any action required by the gas. We only start to reliably (more than 50% of the time) find the weight below the shelf height if the temperature of the weight is below that of the gas - in which case we are simply arranging for heat to flow from a hotter to a colder body, in agreement with the second law.

¹¹This is the same as the Boltzmann distribution for a classical gas in a gravitational field.

If we try to run the machine in reverse, we need to be able to reliably capture fluctuations in the height of the weights and use them to compress the gas. To compress the gas, the weight must be caught above the height h_T . To be reliably (ie. with probability greater than 50%) caught above this height, then $h_m > h_T$. Again, we find the balance between h_m and h_T implies $T_W > T_G$, so that the heat flows from the hotter to the colder heat bath.

There are two key elements we have found. Firstly, unitarity constrains the operation of the Engine. We are not able to ensure the machine stays on one cycle (raising or lowering) because the resetting operation U_{RES} must be unitary and cannot map orthogonal to non-orthogonal states. Furthermore, unitarity requires we define the operation over the entire Hilbert space of the Engine. Once we define the operation of the Engine for one cycle, we find we have completely defined the operation of the Engine on the reversed cycle. The way we attempt to extract Engine in one direction automatically implies a flow of energy in the opposite direction.

The second element is the subtle balance between the thermal states of the two systems. When we try to capture a fluctuation in the gas, and use it to lift the weight through some height, we found that, unless the gas was hotter than the weight, then we were at least as likely to find the weight already above that height, due to its own thermal state. Similarly, when we capture a fluctuation in the height of the weight, and use the lowering of it to compress the gas, we find that, unless the weight is hotter than the gas, probability of capturing the weight above the height is less than the probability of finding the gas spontaneously in the compressed state.

In Chapter 8 we will show the general physical principles which underly these two elements. This will enable us to generalise the conclusion of our analysis of the Popper-Szilard Engine.

Chapter 7

The Thermodynamics of Szilard's Engine

Chapters 5 and 6 present a detailed analysis of the operation of the quantum Popper-Szilard Engine. The conclusion showed that no operation of the Engine compatible with unitary dynamics was capable of transferring energy from a colder to a hotter heat bath. It was not found necessary to make any reference to information theory to reach this conclusion.

However, little reference has been made to thermodynamics either, so one might wonder if one could equally abandon the concepts of entropy or free energy. In fact, the reason why we were able to avoid referring to these is because the system studied is sufficiently idealised that it was possible to explicitly construct operators upon the microstates and analyse statistical behaviour of an ensemble of microstates. The only thermodynamic concept introduced was temperature, to describe the statistical ensembles and the heat baths. This will not be possible for more complex systems, involving many degrees of freedom. For such systems it will only be possible to usefully describe them by aggregate properties, associated with an ensemble. However, this does *not* mean, as it is sometimes asserted, that these ensemble properties are only *valid* for complex, many body systems. The thermodynamic, ensemble properties can still be defined for simple, single body systems.

In this Chapter we will analyse the thermodynamic properties of the Szilard Engine, and show the extent to which they can be considered valid. We will be principally concerned with the properties of entropy and free energy. This will give us a deeper understanding of the reason why the Popper-Szilard does not operate in an anti-entropic manner, and will form the basis of the general resolution of the problem in the next Chapter.

In Section 7.1 the concepts of free energy and entropy will be derived from the statistical ensemble mean energy and pressure, for a system in thermal equilibrium at some temperature T . This demonstrates that these concepts are quite valid for single atom systems. We will then give some consideration to the meaning of these terms for systems exhibiting non-equilibrium mixing

and for correlations between different systems. It will be shown that in some circumstances the concept of free energy must be modified, and in other circumstances cannot be applied at all. Entropy, on the other hand, remains well defined at all times.

Section 7.2 steps through the six stages of the raising cycle, given in Sections 5.6 and 6.6. The entropy and free energy are tracked throughout the cycle. Section 7.3 then does the same for the lowering cycle (Sections 5.6 and 6.7). It will be shown here that the entropy is always constant or increasing, at all stages of the operation of the Engine. This conclusion is derived solely from the will appye thsee de-satioisl to the of the sinlce ned to the

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tis(eng)4320(is)4620)2843(namicn)-321(ermse.)7072(This)4321(will)4321j(usify)4321ourlt
thr(mo)-78(ynamicn)-333(conceptsn)-333(are)4334(appticlthe)-333(for)-333(sinlce)-333(trom)-333(sy
ths comes to the most thenon-equilibriume ixsingof staecs, and the

The mean energy of the system is, of course,

$$E = \frac{1}{Z} \sum_n e^{i \frac{E_n}{kT}} E_n$$

so the difference between the mean and free energy is given by the 'heat'

$$\begin{aligned} Q &= \frac{1}{Z} \sum_n e^{i \frac{E_n}{kT}} E_n + kT \ln Z \\ &= -kT \sum_n \frac{e^{i \frac{E_n}{kT}}}{Z} \ln \left(\frac{e^{i \frac{E_n}{kT}}}{Z} \right) \\ &= -kT \text{Tr} [\rho \ln \rho] \end{aligned}$$

with $\rho = \frac{1}{Z} e^{i H/kT}$, as the density matrix of the system in equilibrium, thus confirming that the Gibbs-von Neumann entropy $S_{VN} = -k \text{Tr} [\rho \ln \rho]$ exactly satisfies the *statistical* equation $E = F + TS_{VN}$, for systems in equilibrium. We will therefore always use this to define the quantum mechanical entropy of a system. This gives us a physical basis for understanding the thermodynamic quantities F and S . These properties must be understood as properties of the statistical ensemble itself, introduced at the start of Chapter 6. Unlike the mean energy and pressure, they do not correspond to the average of any property of the individual systems.

It should be carefully noted that the free energy and entropy have been given significance only for ensembles of systems at a specific temperature T . The entropy S_{VN} , however, is not dependant upon the given temperature, and does not even require the system to be in thermodynamic equilibrium to be calculated. We will therefore assume that S_{VN} is always valid.

Free energy, however, has been defined with respect to thermal equilibrium at a particular temperature. In Appendix G it is argued that the free energy can still be defined where there is more than one temperature, but that it is not conserved. When a quantity of entropy S is transferred reversibly, within a system, through a temperature difference ΔT , then the free energy changes by a quantity $-S\Delta T$. This characteristic equation will occur at several points in our understanding of the Popper-Szilard Engine.

7.1.1 One Atom Gas

We will now apply these concepts to the one atom gas, confined within a box. We will consider here only the situation where the one atom gas is confined entirely to the left of a piston at location Y . The changes in thermodynamics properties of the single atom gas will be shown to be consistent with an ideal gas, even though there is a single particle involved.

Free Energy

The density matrix of the gas is given in Equation 6.7 by $\rho_{G6}^\lambda(Y)$. This has function

$$Z_{G6}^\lambda(Y) = \sum_n e^{i \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} \approx \frac{Y+1-p}{4} \sqrt{\frac{\pi kT_G}{\epsilon}}$$

giving a free energy

$$F_{G6}^\lambda(Y) = \frac{kT_G}{2} \left(4 \ln 2 - \ln \left(\frac{\pi k T_G}{\epsilon} \right) - 2 \ln(Y + 1 - p) \right)$$

It will be convenient to also calculate the free energy for the gas when there is no partition present at all. This has density matrix ρ_{G0} , in Equation 6.4 with

$$\begin{aligned} Z_{G0} &= \sum_n e^{j \frac{\epsilon n^2}{kT_G}} \\ &\approx \int e^{j \frac{\epsilon n^2}{kT_G}} dn = \frac{1}{2} \sqrt{\frac{\pi k T_G}{\epsilon}} \end{aligned}$$

so has free energy

$$F_{G0} = \frac{kT_G}{2} \left(2 \ln 2 - \ln \left(\frac{\pi k T_G}{\epsilon} \right) \right) \quad (7.1)$$

This gives

$$F_{G6}^\lambda(Y) = F_{G0} + kT_G \ln \left(\frac{2}{Y + 1 - p} \right) \quad (7.2)$$

If we neglect terms of order $k \ln(1 - p)$, this gives us the results

$$\begin{aligned} F_{G6}^\lambda(0) &\approx F_{G0} + kT_G \ln 2 \\ F_{G6}^\lambda(1 - p) &\approx F_{G0} \end{aligned}$$

As we saw in Section 6.2, the work performed upon the piston by the expansion of the one atom gas is simply

$$\Delta W = kT_G \ln \left(\frac{Y + 1 - p}{2} \right)$$

so this confirms

$$F_{G6}^\lambda(Y) + \Delta W = \text{constant}$$

or equivalently, the change in free energy of the system is equal to the work performed upon the system.

Entropy

We calculate the entropies directly from the density matrix

$$\begin{aligned} S_{G0} &= \frac{k}{2} \left(1 + \ln \left(\frac{\pi k T_G}{\epsilon} \right) - 2 \ln 2 \right) \\ S_{G6}^\lambda(Y) &= \frac{k}{2} \left(1 + \ln \left(\frac{\pi k T_G}{\epsilon} \right) - 4 \ln 2 + 2 \ln(Y + 1 - p) \right) \\ &= S_{G0} - k \ln \left(\frac{2}{Y + 1 - p} \right) \end{aligned} \quad (7.3)$$

which gives the approximate results for the piston in the center and end of the box

$$\begin{aligned} S_{G6}^\lambda(0) &\approx S_{G0} - k \ln 2 \\ S_{G6}^\lambda(1 - p) &\approx S_{G0} \end{aligned}$$

The entropy of the gas increases by $k \ln 2$ as it expands to fill approximately twice its initial volume.

Heat Bath

The internal energy of the gas, given in Equation 6.7, is constant at $\frac{1}{2}kT_G$. The free energy extracted from the expansion must be drawn from the contact the gas has with the heat bath. This means an energy of $kT_G \ln\left(\frac{Y+1-p}{2}\right)$ comes out of the T_G heat bath.

It can be readily be shown that when the energy change in the heat bath is small compared to it's total energy, then the entropy change in the heat bath is given by

$$dS = \frac{dE}{T}$$

We include this entropy change in the heat bath

$$S_{T_G}(Y) = -k \ln\left(\frac{Y+1-p}{2}\right)$$

to our analysis. This gives a combined entropy of

$$S_{T_G}(Y) + S_{G6}^\lambda(Y) = \frac{k}{2} \left(1 + \ln\left(\frac{\pi k T_G}{\epsilon}\right) - 4 \ln 2\right)$$

which is a constant. This confirms our expectations for a reversible process.

We may also note that, in Section 6.2 the pressure obeys the relationship

$$P(Y)V(Y) = kT_G$$

where we define the 'volume' of the gas as the length of the box

$$V(Y) = Y + 1 - p$$

that gas occupies. This relationship hold for isothermal expansion and compression, where the temperature is constant. For isolated expansion and compression, where the temperature is variable

$$P(Y)V(Y) = kT$$

still holds, but in addition, the one atom adiabatic relationship

$$P(Y)V(Y)^3 = \text{constant}$$

hold true (see also [BBM00]). The single atom gas therefore acts in exactly the manner we would expect from the thermodynamic analysis of an ideal gas.

7.1.2 Weight above height h

We now calculate the thermodynamics properties of a single atom weight, supported at a height h . Again, we will analyse how the free energy and entropy changes as the height is changed, and we will connect this to the thermodynamic state of the one atom gas, being used to lift a weight through the pressure it exerts upon a piston.

Free Energy

In Section 6.3 the thermal state of the weight is given in Equation 6.9. The free energy may be calculated directly from $Z_{W1}(h)$ as

$$\begin{aligned} F_{W1}(h) &= M_W g h - kT_W \left(\frac{3}{2} \ln \left(\frac{kT_W}{M_W g H} \right) - \ln(2\sqrt{\pi}) \right) \\ &= F_{W1}(0) + M_W g h \end{aligned}$$

As was noted before, the work done in raising a weight through a height h is always $M_W g h$, regardless of the ensemble, so again we confirm the status of the free energy.

Substituting the isothermal gearing ratio $h(Y) = \frac{kT_G}{M_W g} \ln \left(1 + \frac{Y}{1-p} \right)$ gives

$$F_{W1}(h(Y)) = F_{W1}(0) + kT_G \ln \left(1 + \frac{Y}{1-p} \right) \quad (7.4)$$

which produces

$$F_{W1}(h_T) = F_{W1}(0) + kT_G \ln 2$$

If we use the expansion of the one atom gas to lift the weight, (or the compression of the weight lifting the gas) then

$$F_{W1}(h(Y)) + F_{G6}^\lambda(Y) = \text{constant}$$

Entropy

Taking the density matrix $\rho_{W1}(h)$, we calculate the entropy to be

$$S_{W1} = \frac{3k}{2} \left(1 + \ln \left(\frac{kT_W}{M_W g H} \right) - \frac{2}{3} \ln(2\sqrt{\pi}) \right) \quad (7.5)$$

This is independent of the height h of the weight. As the entropy of the weight does not change, it is easy to see from $E = F + TS$ that the change in internal energy of a raised weight is exactly equal to its change in free energy, and therefore equal to the work done upon the weight. This agrees with the conclusion in Section 6.3 that no heat need be drawn from or deposited within a heat bath, for a weight to be raised or lowered in thermal equilibrium.

The combination of the one atom gas and the quantum weight behaves exactly as we would expect for a reversible thermodynamic system. The application of the thermodynamic concepts of free energy and entropy to these systems have presented no special problems.

7.1.3 Correlations and Mixing

The systems considered in the previous Subsection are always described by a product of density matrices

$$\rho = \rho_{W1}(h(Y)) \otimes \rho_{G6}^\lambda(Y)$$

For the Popper-Szilard Engine, we will have to consider more complex density matrices, were the subsystem density matrices are not product density matrices, but instead have correlations

between their states. We must now address the behaviour of thermodynamic properties where systems become correlated. To do this we must consider two different features: the mixing of an ensemble from two or more subensembles¹, and the correlation of two or more subsystems.

Entropy

The entropy of composite systems can be defined directly from the properties of S_{VN} [Weh78]. If there are two independent systems, with a total density matrix $\rho = \rho_1 \otimes \rho_2$ then the total entropy is additive, $S = S_1 + S_2$, where $S_1 = k\text{Tr}[\rho_1 \ln \rho_1]$ etc. When the total density matrix is given as the sum of two orthogonal subensembles, so that $\rho = p_a \rho_a + p_b \rho_b$ where $p_a + p_b = 1$ and $\rho_a \rho_b = 0$, then the total entropy is given by the formula $S = p_a S_a + p_b S_b - k p_a \ln p_a - k p_b \ln p_b$. This can be generalised to

$$S = \sum p_i S_i - k \sum p_i \ln p_i \quad (7.6)$$

These two results may be combined to calculate the entropy of correlated systems, such as $\rho = p_a \rho_{a1} \otimes \rho_{a2} + p_b \rho_{b1} \otimes \rho_{b2}$, which has an entropy of $S = \sum p_i (S_{i1} + S_{i2}) - k \sum p_i \ln p_i$.

Free Energy

For free energy, the problem is more subtle. We can consistently assume that the free energy of two independent systems are additive, so that $F = F_1 + F_2$. However, we must be careful when considering a mixture, if it is not an equilibrium mixture. If we suppose we have a system in equilibrium at temperature T , then the free energy is given by

$$F = -kT \ln \left(\sum e^{i \frac{E_i}{kT}} \right)$$

Now let us consider the effect of splitting the system into two orthogonal subspaces, with equilibrium density matrices ρ_a and ρ_b . These density matrices have partition functions

$$\begin{aligned} Z_a &= \sum_{i \in \mathcal{I}_a} e^{i \frac{E_i}{kT}} \\ Z_b &= \sum_{i \in \mathcal{I}_b} e^{i \frac{E_i}{kT}} \\ Z &= Z_a + Z_b \end{aligned}$$

It can be readily shown that for the combined density matrix $\rho = p_a \rho_a + p_b \rho_b$ to be in thermal equilibrium, then $Z_a = p_a Z$ and $Z_b = p_b Z$. This allows us to calculate the free energy of the subensembles using the formula

¹Throughout we will refer to the combination of subensembles as a ‘mixture’ or ‘mixing’. Unfortunately this term is used in several different ways when associated with entropy. Here we will use it exclusively to refer to the relationship between an ensemble and its subensembles, that the density matrix of an ensemble is a ‘mixed state’ of the density matrices of its subensembles. This should not be confused with the ‘entropy of mixing’ that occurs when ‘mixtures’ of more than one substance is considered [Tol79][Chapter XIV] or the ‘mixing’ or ‘mixing enhancement’ associated with coarse graining [Weh78].

$$F_a = -kT \ln Z_a = F - kT \ln p_a \quad (7.7)$$

and similarly for ρ_b . This will turn out to be a key relationship in understanding the thermodynamic explanation for the failure of the Popper-Szilard Engine.

Using Equation 7.7 we can re-write F as

$$F = \sum p_i F_i + kT \sum p_i \ln p_i \quad (7.8)$$

or equivalently

$$F = -kT \ln \left(\sum e^{i \frac{F_i}{kT}} \right)$$

and we also find that

$$p_a = \frac{e^{-\frac{F_a}{kT}}}{\sum e^{-\frac{F_i}{kT}}} = e^{\frac{F - F_a}{kT}} \quad (7.9)$$

It is important to note that these relationships are no longer a sum over the individual eigenstates. They are summations over the orthogonal subspaces, or the subensembles. Rather than relating the total free energy to the logarithmic averaging over the individual energies, they relate the free energy to the logarithmic averaging over the *free* energies of the subensembles. Similarly, the probabilities are not those of the individual eigenstates, depending upon the individual energies, they are the probabilities of the subensemble, and they depend upon the *free* energy of that subensemble.

Equation 7.7 will turn out to be very important in the next Chapter. The value of $-kT \ln p$ is always positive, so the free energy of a subensemble is always greater than the free energy of the ensemble from which it is taken. Despite the similarity of the equations $S = \sum p_i S_i - k \sum p_i \ln p_i$ and $F = \sum p_i F_i + kT \sum p_i \ln p_i$, it should be noted that there is no equivalent relationship to (7.7) between the entropy of an ensemble and the entropy of its subensembles. While the entropy of an ensemble must be greater than the *mean* entropy of its subensembles ($S \leq \sum p_i S_i$), there is no such restriction upon its relationship to the entropies of the individual subensembles.

While we have

$$F \leq F_a$$

for all a for free energies, we only have

$$\min(S_a) \leq S \leq \max(S_a) + \ln N$$

where N is the dimension of the Hilbert space of the system, for entropy. It may be higher than all the subensemble entropies, but may also be lower than any but the minimum entropy.

We now must understand how the free energy is affected when we form the *non-equilibrium* density matrix $\rho^0 = p_a^0 \rho_a + p_b^0 \rho_b$ where $p_a^0 \neq p_a$ (we will assume that the subensembles ρ_a and ρ_b are themselves in thermal equilibrium at temperature T , and that it is only their mixing that is not in proportion).

This is a subtle problem and is addressed in Appendix H. There it is shown that free energy can be meaningful for such mixtures, and that the relation

$$F = \sum p_i F_i + kT \sum p_i \ln p_i$$

is still valid, but that the equations $F_a = F - kT \ln p_a$ and $F = -kT \ln \left(\sum e^{i \frac{F_i}{kT}} \right)$ cannot be used directly². We can therefore calculate the free energy of a non-equilibrium mixture, at a given temperature, but we cannot use the free energy of the subensemble to calculate its probability, in the manner Equation 7.9 allows.

While we have defined free energy for non-equilibrium mixtures at a specific temperature, we should notice that the temperature plays a key role in the change of the free energy with mixing. For this equation to be valid, the relevant subensembles must themselves be in thermal equilibrium at some temperature T . In particular, when we have a correlated density matrix $\rho = p_a \rho_{a1} \otimes \rho_{a2} + p_b \rho_{b1} \otimes \rho_{b2}$ and systems 1 and 2 are at different temperatures to each other, there is clearly no well defined temperature T for the mixture between p_a and p_b . In this situation it appears that the concept of free energy has been stretched to its limit and can no longer be regarded as a well defined, or meaningful, quantity. This is significant, as at several points in the cycle of the Popper-Szilard Engine, the system will be described by precisely such a correlated density matrix. We will not be able to assume that the free energy remains well defined throughout the operation of the Engine.

7.2 Raising cycle

We will now apply these results to the raising cycle of the Szilard Engine, to parallel the statistical mechanical analysis in Section 6.5. The density matrices ρ_{T0} to ρ_{T5} are given in that Section. The raising cycle is shown in Figure 4.5.

Stage a In the initial state of the raising cycle, the density matrix is

$$\rho_{T0} = \rho_{G0} \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\phi_0\rangle \langle \phi_0|$$

To maintain a certain level of generality we will assume that the piston states all have a notional internal free energy F_P and entropy S_P .

The initial entropy and free energy is given by

$$S_{T0} = S_P + S_{G0} + 2S_{W1}$$

²Combining the results for this non-equilibrium mixing of F and S , it can be shown that the statistical equation $E = F + TS$ is still valid

$$F_{T0} = F_P + F_{G0} + 2F_{W1}$$

On raising the partition and inserting the piston in the center of the box, we have a new density matrix

$$\rho_{T1}(0) = \frac{1}{2} (\rho_{G6}^\lambda(0) + \rho_{G6}^\rho(0)) \otimes \rho_{W0}^\lambda \otimes \rho_{W0}^\rho \otimes |\Phi(0)\rangle \langle \Phi(0)|$$

Mixing the entropy and the free energies of the gas subensembles $\rho_{G6}^\lambda(0)$ and $\rho_{G6}^\rho(0)$ at temperature T_G gives

$$\begin{aligned} S_{G1} &= \left(\frac{1}{2} S_{G6}^\lambda(0) + \frac{1}{2} S_{G6}^\rho(0) \right) - k \left(\frac{1}{2} \ln \frac{1}{2} + \frac{1}{2} \ln \frac{1}{2} \right) \\ &= \frac{k}{2} \left(1 + \ln \left(\frac{\pi k T_G}{\epsilon} \right) - 2 \ln 2 + 2 \ln(1-p) \right) \\ F_{G1} &= \left(\frac{1}{2} F_{G6}^\lambda(0) + \frac{1}{2} F_{G6}^\rho(0) \right) + k T_G \left(\frac{1}{2} \ln \frac{1}{2} + \frac{1}{2} \ln \frac{1}{2} \right) \\ &= \frac{k T_G}{2} \left(2 \ln 2 - \ln \left(\frac{\pi k T_G}{\epsilon} \right) - 2 \ln(1-p) \right) \end{aligned}$$

Neglecting terms of order $\ln(1-p)$ we have $S_{G1} \approx S_{G0}$, $F_{G1} \approx F_{G0}$ so the total entropy S_{T1} and free energy F_{T1} are unchanged from S_{T0} and F_{T0} . The insertion of the piston requires negligible work and is reversible.

Stage b During the expansion phase of the raising cycle, the density matrix of the system $\rho_{T1}(Y)$ is a correlated mixture of subensembles at different temperatures T_G and T_W . It follows that the free energy is not well defined during this expansion phase. At the end of the expansion the density matrix becomes

$$\begin{aligned} \rho_{T1}(1-p) &= \frac{1}{2} (\rho_{G6}^\lambda(1-p) \otimes \rho_{W1}^\lambda(h_T) \otimes \rho_{W0}^\rho \otimes |\Phi(1-p)\rangle \langle \Phi(1-p)| \\ &\quad + \rho_{G6}^\rho(-1+p) \otimes \rho_{W0}^\lambda \otimes \rho_{W1}^\rho(h_T) \otimes |\Phi(-1+p)\rangle \langle \Phi(-1+p)|) \end{aligned}$$

Examining these terms we note that $\rho_{G6}^\lambda(1-p) \approx \rho_{G6}^\rho(1-p) \approx \rho_{G0}$, so the gas can be factored out of the correlation, and only the weight temperature T_W is involved in the mixing.

The raised weight subensemble $\rho_{W1}^\lambda(h_T)$ is not orthogonal to the unraised $\rho_{W1}^\lambda(0)$, but the piston states $|\Phi(1-p)\rangle \langle \Phi(1-p)|$ and $|\Phi(-1+p)\rangle \langle \Phi(-1+p)|$ are orthogonal, so we can use the mixing formula for the entropy and free energy, to get

$$\begin{aligned} S_{T1} &= S_{G0} + S_P + 2S_{W1} + k \ln 2 \\ F_{T1} &= F_{G0} + F_P + 2F_{W1} + k T_G \ln 2 - k T_W \ln 2 \\ &= F_{G0} + F_P + 2F_{W1} - k T_W \ln(2P_1) \end{aligned}$$

where we have used the relationship $P_1 = \left(\frac{1}{2}\right)^{\frac{T_G}{T_W}}$ to substitute $k T_G \ln 2 = -k T_W \ln(P_1)$.

During the course of the expansion, $k T_G \ln 2$ heat is drawn from the T_G heat bath, causing an decrease in entropy of $k \ln 2$. This compensates for the increase in the entropy of the engine, and confirms that the process so far has been thermodynamically reversible.

During the expansion phase the free energy becomes undefined. At the end of this phase, it has changed by an amount $F_{T1} - F_{T0} = -kT_W \ln(2P_1) = -(T_W - T_G)k \ln 2$. This is just a free energy change of $\Delta F = -S\Delta T$, where the entropy $k \ln 2$ has been transferred from the T_G heat bath to the weights and piston at T_W . This is the occurrence of the characteristic equation discussed in Appendix G.

Stage c Shelves now come out on both sides of the machine, at a height h_T to support a raised weight. This divides an unraised density matrix into the subensembles for above and below the shelf. In Sections 6.5 and 6.6 it was assumed that the unraised density matrix divides into two orthogonal subensembles

$$\rho_{W1}(0) = P_1 \rho_{W0}(h_T)^{00} + P_2 \rho_{W0}(0)^{00}$$

without interference terms.

This implies the entropies and free energies combine according to

$$\begin{aligned} S_{W1} &= (P_1 S_{W0}(h_T)^{00} + P_2 S_{W0}(0)^{00}) - k(P_1 \ln P_1 + P_2 \ln P_2) \\ F_{W1}(0) &= (P_1 F_{W0}(h_T)^{00} + P_2 F_{W0}(0)^{00}) + kT_W(P_1 \ln P_1 + P_2 \ln P_2) \end{aligned} \quad (7.10)$$

$$(7.11)$$

and so inserting the shelves would be both reversible, and involve negligible work.

Unfortunately, it is not possible to directly confirm these relations. We can estimate the free energy and entropy of $\rho_{W0}(h_T)^{00}$ as the same as the free energy and entropy of the raised weight $\rho_{W1}(h_T)$. However, as we do not have suitable approximations for the wavefunctions trapped below the shelf, we cannot calculate the entropy or free energy for $\rho_{W0}(0)^{00}$.

For the reasons given in Appendix E, if $kT_W \gg M_W g h_T$ or $kT_W \ll M_W g h_T$ the insertion of the shelf should be reversible and involve negligible work, and it is reasonable to assume that this will also be true at intermediate heights for high temperature systems ($kT_W \gg M_w g H$, the characteristic energy of the ground state). If this is the case, Equations 7.11 will then be true.

This assumption simply allows us to continue to calculate entropy and free energies during Stages (c-e) of the cycle. It does not affect the behaviour of the Engine itself, as the interference terms will disappear in Stage (f) of the cycle. The only part of the assumption that is significant is that the insertion of the shelf requires negligible work. This is similar to inserting the narrow barrier into the one atom gas, which was proved to require negligible work in Section 6.2³.

We will therefore assume that Equations 7.11 are true, from which it can immediately be seen that the free energy and entropy of ρ_{T2} is the same as for ρ_{T1} .

Stage d The piston is now removed from the box. The only affect of this is to change $\rho_{G6}^\rho(1-p)$ and $\rho_{G6}^\lambda(-1+p)$ into ρ_{G0} . This has negligible effect upon the free energy or entropy of the gas states, so the thermodynamic properties of ρ_{T3} are also unchanged from ρ_{T1} .

³It should also be noted that if this assumption is false, it would imply a difference between the quantum and classical thermodynamics of a particle in a gravitational field, even in the high temperature limit.

Stage e The operation of U_{reset} then takes the density matrix on the raising cycle to ρ_{T4} . Only the piston states are changed by this, and so again, there is no change in entropy or free energy.

Stage f The shelves are removed and the system is allowed to thermalise, leading to a final density matrix of

$$\begin{aligned} \rho_{T5} = & \rho_{G0} \otimes (w_1 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \otimes |\phi_0\rangle \langle \phi_0| + w_2 \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| \\ & + w_3 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L|) \end{aligned} \quad (7.12)$$

from Equation 6.15.

In the w_1 portion of the density matrix, $M_w g h_T$ energy is dissipated into the T_W heat bath, increasing its entropy. The total entropy is therefore

$$\begin{aligned} S_{T5} = & S_{G0} + w_1 \left(2S_{W0} + S_P + \frac{M_w g h_T}{T_w} \right) + w_2 (S_{W0} + S_{W1}(h_T) + S_P) \\ & + w_3 (S_{W0} + S_{W1}(h_T) + S_P) - k \sum_{n=1,3} w_n \ln w_n - k \ln 2 \\ = & S_{T0} - k \sum_{n=1,3} w_n \ln w_n - k \ln 2 - k \ln P_1 \end{aligned}$$

where we have included the /

	T_G	Gas	Piston	Weight 1	Weight 2	T_W
Stage a						
Energy	/	$\frac{1}{2}kT_G$	/	$\frac{3}{2}kT_W$	$\frac{3}{2}kT_W$	/
Entropy	/	S_{G0}	S_p	S_{W1}	S_{W1}	/
Free Energy	/	F_{G0}	F_P	F_{W1}	F_{W1}	/
Stage b						
Energy	$-kT_G \ln 2$	$\frac{1}{2}kT_G$	/	$3kT_W + M_W gh_T$		/
Entropy	$-k \ln 2$	S_{G0}		$S_p + 2S_{W1} + k \ln 2$		/
Free Energy	/	F_{G0}		$F_P + 2F_{W1} - kT_W \ln(2P_1)$		/
Stage f						
Energy	$-kT_G \ln 2$	$\frac{1}{2}kT_G$	/	$3kT_W - (w_2 + w_3)kT_W \ln P_1$		$-kw_1 T_W \ln P_1$
Entropy	$-k \ln 2$	S_{G0}		$S_p + 2S_{W1} - k \sum w \ln w$		$-kw_1 \ln P_1$
Free Energy	/	F_{G0}		$F_P + 2F_{W1} + kT_W (\sum w \ln w - (w_2 + w_3) \ln P_1)$		/

Table 7.1: Thermodynamic Properties of the Raising Cycle

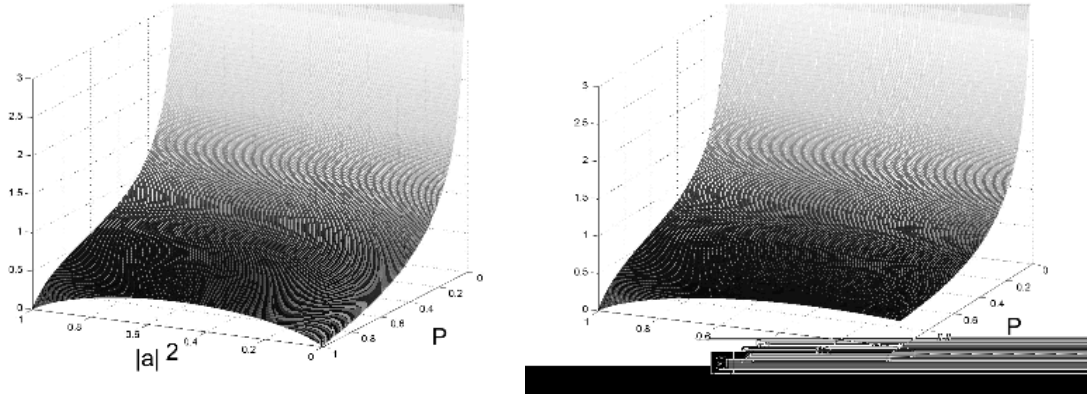


Figure 7.1: Change in Entropy on Raising Cycle for (a) $|c_1|^2 = 0$ and (b) $|b_1|^2 = |c_1|^2$

there is negligible increase in entropy due to mixing. However, the entropy decrease when energy is extracted from the T_G heat bath is much less than the entropy increase when that same energy is deposited in the T_W heat bath.

In addition, it can be seen that when either $|a_1|^2 = 1$ or $|b_1|^2 = 1$, and $P_1 = 1$ the net entropy increase is zero. In this case $T_G \ll T_W$ and the unraised weights are always located above the shelf height. The entropy increase here arises only from the decoherence of the superposition of the piston states, $|\phi_2\rangle \langle\phi_2|$ and $|\phi_3\rangle \langle\phi_3|$, after the operation of U_{RES} . When any of $|a_1|^2, |b_1|^2, |c_1|^2 = 1$, the piston is not left in a superposition, so there is no increase in entropy.

The free energy changes by

$$kT_W \ln(2P_1) = k(T_W - T_G) \ln 2$$

during Stage (b), as $k \ln 2$ entropy is transferred from the gas and T_G heat bath to the weights and T_W heat bath. In the final stage it changes again, alongside the entropy increase, to give a net

change of

$$\frac{\Delta F_R}{kT_W} = \sum_{n=1,2,3} w_n \ln w_n - (w_2 + w_3) \ln P_1$$

over the entire cycle. This can be shown to always be negative. We should not be surprised by this, as our objective was to drop the weight we had lifted, and so dissipate the energy used to raise it.

7.3 Lowering Cycle

The lowering cycle is shown in Figure 5.7. Following the stages of this cycle given in Section 6.6, where the density matrices ρ_{T6} to ρ_{T11} are defined, we will now calculate it's thermodynamic properties.

Stage a Assuming the piston starts initially on the right, the initial density matrix is ρ_{T6} and the entropy and free energies are given by

$$\begin{aligned} S_{T6} &= S_P + S_{G0} + 2S_{W1} \\ F_{T6} &= F_P + F_{G0} + 2F_{W1} + kT_G \ln 2 \end{aligned}$$

and will be negligibly affected by the piston being inserted into one end of the box.

Stage b Under the operation of U_{W4} , the raised weight is lowered, compressing the gas. During this stage, the density matrix is

$$\rho_{T7}(Y) = \rho_{G6}^\lambda(Y) \otimes \rho_{W1}^\lambda(h(Y)) \otimes \rho_{W1}^p(0) \otimes |\Phi(Y)\rangle \langle \Phi(Y)|$$

giving entropies and free energies

$$\begin{aligned} S_{T7}(Y) &= S_{G6}^\lambda(Y) + S_P + 2S_{W1} \\ &= S_{T6} - k \ln \left(\frac{2}{Y+1-p} \right) \\ F_{T7}(Y) &= F_{G6}^\lambda(Y) + F_p + F_{W1}(0) + F_{W1}(h(Y)) \\ &= F_{T6} \end{aligned}$$

During the compression, $kT_G \ln \left(\frac{2}{Y+1-p} \right)$ heat is transferred from the gas to the T_G heat bath, giving a compensating rise in entropy. At the end of this stage, the entropy of the gas has reduced by approximately $k \ln 2$, having halved in volume, and the entropy of the T_G heat bath has increased by the same amount. The total free energy remains constant, as the work done by the weight in work done reversibly upon the gas.

Stage c Shelves are inserted into the thermal state of the two weights at height h_T . As explained in Stage c of the raising cycle above, we must assume that this takes place reversibly and with negligible work. The density matrix ρ_{T8} will then have the same entropy and free energy as $\rho_{T7}(0)$ at the end of Stage b.

Stage d The operation of U_{RI} now removes the piston from the center of the box. The gas is now able to freely expand to occupy the entire box, so that $\rho_{G6}^\lambda(0) \rightarrow \rho_{G0}$. This leaves the system in state ρ_{T9} .

The internal energy of these two density matrices are both $\frac{1}{2}kT_G$, and no work is done upon the gas, so no energy is drawn from the T_G heat bath by this free expansion. However, the entropy of the gas increases by $k \ln 2$ and the free energy decreases by a corresponding amount $kT_G \ln 2$. There is no compensating entropy decrease anywhere else in the system.

Stage e The application of U_{RES} takes ρ_{T9} to ρ_{T10} . This changes only the state of the piston, and does not affect the entropy or free energy.

Stage f Finally, the removal of the shelves and contact with the T_W heat bath leaves the system in the state

$$\begin{aligned} \rho_{T11} = & \rho_{G0} \otimes (w_4 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(0) \otimes |\phi_0\rangle \langle \phi_0| + w_5 \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| \\ & + w_6 \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L|) \end{aligned} \quad (7.13)$$

from Equation 6.17.

In the $(w_5 + w_6)$ part of the density matrix, a thermal fluctuation has caught a weight above one of the shelves. This draws $M_W g h_T$ energy from the T_W heat bath, decreasing its entropy. The total entropy and free energy at the end of the lowering cycle is therefore

$$\begin{aligned} S_{T11} &= S_{G0} + S_P + 2S_W - k \sum_{n=4,6} w_n \ln w_n + k(w_5 + w_6) \ln P_1 + k \ln 2 \\ F_{T11} &= F_{G0} + F_P + 2F_W + kT_W \left((w_5 + w_6) \ln P_1 - \sum_{n=4,6} w_n \ln w_n \right) \end{aligned}$$

where we have explicitly included the entropy changes in the two heat baths.

Summary Table 7.2 summarises the changes in energy, entropy and free energy for the lowering cycle. The values are shown at the end of Stages a, b, d and f, and again, where subsystems are correlated, the entropy and free energy are shown as a total across the relevant columns.

Again, we see that the total energy is constant throughout the operation. The entropy changes at two points. During Stage d, when a free expansion of the one atom gas takes place, the entropy of the gas increases by $k \ln 2$. At Stage f, there is a further entropy change when the weights are allowed to thermalise through contact with the T_W heat bath. There is an entropy *decrease* of $(w_5 + w_6) \ln P_1$, where thermal energy from the heat bath is trapped in a fluctuation of the weight, but an increase of $-\sum_{n=4,5,6} w_n \ln w_n$. The change in entropy at this stage is therefore

$$\frac{\Delta S_L}{k} = (w_5 + w_6) \ln P_1 - \sum_{n=4,5,6} w_n \ln w_n$$

which is always positive. This is shown in Figure 7.2, for the two extremes, where $|c_1|^2 = 0$ and

	T_G	Gas	Piston	Weight 1	Weight 2	T_W
Stage a						
Energy	/	$\frac{1}{2}kT_G$	/	$\frac{3}{2}kT_W + M_Wgh_T$	$\frac{3}{2}kT_W$	/
Entropy	/	S_{G0}	S_p	S_{W1}	S_{W1}	/
Free Energy	/	F_{G0}	F_p	$F_{W1} + M_Wgh_T$	F_{W1}	/
Stage b						
Energy	$kT_G \ln 2$	$\frac{1}{2}kT_G$	/	$\frac{3}{2}kT_W$	$\frac{3}{2}kT_W$	/
Entropy	$k \ln 2$	$S_{G0} - k \ln 2$	S_p	S_{W1}	S_{W1}	/
Free Energy	/	$F_{G0} + kT_G \ln 2$	F_p	F_{W1}	F_{W1}	/
Stage d						
Energy	$kT_G \ln 2$	$\frac{1}{2}kT_G$	/	$\frac{3}{2}kT_W$	$\frac{3}{2}kT_W$	/
Entropy	$k \ln 2$	S_{G0}	S_p	S_{W1}	S_{W1}	/
Free Energy	/	F_{G0}	F_p	F_{W1}	F_{W1}	/
Stage f						
Energy	$kT_G \ln 2$	$\frac{1}{2}kT_G$	/	$3kT_W - (w_5 + w_6)kT_W \ln P_1$	$(w_5 + w_6)kT_W \ln P_1$	
Entropy	$k \ln 2$	S_{G0}		$S_p + 2S_{W1} - k \sum w \ln w$	$(w_5 + w_6)k \ln P_1$	
Free Energy	/	F_{G0}		$F_p + 2F_{W1} + kT_W (\sum w \ln w - (w_5 + w_6) \ln P_1)$	/	

Table 7.2: Thermodynamic Properties of Lowering Cycle

$|b_1|^2 = |c_1|^2$. Notice that the net change in entropy over the entire cycle includes an additional increase of $k \ln 2$ from Stage d. The minimum entropy increase on the lowering cycle is therefore $k \ln 2$.

The minimal increase in entropy occurs in two special cases. The first case is the same as on the raising cycle, when $P_1 = 1$ the weights are always located above the shelf height. The decoherence of $|\phi_1\rangle \langle \phi_1|$ when the weights are brought into contact with the T_W creates an entropy increase, unless the operation of U_{RES} is such that $|\phi_1\rangle \langle \phi_1|$ is not a superposition.

The second case is when $P_1 = 0$, regardless of choice of U_{RES} . In this case, at the end of Stage e, both weights will be found unambiguously below the shelf height. The effect of U_{RES} must leave this unchanged, and only $|\phi_0\rangle \langle \phi_0|$, the piston in the center, is compatible with this state. No entropy increase takes place at this stage, and the Engine cycle reverses. However, there is still the $k \ln 2$ entropy increase that occurred during Stage d.

The free energy similarly changes twice, both times as a direct result of the change in entropy. At Stage d, the increase in the gas entropy leads to a reduction in free energy of $kT_G \ln 2$, while during Stage f, the it changes by $-kT_W((w_5 + w_6) \ln P_1 - \sum_{n=4,5,6} w_n \ln w_n)$, giving a net change

$$\frac{\Delta F_L}{kT_W} = w_4 \ln P_1 + \sum_{n=4,5,6} w_n \ln w_n$$

over the complete cycle. All terms in this are negative. The free energy must be reduced over the course of a lowering cycle.

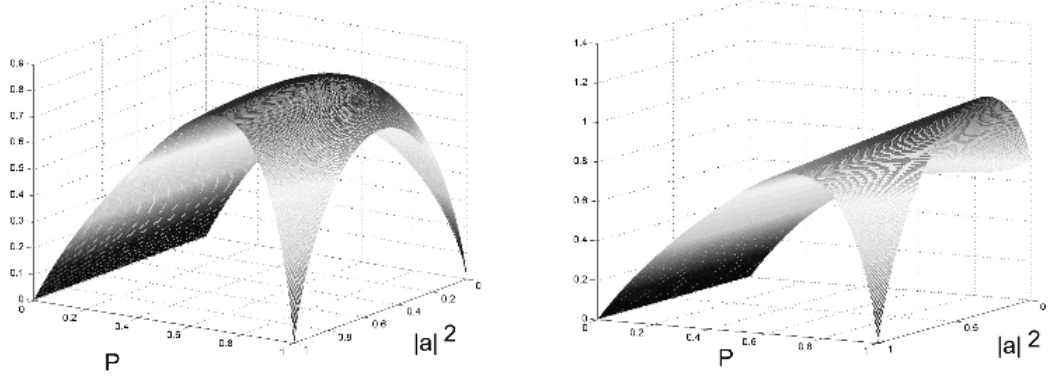


Figure 7.2: Change in Entropy on Lowering Cycle for (a) $|c_1|^2 = 0$ and (b) $|b_1|^2 = |c_1|^2$

7.4 Conclusion

We have now completed a detailed analysis of the thermodynamic quantities associated with the operation of the quantum Szilard Engine.

The free energy becomes undefined at certain stages, and can sometimes increase. However, when such an increase occurs it is compatible with the characteristic equation (G.1), and over the course of an entire cycle, the change in free energy will be negative.

The entropy of the correlated systems also behaves as would be expected. It is constant for all reversible processes, and increases for irreversible processes. Regardless of the choice of the resetting operation, or of the temperatures of the two heat baths, it always increases over the course of a raising or lowering cycle. There is an important subtlety to this result. In Chapter 6 we accepted that an anti-entropic cycle (such as a raising cycle when $T_W > T_C$) may continue, with some probability, despite the fact that the energy flow would be from colder to hotter. All we concluded was that the probability of the anti-entropic flow reversing would ensure the *mean* energy flow, over the long run, would be from hotter to colder. Now we appear to be saying that, even so, the entropy must always increase.

The answer to this apparent contradiction lies in the interpretation of the entropy of the density matrix. In Chapter 6 we assumed that the Engine was always either on a raising or a lowering cycle, and we concerned ourselves with the corresponding transfer of energy between the two heat baths.

To apply the concept of entropy, we must consider the density matrices ρ_{T5} and ρ_{T11} . In these, the Engine is described by a mixture of states, and so is not determinately upon a raising or lowering cycle. This implies an additional entropy of mixing. The results of this Chapter demonstrate that, even when the Engine starts on an anti-entropic cycle, at the completion of that cycle the entropy due to mixing in the final state of the Engine will always be larger than the reduction in entropy we may have achieved from transferring heat between the two baths.

Chapter 8

Resolution of the Szilard Paradox

In Chapters 5, 6 and 7 we have presented a detailed analysis of the operation of the Popper-Szilard Engine. This has shown that, within certain limitations, thermodynamic concepts are applicable to the single atom systems, and that no operation of the Popper-Szilard Engine was capable of violating the second law of thermodynamics. However, we have not as yet gained any real insight into *why* the Engine cannot work, nor why some further modification of the Engine would not be successful. In this Chapter we will attempt to address these issues by uncovering the essential properties of the Engine, demonstrate that these properties are central to the general problem of Maxwell's Demon, and explaining the thermodynamics underlying them.

In Section 8.1, we will consider first part of the role played by the demon. The demon makes a measurement upon the system of interest, and changes the state of the system, conditionally upon the result of that measurement. This attempts to eliminate the mixing entropy of the ensemble. However, the requirement of unitary evolution leads to a change in the state of the demon itself. We will show that the piston plays exactly the role of the demon within the Popper-Szilard Engine. The first stage of the resolution therefore rests in the consideration of the effect the measurement has upon the demon itself.

The second stage of the resolution considers the consequences of the change in the demons state, and the attempts to complete the thermodynamic cycle. This problem is raised, but only partly addressed, by advocates of Landauer's Principle as the resolution to the problem. In Section 8.2, it is shown that the key thermodynamic relationship is one relating the probabilities of thermal fluctuations at different temperatures. This relationship shows why the probabilistic attempt to reset must fail, and why attempts to improve upon this, by performing work upon the system, leads at best to the Carnot cycle efficiency. This cycle differs from the phenomenological Carnot cycle, however, as it operates through correlations in the statistical states of the subsystems, to transfer *entropy*, rather than energy, between subsystems at different temperatures. It is further shown, from this relationship, that the attempt to capture statistical fluctuations will always be an ineffective method of extracting work from a thermal system.

This provides a comprehensive resolution to the general Maxwell's demon problem. In Section 8.3 we will re-examine the arguments offered in Chapter 4 and demonstrate they are, at best, partial resolutions, each focussing upon one aspect of the overall solution.

8.1 The Role of the Demon

We need to understand what are the essential features in the system, that constrains the evolution of the Popper-Szilard Engine in such a way that it fails to operate as intended. The essential restriction placed upon it was that it must be described by a unitary operator. The construction of an appropriate unitary operator in Chapter 5 depended upon the moveable piston in two particular ways. We will now examine this dependancy and show that this captures the essential role played by the Demon.

In Section 5.3 the unitarity of the expansion of the gas states, in Equations 5.12 and 5.13, is guaranteed only through the orthonormality relationship, on the gas and piston states, in Equation 5.14:

$$\langle \Psi_k^\alpha(Y_m)\Phi_A(Y_m) \mid \Psi_l^\beta(Y_n)\Phi_B(Y_n) \rangle = \delta_{nm}\delta_{\alpha\beta}\delta_{kl}\delta_{AB} \quad (8.1)$$

However, this orthonormality does not come from the gas states themselves, as the initially left and right gas states may become overlapping under the action of the unitary operator U_{T2} . It is the orthonormality of the different piston states, in Equation 5.9, that allows us to construct a suitable unitary operator. However, it is also the orthonormality of the final piston states that means we cannot construct a unitary operator to reset the piston states and reliably start another cycle of the Engine.

First we will examine precisely the role of the piston states. This will show that the piston fulfils exactly the same role that is required of a Maxwell's Demon. We will be able to characterise the general role of Maxwell's Demon as an attempt to reverse the mixing between subensembles in Equations 7.6 and 7.8. It is then shown that the Demon can only achieve such a reversal by increasing it's own entropy by at least as much again.

8.1.1 The Role of the Piston

Let us examine the role of the piston, in the Popper-Szilard Engine, in some detail. If we consider the raising cycle, the insertion of the partition into the gas divides it into two orthogonal subensembles

$$\rho_{G1} = \frac{1}{2}\rho_{G6}^\lambda(0) + \frac{1}{2}\rho_{G6}^\rho(0)$$

During the expansion Stage b, the correlated density matrix is

$$\begin{aligned} \rho_{T1}(Y) = & \frac{1}{2}\rho_{G6}^\lambda(Y) \otimes \rho_{W1}^\lambda(h(Y)) \otimes \rho_{W1}^\rho(0) \otimes |\Phi(Y)\rangle \langle \Phi(Y)| \\ & + \frac{1}{2}\rho_{G6}^\rho(Y) \otimes \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h(Y)) \otimes |\Phi(-Y)\rangle \langle \Phi(-Y)| \end{aligned}$$

None of the gas or weight subensembles are orthogonal in this expansion. The left and right gas wavefunctions overlap, as do the raised and unraised weight states. However, the piston states $|\Phi(Y)\rangle \langle \Phi(Y)|$ and $|\Phi(-Y)\rangle \langle \Phi(-Y)|$ are orthogonal. It is this that maintains the orthogonality of the left and right subensembles, and ensures the evolution is unitary.

As the expansion progresses, the overlap between the left and right gas subensembles increases, until the piston reaches the end of the box and is removed, at which point the overlap is complete. The two, initially orthogonal, gas subensembles have been isothermally expanded into the same density matrix. For the weights, the overlap between $\rho_{W1}^\lambda(h(Y))$ and $\rho_{W1}^\lambda(0)$ decreases, but never reaches zero (except in the limit where $T_G \gg T_W$). Although the free energy from the expansion of the gas is picked up by the weights, it is still the piston states that ensures that the final density matrix has orthogonal subensembles:

$$\frac{1}{2}\rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) \otimes |\phi_R\rangle \langle \phi_R| + \frac{1}{2}\rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \otimes |\phi_L\rangle \langle \phi_L| \quad (8.2)$$

When calculating the free energy and entropies in Chapter 7, it was the orthogonality of the piston states that allowed us to apply the mixing formulas. The entropy of mixing between the two gas subensembles has been transferred to the *piston* states. The significance of the piston states can be made clear by considering the density matrix:

$$\frac{1}{2}\rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) + \frac{1}{2}\rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T) \quad (8.3)$$

The correlated weight states in this matrix are not orthogonal, so this density matrix has a lower entropy than the density matrix that includes the piston states. If it were not for the orthogonality of the piston states, the entropy of the Szilard Engine would have been reduced at this stage. Only in the limit of $T_G \gg T_W$ do the weights states become orthogonal, and the entropy of (8.3) becomes equal to (8.2). In this situation the different piston states *can* both be restored to the center (by correlating them to the position of the weights), but this does not reduce the entropy of the Engine as it only takes place where the transfer of heat is from the hotter to the colder system.

For the lowering cycle, the stages described in Section 6.6 do not show correlations. The reason for this is that we started the lowering cycle by assuming the piston is located on one particular side. In general, a lowering cycle can start with the piston at either side of the Engine, and so will have a density matrix of the form

$$p_R |\phi_R\rangle \langle \phi_R| \otimes \rho_{W1}^\lambda(h_T) \otimes \rho_{W1}^\rho(0) + p_L |\phi_L\rangle \langle \phi_L| \otimes \rho_{W1}^\lambda(0) \otimes \rho_{W1}^\rho(h_T)$$

with $p_R + p_L = 1$. This has an additional mixing entropy of $-k(p_L \ln p_L + p_R \ln p_R)$, which has a maximum value of $k \ln 2$, when $p_L = \frac{1}{2}$. Now we have a correlated states with mixing entropy associated initially with the pistons.

The evolution following from this will be the reverse of the raising cycle, and will transfer the entropy of mixing from the piston states, to the gas subensembles. The gas will be left in the state

$p_L \rho_{G6}^\lambda(0) + p_R \rho_{G6}^\rho(0)$ just before the removal of the piston from the center of the box.

After the removal of the piston, the gas returns to the uniform distribution ρ_{G0} . This is an irreversible change, and the entropy of the system increases by the difference between the original entropy of mixing of the piston states, and $k \ln 2$. In Section 7.3 then we have $p_L = 0$ or 1 and the maximum entropy increase of $k \ln 2$ occurs. If $p_L = \frac{1}{2}$, then no entropy increase occurs and we have the exact reverse of the raising cycle¹.

The essential point is that the correlation between the orthogonal piston and weight subensembles is transferred to the orthogonal gas subensembles. This demonstrates the same features as the raising cycle, which highlights the manner in which the Szilard engine is intended to work.

The gas ensemble initially 'occupies' the entire box. When the partition is inserted, it is divided into two orthogonal subensembles. The intention of the engine is to extract useful work from allowing each of these subensembles to expand back to 'occupy' the entire box again.

We have shown that this can be done, by inserting a freely moving piston in the center of the box. The inclusion of the state of this piston is an essential part of the evolution of the system, as the required evolution is not unitary unless the orthogonality of the piston states is taken into account. This transfers the entropy of mixing from the gas subensembles to the piston and weight subensembles. Now the same requirement of unitarity prevents the piston from being restored to its original position, which, if successful would imply a reduction in the entropy of the system.

8.1.2 Maxwell's Demons

It is the orthogonality of the pistons states that are essential to the operation of the Szilard Engine. We will now show how this relates to the Maxwell's Demon.

The original Maxwell's Demon thought experiments did not involve an analysis of work or free energy. Maxwell described two systems, a pressure demon and a temperature demon, using a trap door which separates a gas into two portions. When an atom approaches, the demon opens or closes the trapdoor, allowing the atom to pass or not. We will present a very simplified analysis of the pressure demon, to illustrate its essential similarity to our analysis of the Szilard Engine.

In the case of the pressure demon, if an atom approaches from the left, it is allowed to pass, while if it approaches from the right, it is reflected elastically. No work is performed upon the system. We represent an atom on left by $|L\rangle$ and on the right by $|R\rangle$.

If U_1 represents the unitary operator for the demon holding the trapdoor open and U_2 the unitary operator for the demon holding the trapdoor closed, we have

$$\begin{aligned} U_1 |L\rangle &= |R\rangle \\ U_2 |R\rangle &= |R\rangle \end{aligned}$$

These cannot be combined into a single unitary operator. To operate the trapdoor the demon must involve its own internal states, or some auxiliary system.

¹The net change in entropy over the cycle will still be positive

The complete specification of the unitary operators is

$$\begin{aligned} U_1 &= |L\rangle \langle R| + |R\rangle \langle L| \\ U_2 &= |L\rangle \langle L| + |R\rangle \langle R| \end{aligned}$$

We now assume the demon has auxiliary states $|\pi_0\rangle$ and $|\pi_1\rangle$, and uses these auxiliary states to produce a combined unitary operation. There is some flexibility in choosing this operator but this is not important, so we choose the fairly simple form, assuming the demon initially in the state $|\pi_0\rangle$ of

$$\begin{aligned} U_a &= |\pi_1 L\rangle \langle \pi_0 L| + |\pi_0 R\rangle \langle \pi_0 R| \\ &\quad + |\pi_0 L\rangle \langle \pi_1 L| + |\pi_1 R\rangle \langle \pi_1 R| \\ U_b &= |\pi_1 R\rangle \langle \pi_1 L| + |\pi_0 R\rangle \langle \pi_0 R| \\ &\quad + |\pi_0 L\rangle \langle \pi_0 L| + |\pi_1 L\rangle \langle \pi_1 R| \\ &= |\pi_1\rangle \langle \pi_1| U_1 + |\pi_0\rangle \langle \pi_0| U_2 \end{aligned}$$

The action of U_a represents the Demon measuring the location of the atom, and then U_b represents the Demon holding the trapdoor open or shut.

The atom may initially be on either side, so is described by

$$\frac{1}{2} |L\rangle \langle L| + \frac{1}{2} |R\rangle \langle R|$$

After the operation of U_a , the demon and atom are in a correlated state

$$\frac{1}{2} |L\pi_1\rangle \langle L\pi_1| + \frac{1}{2} |R\pi_0\rangle \langle R\pi_0|$$

Under U_b , the atom then evolves into $|R\rangle \langle R|$, but leaves the demon in the state $\frac{1}{2} |\pi_0\rangle \langle \pi_0| + \frac{1}{2} |\pi_1\rangle \langle \pi_1|$. Clearly the entropy of the atom has decreased, but the entropy of the demon has correspondingly increased². The demon states play exactly the same role as the piston states in the Popper-Szilard Engine. We will now consider the thermodynamics of this.

8.1.3 The Significance of Mixing

What we have seen above is that the problem involves separating an ensemble into subensembles. By correlating these subensembles to an auxiliary system, such as a Demon or a piston, operations can be performed upon the subensembles that cannot be performed upon the overall ensemble. In other words, we are trying to reverse the mixing of the subensembles. We will now have to consider the physical origin of the mixing entropy, and the role it plays. We will restrict the discussion to the case where there are only two subensembles ρ_1 and ρ_2 , and focus upon the problem of reversibly extracting work from the system.

²If we now bring in a second atom in the state $\frac{1}{2} |L\rangle \langle L| + \frac{1}{2} |R\rangle \langle R|$, the demon fails to sort the atom at all. Having picked up the mixing entropy of the atom, it is no longer able to function as intended.

To understand the significance of this requires us to explain the physical origin of the mixing relationships

$$F_i = F - kT \ln p_i$$

$$S = \sum_i p_i (S_i - k \ln p_i)$$

where an equilibrium density matrix may be decomposed into orthogonal subensembles

$$\rho = \sum_i p_i \rho_i$$

$$\rho_i \rho_j = (\rho_i)^2 \delta_{ij}$$

If we start with a system in the equilibrium state $\rho = p_1 \rho_1 + p_2 \rho_2$, we will be able to extract work from the mean pressure exerted on some boundary parameter. This is represented by the free energy F which is the work that can be isothermally extracted, when taking the density matrix ρ to some reference state ρ_0 .

Let the free energy F_1 represents the isothermal work extracted taking a density matrix ρ_1 to the reference state ρ_0 . This is given by $F_1 = F - kT \ln p_1 > F$. Similarly for ρ_2 we have $F_2 = F - kT \ln p_2 > F$. In both these cases, the free energy is higher than is obtained by operating directly upon the ensemble, by an amount $-kT \ln p_i$ so the mean gain in free energy from operating upon the subensembles rather than the ensemble is simply $-kT \sum p_i \ln p_i$. This is the free energy that is lost due to the mixing.

In other words, by separating the ensemble into its orthogonal subensembles, we are attempting to avoid the loss of free energy caused by the mixing. Although other versions of Maxwell's demon do not address free energy directly (eg. creating pressure or temperature gradients), they are all illustrated by being connected to heat engines or turbines which extract work, so in one way or another they are all implicitly concerned with increasing the free energy of an ensemble by manipulating its subensembles.

We will now try to explain how mixing causes the free energy to be lost. This will be shown to be a consequence of the unitarity of the evolution operators.

Perfect Isolation First we will consider the situation of perfect isolation. In this case there are no transitions between eigenstates, and the evolution of a density matrix, initially $\rho^\theta(0)$, will be described by

$$\rho^\theta(t) = U(t) \rho^\theta(0) U^\dagger(t)$$

where $U(t)$ is the solution to the operator Schrödinger equation.

Our first result to establish is that there is no operator that is capable of separately operating upon ρ_1 and ρ_2 to take them into the reference state ρ_0 . This can be seen easily from the fact that if we were to find an operator U_1 such that

$$\rho_0 = U_1 \rho_1 U_1^\dagger$$

it cannot be also true that

$$\rho_0 = U_1 \rho_2 U_1^\dagger$$

as this would mean

$$(\rho_0)^2 = U_1 \rho_1 U_1^\dagger U_1 \rho_2 U_1^\dagger = U_1 \rho_1 \rho_2 U_1^\dagger = 0$$

and a density matrix such as ρ_0 cannot be nilpotent.

From this it follows that if we wish to perform an operation where each of the two subensembles are taken to the same reference state, we must involve a second system.

If we take a second operation, U_2 , such that

$$\rho_0 = U_2 \rho_2 U_2^\dagger$$

and introduce an auxiliary system, with orthogonal states³ π_1 and π_0 , initially in the state π_0 , then we can form two unitary operators, containing the operations

$$\begin{aligned} U_a &= |\pi_1\rangle \langle \pi_0| P_1 + |\pi_0\rangle \langle \pi_0| P_2 \\ U_b &= |\pi_1\rangle \langle \pi_1| U_1 + |\pi_0\rangle \langle \pi_0| U_2 \end{aligned}$$

where P_1 and P_2 are projectors onto the subspaces of ρ_1 and ρ_2 respectively.

The effect of U_a is to correlate the auxiliary system with the subensembles. U_b then acts as a conditional unitary operator. If the auxiliary system is in π_1 , then it switches on the Hamiltonian necessary to take ρ_1 to ρ_0 , while if the auxiliary system is in state π_2 , the Hamiltonian for taking ρ_2 to ρ_0 is switched on. This successfully takes each of the subensembles to the reference state, extracting maximum work in the process, but leaves the auxiliary system in the state $p_1 |\pi_1\rangle \langle \pi_1| + p_2 |\pi_2\rangle \langle \pi_2|$. The entropy of mixing has been transferred from the ensemble to the auxiliary. The π_1 and π_2 are orthogonal, and so again there is no unitary operation that is capable of restoring the auxiliary system to its initial state.

Contact with the environment The situation of perfect isolation, however, is too idealised. In general, while the unitary operation is taking place, contact with an environment will cause transitions between eigenstates. The evolution of the density matrix will not, in general, be described by a unitary operation. We cannot assume that the final and initial density matrices are unitarily equivalent, so the proof given above, based upon the preservation of inner products, is no longer valid.

As an example, let us consider the discussion of the Szilard box with the partition raised, and the atom confined to the left. The state is initially

$$|\psi_i^p\rangle = \frac{1}{\sqrt{2}} (|\psi_i^{\text{even}}\rangle + |\psi_i^{\text{odd}}\rangle)$$

³We will always assume that eigenstates of the auxiliary systems are at the same energy.

If the partition is removed, in perfect isolation, the free evolution of the gas leads to the state

$$\frac{1}{2} \left(e^{i \frac{E_i^{\text{even}} t}{\hbar}} |\psi_i^{\text{even}}\rangle + e^{i \frac{E_i^{\text{odd}} t}{\hbar}} |\psi_i^{\text{odd}}\rangle \right)$$

where the energies are now the non-degenerate energies of the unperturbed eigenstates. This leads to a time dependant factor in the phase of the superposition. The state appears reasonably uniformly spread most of the time, but when

$$\frac{(E_i^{\text{even}} - E_i^{\text{odd}}) t}{\hbar} = n\pi$$

for integer n , the atom will be located on a well defined side of the box. If the piston is re-inserted at this time, the atom will always be found on a specific side of the box.

If the atom had initially started confined to the right, it would evolve to

$$\frac{1}{2} \left(e^{i \frac{E_i^{\text{even}} t}{\hbar}} |\psi_i^{\text{even}}\rangle - e^{i \frac{E_i^{\text{odd}} t}{\hbar}} |\psi_i^{\text{odd}}\rangle \right)$$

This will be found on the opposite side of the box at these same well defined times. In fact, at all intervening times, the two states are orthogonal. Although they are *spatially* overlapping most of the time, in principle the interference terms maintain the distinguishability of the two states.

If we construct the density matrices ρ_{G2}^λ and ρ_{G2}^ρ from the right and left wavefunctions, lowering the partition causes these to evolve into states that are still orthogonal to each other. The initially orthogonal subensembles (of gas on the left or gas on the right) remain orthogonal at all times.

If the box is in contact with an environment, however, decoherence effects destroy the superposition between the even and odd wavefunctions. Both $|\psi_i^\rho\rangle$ and $|\psi_i^\lambda\rangle$ will now evolve into the density matrix

$$\frac{1}{2} (|\psi_i^{\text{even}}\rangle \langle \psi_i^{\text{even}}| + |\psi_i^{\text{odd}}\rangle \langle \psi_i^{\text{odd}}|)$$

As the orthogonality between the ρ_{G2}^λ and ρ_{G2}^ρ states depends upon the coherent phase of the superpositions, when there is decoherence the left and right subensembles evolve to the same equilibrium ensemble ρ_{G0} . In this situation, the same unitary operation (lowering the partition) leads to initially orthogonal subensembles evolving into the same density matrix.

Although we must describe the evolution of the system with unitary operators, contact with the environment can allow non-unitary evolution of the system's density matrix. We must now analyse the effect of this upon the mixing relationship.

Isothermal We must take into account the non-unitarity of the evolution, due to interactions with the environment, when considering how to extract the free energy. Our task is to see if the initially orthogonal subensemble states can be taken into non-orthogonal states, using contact with the heat bath, while extracting the free energy that is lost due to mixing.

We will consider the situation where the environment is a heat bath at temperature T . To extract the optimum free energy F_1 , from subensemble ρ_1 , we need to apply a suitable time dependant Hamiltonian (such as the one that leads to U_1) that takes the subensemble to the

reference state (at temperature T). One of the properties of such a optimum path is that it is thermodynamically reversible. This means that if we apply U_1^Y to the reference state, while in contact with a heat bath at temperature T , we will obtain the original subensemble ρ_1 (and will have to perform F_1 work upon the system).

If we now try to extract the free energy F_2 from the subensemble ρ_2 , we clearly require a different time dependant Hamiltonian as we need it to correspond to the adjoint of that unitary operator U_2^Y which, when isothermally applied to the reference state, produces the subensemble ρ_2 . This leaves us in the same situation as with perfect isolation - if we wish to combine the two unitary operations so that the appropriate one is applied to the appropriate subensemble, we need to include an auxiliary system. This auxiliary system correlates itself to the subensemble, and is itself left in a higher entropy state.

It appears that if we wish to extract the $-kT \ln p$ free energy from the subensembles, we cannot combine the operations into a single operator, but must employ an auxiliary. We know that there *is* an operator that can take both the subensembles to the same state, when in contact with a heat bath, but this operator loses the free energy of mixing. We shall refer to this as a 'dissipation' of the mixing free energy $-kT \sum p \ln p$.

Let us try and understand more clearly the underlying reason why the orthogonal subensembles can be decoherently transformed into the same state using a single unitary operator, but if we wish to extract the free energy rather than dissipate it, two different unitary operators are required. We will consider the example of the Szilard box, with a partition raised, where ρ_1 is the atom confined to the left of the partition, ρ_2 the atom confined to the right, and the reference state is the atom unconfined with no partition.

When applying operator U_{RI} to remove the partition, the eigenstates deform continuously between the states Ψ_l^{even} and Ψ_l^{odd} , and the corresponding unperturbed Ψ_n states. If the atom is initially confined to the left, the initial states are Ψ_j^L which are superpositions of Ψ_j^{even} and Ψ_j^{odd} . As the barrier is lowered, the initial states evolve into a superposition of the unperturbed Ψ_{2j} and Ψ_{2j-1} states. The Ψ_j^R states, corresponding to an atom initially confined to the right of the partition, will evolve into an orthogonal superposition of the same states.

The most important feature of this is that the states into which the Ψ_l^L evolve span only half the Hilbert space - the Ψ_l^R evolve into states which span the other half. However, once the barrier has been lowered, all the states are thermally accessible to the atom, through interactions with the heat bath. The evolution given by U_{RI} does not cause the initially confined atom to occupy the full space and become in the state ρ_{G0} . It is the 'free energy dissipating' or decoherent contact with the heat bath which allows the atom to expand to occupy the entire state space.

Now let us consider the situation where the atom is confined to the left, and we wish to extract the free energy of the expansion to fill the entire box. Again, the atom starts in the Ψ_l^L states. Now the evolution U_1 , however it is implemented, to extract the optimum work, must take the atom into ρ_{G0} , occupying the complete set of the unperturbed Ψ_l states - which span the entire

Hilbert space⁴.

Suppose the effect of U_1 left some of the final Hilbert space unoccupied, but thermally accessible. Then, decoherence from contact with the heat bath would lead to that portion of Hilbert space becoming occupied, dissipating some free energy in the process. To extract maximum work, or equivalently, to eliminate the dissipation of free energy, the operation of U_1 must be a one-to-one mapping of the Ψ_l^L Hilbert space onto the Ψ_l Hilbert space.

Now, the same must also be true for the optimum extraction, using U_2 , of free energy from an atom initially confined on the right. However, this means that U_1 and U_2 are attempting to map initially orthogonal sets of eigenstates Ψ_l^L and Ψ_l^R onto the same set of states Ψ_l . This is the reason that U_1 and U_2 cannot be combined into a single operator, as such a mapping cannot be unitary.

This significantly improves the result derived in the case of perfect isolation above. For perfect isolation, we can rely upon the unitary equivalence of the transformed *density matrices*, and the invariance of their inner product. This cannot be relied upon when there are interactions with an environment. Instead, we have used the properties of the unitary operation, as a mapping upon the *space of states* that the density matrix occupies.

If we were to use a U_1 operator that mapped the Ψ_l^L only onto some subset of the Ψ_l , then that would leave the complementary subset available for some of the Ψ_l^R under U_2 . This would allow some portion of U_1 and U_2 to be combined. However, the atom initially confined to the left, would come to occupy the entire Hilbert space, including that portion of the Hilbert space left unoccupied by U_1 through decoherent contact with the heat bath. The same would take place for the atom initially confined to the right. In other words, the extent to which the U_1 and U_2 operators may be combined is directly linked to the amount of free energy that is dissipated rather than extracted. The operator U_{RI} maps the Ψ_l^L and Ψ_l^R onto entirely orthogonal sets of states, but which are accessible to the same set of states by a decoherent process. This allows a single operator to take the left and right density matrices into occupying the whole space, but at the cost of dissipating the entire free energy of mixing.

The conclusion of this is that it is the requirement of unitarity that prevents us from extracting the optimum free energy from the subensembles. A unitary operator that acts upon both subensembles will fall short of optimum by at least that amount of free energy given by the mixing formula. We can use a different unitary operator upon each subensemble only if we correlate an auxiliary system to the subensembles. However, the consequence is that the auxiliary system picks up precisely that entropy of mixing that compensates for the increase in work we are now able to extract from the subensembles.

⁴This difference between U_1 and U_{RI} , mapping the same initial states to all, and one-half of the final Hilbert space, respectively, is possible because there is a countable infinity of states available.

8.1.4 Generalised Demon

We have argued that it is the relationship between the mixing and correlations that both gives rise to, and resolves, the Maxwell's Demon problem. Let us examine this in more detail, and greater generality. Our intention here is to highlight the role of the unitary operations upon the subspaces and the effect of introducing an auxiliary system. Our argument is that the mixing entropy is a consequence of unitarity. Reversing this mixing, separating the ensemble into subensembles, can only be achieved by introducing an auxiliary system. However, any gain in the free energy or entropy due to this separation is offset by at least as large an increase in the entropy of the auxiliary system.

We assume the initial Hilbert space is formed from two orthogonal subspaces $\Gamma = \Gamma_1 \oplus \Gamma_2$. The initial, equilibrium ensemble may be written in terms of the orthogonal subensembles $\rho = p_1\rho_1 + p_2\rho_2$. The subensemble ρ_1 initially occupies⁵ the subspace Γ_1 of the Hilbert space and ρ_2 occupies the orthogonal subspace Γ_2 . They occur with probability p_1 and p_2 in the initial equilibrium ensemble, and $p_1 + p_2 = 1$. The unitary operator U_1 maps Γ_1 to some subspace Γ_1^ℓ of Γ and U_2 maps Γ_2 to Γ_2^ℓ . We will assume that contact with a thermal heat bath will cause an ensemble initially localised in Γ_1^ℓ to decoherently spread throughout Γ , returning the system to the initial equilibrium ensemble ρ , and similarly for Γ_2^ℓ .

The probability of an equilibrium system ρ being spontaneously found in the Γ_1^ℓ subspace is p_1^ℓ and the probability of the system being similarly in Γ_2^ℓ is p_2^ℓ . As we do not assume that Γ_1^ℓ and Γ_2^ℓ are orthogonal subspaces, there is no restriction on $p_1^\ell + p_2^\ell$.

The free energy of the subensembles can be calculated from their probabilities, and the free energy of the initial ensemble F

$$\begin{aligned} F_1 &= F - kT \ln p_1 \\ F_1^\ell &= F - kT \ln p_1^\ell \\ F_2 &= F - kT \ln p_2 \\ F_2^\ell &= F - kT \ln p_2^\ell \end{aligned}$$

We now wish to see how we can extract the extra free energy from the subensembles.

In p_1 proportion of the cases, the system is in subensemble ρ_1 . Under the operation of U_1 , it isothermally expands to occupy Γ_1^ℓ , becoming ρ_1^ℓ . This extracts $kT \ln(p_1^\ell/p_1)$ free energy. The density matrix ρ_1^ℓ then expands freely into ρ , and $-kT \ln(p_1^\ell)$ notional free energy is dissipated.

In p_2 cases, the initial subensemble is ρ_2 . Isothermally expanding this with the operation of U_2 extracts $kT \ln(p_2^\ell/p_2)$ and then dissipates the notional free energy $-kT \ln(p_2^\ell)$.

The mean free energy gained is

$$\frac{\Delta F_G}{kT} = p_1 \ln \left(\frac{p_1^\ell}{p_1} \right) + p_2 \ln \left(\frac{p_2^\ell}{p_2} \right)$$

⁵When we say a density matrix 'occupies' a subspace, we mean that those eigenvectors of the density matrix which have non-zero eigenvalues, form a basis for the subspace.

and the subensemble free energy which may be regarded as dissipated is

$$\frac{\Delta F_D}{kT} = -p_1 \ln p_1^\ell - p_2 \ln p_2^\ell \geq 0$$

giving

$$\frac{\Delta F_G + \Delta F_D}{kT} = -p_1 \ln p_1 - p_2 \ln p_2 \geq 0$$

which is equal to the entropy of mixing of the two subensembles. As the free energy dissipated is never negative, it is immediately apparent that the free energy gained cannot exceed the entropy of mixing.

When we wish to distinguish between the actual free energy of an ensemble, F , and the mean free energy of its subensembles $\sum p_i F_i$ we shall refer to the additional free energy $-kT \sum p_i \ln p_i$ of the subensembles as a 'notional' free energy. This is the free energy we would *like* to be able to extract by splitting the ensemble into subensembles. The sense in which this 'notional' free energy is 'dissipated' is simply that we have failed to extract it. This is not the same as the situation where the initial matrix is actually ρ_1 say, and it is allowed to expand freely to ρ in which case an actual, rather than notional, free energy $-kT \ln p_1$ would have been lost.

No overlap in final subspaces In the case where Γ_1^ℓ and Γ_2^ℓ are complementary⁶ orthogonal subspaces, then U_1 and U_2 may be combined into a single unitary operator U_3 and $p_1^\ell + p_2^\ell = 1$. This yields a value of

$$\frac{\Delta F_G}{kT} = p_1 \ln \left(\frac{p_1^\ell}{p_1} \right) + (1 - p_1) \ln \left(\frac{1 - p_1^\ell}{1 - p_1} \right) \leq 0$$

with equality occurring only for $p_1 = p_1^\ell$.

To understand this we must consider what is happening to the two respective subensembles. As $p_1 + p_2 = p_1^\ell + p_2^\ell$ any 'expansion' of one subensemble is paid for by a 'compression' of the other. What the relationship above shows, is that when we divide an equilibrium ensemble into subensembles, the work required to perform the compression on one will always outweigh the work gained from the expansion on the other.

It is important to remember the values of p_1^ℓ and p_2^ℓ are the equilibrium probabilities that initial density matrix would have spontaneously been found in Γ_1^ℓ or Γ_2^ℓ , while p_1 and p_2 are the probabilities of spontaneously finding the system in a subensemble that is isothermally moved into those subspaces. Unless these probabilities are the same, the final density matrix will not be in equilibrium. This result tells us that any attempt to rearrange an equilibrium distribution into a non-equilibrium distribution requires work.

For the case of the Szilard Box, we divide the gas ensemble ρ_{G0} into the two subensembles ρ_{G2}^λ and ρ_{G2}^ρ by inserting a partition. This gives us $p_1 = p_2 = \frac{1}{2}$. If we simply remove the piston, we 'dissipate' the notional $kT \ln 2$ energy we could have extracted from expanding either of the

⁶If we were to use subensembles which were orthogonal, but not complementary, then $p_1' + p_2' < 1$. The only effect of this would be to reduce the amount of free energy that could be extracted.

subensembles, as we do not have an operator that, acting upon the gas alone, can extract this as work.

Complete overlap in final subspaces Now let us consider the case where Γ_1^ℓ and Γ_2^ℓ have an overlapping subspace Γ_{12}^ℓ . We are not restricted to $p_1^\ell + p_2^\ell = 1$ anymore, but we can no longer combine U_1 and U_2 into a single operator, so must employ an auxiliary system. The increase in entropy of the auxiliary system is

$$\frac{\Delta S_{aux}}{k} = -p_1 \ln p_1 - p_2 \ln p_2$$

which is the same as the entropy of mixing of the subensembles, and equal to the total free energy that is available to extraction and dissipation.

As we have no restrictions upon p_1^ℓ and p_2^ℓ , we obtain minimum 'dissipation', and extract maximum free energy, by setting $\Gamma_1^\ell = \Gamma_2^\ell = \Gamma_{12}^\ell = \Gamma_1 \oplus \Gamma_2$ so that $p_1^\ell = p_2^\ell = 1$. This allows us to extract the free energy $-kT \ln p_1$ with probability p_1 and $-kT \ln p_2$ with probability p_2 . Each subensemble has been allowed to expand to fill the entire space, extracting maximum free energy. However, the auxiliary system has had an equivalent increase in entropy.

This corresponds to the isothermal expansion of the Szilard box, where the piston plays the role of the auxiliary system. The free energy is extracted from each of the gas subensembles, but the piston is left in a mixture of states.

Partial overlap in final subspaces We might now ask that if Γ_1^ℓ and Γ_2^ℓ are not completely overlapping but not completely orthogonal, is there some way we can avoid the auxiliary system picking up the entire entropy of mixing. If we assume that $p_2 \leq p_1$, without loss of generality, we start by separating Γ_2^ℓ into orthogonal subspaces Γ_{12}^ℓ and Γ_{2a}^ℓ , where Γ_{2a}^ℓ does not overlap with Γ_1^ℓ .

We now need to separate the initial density matrix ρ_2 into the orthogonal subensembles ρ_{2a} and ρ_{2b} , where the subspace containing ρ_{2a} is mapped onto Γ_{2a}^ℓ and ρ_{2b} onto Γ_{12}^ℓ by U_2 . The probabilities of these subensembles will be p_{2a} and p_{2b} and the probabilities associated with Γ_{12}^ℓ and Γ_{2a}^ℓ are p_{12}^ℓ and $p_{2a}^\ell = p_2^\ell - p_{12}^\ell$. Finally, we split U_2 into an operator U_{2a} acting upon ρ_{2a} and an operator U_{2b} acting on ρ_{2b} .

We are now able to combine U_1 with U_{2a} , as Γ_{2a}^ℓ and Γ_1^ℓ do not overlap, into a single operator $U_A = U_1 \otimes U_{2a}$. This allows us to reformulate the problem as involving the two complementary orthogonal subspaces Γ_A and Γ_B with

$$\begin{aligned} \rho_A &= \frac{p_1 \rho_1 + p_{2a} \rho_{2a}}{p_1 + p_{2a}} \\ \rho_B &= \rho_{2b} \\ \Gamma_A &= \Gamma_1 \oplus \Gamma_{2a} \\ p_A &= p_1 + p_{2a} \\ \Gamma_B &= \Gamma_{2b} \\ p_B &= p_{2b} \end{aligned}$$

$$\begin{aligned}
\Gamma_A^\ell &= \Gamma_1^\ell \oplus \Gamma_{2a}^\ell \\
p_A^\ell &= p_1^\ell + p_2^\ell - p_{12}^\ell \\
\Gamma_B^\ell &= \Gamma_{12}^\ell \\
p_B^\ell &= p_{12}^\ell
\end{aligned}$$

Now the final entropy of the auxiliary system

$$\frac{\Delta S_{aux}}{k} = -p_A \ln p_A - p_B \ln p_B$$

is lower than the increase that would have occurred based upon p_1 and p_2 , so we have reduced it's increase in entropy. However, now we still have a dissipation of

$$\frac{\Delta F_D}{kT} = -p_A \ln p_A^\ell - p_B \ln p_B^\ell \geq 0$$

notional free energy and an extraction of only

$$\frac{\Delta F_G}{kT} = p_A \ln \left(\frac{p_A^\ell}{p_A} \right) + p_B \ln \left(\frac{p_B^\ell}{p_B} \right)$$

so the gain in free energy is still less than the equivalent increase in entropy of the auxiliary.

In the special case where $p_{2b} = p_{12}^\ell = 0$, there is no overlap between Γ_1^ℓ and Γ_2^ℓ

It is important to note that the correlation between the auxiliary and the subensembles must be carefully controlled. If we have complete overlap in the final subspaces, then the operator U_1 , which maps Γ_1 onto Γ , will map Γ_2 onto a space which occurs with $p = 0$. If the auxiliary becomes correlated to the wrong subensemble, the conditional operation may attempt to apply U_1 to ρ_2 . Instead of extracting free energy, this will attempt to compress the system into a zero volume. This would require an infinite amount of work. Obviously this is not physically possible, and so would lead to the engine breaking down in some way. If there is any possibility of the auxiliary being in the wrong state, therefore, this imposes an additional constraint upon the unitary operations that may be conditionalised upon it. In the Szilard Engine, for example, this leads to the restriction on the four subspaces of the piston and weights, for U_{RES} in Equation 5.25.

8.1.5 Conclusion

We believe this has brought out one of the essential features of the general Maxwell's demon problem, and shown why it does not constitute a problem for the second law of thermodynamics. In essence, the problem arises from the increase in entropy that comes about when subensembles are mixed. The demon Maxwell proposed was able to examine each atom, and sort the ensemble into its subensembles. This reverses the entropy increase due to the mixing, in apparent violation of the second law of thermodynamics.

However, we have seen that this sorting cannot be implemented by any unitary operation acting only upon the space of the gas⁷. Instead, it must include an auxiliary system. This auxiliary system increases in entropy to match the decrease in entropy of the gas.

When we consider the change in free energy from mixing, we find the same problem. To extract the free energy from each subensemble, we must employ an auxiliary system, whose entropy increases in direct relation to the gain in free energy. For the Szilard Engine, this auxiliary system is clearly the piston system.

This completes the first stage of the resolution to the Maxwell's Demon problem. The 'measurement' of the system by the 'Demon' (or equivalently, the correlation of the auxiliary to the system) does not decrease entropy, as there is a compensating increase in entropy of the auxiliary system.

However, this does not constitute the whole resolution. In the Popper version of Szilard's Engine, there are also weights whose state is imperfectly correlated to the auxiliary state. This suggests that it is possible to imperfectly reset the auxiliary. Although we have shown that, in the case of the Popper-Szilard Engine, this resetting cannot succeed, we need to understand why such a resetting mechanism cannot succeed in general, and how this resetting relates to the $kT \ln 2$ energy that Landauer's Principle suggests is necessary to reset the state of the auxiliary.

⁷Maxwell argued that his demon proves the second law of thermodynamics cannot be derived from Hamiltonian mechanics. Clearly this is mistaken. The demon Maxwell envisages is able to violate the second law only because it is a non-Hamiltonian system.

8.2 Restoring the Auxiliary

We now must consider means by which the auxiliary system may be restored to its initial state. This would allow the system to continue extracting energy in cyclic process. For the Popper-Szilard Engine this involves attempting to reset the piston state by correlating it to the location of the two weights.

The essential point to note here is that it was necessary to include the quantum description of the weights as a thermodynamic system at some temperature T_W , rather than simply as a 'work reservoir'. Although we noted certain properties of the thermodynamic weight⁸, in Sections 6.3 and 7.1 that make the weight in a gravitational field a very convenient system to use as a 'work reservoir', our treatment of it was as an isothermal compression.

In the previous Section we showed how the correlation of an auxiliary could be used to extract work from the mixing free energy of the system. To complete the analysis we must also take into account the effect of this work on a second system, and the possible correlations this second system can have with the auxiliary.

First we will derive a general relation, which we will refer to as the 'fluctuation probability relation', which characterises the effect upon one system that can be achieved from a thermal fluctuation in a second. We will then apply this relation to the generalisation of the Popper-Szilard Engine. The fluctuation probability relation will be shown to govern the long term energy flows in such a way as to ensure that any attempt to reset the Engine must fail in exactly such a way as to ensure that the mean flow of energy is always in an entropy increasing direction. We will also show how, by performing work upon the system, the Engine can be made to operate without error, but only at the efficiency of the Carnot Cycle.

8.2.1 Fluctuation Probability Relationship

We will now calculate the key relationship governing the work that may be extracted from a thermal fluctuation. We must first discuss what we mean by a fluctuation within the context of the Gibbs ensemble. Generally, the equilibrium density matrix

$$\rho = \frac{e^{-i \frac{H}{\hbar T}}}{\text{Tr} \left[e^{-i \frac{H}{\hbar T}} \right]}$$

may be interpreted as the system being in one of the eigenstates of the Hamiltonian with probability

$$p_i = \frac{e^{-i \frac{E_i}{\hbar T}}}{\text{Tr} \left[e^{-i \frac{H}{\hbar T}} \right]}$$

and that contact with a heat bath at temperature T completely randomises the state of the system, on a timescale of order τ , the thermal relaxation time. The system jumps randomly between the available states. These are the thermal 'fluctuations'.

⁸The equivalence of perfect isolation, essential isolation and isothermal lifting, and also the constancy of entropy as it is raised

If we had a macroscopic system, we could partition the Hilbert space into macroscopically distinct subspaces. From the perspective of the Gibbs ensemble, this is the separation of the density matrix into subensembles

$$\rho = \sum_{\alpha} p_{\alpha} \rho_{\alpha}$$

where ρ_{α} is the equilibrium density matrix occupying the subspace and p_{α} is the probability that the system state is in the subspace.

For macroscopic systems, the majority of states will be in one large subspace, which will have approximately the same entropy as the ensemble. However, there will be some states in small subspaces that correspond to situations with lower entropy, such as the atoms of a macroscopic gas all located in one half of a room. At any point there will be a small probability that the thermal fluctuations will lead to such a subspace being occupied. As we have seen in Equation 7.7, these fluctuations will have a free energy given by

$$F_i = F - kT \ln p_i$$

If the fluctuation is very rare ($p_i \ll 1$) the increase in free energy will be large in comparison to *macroscopic* quantities.

For microscopic systems, such as the single atom Szilard Engine, the ensemble free energy may well be of the order of kT . If this is the case, reasonably common fluctuations may show an increase in free energy comparable to the free energy of the ensemble itself. We are now going to consider trying to harness this gain in free energy, and put it to use on some other system, such as by lifting a weight.

If we find a system at temperature T_1 in a subensemble which spontaneously occurs with probability p_1 , we can extract $-kT_1 \ln p_1$ work from allowing the subensemble to expand back to the equilibrium. We wish to use this work to perform some action upon a second system. If treat this as storing the energy in a work reservoir, such as a weight, we have noted this is exactly equivalent to isothermally compressing the second system (lifting the weight).

The free energy F_2^{θ} of the compressed state of the second system will differ from the free energy F_2 of it's original state by

$$F_2^{\theta} = F_2 - kT_1 \ln p_1$$

Now, we know that the second system will spontaneously occur in a fluctuation state with free energy F_2^{θ} with a probability p_2 , where

$$F_2^{\theta} = F_2 - kT_2 \ln p_2$$

and T_2 is the temperature of the second system.

The Fluctuation Probability Relation

Equating these we reach the essential result⁹ of this section, the fluctuation probability relation:

$$(p_1)^{T_1} = (p_2)^{T_2} \tag{8.4}$$

We are now going to examine a key consequence of this result:

$$p_1 > p_2$$

only if

$$T_1 > T_2$$

The probability of the second system to be spontaneously found in the desired state is less than the probability of the original fluctuation occurring, only if the second system is at a lower temperature.

Let us consider what this means. We have some system, at temperature T_2 , and we wish to perform some action upon it, that requires work. We wish to obtain this work from a thermal fluctuation in another system, at temperature T_1 .

Now, if $T_1 > T_2$, we could simply connect a heat engine between the two and reliably compress the second system without having to bother with identifying what fluctuations were occurring in system one (remember - although we are not considering it here, we will have to introduce an auxiliary system to determine which fluctuation has taken place in system one, and this auxiliary suffers an increase in entropy). Unfortunately, if system one is not at a higher temperature than system two, then the probability of system two spontaneously being found in the desired state is at least as high as the probability that the fluctuation occurs in system one.

The most effective way of obtaining a desired result from thermal fluctuations is to wait for the fluctuation to occur in the system of interest, rather than in any other system. Other systems will only give a higher probability of being able to achieve the desired result if they are at a higher temperature than the system of interest, and so can achieve the result more reliably by more conventional methods, and without involving auxiliaries. So the most effective means of boiling a kettle by thermal fluctuations is to unplug it and wait for it to spontaneously boil. This is an important result, which is perhaps not well appreciated. In [Cav90], for example, it is suggested that it may be possible to build a demon capable of

”violating” the second law by waiting for rare thermal fluctuations

while from the opposite point of view in [EN99] it is argued

⁹For the Popper-Szilard Engine, this gives us $P_1 = \left(\frac{1}{2}\right)^{(T_G/T_W)}$, which we saw in Chapter 6 was the key relationship in the failure of the Engine.

the result assures us that over the longer term, no . . . demon can exploit this fluctuation. But it can make no such assurance for the shorter term. Short term and correspondingly improbable violations of the Second Law remain.

The result we have obtained here suggests that there is nothing to be gained even from waiting for such improbable fluctuations to occur - as any objective we could achieve by exploiting such a rare fluctuation would be more likely to occur spontaneously than the fluctuation itself!

8.2.2 Imperfect Resetting

We will now combine the results just obtained, with those of Section 8.1. This will demonstrate the significance of the fluctuation probability relationship, completing our understanding of why the Popper-Szilard Engine must fail.

Let us recall some of the key features of the resetting of the piston in Chapter 5 and 6. There are two weights, but only one is raised, depending upon which side of the piston that the gas is initially located. This leaves a correlation between the position of the raised and unraised weights and the position of the piston. We attempted to make use of this correlation to reset the piston, but found that the thermal state of the weights themselves defeated this attempt. The result was that a mean flow of heat would occur only in the direction of hot to cold.

When work was extracted from the expansion of the subensemble it was assumed that this was simply absorbed by a suitable work reservoir, such as a raised weight. Note, however, that this raising of a weight can equally well be regarded as the isothermal compression of the weight system, once we take into account the fact that the weight must itself be at some temperature. Having noted that the raising of the weight may be regarded as an isothermal compression, we see that the fluctuation relation above applies and

$$(P_W)^{T_W} = (P_G)^{T_G}$$

For the Popper-Szilard Engine, $P_W = P_1$ and $P_G = \frac{1}{2}$. This leads directly to the relationship in Equation 6.12

$$P_1 = \left(\frac{1}{2}\right)^{\frac{T_G}{T_W}}$$

We saw in Section 6.7 that this equation plays the key role in ensuring that the mean flow of energy in the Popper-Szilard Engine is in an entropy increasing direction, regardless of the choice of T_W and T_G .

We must now try to understand how this relationship enters into the attempt to reset a general Maxwell Demon. The key is the additional feature that the arrangement of the weights makes to the standard Szilard Engine. This feature is that the work extracted from the gas is used to compress the weights in a *different* manner, depending upon which subensemble of the gas is selected. A different weight is lifted, depending upon which side of the piston the one-atom gas is located. This produces the correlation between weights and piston states at the end of the raising

cycle, and it is this correlation that enables an imperfect resetting to be attempted. We need to understand how the relationship between the fluctuation probabilities ensures that this correlation is just sufficiently imperfect to prevent a mean flow of energy from the colder to the hotter heat bath.

To do this we must add a second system, at a second temperature, to the analysis of Section 8.1. When the auxiliary draws energy from the expansion of the subensembles of the first system, it uses it to compress the second system in such a way that there is a correlation between the final state of the second system and the final state of the auxiliary. This correlation will be used to reset the state of the auxiliary, in an attempt to complete the engine cycle.

If the first system is at a higher temperature, we will see the auxiliary can be reset by a correlation to the compression of the second system, allowing the engine cycle to continue. However, this is a flow of energy from a hotter to colder heat bath, so is in an entropy increasing direction.

When the transfer of energy is in an anti-entropic direction, the correlation between the second system and the auxiliary will be shown to be imperfect. This leaves a mixture, whose entropy offsets the transfer of energy between the heat baths. If we attempt to reset the auxiliary imperfectly, the consequences of the resetting failing are determined by the unitarity of the evolution operators. It is shown that this leads inevitably to a reversal of the direction of operation of the engine.

We will calculate general expressions for the mean number of cycles the engine spends in each direction, and the mean energy transferred between the heat baths per cycle. This will allow us to show, quite generally, that the mean flow of energy will always be in an entropy increasing direction.

Expansion and Compression

We start with the system from which we wish to extract free energy. Assuming this system to be in thermal equilibrium at some temperature T_G , it's density matrix is separated into orthogonal subensembles

$$\rho_G = p_A \rho_{GA} + p_B \rho_{GB}$$

which have free energies which differ from the ensemble free energy by $kT_G \ln p_A$ and $kT_G \ln p_B$. We will not be assuming that the two subensembles occur with equal probability. This differs from the Szilard Engine, but is necessary to ensure the generality of the results.

To extract the maximum amount of free energy, we need to expand each subensemble to occupy the entire space, isothermally, leaving it in the state ρ_G . We use the energy extracted from this to compress a second system, at a temperature T_W (if $p_A \neq p_B$ then this second system will be compressed by different amounts). If the equilibrium density matrix of the second system is ρ_W , then ρ_{WA} and ρ_{WB} will represent the density matrices it is isothermally compressed into by ρ_{GA} and ρ_{GB} , respectively. From the fluctuation probability relationship, the ρ_{WA} and ρ_{WB} density matrices would occur *spontaneously* in ρ_W with probabilities $p_\alpha = (p_A)^\top$ and $p_\beta = (p_B)^\top$ where

$\tau = T_G/T_W$. We may write the initial density matrix of the second system in two different ways:

$$\begin{aligned}\rho_W &= p_\alpha \rho_{WA} + (1 - p_\alpha) \rho_{W\bar{A}} \\ \rho_W &= p_\beta \rho_{WB} + (1 - p_\beta) \rho_{W\bar{B}}\end{aligned}$$

As shown in Section 8.1 above, we must also employ an auxiliary system, which is initially in a state $|\pi_0\rangle \langle \pi_0|$. This system is required as the initially orthogonal states ρ_{GA} and ρ_{GB} cannot be mapped to the same space ρ_G , while extracting free energy. We cannot use the second system as the auxiliary, as we do not yet know if the states ρ_{WA} and ρ_{WB} can be made orthogonal. It is also helpful to regard the auxiliary as representing the state of the pistons, pulleys, and other mechanisms (such as demons and memory registers, if they are considered necessary) by which the subensembles of the first system are selected, and used to compress the second system.

The initial evolution of the system is from

$$\rho_1 = \{p_A \rho_{GA} + p_B \rho_{GB}\} \otimes \rho_W \otimes |\pi_0\rangle \langle \pi_0|$$

to

$$\rho_2 = \rho_G \otimes \{p_A \rho_{WA} \otimes |\pi_A\rangle \langle \pi_A| + p_B \rho_{WB} \otimes |\pi_B\rangle \langle \pi_B|\}$$

through intermediate stages

$$\rho_1^0 = p_A \rho_{GA}(Y) \rho_{WA}(Y) |\pi_A(Y)\rangle \langle \pi_A(Y)| + p_B \rho_{GB}(Y) \rho_{WB}(Y) \otimes |\pi_B(Y)\rangle \langle \pi_B(Y)|$$

where Y is a parameter varying from 0 to 1, and

$$\begin{aligned}|\pi_A(0)\rangle \langle \pi_A(0)| &= |\pi_B(0)\rangle \langle \pi_B(0)| = |\pi_0\rangle \langle \pi_0| \\ |\pi_A(1)\rangle \langle \pi_A(1)| &= |\pi_A\rangle \langle \pi_A| \\ |\pi_B(1)\rangle \langle \pi_B(1)| &= |\pi_B\rangle \langle \pi_B| \\ \rho_{GA}(1) &= \rho_{GB}(1) = \rho_G \\ \rho_{GA}(0) &= \rho_{GA} \\ \rho_{GB}(0) &= \rho_{GB} \\ \rho_{WA}(0) &= \rho_{WB}(0) = \rho_W \\ \rho_{WA}(1) &= \rho_{WA} \\ \rho_{WB}(1) &= \rho_{WB}\end{aligned}$$

In the process of this evolution, either $-kT_G \ln p_A$ or $-kT_G \ln p_B$ energy is drawn from a heat bath at T_G .

The Hilbert space Γ_G of the first system can be partitioned into complementary subspaces as

$$\begin{aligned}\Gamma_G &= \Gamma_{GA}(Y) \oplus \Gamma_{G\bar{A}}(Y) \\ &= \Gamma_{GB}(Y) \oplus \Gamma_{G\bar{B}}(Y)\end{aligned}$$

where $\Gamma_{GA}(Y)$ is the space occupied by the density matrix $\rho_{GA}(Y)$ etc.

The Hilbert space Γ_W of the second system has a more complicated partition. Let $\Gamma_{WA}(Y)$ be the subspace occupied by the density matrix $\rho_{WA}(Y)$, $\Gamma_{WB}(Y)$ the subspace occupied by $\rho_{WB}(Y)$ and $\Gamma_{WAB}(Y)$ is the subspace of the overlap between these two, then

$$\Gamma_W = \Gamma_{WA}^\emptyset(Y) \oplus \Gamma_{WB}^\emptyset(Y) \oplus \Gamma_{WAB}(Y) \oplus \Gamma_{W\overline{AB}}(Y)$$

where

$$\begin{aligned}\Gamma_{WA}(Y) &= \Gamma_{WA}^\emptyset(Y) \oplus \Gamma_{WAB}(Y) \\ \Gamma_{WB}(Y) &= \Gamma_{WB}^\emptyset(Y) \oplus \Gamma_{WAB}(Y)\end{aligned}$$

while $\Gamma_{W\overline{AB}}(Y)$ is the space occupied by neither density matrix. The complementary subspaces are

$$\begin{aligned}\Gamma_{W\overline{A}}(Y) &= \Gamma_{WB}^\emptyset(Y) \oplus \Gamma_{W\overline{AB}}(Y) \\ \Gamma_{W\overline{B}}(Y) &= \Gamma_{WA}^\emptyset(Y) \oplus \Gamma_{W\overline{AB}}(Y)\end{aligned}$$

When $Y = 1$ we will simply refer to Γ_{WA} , Γ_{WB} etc. Projectors onto the subspaces are denoted by P_{WA} , P_{GA} and so forth.

To ensure the isothermal expansion is optimal, the systems have internal Hamiltonians conditional upon discrete Y_n states of the auxiliary system

$$\begin{aligned}H_G &= \sum_n |\pi_A(Y_n)\rangle \langle \pi_A(Y_n)| \{H_{GA}(Y_n) + H_{G\overline{A}}(Y_n)\} \\ &\quad + |\pi_B(Y_n)\rangle \langle \pi_B(Y_n)| \{H_{GB}(Y_n) + H_{G\overline{B}}(Y_n)\} \\ H_W &= \sum_n |\pi_A(Y_n)\rangle \langle \pi_A(Y_n)| \{H_{WA}(Y_n) + H_{W\overline{A}}(Y_n)\} \\ &\quad + |\pi_B(Y_n)\rangle \langle \pi_B(Y_n)| \{H_{WB}(Y_n) + H_{W\overline{B}}(Y_n)\}\end{aligned}$$

where $H_{W\overline{A}}(Y_n)$ represents the Hamiltonian for the subspace $\Gamma_{W\overline{A}}$ (complementary to the subspace occupied by $\rho_{WA}(Y)$) and so on. When the auxiliary is in the state $|\pi_A(Y_n)\rangle \langle \pi_A(Y_n)|$, then transitions between states in $H_{GA}(Y_n)$ and states in $H_{G\overline{A}}(Y_n)$ are forbidden, and similarly for $H_{WA}(Y)$, $H_{GB}(Y)$ and $H_{WB}(Y)$. As compression and expansion takes place isothermally, the subensembles are equilibrium density matrices for their respective subspaces.

Perfect Correlation

If $T_G \geq T_W$ then

$$p_\alpha + p_\beta \leq 1$$

This means that Γ_{WA} and Γ_{WB} can be non-overlapping, so that $\Gamma_{WAB} = 0$, and the density matrices ρ_{WA} and ρ_{WB} can be orthogonal.

If we use a reset operation which includes

$$U_{r1} = |\pi_0\rangle \langle \pi_A| P_{WA} + |\pi_0\rangle \langle \pi_B| P_{WB} + \dots$$

where P_{WA} is the projector onto Γ_{WA} , and P_{WB} onto Γ_{WB} , then we can reset the auxiliary state to $|\pi_0\rangle \langle\pi_0|$ and begin a new cycle, with perfect accuracy.

Restoring the auxiliary will make the second system internal Hamiltonian $H_W(0)$, which has the equilibrium density matrix ρ_W . This leads to a dissipation of the notional free energy, $-kT_W \ln p_\alpha = -kT_G \ln p_A$ from ρ_{WA} , with probability p_A , and dissipation of $-kT_W \ln p_\beta = -kT_G \ln p_B$ from ρ_{WB} with probability p_B . The mean dissipation of notional free energy is then

$$Q = -kT_G(p_A \ln p_A + p_B \ln p_B)$$

which equals the heat drawn from the T_G heat bath. In other words, a quantity of heat Q can be reliably and continuously drawn from one heat bath at T_G and deposited at a colder heat bath at T_W . This simply represents a flow of heat from the hotter to the colder heat bath, and so presents no particular problem for thermodynamics.

Imperfect Correlation

We now turn to the more interesting case, where the second system, which is initially receiving energy, is at a higher temperature than the first system, $T_W > T_G$, and so

$$p_\alpha + p_\beta > 1$$

In this case the subspace occupied by ρ_{WA} and that occupied by ρ_{WB} will be overlapping. The projectors P_{WA} and P_{WB} in U_{r1} will not be orthogonal so the operation U_{r1} is no longer unitary.

To reduce the overlap, ρ_{WA} and ρ_{WB} should leave no portion of the Hilbert space unoccupied, so that $\Gamma_{W\overline{AB}} = 0$ and

$$\Gamma_W = \Gamma_{WA}^\circ \oplus \Gamma_{WB}^\circ \oplus \Gamma_{WAB}$$

The probabilities of an equilibrium density matrix ρ_W being found in these subspaces are p_α° , p_β° and $p_{\alpha\beta}$, with $p_\alpha^\circ + p_\beta^\circ + p_{\alpha\beta} = 1$, so that

$$\begin{aligned} \rho_W &= p_\alpha^\circ \rho_{WA}^\circ + p_\beta^\circ \rho_{WB}^\circ + p_{\alpha\beta} \rho_{WAB} \\ \rho_{WA} &= \left(1 - \frac{p_{\alpha\beta}}{p_\alpha}\right) \rho_{WA}^\circ + \left(\frac{p_{\alpha\beta}}{p_\alpha}\right) \rho_{WAB} \\ \rho_{WB} &= \left(1 - \frac{p_{\alpha\beta}}{p_\beta}\right) \rho_{WB}^\circ + \left(\frac{p_{\alpha\beta}}{p_\beta}\right) \rho_{WAB} \end{aligned}$$

Using $\tau = T_G/T_W$, the probabilities are related by

$$\begin{aligned} p_\alpha &= (p_A)^\tau \\ p_\beta &= (p_B)^\tau \\ p_{\alpha\beta} &= p_\alpha + p_\beta - 1 \\ p_\alpha^\circ &= p_\alpha - p_{\alpha\beta} = 1 - p_\beta \\ p_\beta^\circ &= p_\beta - p_{\alpha\beta} = 1 - p_\alpha \end{aligned}$$

Now, if the second system is located in either Γ_{WA}^θ or Γ_{WB}^θ , then there is a correlation between that system and the auxiliary system. The auxiliary system may be restored to its initial state $|\pi_0\rangle \langle\pi_0|$, by a correlated unitary operation.

However, if the second system is located in Γ_{WAB} , the auxiliary may be in either position, and there is no correlation. The resetting is now not possible. This is equivalent to the situation in the Popper-Szilard Engine when both weights are located above the shelf height.

As we can only unambiguously identify the state of the auxiliary from the state of the second system when the second system is located in a non-overlapping portion of the Hilbert space, we choose to reset the auxiliary when the second system is in Γ_{WA}^θ or Γ_{WB}^θ , but perform no resetting when the second system is in Γ_{WAB} . The conditional unitary operation for this is

$$U_{r2} = P_{WA}^\theta U_{RA} + P_{WB}^\theta U_{RB} + P_{WAB} U_{AB}$$

where P_{WA}^θ etc. are projection operators onto the relevant subspace of the second system, and the U_{RA} are unitary operators¹⁰ on the auxiliary space of the form

$$\begin{aligned} U_{RA} &= |\pi_0\rangle \langle\pi_A| + |\pi_A\rangle \langle\pi_0| + |\pi_B\rangle \langle\pi_B| \\ U_{RB} &= |\pi_0\rangle \langle\pi_B| + |\pi_B\rangle \langle\pi_0| + |\pi_A\rangle \langle\pi_A| \\ U_{AB} &= |\pi_0\rangle \langle\pi_0| + |\pi_A\rangle \langle\pi_A| + |\pi_B\rangle \langle\pi_B| \end{aligned}$$

When the second system can be reliably correlated to the state of the auxiliary, these operators will restore the auxiliary to its initial state. Following this, the notional free energy of the subensemble is dissipated, and a net transfer of heat from the T_G to the T_W heat bath has taken place. However, in those cases where the second system is found in Γ_{WAB} , the system has not been restored to its initial condition.

Raising Cycle

We can summarise the evolution so far, which we shall call the 'raising cycle' as it corresponds to the raising cycle of the Szilard Engine:

$$\begin{aligned} \rho_1 &= \rho_G \Pi_0 \rho_W = \{p_A \rho_{GA} + p_B \rho_{GB}\} \Pi_0 \rho_W \\ \rho_2 &= p_A \rho_G \Pi_A \rho_{WA} + p_B \rho_G \Pi_B \rho_{WB} \\ &= p_A \rho_G \Pi_A \left\{ \left(1 - \frac{p_{\alpha\beta}}{p_\alpha}\right) \rho_{WA}^\theta + \left(\frac{p_{\alpha\beta}}{p_\alpha}\right) \rho_{WAB} \right\} \\ &\quad + p_B \rho_G \Pi_B \left\{ \left(1 - \frac{p_{\alpha\beta}}{p_\beta}\right) \rho_{WB}^\theta + \left(\frac{p_{\alpha\beta}}{p_\beta}\right) \rho_{WAB} \right\} \\ \rho_3 &= \rho_G \Pi_0 \left\{ p_A \left(1 - \frac{p_{\alpha\beta}}{p_\alpha}\right) \rho_{WA}^\theta + p_B \left(1 - \frac{p_{\alpha\beta}}{p_\beta}\right) \rho_{WB}^\theta \right\} \\ &\quad + \rho_G \left\{ p_A \frac{p_{\alpha\beta}}{p_\alpha} \Pi_A + p_B \frac{p_{\alpha\beta}}{p_\beta} \Pi_B \right\} \rho_{WAB} \end{aligned}$$

¹⁰Similar to the U_{RES} in Section 5.5 there is some flexibility in the choice of U_{RA} , U_{RB} , and U_{AB} , so the ones chosen here are not the only ones possible. However, they are the simplest choice, and a more complicated expression would not essentially affect the outcome.

$$\begin{aligned} \rho_4 = & \left\{ p_A \left(1 - \frac{p_{\alpha\beta}}{p_\alpha} \right) + p_B \left(1 - \frac{p_{\alpha\beta}}{p_\beta} \right) \right\} \rho_G \Pi_0 \rho_W \\ & + \rho_G \left\{ p_A \frac{p_{\alpha\beta}}{p_\alpha} \Pi_A \rho_{WA} + p_B \frac{p_{\alpha\beta}}{p_\beta} \Pi_B \rho_{WB} \right\} \end{aligned}$$

The initial density matrix is ρ_1 , in equilibrium. The first stage correlates the auxiliary to the subensembles of system one, extracts free energy from their conditional expansion, and uses the same free energy to compress the second system. However, the compression of the second system is also conditional upon the auxiliary, so that at the end of the expansion-compression stage the auxiliary and the second system are correlated, in density matrix ρ_2 . An amount of heat equal to $Q = -kT_G (p_A \ln p_A + p_B \ln p_B)$ has been drawn from the T_G heat bath, and used to compress the second system.

The next stage uses the operator U_{r2} . This utilises the correlation between the auxiliary and the second system to restore the auxiliary to its initial state. When the second system is located in the Γ_{WAB} subspace, however, the imperfect correlation does not allow the auxiliary to be reset. The final state of the system is ρ_3 .

Finally, the contact with the T_W heat bath causes the second system subensembles to thermally expand throughout their accessible Hilbert space, leading to ρ_4 .

With a probability given by

$$p_C = \left\{ p_A \left(1 - \frac{p_{\alpha\beta}}{p_\alpha} \right) + p_B \left(1 - \frac{p_{\alpha\beta}}{p_\beta} \right) \right\}$$

the system will be ready to start another raising cycle. However, in the final line of ρ_4 we find that the system has a probability of not being restored, with probability

$$p_R = p_{\alpha\beta} \left(\frac{p_A}{p_\alpha} + \frac{p_B}{p_\beta} \right)$$

Lowering Cycle

We now need to consider what must happen to the unrestored system at the start of a new cycle. We must be very careful when doing this. As noted towards the end of Section 8.1, if the auxiliary is in the wrong state, the expansion/compression unitary operation may attempt to compress a density matrix into a zero volume. In such situations the operation of the engine would break down. Avoiding such situations occurring constrains the form of the operation upon the reversed cycle. We must always be sure that the energy extracted from one system is equal to the energy added to the other.

The conditional internal Hamiltonians H_G and H_W shows that the states consistent with the different positions of the auxiliary are

$$\begin{array}{ll} \rho_{GA} \Pi_0 \rho_W & \rho_{GB} \Pi_0 \rho_W \\ \rho_G \Pi_A \rho_{WA} & \rho_G \Pi_B \rho_{WB} \\ \rho_G \Pi_A \rho_{W\bar{A}} & \rho_G \Pi_B \rho_{W\bar{B}} \end{array}$$

The expansion/compression operation must map the space of $\rho_{GA}\Pi_0\rho_W$ to $\rho_G\Pi_A\rho_{WA}$ and $\rho_{GB}\Pi_0\rho_W$ to $\rho_G\Pi_B\rho_{WB}$. The states $\rho_G\Pi_A\rho_{W\bar{A}}$ and $\rho_G\Pi_A\rho_{W\bar{B}}$ are inaccessible, and would lead to a breakdown of the engine, should they occur.

The unitary operation for the expansion and compression phase must therefore map the space $\rho_G\Pi_A\rho_{WA}$ onto $\rho_{GA}\Pi_0\rho_W$ and $\rho_G\Pi_B\rho_{WB}$ onto $\rho_{GB}\Pi_0\rho_W$, and then allow ρ_{GA} and ρ_{GB} to dissipate into ρ_G (which corresponds to the piston being removed from the Szilard box) when the auxiliary system is reset. This is a 'lowering cycle' where the expansion of ρ_{WA} or ρ_{WB} is used to compress ρ_G , in a reverse direction to the 'raising cycle'.

The energy $Q_A = -kT_G \ln p_A$ is transferred to the first system, on a lowering A -cycle' and $Q_B = -kT_B \ln p_B$ on a 'lowering B -cycle'. If we follow the stages of the 'lowering A -cycle' for a system initially in state $\rho_G\Pi_A\rho_{WA}$ we have

$$\begin{aligned}\rho_1^0 &= \rho_G\Pi_A\rho_{WA} \\ \rho_2^0 &= \rho_{GA}\Pi_0\rho_W \\ &= \rho_{GA}\Pi_0 \{p_\alpha^0\rho_{WA}^0 + p_\beta^0\rho_{WB}^0 + p_{\alpha\beta}\rho_{WAB}\} \\ \rho_3^0 &= \rho_G \{p_\alpha^0\Pi_A\rho_{WA}^0 + p_\beta^0\Pi_B\rho_{WB}^0\} + p_{\alpha\beta}\rho_{GA}\Pi_0\rho_{WAB} \\ \rho_4^0 &= \rho_G \{p_\alpha^0\Pi_A\rho_{WA}^0 + p_\beta^0\Pi_B\rho_{WB}^0\} + p_{\alpha\beta}\rho_{GA}\Pi_0\rho_W\end{aligned}$$

These follow the same stages as the 'raising cycle' above. Initially, the density matrix ρ_1^0 compresses the first system, through the expansion of the second, leaving the system in state ρ_2^0 . Now we must apply the reset operation U_{r2} , which leaves the system in state ρ_3^0 . Finally, contact with the T_W heat bath leads to state ρ_4^0 .

Now the probability of a 'reversal' back onto the 'raising cycle' is $p_{\alpha\beta}$. For a system initially in $\rho_G\Pi_B\rho_{WB}$, the dissipation of ρ_{GB} to ρ_G between ρ_2^0 and ρ_3^0 leads to the same probability of reversing, only now starting the raising cycle on $\rho_{GB}\Pi_0\rho_W$.

This completes the optimal design for attempting to imperfectly reset the auxiliary system, using correlations with the second system, and the effect of the imperfect resetting. We have found that, quite generally, the same considerations that constrained the design of the Popper-Szilard Engine have arisen.

The compression of the second system, by expansion of subensembles in the first system, is governed by the fluctuation probability relation

$$(p_G)^{T_G} = (p_W)^{T_W}$$

When the flow of energy is in an anti-entropic direction, then $\tau = \frac{T_G}{T_W} < 1$. The compression of the second system is into subensembles $\rho_{W\alpha}$ which would spontaneously occur with probabilities $p_{W\alpha}$. This gives

$$\sum_{\alpha} p_{W\alpha} = \sum_{\alpha} (p_{G\alpha})^{\tau} > 1 \quad (8.5)$$

as $(p_{G\alpha})^{\tau} > p_{G\alpha}$ and $\sum_{\alpha} p_{G\alpha} = 1$. There must be overlaps between the compressed subensembles of the second system. Should the second system be in one of the non-overlapping regions of the

Hilbert space, then there will be a correlation between the auxiliary and the second system that allows the auxiliary to be reset. If, instead, the second system is located in one of the overlapping regions, then there is more than one auxiliary state possible, and a unitary resetting operation does not exist.

The imperfect correlations lead to a failure to reset the auxiliary, so we must consider the effect of starting a new cycle with the auxiliary in the other states. The constraints upon this is that the evolution of the system be described by a unitary operation and no work is performed upon the system. When the auxiliary has not been reset this forces the engine to reverse direction.

Average length of cycles

We have shown that the engine must switch between 'raising' and 'lowering' cycles. We now need to demonstrate that this switching will lead to a mean flow of heat in the entropy increasing direction. There are two factors which need to be evaluated to calculate this: the mean number of raising or lowering cycles before a reversal takes place, and the average amount of energy transferred per cycle.

The average length of a complete run of raising or lowering cycles is simply given by the reciprocal of the probability of it reversing. The total probability of reversal from a raising cycle is

$$\begin{aligned}
 P_R &= p_A \frac{p_{\alpha\beta}}{p_\alpha} + p_B \frac{p_{\alpha\beta}}{p_\beta} \\
 &= p_{\alpha\beta} \left(\frac{p_A}{p_\alpha} + \frac{p_B}{p_\beta} \right) \\
 &= ((p_A)^\tau + (p_B)^\tau - 1) \left((p_A)^{1-i\tau} + (p_B)^{1-i\tau} \right)
 \end{aligned}$$

while the probability of reversal from a lowering cycle is

$$\begin{aligned}
 P_L &= p_{\alpha\beta} \\
 &= ((p_A)^\tau + (p_B)^\tau - 1)
 \end{aligned}$$

The mean number of cycles for the raising and lowering cycles, N_R and N_L are then related by

$$N_L = \left((p_A)^{1-i\tau} + (p_B)^{1-i\tau} \right) N_R$$

This is the essential relationship between the relative temperatures of the systems, and the mean length of time spent on the raising and lowering cycles.

As $0 \leq 1 - \tau \leq 1$ then we have

$$1 \leq \left((p_A)^{1-i\tau} + (p_B)^{1-i\tau} \right) \leq 2$$

This produces the result that

$$N_L \geq N_R$$

so that the engine will, on average, spend more cycles transferring energy from the hotter to the colder heat bath, on the lowering cycle, than it will transferring energy in the from the colder to the hotter, on the raising cycle. The engine spends a proportion

$$\frac{N_L}{N_L + N_R} = \frac{(p_A)^{1/\tau} + (p_B)^{1/\tau}}{(p_A)^{1/\tau} + (p_B)^{1/\tau} + 1}$$

of the time on the lowering cycle, and the remaining

$$\frac{N_R}{N_L + N_R} = \frac{1}{(p_A)^{1/\tau} + (p_B)^{1/\tau} + 1}$$

of the time on the raising cycle. The limit that $T_G \approx T_W$ leads to $N_L = 2N_R$. This spends one-third of the time on a raising cycle, and two-thirds of the time on a lowering cycle. In the limit $T_G \ll T_W$, the engine approaches half the time on each cycle. Surprisingly, as the temperature difference increases, the proportion of the time on the anti-entropic cycle goes up. This is because with large temperature differences, both cycles are highly likely to go into reverse, until at the limit the auxiliary is never reliably reset and the engine switches with certainty between the two cycles.

It is interesting to note that if T_G is only slightly lower than T_W , the initial run of raising cycle can last for a very long time (both N_L and N_R become very large). However, the apparent entropy increase implied by this transfer of energy from the colder to the hotter is very small, precisely because the temperature difference is so small, and will be more than offset by the increase in entropy that comes about from the small probability of the cycle reversing, and the effect this has on the mixing entropy of the auxiliary system. Once a reversal has occurred, of course, the probability is that the Engine will stay on the lowering cycle, for an even longer period of time.

Mean energy per cycle

To complete the analysis, we must calculate the mean energy per cycle. It is not generally the case that the same mean amount of energy is transferred on a lowering cycle as on a raising cycle.

On a raising cycle, the mean energy transfer is

$$Q_R = -kT_G (p_A \ln p_A + p_B \ln p_B)$$

On a lowering A -cycle, the energy transfer is $Q_A = -kT_G \ln p_A$ and on a lowering B -cycle it is $Q_B = -kT_G \ln p_B$, but the probabilities of a lowering cycle being an A or B cycle are *not* p_A and p_B . The mean energy transfer will therefore be different to a raising cycle.

For the initial lowering cycle, which follows from a reversal from the raising cycle, the probabilities of the A or B cycles are

$$\begin{aligned} p_{A1} &= \frac{p_A \frac{p_{\alpha\beta}}{p_\alpha}}{p_A \frac{p_{\alpha\beta}}{p_\alpha} + p_B \frac{p_{\alpha\beta}}{p_\beta}} \\ &= \frac{p_A p_\beta}{p_A p_\beta + p_B p_\alpha} \end{aligned}$$

$$\begin{aligned}
&= \frac{(p_A)^{1_i \tau}}{(p_A)^{1_i \tau} + (p_B)^{1_i \tau}} \\
p_{B1} &= \frac{p_B \frac{p_{\alpha\beta}}{p_\beta}}{p_A \frac{p_{\alpha\beta}}{p_\alpha} + p_B \frac{p_{\alpha\beta}}{p_\beta}} \\
&= \frac{p_B p_\alpha}{p_A p_\beta + p_B p_\alpha} \\
&= \frac{(p_B)^{1_i \tau}}{(p_A)^{1_i \tau} + (p_B)^{1_i \tau}}
\end{aligned}$$

while a continuation of the lowering cycle will give probabilities

$$\begin{aligned}
p_{A2} &= \frac{p_\alpha^\theta}{p_\alpha^\theta + p_\beta^\theta} \\
p_{B2} &= \frac{p_\beta^\theta}{p_\alpha^\theta + p_\beta^\theta}
\end{aligned}$$

The mean energy transfer on the first lowering cycle is then

$$Q_1 = -kT_G (p_{A1} \ln p_A + p_{B1} \ln p_B)$$

and on subsequent lowering cycles

$$Q_2 = -kT_G (p_{A2} \ln p_A + p_{B2} \ln p_B)$$

To calculate the mean energy transfer, per cycle, over the course for a complete run of lowering cycles, we need to include both these results. Any run of lowering cycles starts with one Q_1 cycle. If it continues, with probability $(p_\alpha^\theta + p_\beta^\theta)$, then the mean energy per cycle after that is Q_2 . The probability of reversal is the same on all cycles, so, if we are given that it does continue beyond the Q_1 cycle, then the mean number of Q_2 cycles will be N_L . The mean energy transferred over the course of an entire run of lowering cycles will be

$$Q_1 + (p_\alpha^\theta + p_\beta^\theta) (N_L Q_2)$$

As the mean number of cycles is still N_L , the mean energy transfer, per cycle is

$$\begin{aligned}
Q_L &= \frac{Q_1 + (p_\alpha^\theta + p_\beta^\theta) (N_L Q_2)}{N_L} \\
&= p_{\alpha\beta} Q_1 + (p_\alpha^\theta + p_\beta^\theta) Q_2 \\
\frac{Q_L}{-kT_G} &= \left(p_{\alpha\beta} \frac{(p_A)^{1_i \tau}}{(p_A)^{1_i \tau} + (p_B)^{1_i \tau}} + p_\alpha^\theta \right) \ln p_A + \left(p_{\alpha\beta} \frac{(p_B)^{1_i \tau}}{(p_A)^{1_i \tau} + (p_B)^{1_i \tau}} + p_\beta^\theta \right) \ln p_B
\end{aligned}$$

which can be rearranged to give

$$Q_L = -\frac{kT_G ((p_A - p_B + (p_B)^{1_i \tau}) \ln p_A + (p_B - p_A + (p_A)^{1_i \tau}) \ln p_B)}{(p_A)^{1_i \tau} + (p_B)^{1_i \tau}}$$

Long Term Mean We are now in a position to complete the analysis of the mean heat flow for the imperfect resetting of the generalised Szilard Engine. The mean flow of energy, per cycle, from the T_G heat bath to the T_W heat bath is

$$\begin{aligned}
Q &= \frac{N_R Q_R - N_L Q_L}{N_R + N_L} \\
&= kT_G \frac{((p_B)^{1-i\tau} - p_B) \ln p_A + ((p_A)^{1-i\tau} - p_A) \ln p_B}{(p_A)^{1-i\tau} + (p_B)^{1-i\tau} + 1}
\end{aligned}$$

We know that $(1 - \tau) \leq 1$ so

$$(p_A)^{1-i\tau} > p_A$$

$$(p_B)^{1-i\tau} > p_B$$

The value of Q is always negative¹¹. The mean flow of energy must go from the hotter heat bath to the colder heat bath.

This generalises the conclusion to Chapters 5, 6 and 7 and is independant of any particular physical model. We have demonstrated that, even when we attempt to correlate an auxiliary to a second system, the correlation must always fail sufficiently often to prevent a long term anti-entropic energy flow.

Summary

We have seen that, when $T_G < T_W$ it is impossible to create a perfect correlation between the auxiliary and the subensembles of the T_W system. The requirement that the resetting operation be unitary then leads to the engine switching from a 'raising' to a 'lowering' cycle. However, this also leads to a 'lowering' cycle switching back to a 'raising' cycle.

The key result we have shown here, is that the engine must, in the long run, transfer more energy on the 'lowering' cycles, than on the 'raising' cycles. The reason for this lies in the average length of the cycles. On the entropic lowering cycle, the probability of reversal is

$$p_{\alpha\beta}$$

which comes from the subspace Γ_{WAB} , representing the overlap between the compressed subensembles. This is the probability of finding an equilibrium system in the overlap region, out of the entire Hilbert space Γ_W .

On the anti-entropic raising cycle, the probability of reversal depends upon which subensemble was selected. With probability p_A the subensemble was ρ_{GA} . In this case the reversal occurs if the second system is located within Γ_{WAB} , but now it is out of the compressed subspace Γ_{WA} . The probability

$$\frac{p_{\alpha\beta}}{p_\alpha}$$

must be higher than the probability of reversal from the raising cycle.

The same will be true had the subensemble selected been ρ_{GB} , which has probability $\frac{p_{\alpha\beta}}{p_\beta}$. Clearly, therefore, the mean reversal probability

$$p_A \left(\frac{p_{\alpha\beta}}{p_\alpha} \right) + p_B \left(\frac{p_{\alpha\beta}}{p_\beta} \right) = p_{\alpha\beta} \left(\frac{p_A}{p_\alpha} + \frac{p_B}{p_\beta} \right)$$

¹¹In the limit of $T_G \ll T_W$ the value approaches zero as the engine reverses between cycles with certainty

will always be at least as large as the reversal probability for the lowering cycle. It is therefore unavoidable that the engine will spend more time, in the long run, on the lowering cycles, and so will lead to a long term energy flow from the hotter to the colder heat bath.

8.2.3 The Carnot Cycle and the Entropy Engine

We saw that when $T_G \geq T_W$ there was a perfect correlation between the auxiliary and the second system, that could be used to perfectly reset the auxiliary. However, this only leads to a transfer of heat from the hotter to the colder heat bath.

In this Subsection we will see how we can extract work from the second system, before the auxiliary is reset, without losing the correlation. After the auxiliary is reset, we will discover that this leads to heat engine operating at Carnot Cycle efficiency. We will then apply the same method to the case where $T_G < T_W$. By performing work upon the second system, we will show that the imperfect correlation can be made perfect, allowing the auxiliary to be reset without error. Again, when we take the complete cycle of this, we will have a heat pump, operating at the Carnot Cycle efficiency, so we still will not have succeeded in violating the second law of thermodynamics. The resulting cycle is a form of the Entropy Engine considered in Appendix G.

$$T_G \geq T_W$$

As $p_\alpha + p_\beta \leq 1$ there is no overlap between the subspaces Γ_{WA} and Γ_{WB} , so we can write

$$\Gamma_W = \Gamma_{WA} \oplus \Gamma_{WB} \oplus \Gamma_{W\overline{AB}}$$

The space $\Gamma_{W\overline{AB}}$ represents an unoccupied portion of the Hilbert space. By allowing the second system to isothermally expand into this space, we can extract some energy as work, without creating an overlap and so without losing the correlation with the auxiliary.

To do this, the two subensembles ρ_{WA} and ρ_{WB} must isothermally expand to ρ_{WA}^{00} and ρ_{WB}^{00} respectively. These density matrices spontaneously occur with probabilities p_α^{00} and p_β^{00} in the equilibrium density matrix ρ_W .

Provided the expansion leaves $p_\alpha^{00} + p_\beta^{00} \leq 1$, we do not need to have any overlap between ρ_{WA}^{00} and ρ_{WB}^{00} , and we will still have perfect correlation with the auxiliary, and we will be able to reset the system. The expansion of the system has allowed us to extract some of the heat flow from the hotter to the colder bath, and turn it into useful work.

The most energy can be extracted, without allowing the density matrices to overlap, will be when $p_\alpha^{00} + p_\beta^{00} = 1$, so that

$$\rho_W = p_\alpha^{00} \rho_{WA}^{00} + p_\beta^{00} \rho_{WB}^{00}$$

After the second system expands and the auxiliary is reset, the second system density matrix is

$$\rho_W^{00} = p_A \rho_{WA}^{00} + p_B \rho_{WB}^{00}$$

The second system will then return to the equilibrium distribution ρ_W .

Using the results in Section 8.1, there is a dissipation of notional free energy into the T_W heat bath of

$$\frac{\Delta F_D}{kT_W} = -(p_A \ln p_\alpha^{00} + p_B \ln p_\beta^{00})$$

and mean work extracted of

$$\begin{aligned} \Delta F_G &= kT_W \left(p_A \ln \left(\frac{p_\alpha^{00}}{p_A} \right) + p_B \ln \left(\frac{p_\beta^{00}}{p_B} \right) \right) \\ &= -kT_G (p_A \ln p_A + p_B \ln p_B) + kT_W (p_A \ln (p_\alpha^{00}) + p_B \ln (p_\beta^{00})) \end{aligned}$$

The first term in this is simply the heat extracted from the T_G heat bath. The second term is the notional dissipation, and has a minimum value (subject to $p_\alpha^{00} + p_\beta^{00} \leq 1$) when $p_\alpha^{00} = p_A$, and $p_\beta^{00} = p_B$. This gives

$$\begin{aligned} \Delta F_G &\leq k(T_W - T_G) (p_A \ln p_A + p_B \ln p_B) \\ &\leq -S\Delta T \end{aligned}$$

where S is the mixing entropy transferred from the system at temperature T_G to the system at temperature T_W .

This gives a heat engine efficiency of

$$\frac{\Delta F_G}{Q} \leq 1 - \frac{T_W}{T_G}$$

which is in complete agreement with the efficiency of a Carnot cycle.

$T_G < T_W$

We will now use the same approach for the case where the first heat bath is colder than the second heat bath, and we have extracted energy from the colder system to compress the hotter system. As we saw above, the compression of the second system will lead to an imperfect correlation with the auxiliary, as there will be an overlap between the ρ_{WA} and ρ_{WB} density matrices.

To remove the overlap, we must compress ρ_{WA} and ρ_{WB} further, performing work upon the system, until they are no longer overlapping. This will allow us to reset the auxiliary system without error using U_{r1} above. This will lead to the density matrices ρ_{WA}^{00} and ρ_{WB}^{00} as before, only now, as $p_\alpha + p_\beta > p_\alpha^{00} + p_\beta^{00} = 1$, the mean work 'extracted'

$$\begin{aligned} \Delta F_G &= kT_W \left(p_A \ln \left(\frac{p_\alpha^{00}}{p_A} \right) + p_B \ln \left(\frac{p_\beta^{00}}{p_B} \right) \right) \\ &= -kT_G (p_A \ln p_A + p_B \ln p_B) + kT_W (p_A \ln (p_\alpha^{00}) + p_B \ln (p_\beta^{00})) \end{aligned}$$

is negative, and is least negative when $p_\alpha^{00} = p_A$ and $p_\beta^{00} = p_B$.

Re-expressing this as work, $W = -\Delta F_G$, required to pump heat $Q = -kT_G (p_A \ln p_A + p_B \ln p_B)$ from a heat bath at T_G to a hotter heat bath at T_W , we have

$$\frac{W}{Q} \geq \frac{T_W}{T_G} - 1$$

once again agreeing with the Carnot efficiency.

8.2.4 Conclusion

In Section 8.1 we examined how the mixing of subensembles lead to an increase in entropy, and corresponding reduction in free energy of the ensemble. We demonstrated that this loss of free energy is because of the restriction of unitarity upon the evolution operators. The optimal operations cannot be applied to their respective subensembles, as this would require mappings of orthogonal to non-orthogonal states. If an auxiliary system is introduced, the optimal operators can be applied, by a conditional interaction with the auxiliary system. However, this leads to a compensating increase of the entropy of the auxiliary system.

The two-weight Szilard Engine suggested that the work extracted from the subensembles could be used to correlate a second system to the auxiliary, and that this correlation could be used to reset the auxiliary, if imperfectly. However, it was found that the relationship $P_1 = \left(\frac{1}{2}\right)^{T_G/T_W}$ played a critical role, preventing the correlation from being sufficient to allow heat to flow in an anti-entropic direction. In this section we have examined the origin of this, in terms of the free energy subensemble formula (7.7)

$$F_i = F - kT \ln p_i$$

which leads to the probability fluctuation relationship (8.4)

$$(p_1)^{T_1} = (p_2)^{T_2}$$

This relationship plays a key role in preventing the violation of the statistical second law of thermodynamics. It is this relationship that ensures that correlations are imperfect when the heat flow would otherwise be anti-entropic. When we try to use an imperfect resetting, this relationship then also guarantees that the switching between raising and lowering cycles will always prefer the lowering cycle.

The fluctuation probability relationship also ensures that thermal fluctuations are ineffective as a means of performing work upon other systems. Any objective, such as boiling a kettle, that could be achieved through capturing a rare thermal fluctuation, will be more likely to occur spontaneously, by unplugging it and leaving it, or else could be achieved reliably without resort to fluctuations.

Finally, when we attempt to improve the correlation with the auxiliary, by performing work upon the second system, we find that we recover a heat pump or heat engine operating at the Carnot Cycle efficiency. It should be noted, however, that the cycle we have here is not the same as the phenomenological Carnot Cycle, using adiabatic and isothermal expansion and compression. At several stages in this cycle we find key thermodynamic concepts, such as the free energy, become undefined, as we have a correlated mixture of systems at different temperatures. In fact, we have here an example of the Entropy Engine, considered in Appendix G. The origin of the work extracted is the transfer of mixing entropy between systems at different temperatures.

8.3 Alternative resolutions

Having thoroughly investigated the physics of the quantum Szilard Engine, we now wish to re-examine the arguments and resolutions put forward by other authors, and explored in Chapter 4. We will use the simplest models possible to demonstrate how these relate to our own conclusions. We will find that, where these resolutions are not flawed, they are physically equivalent to some aspect of our resolution, and so represent only partial resolutions.

8.3.1 Information Acquisition

The first argument we will review will be that of Gabor and Brillouin. We will examine this because, although, in its information theoretic form, it is no longer supported, its physical basis has been defended by opponents of the resolution based upon Landauer's Principle. We will find that Gabor and Brillouin did make unnecessary assumptions in their analysis, and without these assumptions, their explanation of the resolution does not hold. It will be instructive to examine the basis of this when considering later arguments.

The key suggestion they made was that the demon was required "to make some physical means of distinguishing between the gas molecules" [DD85] and that this physical means of acquiring information inevitably lead to a dissipation of $kT \ln 2$ energy. In the context of Szilard's Engine, it was the demon using a light source to illuminate the location of the atom that would dissipate the energy. Brillouin went on to argue that each elementary act of information acquisition was associated with such a dissipation of energy.

If we start by considering the physical connection between the demon and the gas, we must consider three systems

- A gas, initially in a mixture of two subensembles $\rho_G = \frac{1}{2}(\rho_G(A) + \rho_G(B))$
- A physical connection (such as a photon), initially in the unscattered state $\rho_{Ph}(Un)$, but which will be scattered into a different state, $\rho_{Ph}(Sc)$, if the gas is in the particular subensemble $\rho_G(B)$.
- the demon, initially in state $\rho_D(A)$, but which will move into state $\rho_D(B)$ if it sees the photon in the scattered state.

The system is initially in the state

$$\rho_1 = \frac{1}{2}(\rho_G(A) + \rho_G(B))\rho_{Ph}(Un)\rho_D(A)$$

If the photon encounters the state $\rho_G(B)$, it is scattered into a new state, creating a correlation

$$\rho_2 = \frac{1}{2}(\rho_G(A)\rho_{Ph}(Un) + \rho_G(B)\rho_{Ph}(Sc))\rho_D(A)$$

and then the demon sees the photon, creating a correlation to its own state

$$\rho_3 = \frac{1}{2}(\rho_G(A)\rho_{Ph}(Un)\rho_D(A) + \rho_G(B)\rho_{Ph}(Sc)\rho_D(B))$$

Gabor and Brillouin now argue that the mean entropy of the gas has been reduced by a mean factor of $k \ln 2$ on the basis that the demon, by inspecting its own state, knows which of the subensembles the gas lies in. As a compensation, however, the energy of the scattered photon is dissipated. They then argue that the energy of the photon must be at least $kT \ln 2$, and this completes the entropy balance.

There are two assumptions that they must make for this argument to hold. Firstly, the demon must be able to identify the entropy reduction only when the photon is scattered, otherwise the entropy reduction would take place each time, while the dissipation of the photon energy takes place only on the 50% of occasions in which it is scattered. Secondly, the energy of the scattered photon must be dissipated.

There seems little real basis for either assumption. The demon's actions are determined by its state, so it can perform a conditional unitary operation upon the gas, to produce

$$\rho_4 = \frac{1}{2} \rho_G(A) (\rho_{Ph}(Un) \rho_D(A) + \rho_{Ph}(Sc) \rho_D(B))$$

reducing the entropy of the gas for either outcome. Secondly, there appears no reason why the detection of the scattered photon must be dissipative. A suitably quick and idealised demon could detect the photon through the recoil from its deflection from a mirror, rather than absorption by a photodetector, and by a rapid adjustment of the apparatus effect a conditional operation upon the photon to restore it to the unscattered state, giving

$$\rho_5 = \frac{1}{2} \rho_G(A) \rho_{Ph}(Un) (\rho_D(A) + \rho_D(B))$$

These operations are quite consistent with unitary evolution. The entropy of the gas has been reduced, and the photon energy has not been dissipated.

Finally, as the example of the piston in the Popper-Szilard Engine above shows, there is no necessary reason why a physical intermediary is even needed between the gas and the demon. The essential issue, as we have seen, is not the energy of the photon, but the fact that the demon itself, in ρ_5 , is described by a mixture, whose increase in entropy matches the reduction in entropy of the gas.

We will now examine the conceptual difficulties this brings, and where the error in thinking comes about. The problem lies in the interpretation of the density matrix of the demon. The demon, of course, does not regard itself as being in a mixture, as it should be quite aware that it is in either the state $\rho_D(A)$ or the state $\rho_D(B)$. This cuts to the heart of the statistical nature of the problem. The density matrix ρ_5 is interpreted as meaning that the state of the system, in reality, is either

$$\rho_5^\theta = \rho_G(A) \rho_{Ph}(Un) \rho_D(A)$$

or

$$\rho_5^{\theta\theta} = \rho_G(A) \rho_{Ph}(Un) \rho_D(B)$$

In each of these cases the entropy is reduced by $k \ln 2$ from its initial value.

The compensation is in the mixing entropy of the demon. However, if we interpret this mixing entropy as a measure of ignorance, we are left with the awkward fact that the demon is quite aware of it's own state. From the perspective of the demon, the entropy would have appeared to have decreased. Unfortunately the demon is simply a particularly efficient observer, and there is nothing in principle to stop us substituting a human being in it's place. This brings us right back to Szilard's original problem - that the intervention of an intelligent being, by making a measurement upon a system, appears to be able to reduce it's entropy.

The error lies in the fact that we have abandoned the ensemble, and with it the entropy of mixing, as soon as we correlate an intelligent being to the system. We are led into this error by the belief that the entropy of mixing represents ignorance about the exact state of a system, and an intelligent being is certainly not ignorant about it's own state. Thus we substitute for the ensemble density matrix ρ_5 the particular subensemble ρ_5^l or ρ_5^o that the intelligent being knows to be the case.

The flaw in this reasoning only comes about when we consider the future behaviour of the demon, and the requirement of unitarity, For example, we wish the demon to extract the energy from expanding the one atom gas, and then start a new cycle. If we think of the demon in state ρ_5^l , then it is a simple matter to construct a unitary operation that achieves this. The same holds true for ρ_5^o . The problem lies in the fact that these operations cannot be combined into a single unitary operation. The unitary operator to complete the cycle *must* be defined for the entire ensemble ρ_5 . By implicitly abandoning the description of the system in terms of ensembles, we are led to construct unitary operations that do not, in fact, exist. We will find ourselves returning to this point.

8.3.2 Information Erasure

We have found that, contrary to [DD85, EN99], Gabor and Brillouin do not provide a resolution to the problem. Information acquisition need not be dissipative. In this we are in agreement with Landauer [Lan61]. We must now examine how Bennett's resolution [Ben82] using Landauer's Principle of information erasure relates to our analysis. It will be shown that Bennett's analysis is a special case of the Entropy Engine discussed above in Section 8.2.3 and in Appendix G. It is therefore only a partial resolution.

Dispensing with the need for a physical intermediary between demon and system, we have the simple process

$$\begin{aligned}\rho_1 &= \frac{1}{2}(\rho_G(A) + \rho_G(B))\rho_D(A) \\ \rho_2 &= \frac{1}{2}(\rho_G(A)\rho_D(A) + \rho_G(B)\rho_D(B)) \\ \rho_3 &= \rho_G(A)\frac{1}{2}(\rho_D(A) + \rho_D(B))\end{aligned}$$

Bennett, in essence, accepts the argument that entropy represents ignorance and the demon has reduced the entropy of the system, as it is not ignorant of it's own state, but realises that the

future behaviour of the system depends upon the state the demon is left in. The cycle must be completed.

The two different states $\rho_D(A)$ and $\rho_D(B)$ are taken to represent the demon's own knowledge, or memory, of the measurement outcome. To complete the cycle, and allow the Engine to extract further energy, the demon must 'forget' this information. This will return the demon to its initial state and allow the cycle to continue. It is the erasure of the information, Bennett argues, that dissipates $kT \ln 2$ energy, and saves the second law of thermodynamics.

This dissipation is based upon Landauer's Principle, that the erasure of 1 bit of information requires the dissipation of $kT \ln 2$ energy. The basis of Landauer's Principle may be summarised as:

1. Information is physical. It must be stored and processed in physical systems, and be subject to physical laws.
2. Distinct logical states must be represented within the physical system by distinct (orthogonal) states.

from which it is derived that the erasure of one bit of logical information requires the dissipation of $kT \ln 2$ free energy, or work.

There is an additional assumption, which is physically unnecessary and usually unstated, which is also necessary to Landauer's Principle

3. The physical states that are used represent the logical states all have the same internal entropy, and mean energy.

and the denial of this forms the basis of Fahn's critique[Fah96]¹². Removing this assumption generalises the principle, and requires taking note of the thermodynamic expansion and compression between different states as part of the physical operations by which the logical states are manipulated. As the effect of this is only to make the relationship between information and thermodynamics more complex, we will adopt Assumption 3 as a simplification.

It is an immediate consequence of these assumptions that the physical storage of 1 bit of Shannon information requires a system to have $k \ln 2$ entropy. The reason for this is simple. 1 bit of Shannon information implies two logical states (such as true or false), occurring with equal probability, so that the Shannon information $I_{Sh} = \frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{2} \log_2 \frac{1}{2} = 1$. To store this in a physical system takes two orthogonal physical states, which will be occupied with equal probability, giving an ensemble mixing entropy of $S = k \left(\frac{1}{2} \ln \frac{1}{2} + \frac{1}{2} \ln \frac{1}{2} \right) = k \ln 2$. Now, to eliminate this bit, the logical state must be restored to a single state. The Shannon information of this is zero, and the mixing entropy is zero. As Assumption 3 requires the mean energy to be unaffected by this, a simple manipulation of the formula $E = F + TS$ demonstrates that the reduction of entropy by

¹²Fahn considers states with different entropies, but neglects the possibility of different energies. In other respects his resolution is equivalent to Bennett's.

$k \ln 2$ required to 'erase' the bit of information isothermally requires $kT \ln 2$ work to be done upon the system.

In this there is nothing controversial about Landauer's Principle. However, it clearly rests upon the assumption that the second law of thermodynamics is valid, which was precisely the point at issue. To examine the Principles's relevance to the Szilard engine we must consider how the erasure is to be achieved. Our demon will be identified with the piston state, extracted from the box in a mixed state.

As shown in Appendix G, there is a procedure by which the piston may be restored to it's original state. This is equivalent to inserting the piston into a second Szilard box at some 'erasure' temperature T_E . This corresponds to the piston alternating between a raising cycle, at temperature T_G and a lowering cycle at temperature T_E . The work extracted from the T_G heat bath on the raising cycle is $kT_G \ln 2$, and the work dissipated into the T_E heat bath is $kT_E \ln 2$. There is an entropy increase of $k \ln 2$ in the T_E heat bath, and decrease of $k \ln 2$ in the T_G heat bath. It should be immediately apparent that this reversible cycle is equivalent to a Carnot cycle, with efficiency

$$\frac{W}{Q} = 1 - \frac{T_E}{T_G}$$

Whether this cycle is acting as a heat pump or a heat engine naturally depends upon which of T_E or T_G is the hotter.

Bennett assumes that the second heat bath is at $T_E = T_G$, so the system acts as neither pump nor engine - the work extracted from the raising cycle is used up on the lowering cycle. This cycle is clearly the same as the Entropy Engine considered in Section 8.2.3 and Appendix G, when restricted to the case $T_W = T_G$. Removing this restriction, the Engine operates at a Carnot cycle efficiency.

It is nevertheless operating on a quite different principle to the more standard Carnot engine, which is based upon the isothermal and adiabatic compression and expansion of a gas. No heat energy actually flows directly between the two heat baths. Rather, it is the piston (or 'demon') that transfers $S = k \ln 2$ entropy through a temperature difference of $\Delta T = T_G - T_E$, and produces the characteristic gain in free energy, $\Delta F = -S\Delta T$.

To obtain this gain, the temperature of erasure must be different to the temperature at which the free energy is extracted from the Szilard Box. This raises an issue that is not often addressed by the information theoretic analysis of Maxwell's demon and thermodynamics - there is no relationship between the entropy involved in information storage and manipulation, and thermodynamic temperature. Although Landauer's Principle is framed in terms of an isothermal erasure process, such as that used for the Szilard box above, the discussion of the 'fuel value' of blank tapes [Ben82, Fey99] rarely makes clear how this temperature is to be identified, as a purely information theoretical blank tape has no temperature associated with it. For example, if we represent the states by the spin up and spin down states of an array of electrons, and there is no magnetic field, then all possible logical states have the same energy, and the temperature is undefined. By

emphasising the role of information, the additional role of temperature has been missed. An exception is Schumacher[Sch94] whose information theoretic heat engine may be compared to the more physically explicit arrangement considered here.

The information erasure argument can now be seen to be insufficient to produce a complete resolution, and unnecessary even where it is valid. It's physical basis is sound, but it is not general enough, and information theory is not necessary to understand it once the physical principles are correctly understood.

Let us examine how it works as a resolution. First, we create the problem by abandoning the ensemble of the states of the auxiliary system. Then we characterise the different auxiliary states as information. To quantify the information, however, we must use the Shannon formula, and this just reintroduces the ensemble we abandoned. We then try to connect the Shannon information back to thermodynamics by appealing to the Landauer Principle, which is itself derived from an assumption that the second law of thermodynamics is universally valid. Had we not abandoned the ensemble of auxiliary states in the first place, no reference to information would have been necessary.

Finally, we note that information erasure has nothing to say about the imperfect resetting considered in Section 8.2.2, and so, as it does not apply to the Popper-Szilard Engine, it is also insufficient to completely resolve the paradox.

8.3.3 'Free will' and Computation

There have recently been criticisms of the information erasure resolution by Earman and Norton [EN98, EN99], and by Shenker[She99]. Although we agree with the general tenor of both papers, we believe that, unfortunately, both of them misunderstand the nature of the Bennett-Landauer resolution. This leads them to suspect that there are faults to be uncovered in the Landauer principle, and to suggest that the true resolution should be found in thermal fluctuations, with a similar physical basis to Gabor and Brillouin's work, but that these fluctuations need not be interpreted in any information theoretic manner. Thus, in Earman and Norton we read

[Bennett's] devices can only succeed in so far as we presume that they are not canonical thermal systems. Thus Bennett's logic is difficult to follow. Landauer's Principle is supported by arguments that require memory devices to be canonical thermal systems, but Szilard's Principle is defeated by the expedient of ignoring the canonical thermal properties of the sensing device.

and in Shenker

[The resolution] sacrifices basic ideas of statistical mechanics in order to save the Second Law of Thermodynamics. Szilard and his school claim that if we add the dissipation ... then the Demon *never* reduces the entropy of the universe ... This way the Second Law is invariably obeyed. The principles of statistical mechanics, however,

are violated. According to these principles, entropy can decrease as well as increase, with some non-zero probability.

Thermal Fluctuations

It is unclear what Earman and Norton mean when they suggest Bennett ignores 'canonical thermal properties of the sensing device'. It is clearly the case that the auxiliary starts in only one of the states that is possible, so is not in a full thermal equilibrium. However, this depends upon the thermal relaxation times. There is no reason why selecting systems with large thermal relaxation times, for transitions between some subspaces, and preparing them initially in one of the subspaces, does not constitute a 'canonical thermal system', or that use of such a system is illegitimate.

In [EN99][Appendix 1] they claim to present a resolution, equivalent to information theoretic arguments, in terms of thermal fluctuations. However, their analysis rests upon the two equations

$$\begin{aligned} S[O, D] &= S[O] + S[D] \\ \Delta S &= 0 \end{aligned}$$

where $S[O]$ is the entropy of the object subsystem and $S[D]$ is the entropy of the demon. From this they deduce $\Delta S[D] = -\Delta S[O]$ and conclude that, as the entropy of the system is reduced by the measurement, the entropy of the demon must have increased.

The problem with this analysis is that these equations are simply wrong when applied to correlated systems. The correct equation is given in Equation 2.5 as

$$S^\theta[O, D] = S[O] + S[D] + S[O : D]$$

where $S[O : D]$ is the correlation between the subsystems. The value of S^θ will be constant, while Earman and Norton's S will increase by $k \ln 2$ when the demon measures the state of the gas, then *decrease* by the same amount when the demon uses this correlation to change the state of the gas. Thus Earman and Norton's argument that

A demon closing the door at this moment has effected a reduction in entropy. $[\Delta S[O] = -\Delta S[D]]$ assures us that this reduction must be compensated by a corresponding dissipation of entropy in the demonic system

is incorrect, and it is unsurprising they are unable to offer an account of how this dissipation occurs. While it is true that an increase in entropy of the demon system takes place, it does not do so for the reason, or in the manner that Earman and Norton appear to think.

Earman and Norton proceed to suggest that, if the demon can non-dissipatively measure the location of the atom in the box, then an erasure *can* take place non-dissipatively, allowing the second law to be violated. As this criticism would seem to be applicable to our analysis of the Szilard Engine above, we must consider it carefully below. It will be useful to examine Shenker's arguments first, though.

Free Will

Shenker presents a different resolution, based upon the issue of whether the demon may be considered to have 'free will'. If we strip this of its philosophical connotations, we find that the specific property Shenker makes use of is more or less equivalent to the absence of 'self-conditional' operations in unitary dynamics, and that this is the same reason why Earman and Norton's suggestion fails. Specifically, she refers to

a system has free will if it is capable of choosing and controlling its own trajectory
in the state space

Now, to represent this in terms of unitary dynamics this would correspond to an operation where

$$\begin{aligned} U|0\rangle &= |0\rangle \\ U|1\rangle &= |0\rangle \end{aligned}$$

and we have seen before, this is not a unitary operation. It will be useful now to elaborate this with the help of the conditional dynamics on an auxiliary system

$$\begin{aligned} U_a &= |\pi_1\rangle \langle \pi_0| P_0 + |\pi_0\rangle \langle \pi_0| P_1 \\ &\quad + |\pi_0\rangle \langle \pi_1| P_0 + |\pi_1\rangle \langle \pi_1| P_1 \\ U_b &= \Pi_0 U_1 + \Pi_1 U_2 \end{aligned}$$

with P_0 and P_1 are projectors on the system of interest, Π_0 and Π_1 are projectors onto the states of the auxiliary system, and $U_1 = |1\rangle \langle 0| + |0\rangle \langle 1|$, $U_2 = |1\rangle \langle 1| + |0\rangle \langle 0|$.

The system is initially in the state $\rho = \frac{1}{2}(P_0 + P_1)$ and the auxiliary is in the state Π_0 . The auxiliary examines the object, and goes into a correlated state. It then refers to its own state and sets the object system to P_0 . As noted before, this conditional operation leaves the auxiliary system in a higher entropy state, which compensates for the manner in which the entropy of the system of interest has been reduced.

Shenker's characterisation of the absence of 'free will' amounts to the statement that a system cannot refer to its own state to reset itself. A unitary operation cannot be conditionalised upon the state of the system it acts upon. There are no 'self-conditional' unitary interactions. If we attempt to construct such an operator, we must identify the auxiliary with the system of interest. Terms such as $|\pi_1\rangle \langle \pi_0| P_0$ would 'collapse' as the operators act upon each other. Even assuming such a 'collapse' is well defined, the two conditional operators would become operators such as

$$\begin{aligned} U_a^\theta &= |1\rangle \langle 0| + |1\rangle \langle 1| \\ U_b^\theta &= |1\rangle \langle 0| + |0\rangle \langle 0| \end{aligned}$$

neither of which are unitary. A system which could exercise 'free will', in this sense, would be able to violate the second law of thermodynamics by resetting its own state.

However, this is not the whole story. In [ZZ92], it is demonstrated that there are classical, deterministic systems which can be rigorously entropy decreasing. None of the elements in the system can be regarded as exercising 'free will' in Shenker's terminology. Nevertheless, the second law of thermodynamics is broken. The reason for this is that the forces considered in [ZZ92] are Non-Hamiltonian. This is equivalent to a form of non-unitary dynamics in quantum theory. In [Per93, Chapter 9] Peres shows how such a non-unitary modification to quantum theory will also lead to situations where entropy can decrease. Clearly, the absence of free will is not enough to completely resolve the problem.

Computation

Earman and Norton argue that a computer resetting non-dissipatively should be possible. Their argument turns upon the fact that there exists a non-dissipative program by means of which a bit may be switched from one state to the other. This is simply the operation U_1 . There is a second program, represented by operation U_2 which leaves the bit unchanged. Neither of these operations are dissipative. They now propose a program in which the bit is used to store the location of the atom in the Szilard Engine. The computer then goes into one of two subprograms, depending upon the state of the bit, which extracts the energy from expanding the state of the atom.

Programme-L leaves the memory register unaltered [U_2 is applied] as it directs the expansion that yields a net reduction of entropy. Programme-R proceeds similarly. However, at its end Programme-R resets the memory register to L [U_1 is applied]. This last resetting is again not an erasure.

The flaw is that the choice of whether to execute Programme-R or Programme-L (which are, of course, just unitary operations), is made by a unitary operation that must be conditionalised upon the state of the memory register itself. As we have seen, such an operation *cannot* include the U_1 or U_2 operations, as this would be a 'self-conditionalisation' and would result in a non-unitary operation. A similar confusion affects their later argument, where they combine several Szilard Engines, and attempt to extract energy only when 'highly favourable' (and correspondingly rare) combinations of atom positions occur. In this argument, they propose to only perform the 'erasure' when those favourable combinations occur, thereby incurring a very small mean erasure cost. Again, however, the choice of whether to perform the 'erasure' operation or not cannot be made conditional upon the state of the very bit it is required to erase, and their argument fails. This is not some "details of computerese", but due to the requirement that the evolution of any system be described by a unitary operation.

8.3.4 Quantum superposition

We now return to the quantum mechanical arguments put forward by Zurek[Zur84] and Biedenharn and Solem[BS95]. They argue that the gas, being in a quantum superposition of both sides of the

partition, exerts no net pressure upon the piston, and so the piston cannot move until the gas is localised by a quantum measurement by the demon. Clearly, the piston arrangement considered in Chapters 5 and 6 provides a decisive counterexample to this argument. In fact, as we have argued in Section 5.3.3, the opposite conclusion, that the piston must move, can be reached purely from consideration of the linearity of quantum evolution.

However, it is now possible, and informative, to consider how such a mistake could have been made. We believe that the reason for this can be understood from the discussion of Section 8.1. This mistake, we will find, has been at the heart of much of the confusion surrounding the operation of the Szilard Engine, applies to the classical as well as the quantum description and is responsible for making the information theoretic analysis seem more plausible. By removing this mistake, we can even apply this analysis of the Szilard Engine to the expansion of a macroscopic N-atom gas, and we will find the same issues are raised, and resolved, as for the one atom gas.

We start with the Hamiltonian in Section 5.1, with an infinitely high potential barrier. We now consider a modification of this Hamiltonian, with the potential barrier displaced by a distance Y

$$H^0(Y)\Psi_n = \left(-\frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} + V^0(x, Y) \right) \Psi_n$$

with

$$V^0(x, Y) = \left\{ \begin{array}{ll} \infty & (x < -L) \\ 0 & (-L < x < Y - d) \\ \infty & (Y - d < x < Y + d) \\ 0 & (Y + d < x < L) \\ \infty & (x > L) \end{array} \right\}$$

The eigenstates of this gas are the same as the internal eigenstates of the gas, with a piston located at position Y , denoted by $|\Psi_l^\lambda(Y)\rangle$ and $|\Psi_l^\rho(Y)\rangle$, for states located entirely to the left or right of the partition, respectively. The density matrix of the gas with $Y = 0$ is

$$\begin{aligned} \rho_{P0} &= \frac{1}{2} (\rho^\lambda + \rho^\rho) \\ \rho^\lambda &= \frac{1}{Z_{P0}} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} |\Psi_l^\lambda(0)\rangle \langle \Psi_l^\lambda(0)| \\ \rho^\rho &= \frac{1}{Z_{P0}} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} |\Psi_l^\rho(0)\rangle \langle \Psi_l^\rho(0)| \\ Z_{P0} &= \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{1-p} \right)^2} \end{aligned}$$

If we now consider $H^0(Y)$ as a time dependant Hamiltonian, with a changing parameter Y , we can apply the analysis of Section 6.2 to the movement of the potential barrier, rather than the movement of the piston (this will involve ignoring or suppressing the piston states where they occur). As Y moves, the density matrix ρ_{P0} will evolve into

$$\begin{aligned} \rho_{P1}^\theta(Y) &= \frac{1}{Z_{P1}^\theta} \left\{ \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \right. \\ &\quad \left. + e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} |\Psi_l^\rho(Y)\rangle \langle \Psi_l^\rho(Y)| \right\} \end{aligned}$$

$$Z_{P1}^0 = \sum_l \left\{ e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} + e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} \right\}$$

This is a significantly different density matrix to the density matrix the gas evolves into when the moveable piston is present. If we trace out the weight and piston states from $\rho_{T1}(Y)$ in Equation 6.14, we find

$$\begin{aligned} \rho_{P1}(Y) &= \frac{1}{Z_{P1}} \left\{ \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \right. \\ &\quad \left. + e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} |\Psi_l^\rho(Y)\rangle \langle \Psi_l^\rho(Y)| \right\} \\ Z_{P1} &= \sum_l \left\{ e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} + e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} \right\} \end{aligned}$$

Let us consider the behaviour of ρ_{P1}^0 , supposing Y has moved to the right. The $|\Psi_l^\lambda(Y)\rangle$ states will have expanded, giving up energy as before, through pressure exerted upon the potential barrier (this energy must be absorbed by a work reservoir, as before). However, the $|\Psi_l^\rho(Y)\rangle$ states have been compressed, which requires energy to be extracted from the work reservoir. The pressure from the left is $-\frac{kT_G}{Y+1-p}$ and that from the right $-\frac{kT_G}{Y-1+p}$, giving a mean pressure on the co-ordinate Y of

$$P_{P1}^0 = -kT_G \left(\frac{Y}{Y^2 - (1-p)^2} \right)$$

Now, this pressure is zero when $Y = 0$, is positive (pushing in the positive Y direction) when Y is negative and vice versa. This appears to be a restoring force, which if applied to a piston, would keep it located in the center! Yet we saw from $\rho_{T1}(Y)$ that the piston moves.

The reason for this apparent paradox is that Y is used quite differently in $\rho_{P1}^0(Y)$ compared to $\rho_{P1}(Y)$. In $\rho_{P1}(Y)$, for the wavefunctions on the right of the piston Y represents the piston at a position $-Y$. The result of this change of sign is that, when the pressure exerted upon the moving piston is calculated from $\rho_{P1}(Y)$, it is always in the direction of increasing Y (which for the gas on the right represents $-Y$ becoming more negative). The freely moving piston represents a physically very different situation to the constrained potential barrier.

Let us consider the difference between the two situations. The density matrices are represented by

$$\begin{aligned} \rho_{P1}(Y) &= \frac{1}{2} \rho^\lambda(Y) + \frac{1}{2} \rho^\rho(-Y) \\ \rho_{P1}^0(Y) &= \frac{1}{2} \rho^\lambda(Y) + \frac{1}{2} \rho^\rho(Y) \\ \rho^\lambda(Y) &= \frac{1}{Z^\lambda(Y)} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} |\Psi_l^\lambda(Y)\rangle \langle \Psi_l^\lambda(Y)| \\ Z^\lambda(Y) &= \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y+1-p} \right)^2} \\ \rho^\rho(Y) &= \frac{1}{Z^\rho(Y)} \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} |\Psi_l^\rho(Y)\rangle \langle \Psi_l^\rho(Y)| \\ Z^\rho(Y) &= \sum_l e^{j \frac{\epsilon}{kT_G} \left(\frac{2l}{Y-1+p} \right)^2} \end{aligned}$$

Note that $\rho_{P1}(0) = \rho_{P1}^{\ell}(0) = \rho_{G1}$, so the system starts in equilibrium

We represent the unitary evolution operator associated with $H^{\theta}(Y)$ where Y is moving slowly to the right by U_R and where Y is moving slowly to the left by U_L . Now U_R is the optimum operator for extracting energy from $\rho^{\lambda}(Y)$, while U_L is the optimum operator for extracting energy from $\rho^{\rho}(Y)$. As discussed in Section 8.1, these cannot be combined into a single operator. The application of either U_R or U_L to ρ_{G1} will lead to $\rho_{P1}^{\theta}(Y)$. This is not the equilibrium distribution that would be reached had we started by inserting the potential barrier at Y .

The equilibrium distribution of $\rho^{\lambda}(Y)$ and $\rho^{\rho}(Y)$ is

$$\rho(Y) = p_1^{\ell} \rho^{\lambda}(Y) + p_2^{\ell} \rho^{\rho}(Y)$$

where $p_1^{\ell} + p_2^{\ell} = 1$, but $p_1^{\ell} \neq \frac{1}{2}$ unless $Y = 0$. This evolution moves the density matrix away from equilibrium. As was shown in Section 8.1, this requires a mean work expenditure. Note, however, that this work expenditure is only expressed as an average. We are still able to regard this as gaining energy on some attempts, but losing more energy on others.

In order to gain energy reliably, we must employ an auxiliary system, and correlate this to the application of U_R or U_L , depending upon the location of the one atom gas. This leads to the density matrix of the gas to become $\rho_{P1}(Y)$, instead of $\rho_{P1}^{\theta}(Y)$. The mistake is to assume that this auxiliary requires the act of observation by an external 'demon'. As we have noted, the piston itself constitutes an auxiliary system, so no external observer is required to 'gather information'.

The conditionalisation of the evolution operator upon the piston is related to the conditionalisation of the internal Hamiltonian of the gas. The constrained potential barrier Hamiltonian breaks down into right and left subspaces $H^{\theta}(Y) = H^{\lambda}(Y) \oplus H^{\rho}(Y)$, between which there are no transitions, with Y as the externally constrained parameter. The internal Hamiltonian for the gas, when the piston is taken into account, however, is always a conditional Hamiltonian

$$H = \sum_n \Pi(Y_n) (H^{\lambda}(Y_n) \oplus H^{\rho}(Y_n))$$

where $\Pi(Y_n)$ are projectors on the position of the piston.

If we demand that the position of the piston is an externally constrained parameter, then we find that [Zur84, BS95] would be correct. Nonetheless, this is not a quantum effect, *as the same result would also hold for a classical one-atom gas*. Thus, even to the extent to which their contention is true, it is nothing to do with quantum superpositions. However, the most important conclusion is that this demand is simply unreasonable. It does not correspond to any standard practice in thermodynamics. This point Chambadal[Cha73] argues is the key error in the 'paradox' of the Szilard Engine

In all piston engines work is supplied by the movement of a piston under the action of an expanding fluid. Here, though, it is the operator who displaces the piston... It is clear that this strange mode of operation was imagined only to make it necessary to have information about the position of the molecule.

It is hard to disagree with this sentiment¹³. In fact, we can now go further and consider how this 'mode of operation' would affect an N-atom gas. Let us examine the situation where $\rho_N^\lambda(Y)$ corresponds to N atoms confined to the left of a piston at Y, and $\rho_N^\rho(Y)$ with them confined to the right. Obviously such a situation would not be likely to arise from the insertion of a piston into an N-atom gas, but we can still consider a situation where there are two boxes, one of which encloses a vacuum, and one contains an N-atom gas, and some randomising process in the stacking of the boxes makes it equally likely which box contains the gas.

In an ensemble of such situations, the mixing entropy is still $k \ln 2$. If N is large, this will be negligible compared to the entropy of the gas. It is unsurprising that this negligible mixing entropy will pass unnoticed by macroscopic experiments. However, if we wish to place the two boxes side by side, and replace their shared wall with a moveable piston, we can extract energy of expansion by connecting the piston to some arrangement of weights, similar to that considered for the Popper-Szilard Engine. No-one, under such circumstances, could seriously believe that the piston would not move, without an external observation to determine on which side of the piston the N-atom gas is located, or that an operator is required to know in which direction the piston should be moved¹⁴. The 'strange mode of operation' is seen to be quite unnatural and unnecessary.

Nevertheless, if we consider the work we gain from the expansion, $NkT \ln 2$, and the change in entropy of the gas $\Delta S = (N - 1) k \ln 2$, we find we have gained the tiny amount $kT \ln 2$ more than we should have done. No information gathering of any kind has taken place, and no observation was necessary. The reason for this gain is that the mixing entropy of $k \ln 2$ has been eliminated from the gas. However, the piston is now in a mixture of states, having increased its own entropy by $k \ln 2$. As this is a negligible quantity, compared to the dissipation of macroscopic processes, it would naturally seem a simple matter to restore the piston to its original condition (though, of course, with an N-atom gas, one could not start a new cycle by re-inserting the piston). In fact such a restoration requires some compression of the state of the piston as its entropy must decrease by $k \ln 2$, and so requires some tiny compensating increase in entropy elsewhere. No paradox would ever be noticed for such macroscopic objects, as both the free energy gain, and entropy increase are negligible.

Nevertheless, the situation is otherwise identical, in principle, to the Szilard Engine. No-one, we hope, would suggest that the most sensible resolution is that $k \ln 2$ information must be gathered about the location of the N-atom gas, by some dissipative process, before the expansion can take place, or that thermal fluctuations in the piston prevent its operation! If such interpretations seem absurdly contrived in the N-atom case, they should be regarded as equally contrived in the single atom case.

¹³Although we must then disagree with Chambadal's conclusion that work can be continuously extracted from the Engine.

¹⁴Or even worse, Biedenharn and Solem's suggestion that an observation may be required to 'localise' the N-atom gas to one side or the other, and that this 'observation' involves the thermal compression of the gas!

8.4 Comments and Conclusions

The analysis and resolution of the Szilard Paradox presented in this Chapter addresses all the problems raised in Chapter 4, and shows how the previous resolutions stand in respect to one another. Rather than 'unseating' previous attempts to resolve the problem, we have attempted to show how the resulting partial resolutions fit into a more general structure. Nevertheless, the analysis of this Chapter is not definitively comprehensive. We will now briefly discuss the principal areas where further analysis may be considered to be desirable. We will then conclude by reviewing the reason for the occurrence of the Szilard Paradox, and how our analysis shows this reason to be mistaken.

8.4.1 Criticisms of the Resolution

There are four places in the analysis where we have made assumptions about the physical processes involved, or where we have not analysed the most general situation conceivable. These represent situations where further work could be done to provide a more comprehensive resolution.

These four areas may be summarised as:

- Non-orthogonality of subensembles;
- More than two subensembles;
- Pressure fluctuations;
- Statistical Carnot Cycle.

We will now review each of these areas

Non-orthogonality of subensembles

Throughout Chapter 8 we have assumed that the density matrix of a system is decomposed into orthogonal subensembles:

$$\rho = p_1\rho_1 + p_2\rho_2$$

or if it is not, it can be decomposed into three orthogonal subensembles, where the third is the overlap between the initial two subspaces. This will always be the case for *classical* ensembles.

However, for quantum systems, the problem is more subtle. Let us consider the projection \hat{P} of a density matrix ρ , onto some subspace of the total Hilbert space, and onto its complement $\widehat{1 - P}$.

$$\begin{aligned}\rho_1 &= \hat{P}\rho\hat{P} \\ \rho_2 &= (\widehat{1 - P})\rho(\widehat{1 - P})\end{aligned}$$

The decomposition

$$\rho = \rho_1 + \rho_2$$

will only be true if ρ was diagonalised in a basis for the projected spaces. This can be seen in both the Szilard Box, and the quantum weight. The insertion of the potential barrier, or shelf, must deform the wavefunctions until previously non-degenerate solutions become degenerate (which allows the density matrix to diagonalise in a different basis). Until this degeneracy occurs, there will be phase coherence between the wavefunctions, that means we cannot simply divide the density matrix into two.

For the situations considered here, we have argued that the work required to create this degeneracy is negligible. Naturally there will be situations where this will not be true. As long as this work is applied slowly and isothermally, however, it should always be recoverable at some other point in the cycle. This simply represents an additional, if difficult, energy calculation and so we do not believe it significantly affects our argument.

More than two subensembles

We have only considered situations where the ensemble is separated into two. The most general solution is where the ensemble is separated into a large number of subensembles, and the notional free energy is extracted from each. It can be readily shown that the increase in the entropy of the auxiliary must be at least as large as T times the gain in free energy. However, complications arise when we attempt to consider an imperfect correlation between the auxiliary and a compressed second system, as we must consider all possible overlaps between the compressed states of the second system. For n initial subensembles, there will be $(2^n - 1)$ different correlations between the auxiliary and the second system. Demonstrating that the Engine must, in the long run, go into reverse for all possible unitary operations, for all possible values of n , remains a considerable task.

Pressure fluctuations

We have assumed that the piston moves with a constant speed, under pressure from the gas and that, although the fluctuation in pressure exerted by the gas upon the piston, at any one time, is large, over the course of an entire cycle it is small. A more rigorous approach would be to attribute a kinetic energy to the piston, and allow the pressure fluctuations from the gas to cause this to vary. The result would be a form of Brownian motion in the piston. It might be argued that this is the 'fluctuations in the detector' that should be seen as the real reason the Engine cannot operate, similar to the fluctuating trapdoor. However we believe this is false.

Although such motion would mean the piston would not reach the end of the box at a specific time, we can be certain that it would never reach the 'wrong' end of the box (as this would require compressing the one atom gas to a zero volume). It is a simple matter to create a new set of evolution operators, which, rather than extract the piston at a given time, will extract the piston at any time when it is in one of the three states: at the left end; at the right end, and in the center of the box. This means that sometimes the piston will be inserted and removed without having any net effect, reducing the time it takes for the Engine to operate. However, other than this, it

would not affect the conclusions above.

Statistical Carnot Cycle

Finally, in Section 8.2 we have only considered two extremes: the Entropy Engine, where we perform work upon the system to ensure a perfect correlation between the auxiliary and the second system; and the imperfect correlation, where we perform no work at all. In between there would be the situations where some work is performed to improve the correlation, but not enough to make the correlation perfect. It may be possible to use this to produce a 'Statistical Carnot Cycle', in which the efficiency of the Carnot Engine is exceeded, as long as the cycle continues, but a probability of the Engine going into reverse is allowed. Any initial gains in such an Engine are always more than offset in the short run by the increase in entropy of the auxiliary, and in the long run by the tendency of the machine to go into reverse.

8.4.2 Summary

In Chapter 4 we considered the arguments surrounding the identification of information with entropy. Essentially, these came from a dissatisfaction with the description of physical systems using statistical mechanics, and in particular, the status of entropy. At least part of the problem arises because of confusion between the Boltzmann description of entropy, and the Gibbs description, and how these two descriptions deal with fluctuations.

The system is assumed to be in a particular state, at any one time, but over a period of time comparable to the thermal relaxation time, the state becomes randomly changed to any of the other accessible states, with a probability proportional to $e^{i E/kT}$. The Boltzmann entropy involves partitioning the phase space into macroscopically distinct 'observational states', with entropy $S_B = k \ln W$, where W is the phase space volume of the partition. The system will almost always be found in the high entropy 'observational states', but has some small probability of 'fluctuating' into a low entropy state. Further, if the 'observational states' can be refined, then the entropy of the system will decrease, until, with a completely fine grained description, it appears to become zero!

For the Gibbs entropy, an ensemble of equivalently prepared states must be considered, and the entropy is the average of $-k \ln p$ over this ensemble. A fluctuation is simply the division of the ensemble into subensembles, only one of which will be actually realized in any given system. However, by refining this to the individual states, the entropy of the *subensembles* go to zero. This is not a problem, so long as one does not abandon the ensemble description, as the entropy is still present in the mixing entropy.

The conceptual difficulty arises because the ensemble clearly does not actually exist. Instead there is actually only a single system, in a single state. It should seem that if we could determine the actual state, we could reduce the entropy of the system to zero. This is the origin of Maxwell's Demon and the Szilard Paradox.

The resolution rests upon the fact that the Demon, as an active participant within the system, must be described by the same laws as the rest of the system. We find that, to be subject to a unitary evolution, the Demon can only reduce the observed system's entropy by increasing its own. The fluctuation probability relationship ensures that correlating a second system cannot improve the situation.

Information theory would see the idea that the demon is an intelligent being as central, and that this is different from the 'demonless' auxiliary, such as the fluctuating trapdoor. To resolve this, it is necessary to supply principles to connect the operation of intelligence to the physical system. What are the principles required? No less than the Church-Turing thesis, that

What is human computable is Universal Turing Machine computable [Zur90a]

to be sure that all intelligent creatures can be simulated as a computer, and then Landauer's Principle, to connect the storage of information to thermodynamics. However, if we consider what the net effect of this is, we find it is simply to establish that we must treat the 'intelligent being' as a physical system, subject to unitary evolution and described by an ensemble. As we have shown, the role played by an information processing demon is nothing more or less than that of the auxiliary in the demonless engine, for which no reference to information theory was considered necessary.

Chapter 9

Information and Computation

In Chapters 4 and 8 we made reference to Landauer's Principle, as a means of providing a link between thermodynamics and information. Although we concluded that the Principle was insufficient to provide a complete resolution to the Szilard Paradox, we did not find a problem with the Principle itself.

In this Chapter we will re-examine Landauer's Principle to see if, on its own, it provides a connection between information and thermodynamics. In Section 9.1 we will briefly review the theory of reversible computation. We will show that classical reversible computation can be made very efficient, or 'tidy', by a procedure due to Bennett. However, we will also demonstrate that Bennett's procedure does not work in general for quantum computations. While these must be reversible, there exist quantum computations that cannot be made 'tidy' and this has consequences for the thermodynamics of distributed quantum computations.

Section 9.2 will then consider the different meanings of the information measure and the entropy measure. It will be demonstrated that there are physical processes that are logically reversible but not thermodynamically reversible, and there are physical processes that are thermodynamically reversible, but not logically reversible. It is therefore demonstrated that, although Shannon-Schumacher information and Gibbs-Von Neumann entropy share the same mathematical form, they refer to different physical concepts and are not equivalent.

9.1 Reversible and tidy computations

The theory of reversible computation was developed following the discovery of Landauer's Principle [Lan61], that only logically irreversible operations implied an irretrievable loss of energy (prior to that, it was thought that each logical operation involved a dissipation of $kT \ln 2$ per bit). The amount of lost energy is directly proportional to the Shannon measure of the information that is lost in the irreversible operation.

We will now give a concrete physical example of how this Landauer erasure operates, using the Szilard Box. It will be demonstrated that the dissipation of $kT \ln 2$ work only occurs over a

complete cycle, and not during the actual process of erasing the 'information'. For understanding the thermodynamics of computation we find that this distinction is unimportant, although in the remainder of the Chapter we will see that the distinction can be significant.

In Subsection 9.1.2 we will then show how Landauer's Principle is applied by Bennett to produce thermodynamically efficient classical computations, but in Subsection 9.1.3 we will show that this approach cannot, in general, be applied quantum computations[Mar01].

9.1.1 Landauer Erasure

Landauer's Principle is typically formulated as:

to erase a bit of information in an environment at temperature T requires dissipation of energy $\geq kT \ln 2$ [Cav90]

We will represent the storage of a bit of information by a Szilard Box, with a potential barrier in the center. The atom on the lefthand side of the barrier represents the logical state zero, while the atom on the righthand side represents the logical one. Landauer argues that RESTORE TO ZERO is the only logical operation that must be thermodynamically irreversible¹.

Firstly let us consider how much information is stored in the bit. If the bit is always located in the logical one state, there is an obvious procedure to RESTORE this to the logical zero state:

1. Isothermally move the barrier *and* the righthand wall to the left at the same rate. The work performed upon the barrier by the atom is equal to the work the wall performs upon the atom so no net work is done.
2. When the wall has reached the original location of the barrier, the barrier is by the lefthand wall. Now lower the barrier from the lefthand wall, and raise it by the righthand wall, confining the atom to the left of the barrier,
3. Return the righthand wall to it's original state.

Naturally, if we have the bit in the logical zero state, an operation required to RESTORE it to zero is simply: do nothing. At first, this implies that Landauer's Principle is wrong - a bit may always be RESTORED TO ZERO without any work being done. Of course, we saw the fallacy in this argument in Section 8.3.3, as the two procedures here cannot be combined into a single operation.

What this tells us, however, is that if it *is* certain that the bit is on one side or the other, it may be RESTORED TO ZERO without any energy cost. It is only when the location of the bit is uncertain that there is an energy cost. The information represented by this is

$$I_{Sh} = - \sum_a p_a \log p_a$$

¹For a single bit, the only other logical operation is NOT.

If the location of the bit is certain, it conveys no useful information. It is only if there is a possibility of the bit being in one state or the other that it represents information. In other words, after the performing of some series of logical operations the atom in the Szilard Box will be to the left of the barrier with probability p_0 and to the right with probability p_1 , over an ensemble of such operations. I_{Sh} represents the information the person running the computation gains by measuring which side of the box contains the atom.

We will now show how the RESTORE TO ZERO operation implies an energy cost of $I_{Sh}kT \ln 2$. We are going to assume that the probabilities p_a are known. The information that is unknown is the precise location of the atom in each individual case from the ensemble.

First, let us note that we have already shown above that for $p_0 = 1$ and $p_0 = 0$ we can perform the operation with zero energy cost. These are situations where $I_{Sh} = 0$.

Next, we follow this procedure if $p_0 = p_1 = \frac{1}{2}$, for which $I_{Sh} = 1$:

1. Remove the barrier from the center of the box, and allow the atom to thermalise.
2. Isothermally move the righthand wall to the center of the box. This compresses the atom to the lefthand side, and requires work $kT \ln 2$.
3. Re-insert the potential barrier by the righthand wall, confining the atom to the left of the barrier
4. Return the righthand wall to its initial location.

This has required $kT \ln 2$ work to be performed upon the gas. This energy is transferred into the heat bath, compensating for the reduction in entropy of the atomic state.

If the probabilities are not evenly distributed the Shannon information, $I_{Sh} < 1$ and we must follow a slightly different procedure:

1. While keeping the central barrier raised, isothermally move its location to $Y = 1 - 2p_1$. As shown in Section 8.1 and Appendix H, this extracts a mean energy $(1 - I_{Sh})kT \ln 2$.
2. Remove the barrier from the box and allow the atom to thermalise.
3. Isothermally move the righthand wall to the center of the box. This compresses the atom to the lefthand side, and requires work $kT \ln 2$.
4. Re-insert the potential barrier by the righthand wall, confining the atom to the left of the barrier
5. Return the righthand wall to its initial location.

The net work performed upon the gas is now $I_{Sh}kT \ln 2$.

This shows how the RESTORE TO ZERO operation comes with the work requirement of $kT \ln 2$ per bit of Shannon information. This work is transferred into an environmental heat bath, so represents the heat emitted by a computer. Other logical operations do not give off heat.

However, it is not clear that the work here has been lost, as the key stage (compressions of the atom by the righthand wall) is thermodynamically reversible. Although the energy may be described as dissipated into the heat bath, the entropy of the one atom gas has decreased by $k \ln 2$ in compensation. The free energy of the atom increases by $kT \ln 2$. The work performed upon the system may, it appears, be recovered. The actual erasure of the information occurs when the potential barrier is lowered, and this does not require any work to be performed.

The key to understanding the role of Landauer's Principle in the thermodynamics of computation is to consider the entire computational cycle. At the start of the computation, there will, in general, be large numbers of memory registers. To perform operations upon these, they must all be initially in a known state, which we may by convention choose to be logical zero. So the computation must start by initialising all the memory registers that will be used. If we start with our Szilard Box representing a Landauer Bit, then the atom will be equally likely to be on either side of the box. To initialise it, we must compress the atom to the left. This takes $kT \ln 2$ work. This work has not been lost, as it has been stored as free energy of the atom.

In other words, computation requires an *investment* of $kT \ln 2$ free energy, per bit of information that must be stored in the system. At any time in the computation, any bit that is in a known state can have this free energy recovered, by allowing its state to expand to fill the entire Szilard Box once more. A known state is one that is in a particular value, regardless of the choice of input state, (we may extend this to include the same state as an initial input state).

When we examine a computational network, given the program and the input state, we can recover all the free energy from the bits that are known. Other bits may be in determinate states, well defined functions of the input. It may be argued that these are, therefore, 'known' but, as these states are non-trivially dependent upon the input state (eg. (A OR NOT B) AND (C XOR D)), to extract the energy requires one to find the value of the bit from the input state ie. to recapitulate the calculation on a second system. This requires an investment of an equivalent amount of free energy into the second computation, so no gain is made in terms of recoverable energy.

When a computation is reversible, we can recover all the free energy initially invested in the system by completely reversing the operation of the computation. However, if we have performed the RESTORE TO ZERO operation, we cannot recover the original free energy invested in the system, we only recover the $kT \ln 2$ we invested during the RESTORE TO ZERO operation. So we see that it is only over the course of an entire cycle of computation that the RESTORE TO ZERO operation has a thermodynamic cost. The objective of reversible computing is to reduce the heat emitted during the operation of a computer, and reduce the amount of the free energy invested into the calculation that cannot be recovered at the end, without losing the results of the computation. We will now look at how this is achieved.

9.1.2 Tidy classical computations

A reversible calculation may be defined as one which operates, upon an input state i and an auxiliary system, prepared in an initial state $Aux0$, to produce an output from the calculation $O(i)$, and some additional 'junk' information $Aux(i)$:

$$F : (i, Aux0) \rightarrow (O(i), Aux(i))$$

in such a manner that there exists a complementary calculation:

$$F^\theta : (O(i), Aux(i)) \rightarrow (i, Aux0)$$

The existence of the 'junk' information corresponds to a history of the intervening steps in the computation, so allowing the original input to be reconstructed. A computation that did not keep such a history, would be irreversible, and would have lost information on the way. The information lost would correspond to an amount of free energy invested into the system that could not be recovered.

However, $Aux(i)$ is not generally known, being non-trivially dependant upon the input, i , and so represents free energy that cannot be recovered. A general procedure for discovering the complementary calculation F^θ can be given like this:

- Take all the logical operations performed in F , and reverse their operation and order.

As long as all the logical operations in F are reversible logic gates, this is possible. It is known that the reversible Fredkin-Toffoli gates are capable of performing all classical logical operations, so it is always possible to make a computation logically reversible. However, this is not immediately very useful: although we could recover the energy by reversing the computation, we lose the output $O(i)$ in doing so.

Bennett[Ben73, Ben82] showed that a better solution was to find a different reverse calculation $F^{\theta\theta}$

$$F^{\theta\theta} : (O(i), Aux(i), AuxO) \rightarrow (i, Aux0, O(i))$$

Now the only additional unknown information is $O(i)$, which is simply the output we desired (or extra information we needed to know). A general procedure for $F^{\theta\theta}$, is:

- Copy $O(i)$ into a further auxiliary system $AuxO$ by means of a Controlled-NOT gate;
- Run F^θ on the original system.

This has also been shown to be the optimal procedure[LTV98, LV96] for $F^{\theta\theta}$. We call such a calculation TIDY. All classical reversible computations can be made TIDY.

9.1.3 Tidy quantum computations

We will now show that when we try to apply this procedure to quantum computations, it fails. This fact does not appear to be widely appreciated[BTV01, for example]. The problem is that the Controlled-NOT gate does not act as a universal copying gate for quantum computers. In fact, the universal copying gate does not exist, as a result of the 'no-cloning theorem'[WZ82, BH96b, GM97, BBBH97, Mar01].

Clearly, in the case where the output states from a quantum computer are in a known orthogonal set, then the quantum computation can be made tidy. In fact, for other reasons, having orthogonal output states was initially taken as a requirement on a quantum computer, as it was deemed necessary for reading out the output. This was suggestive not of a general quantum computation, but of limited quantum algorithmic boxes: each connected by classical communication. However, developments in quantum information theory have suggested that distributed quantum information may be desirable - in particular, a more general conception of quantum computation may be required which takes inputs from different sources, and/or at different times. In Figure 9.1 we see an example of this - Alice performs some quantum computation, and stores the result of it in a 'quantum data warehouse'. At some later time, Bob takes part of these results as an input into his own computation.

We are going to take our definition of a quantum computation² as the operation:

$$U_C : |i\rangle |Aux0\rangle \rightarrow |O(i)\rangle |Aux(i)\rangle$$

so that the output is always in a separable state (in other words, we regard the 'output' of the computation as the subsection of the Hilbert space that is interesting, and the 'auxiliary' as everything that is uninteresting. If the 'output' were entangled with the 'auxiliary' space, then there would be additional information relevant to the 'output', contained in the super-correlations between 'output' and 'auxiliary' spaces). As any quantum computation must be performed by a unitary operation, all quantum computers must be reversible. But are they TIDY?

If this model of computation is classical, then each time data is sent to the central database, the local user can copy the data before sending it, and tidy up their computer as they go along. The only energy commitment is: total input, plus stored data. At end of all processing - if it happens - reconstruction of computation from stored input would allow tidying of any stored data no longer needed. The difference between computation using distributed classical algorithmic boxes and a single classical computation is a trivial distinction, as the computation may be tidied up along the way. However, this distinction depends upon the classical nature of the information transferred between the algorithmic boxes.

²There is further complication when entanglement enters the problem. When the output part of an entangled state is non-recoverably transmitted, the loss of free energy in the remainder is always at least equal to the entropy of the reduced density matrix of the output. However, this minimum loss of free energy requires knowledge of an accurate representation of the resulting density matrix - which may not be possible without explicitly calculating the output states.

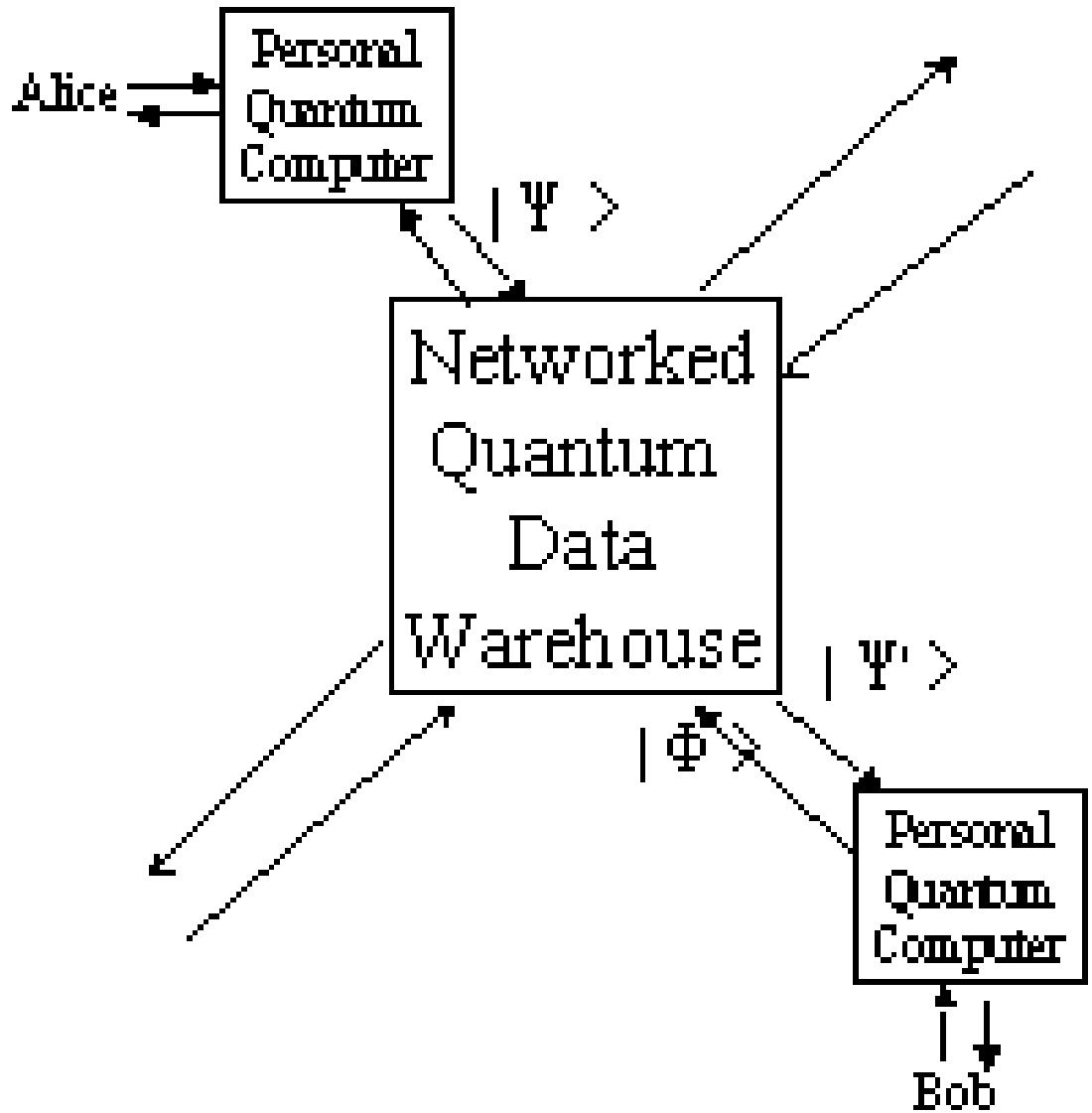


Figure 9.1: Distributed quantum computing

In our generalised quantum computation network, we can no longer guarantee that the operations performed at separate locations are connected by classical signals only. We now need to generalise the definition of reversibility and tidiness to quantum computers.

Considering a general operation, unitarity requires that the inner products between different input states and between the corresponding output states is unchanged by the computation. Reversibility must always hold. This leads to the conditions:

Reversible

$$\langle i | j \rangle \langle Aux0 | Aux0 \rangle = \langle O(i) | O(j) \rangle \langle Aux(i) | Aux(j) \rangle$$

Tidy

$$\langle i | j \rangle \langle Aux0 | Aux0 \rangle \langle AuxO | AuxO \rangle = \langle i | j \rangle \langle O(i) | O(j) \rangle \langle Aux0 | Aux0 \rangle$$

We can eliminate $\langle Aux0 | Aux0 \rangle = 1$ and $\langle AuxO | AuxO \rangle = 1$, leaving only three cases.

Orthogonal Outputs

The output states are orthogonal set:

$$\langle O(i) | O(j) \rangle = \delta_{ij}$$

Reversibility *requires* the input states to be an orthogonal set $|i\rangle \langle j| = 0$, and the TIDY condition will hold. This is not too surprising, as an orthogonal set of outputs *can* be cloned, and so can be tidied using Bennett's procedure.

Orthogonal Inputs

The input states are orthogonal set $\langle i | j \rangle = \delta_{ij}$, but the output states are not.

To satisfy unitarity, this requires the *auxiliary* output states to be orthogonal.

$$\langle Aux(i) | Aux(j) \rangle = \delta_{ij}$$

There does exist a unitary operator (and therefore a computable procedure) for tidying the computation, without losing the output. However, this tidying computation is not derivable from the initial computation by Bennett's procedure. If we were to clone the auxiliary output, and run the reverse operation, we would lose the output, and be left with the 'junk'! Whether there is an equivalent general procedure for obtaining F^{00} is not known.

One obvious method is to examine the resulting auxiliary output states, construct a unitary operator from

$$U_G |Aux(i), O(i)\rangle = |Aux0, O(i)\rangle$$

and decompose U_G into a quantum logic circuit. However, it is not clear whether the operator can be constructed without explicitly computing each of the auxiliary output states - which may entail running the computation itself, for each input, and measuring the auxiliary output basis. Alternatively, examine the form of the auxiliary output (eg. (A OR NOT B) AND (C XOR D)) and devise a logic circuit that reconstructs the input state from this. However, these simply restates the problem: although some such circuit (or U_G) must exist, is there a general procedure for efficiently constructing it from only a knowledge of U_G ?

Non-orthogonal Inputs

The input states are a non-orthogonal set. This corresponds to Bob's position in the quantum distribution network of Figure 9.1.

If we look at the requirements for a tidy computation, this leads to:

$$\langle O(i) | O(j) \rangle = 1$$

The output is always the same, regardless of the input! Obviously for a computation to be meaningful, or non-trivial, at least some of the output states must depend in some way upon the particular input state. So in this case we can say there are NO procedures F^{00} that allow us to tidy our output from F . To state this exactly:

There does not exist any non-trivial ($|O(i)\rangle \neq |O(j)\rangle$) computations of the form

$$G : |i\rangle |Aux0\rangle |AuxO\rangle \rightarrow |i\rangle |Aux0\rangle |O(i)\rangle$$

for which $|i\rangle |j\rangle \neq \delta_{ij}$ ³.

It should be made clear: this does NOT mean useful quantum computations of the form

$$F : |i\rangle |Aux0\rangle \rightarrow |Aux(i)\rangle |O(i)\rangle$$

do not exist if $|i\rangle |j\rangle \neq \delta_{ij}$ - simply that such computations cannot be 'tidy'. For such computations, not only is the free energy used to store the auxiliary output unrecoverable, but also the input state cannot be recovered, except through losing the output. For our distributed network, this means that not only can Bob not 'tidy' his computation, but he cannot restore Alice's data to the database.

9.1.4 Conclusion

We have now seen how Landauer's Principle arises within computation. However we have seen that, strictly speaking, the interpretation of Landauer's Principle as:

To erase information requires one to do $kT \ln 2$ work per bit upon the system

is not strictly justified. A better use of language would be

To erase information requires the loss of $kT \ln 2$ free energy per bit

This applies both in the classical computation (where the information is measured in Shannon bits) and the quantum computation (where information is measured in Schumacher bits). However, the efficient tidying procedure due to Bennett is not applicable to all quantum computations. Some quantum computations may be tidied, but only by using some other procedure, and some cannot be tidied at all.

9.2 Thermodynamic and logical reversibility

We have clarified the significance of Landauer's Principle for the thermodynamics of computation. However, we found that the logical erasure step of the process is at a different stage to the stage that involves the thermodynamic work of $kT \ln 2$ per bit of information. Over the course of a computational cycle, this is of little significance.

³It is interesting to note that the 'no-cloning' theorem is a special case of this theorem.

Nevertheless, when the interpreting the relationship between information and entropy, this is very significant. We are now going to briefly examine the relationship between thermodynamic entropy and logical information. We will find that the two concepts are quite distinct. There are processes that are thermodynamically reversible but logically irreversible and processes that are logically reversible but thermodynamically irreversible.

9.2.1 Thermodynamically irreversible computation

Modern computers gives off heat well in excess of that suggested by Landauer's Principle. They also use irreversible logic gates, such as AND/OR gates. However, these two facts are not related in the manner that Landauer's Principle would suggest.

While it is true that the development of quantum computing requires the heat dissipation of computers to be minimised, the desktop PC does not use anything approximating this kind of technology. The computer gives off heat simply because it is very inefficient.

Now, as Bennett has shown, any logically irreversible computation could be implemented on a reversible computer. It would be perfectly possible, using existing technology, to construct a computer which was based upon reversible logic gates. Such a computer would have to store more bits in it's memory while it was making it's calculations, and would take approximately twice as long to perform a calculation. The storing and reading of all these extra bits would mean that *more* heat was given off than in a corresponding irreversible computer. With current technology, logically reversible computers are thermodynamically *less* efficient than logically irreversible computers.

To put this another way: current computers are implemented using irreversible logic gates *because* they are thermodynamically inefficient, rather than the reverse. In the limit, where the dissipation per bit stored, analysed or transmitted, is significantly less than $kT \ln 2$, a reversible computer would be more thermodynamically efficient than an irreversible one. However, if the technology is such that there is a dissipation per bit stored, transmitted or analysed of more than $kT \ln 2$ per bit, then a logically irreversible computer will be thermodynamically *more* efficient than a reversible one, as it has to store less bits. With current technology, the desktop PC is far more efficient if it is built from irreversible gates.

If we were to construct a desktop PC using reversible gates, they would still give off heat. In short, they would be thermodynamically irreversible, while logically reversible. This demonstrates the first main point of this Section: logical reversibility does not imply thermodynamic reversibility.

9.2.2 Logically irreversible operations

When we examined the Landauer Erasure, from the point of view of the Szilard Box, we found that the logically irreversible stage was distinct from the stage at which work is performed upon the system. From the point of view of efficient computation these distinctions are, perhaps, not very important. However, when we are considering the relationship between information and entropy, we will find this distinction becomes critical.

We are now going to consider very carefully what we mean by logical reversibility, and demonstrate that there are operations which are not logically reversible, but are thermodynamically reversible. The computations will be taking place at the limiting efficiency, where no dissipation takes place.

The information of the represented by the output states of the computation is

$$-\sum_a p_a \ln p_a$$

Now we must ask, where do the p_a come from? If the computation is deterministic then, given a specific input there must be a specific output, and the probabilities are all either zero or one. This would imply that the information contained in the output is zero.

Naturally this is not the case. The computation will typically have a number of possible inputs, and a corresponding number of possible outputs. For a reversible, deterministic computation there will be a one-to-one correspondence between inputs and outputs, and so the p_a in the output bits are simply the probabilities of the corresponding inputs being fed into the computation.

This reminds us that the Shannon information is only defined over an ensemble of possible states. To attempt to compare the Shannon information of a computation to the thermodynamic entropy we must consider an ensemble of computations run with different input states.

Now let us consider how the logical reversibility comes into the computation. The computation is fed an input state I_a . After successive computation it produces the output state O_a . The Shannon information of the ensemble is the same at the end of the computation as at the start of the ensemble. This is only natural, as we could equally well have considered the reverse computation. This takes as it's input the states O_a and produces the output states I_a .

The definition of the logically reversible computation is effectively one where, given the output state O_a we can determine exactly which input state (I_a) was fed into the start of the computation.

Now, this is actually a much stronger condition than thermodynamic reversibility. For a process to be thermodynamically reversible, all that is required is that the entropy of the system, including auxiliaries, is the same before and after the process.

We can now show the simple procedure that is thermodynamically reversible but is not logically reversible. Let us return to our Szilard Box, holding the output of some computation⁴. We suppose that the atom representing the outcome of the computation is located on the left with probability p_a and on the right with probability $1 - p_a$.

1. Move the partition, isothermally, from the center to the location $Y = 1 - 2p$, as described in Section 9.1 above.
2. The partition is removed completely from the Szilard Box and the Box is left in contact with a heat bath for a period of time long with respect to the thermal relaxation time.

⁴As there are only two possible outputs in this case we know there can have only been only two possible inputs. It is a very simple computation we are considering! However, this argument can easily be generalised to computations with any size of output.

3. The partition is reinserted in the box at the location Y . The atom is again located upon the left with probability p_a and on the right with probability $1 - p_a$.
4. The piston can now be isothermally returned to the center of the box, again in connection to a work reservoir.

This process we have described fulfils all the criteria of thermodynamic reversibility.

In fact the thermodynamic description of the Szilard Box and the heat bath is exactly the same at the end of this cycle as at the start. However, there is also clearly no correspondence between the location of the atom at the end of the cycle and the location of the atom at the start of the cycle. If we were to now reverse the cycle completely, and run the original computation in reverse, there is no guarantee that the state we will end up with was the original input state. The process is not logically reversible.

This demonstrates the second main point to this Section: that thermodynamic reversibility does not imply logical reversibility.

9.3 Conclusion

We have looked at the relationship between information and entropy given by Landauer in some more detail in this Chapter. This has lead to a better understanding of the thermodynamics of computation but also has lead to a perhaps surprising conclusion:

- Logically reversible operations do not imply thermodynamic reversibility.
- Thermodynamically reversible operations do not imply logical reversibility.

This pair of conclusions undermines any attempt to connect Shannon information to Gibbs entropy⁵ using Landauer's Principle and computation. We will now see why this is so by considering the conceptual basis of the two terms.

Shannon Information

Shannon information represents a situation where a system is in one of a number of states ρ_a , and over an ensemble of such situations occurs with probability p_a . Logically reversible computations may be performed upon the system, where the state of the system undergoes one-to-one transformations, and it is always possible to reverse the computation and recover exactly the initial state. For this to be possible, *there must be no possibility of spontaneous transitions between the different ρ_a states*. The whole point of Shannon information is that it quantifies the knowledge gained, on discovering that the state is the particular ρ_a , out of the ensemble of possible states.

When sending a signal, or performing a computation, any tendency of the signal states to undergo transitions during transmission is 'noise'. This reduces the information that the receiver

⁵The arguments can be easily generalised to Schumacher information and Von Neumann entropy in quantum systems.

gains about the signal sent, even if the effect of the noise is to leave the *density matrix* over the ensemble unchanged. If the system is allowed to completely randomise during transmission, so that any input state ρ_a leads to the density matrix $\sum_a p_a \rho_a$ by the time it reaches the receiver, then *no* information is conveyed.

Entropy

Thermodynamic entropy, on the other hand, is completely insensitive to such transitions, *so long as* the ensemble density matrix is unchanged. In a thermodynamic system the states ρ_a occur with probability p_a . Assuming the system is in equilibrium at some temperature T , the system can be left in contact with a heat bath at that temperature, and allowed to undergo random transitions between all of the possible states. The final density matrix will be the same as at the start and none of the thermodynamic properties of the system will have changed.

In complete contrast to Shannon information, the exact individual state ρ_a that the system may be occupying has no significance at all.

Summary The fact that signal information and entropy share the same functional form, in both quantum and classical cases, is remarkable. This means that many results derived in information science will be applicable in thermodynamics, and vice versa. It also means that, as information processing must take place on physical systems, there are limiting cases where the two terms will appear to coincide. However, despite their functional similarity they refer to quite different concepts. They are not the same thing.

Chapter 10

Active Information and Entropy

In Chapters 4 and 8 we examined the arguments surrounding the Szilard Engine thought experiment and the role of information in its resolution. We found that the intrusion of information into the problem came about only because of the failure to follow through with the ensemble description of a thermodynamic system when that ensemble includes intelligent beings. However, the reason for that failure can be traced, not to a specific property of the intelligent beings, as such, but rather a dissatisfaction with the ensemble description.

In this final Chapter we are going to briefly discuss this dissatisfaction with the ensemble description. This has led some to suggest that the quantum density matrix should be treated as a description applying to an individual system, rather than a statistical ensemble of systems. We will argue that the attempt to do this, rather than resolving the problem, simply imports the quantum measurement problem into statistical mechanics.

However, we will then show that the Bohm approach to quantum theory may be used to resolve this problem, by extending the concept of active information to apply to the density matrix. This resolves the tension in thermodynamics between the statistical description and the individual system. We will construct a very simple model suggesting how this approach could work, and how it would be applied in the case of the interferometer and the Szilard Engine.

10.1 The Statistical Ensemble

The statistical ensemble,

$$\rho = \sum_a p_a |a\rangle \langle a|$$

as introduced in Chapters 2 and 6, is a description of the limiting case where an experiment is run an infinitely large number of times, on a system that is prepared in such a manner that state $|a\rangle$ occurs with the relative frequency p_a . As noted before, if the $|a\rangle$ do not form an orthogonal basis then they do not diagonalise ρ , and the Schumacher information of the ensemble is less than the

Shannon information

$$S[\rho] < - \sum_a p_a \log_2 p_a$$

In reality, of course, there is no such limiting case. We never have an infinite number of systems to act upon. The actual physical situation should then be represented by a finite ensemble or assembly¹. This is a sequence of systems, i , each in a particular state $|a_i\rangle$. The correct way to represent this would be in a product of the Hilbert spaces of the individual systems

$$\begin{aligned} |\Psi\rangle \langle\Psi| &= |a_1\rangle \langle a_1| \otimes |a_2\rangle \langle a_2| \otimes |a_3\rangle \langle a_3| \otimes \dots \\ &= \prod_i |a_i\rangle \langle a_i| \end{aligned}$$

If there are N such systems, and the state $|a\rangle$ occurs n_a times, the relative frequency of $|a\rangle$ is

$$f_a = \frac{n_a}{N}$$

In the limit $N \rightarrow \infty$, then $f_a \rightarrow p_a$ ².

The properties of an assembly differ from the statistical ensemble in a number of ways.

Ordered systems The individual systems occur in a particular order, and this order may display a pattern in the occurrence of the particular states. It is generally assumed that the particular state $|a\rangle$ is randomly selected with probability p_a , and this will be unlikely to produce a pattern in the appearance of the states. Such patterned assemblies are less likely to occur the larger the value of N , and become a set of measure zero as $N \rightarrow \infty$, assuming that the states are indeed, probabilistically generated. However, for a finite system, there is still a non-zero probability of such order occurring. Of course, if the states are not randomly generated (and it remains an open problem of how to generate truly random states) then there may be an order in the assembly even when N becomes infinitely large.

An example of such a pattern is the assembly of spin- $\frac{1}{2}$ particles, where the even numbered states are in the spin-up state, while the odd numbered states are in the spin-down state. This represents information, or a pattern, within the assembly, that could be revealed by the appropriate measurements. Such information is not represented in the statistical ensemble.

Joint measurements Measurements performed upon the system represented by the statistical ensemble must be designed as a single POVM experiment. This experiment is repeated for each system in turn, and the relative frequencies of the POVM outcomes, B_b , occur. As the value of N gets large, these relative frequencies will approach the values

$$p_b = \text{Tr}[B_b \rho]$$

However, this is *not* the most efficient method for gathering information, given an assembly.

¹The terminology *assembly* is due to Peres[Per93].

²Although the probability that the relative frequencies match the probabilities exactly, $f_a = p_a$, approaches zero as N becomes large!

Firstly, one has the classically available option to correlate the measurements performed upon a given system to the outcomes of previous measurements. A given measurement is performed upon system 1, then the outcome of this measurement is used to modify the experiment performed upon system 2. The outcome of both measurements can be used to perform an experiment upon system 3, and so forth. It is even possible, if one performs measurements that do not completely collapse the state of the system measured ('weak' measurements), to go back and perform further measurements upon system 1, correlated to the outcomes of the measurements on system 2 and 3. Such a scheme is referred to as 'Local operations and classical communications' or LOCC measurements, as it can be implemented by a separate experimentalist acting with locally defined operations upon their own system, and communicating with each other using classical information obtained from their measurements.

Secondly, for quantum systems it is possible to improve upon LOCC measurements by performing a joint measurement upon the combined Hilbert space of the entire assembly [MP95, LPT98, BDE98, LPTV99, TV99]. Although joint measurements have long been known to be required for entangled systems, it has recently been discovered that such joint measurements can have surprising consequences [BDF⁺99, GP99, Mas00, for examples] even for systems constructed entirely out of separable states, such as the assemblies considered here.

Entropy of the universe The issues considered above arise because the assembly $|\Psi\rangle\langle\Psi|$ describes, not a statistical ensemble, but a *single state* albeit one with a very large number of constituent subsystems. This remains the case even if N is allowed to become infinitely large³.

When we consider the entropy of the *assembly*, we find

$$S[|\Psi\rangle\langle\Psi|] = 0$$

as it is a pure state! Apparently, no matter how large we make the assembly, it will have an entropy of zero. How do we reconcile the entropy of the assembly with the entropy of the ensemble?

We have seen before that, for any given state $|a\rangle$, there exists a unitary operator that will take it to a reference state $|0\rangle$. A simple example of this is

$$U_a = |0\rangle\langle a| + |a\rangle\langle 0| + \sum_{\alpha \notin 0,a} |\alpha\rangle\langle\alpha|$$

If we use U^1 to represent an operator acting on the Hilbert space of the first subsystem in the assembly, then the combined unitary operation

$$\begin{aligned} U_A &= U_{a_1}^1 \otimes U_{a_2}^2 \otimes U_{a_3}^3 \otimes \dots \\ &= \prod_i U_{a_i}^i \end{aligned}$$

will convert the entire assembly to the state $|0\rangle$. The equivalent ensemble is now $|0\rangle\langle 0|$, which has an entropy of zero. Thus, although there is no unitary operation which can act upon the ensemble

³Although if the universe is finite, then this will not be possible.

to reduce its entropy, there do exist unitary operations that can act upon assemblies, that reduce the entropy of their equivalent ensembles.

What we have seen here is the 'global entropy problem'. The universe does not occur as a statistical ensemble, it occurs once only, and so has an entropy of zero. Naively, this might suggest that we could exploit this to extract work from heat, somehow. This is not the case. To implement an operation such as U_A , we must apply the correct U_a to each i subsystem. This requires a conditionally correlated system B to the original assembly A , and when we find the equivalent ensemble to the joint system, the entropy we gain from the ensemble of the first system is just the correlation entropy $-S[A : B]$, in

$$S[A, B] = S[A] + S[B] + S[A : B]$$

The overall entropy $S[A, B]$ of the joint ensemble remains constant⁴.

10.2 The Density Matrix

Although we have seen that the finite assembly does not imply we can violate the second law of thermodynamics, we are still left with an uncomfortable situation. To express thermodynamic properties, such as entropy and temperature, we must move from the physically real assembly to a fictitious ensemble. This calls into question whether the thermodynamic properties are physically real.

In addition to this, in Chapter 2 we saw that the statistics of measurement outcomes were defined in terms of the ensemble. The density matrix of the ensemble represents all the information that can be gained from a measurement⁵. There is no measurement that we can perform that reveals the actual structure of the randomly generated assembly, as opposed to the 'fictitious' ensemble, as the statistics of measurements performed upon such an assembly can only be expressed in terms of the ensemble density matrix.

As we cannot discover which states actually went into composing a given density matrix, it is surely a matter of choice as to whether we consider it to be constructed from individual pure states, or not. Could we not abandon the idea that the density matrix is composed of actual pure states? Can we treat the density matrix as the fundamental description of a state, and the pure states as simply representing the special cases of zero entropy?

If we could consistently make this assumption, then the density matrix would no longer represent a 'fictitious' ensemble and instead represents the actual state of a physically real system. The thermodynamic quantities would then be undoubtedly physically real properties rather than

⁴The operation U_A may also come about through some fundamentally random process, that fortuitously happens to apply the correct operator to each system. Such a situation is a form of fluctuation, and the probability becomes negligible as N becomes large.

⁵This may appear to contradict the joint measurements on the assembly considered above. This is not the case. The statistics on the outcomes of these measurements turns out to be defined in terms of an ensemble of assemblies!

statistical properties. This would significantly affect our discussion of Maxwell's Demon and the Szilard Engine.

This question has been raised recently by [AA98]. We will find that their suggestion is only valid if the measurement problem is assumed solved, and their suggestion does not provide a solution to this. On the contrary, we find instead that the general agreement that a measurement can be said to have taken place when there has been a, for all practical purposes, irreversible loss of phase coherence, can no longer be relied upon.

10.2.1 Szilard Box

Let us be very clear what is being suggested here. Aharanov and Anandan suggest taking the density matrix as the fundamental expression of a *single* system with

the same ontological status as the wavefunction describing a pure state[AA98]

This is a very different situation to the statistical density matrices in Chapter 2. The density matrices there do indeed represent an absence of knowledge of the exact state of the system, while the system is actually in a definite state. To distinguish between the two cases, we will continue to use ρ to represent statistical ensembles, but will now use ϱ to represent the kind of ontological density matrices suggested by [AA98].

The obvious situation to apply the ontological density matrix is to thermodynamic systems. If we can do this, then the entropy

$$S[\varrho] = \text{Tr} [\varrho \ln \varrho]$$

can be associated with an individual system, rather than with a representative, or fictitious, ensemble of equivalently prepared systems. If the system is in a thermal equilibrium then it also has a temperature T , and a free energy F , expressed as physically real properties of the individual system, in much the same manner as mass, or energy.

We will now consider the consequences of this by applying it to the Szilard Box. We start with the one atom gas occupying the entire box, with a density matrix

$$\varrho_{G0} = \frac{1}{Z_{G0}} \sum_n e^{j \frac{\epsilon_n^2}{kT_G}} |\psi_n\rangle \langle \psi_n|$$

as in Equation 6.4. However, this no longer represents a statistical mixture of $|\psi_n\rangle$ states, with the atom in a particular, but unknown state. Rather, it represents the actual state of the individual atom. Clearly the probability distribution of the particle throughout the box is given by

$$\begin{aligned} P_{G0}(x) &= \langle x | \varrho_{G0} | x \rangle \\ &= \frac{1}{Z_{G0}} \sum_n e^{j \frac{\epsilon_n^2}{kT_G}} |\psi_n(x)|^2 \\ &= \frac{1}{Z_{G0}} \sum_n e^{j \frac{\epsilon_n^2}{kT_G}} R_n(x)^2 \end{aligned}$$

where we have used the polar decomposition $\psi_n(x) = \langle x | \psi_n \rangle = R_n(x)e^{iS_n(x)}$, to emphasise this is now just a real probability distribution. If we follow standard quantum theory, this represents the probability of finding the atom at a particular location x , if it is measured. It is important to be clear that no possible measurement could distinguish between this point of view and the statistical point of view, where the probability density P_{G0} represents the probability of finding an atom at a location x only over an *ensemble* of measurements, as in each case the system would be in a pure state.

If the partition is inserted into the center of the box, the density matrix splits into two

$$\begin{aligned} \varrho_{G1} &= \frac{1}{Z_{G1}} \sum_l e^{i \frac{\epsilon}{\kappa T_G} \left(\frac{2l}{1-p}\right)^2} (|\Psi_l^\lambda\rangle \langle \Psi_l^\lambda| + |\Psi_l^\rho\rangle \langle \Psi_l^\rho|) \\ &= \frac{1}{2} (\varrho_{G2}^\lambda + \varrho_{G2}^\rho) \end{aligned}$$

Now we cannot interpret this as the atom being on one side or the other of the partition, any more than we could interpret the wavefunction

$$\frac{1}{\sqrt{2}} (\Psi_l^\rho(x) + \Psi_l^\lambda(x))$$

as a statistical mixture. However, the reason for this is now entirely interpretational: we are no longer assuming ϱ_{G1} represents a statistical mixture as a matter of principle. Unlike interference in the wavefunction, there are *no observable consequences* that tell us that the statistical mixture is an untenable point of view.

10.2.2 Correlations and Measurement

Now let us suppose an auxiliary system (or Demon) attempts to observe the box to determine on which side of the partition the atom lies. The auxiliary is originally in the state $\varrho_0(Aux)$. We wish an interaction so that, if the atom is *actually* on the left, the auxiliary state changes to $\varrho_L(Aux)$, and similarly $\varrho_R(Aux)$ if the atom is *actually* on the right.

When we apply this interaction to the density matrix ϱ_{G1} , the joint system evolves into:

$$\varrho_2 = \frac{1}{2} (\varrho_{G2}^\lambda \otimes \varrho_L(Aux) + \varrho_{G2}^\rho \otimes \varrho_R(Aux))$$

How are we to understand this correlated matrix? For a statistical ensemble ρ_2 , the situation would be very clear. The ensemble represents the situation where the system is either

$$\rho_{G2}^\lambda \otimes \rho_L(Aux)$$

or

$$\rho_{G2}^\rho \otimes \rho_R(Aux)$$

The demon is in a particular state, and observes the atom to be in the correlated state.

However, [AA98] cannot make use of this interpretation of the correlated density matrix. To be consistent in the interpretation of a density matrix ϱ_2 , the correlated state simply represents

a joint probability density for finding the atom on one side and the demon observing it, *when a measurement is performed*. For the measurement to be brought to a closure, and a *particular* outcome be observed, we must change from the ontological density matrix ϱ_2 to the statistical ensemble ρ_2

$$\varrho_2 \rightarrow \rho_2$$

and no process has been suggested through which this change will occur.

Even if we include ourselves within the description, as Demon states, we do not produce a well defined measurement procedure. Instead we simply include ourselves in the quantum uncertainty, exactly as if we were Schrödinger cats. Nevertheless, we know, from our own experience, that specific outcomes of measurements *do* occur. Even if we are able to interpret the density matrix as a single system, at some point it *must* cease to be physically real and become a statistical ensemble.

We notice that this new problem of measurement is even more intractable than the old measurement problem of quantum theory! It includes the old measurement problem, as a special case involving pure states. The old problem consists of the fact that no unitary transformation exists to convert the entangled pure state into the physically real density matrix. On top of this, we then have the fact that, even where we do not start with pure states, there is no clear process by which the physically real density matrix becomes a statistical ensemble.

In the case of the old measurement problem, there is at least general agreement on when a measurement can, for all practical purposes, be said to have taken place. When there has been a practically irreversible loss of phase coherence between two elements of a superposition, the wavefunction may be replaced by

$$\frac{1}{2} (|\Psi_l^\rho\rangle \langle \Psi_l^\rho| + |\Psi_r^\rho\rangle \langle \Psi_r^\rho|)$$

which is then interpreted as a statistical mixture ρ .

Now, even when the phase coherence has gone, we may still be left with an ontological density matrix ϱ . A further process appears necessary to complete the measurement, but this further process, unlike the loss of phase coherence, has no observable consequences⁶!

10.3 Active Information

We saw in Chapter 3 how the Bohm approach to quantum theory resolves the measurement problem. In addition to the wavefunction, there is an actual trajectory (whether 'particle' or 'center of activity'), and it is the location of the trajectory within the wavepacket that determines which of the measurement outcomes is realized.

We now find a similar *interpretational* problem in thermodynamics. We would like to be able to apply thermodynamic concepts to individual systems. However, the only way we know how to

⁶This is not strictly correct. Without such a process, measurements cannot be said to actually have outcomes. The fact that measurements actually *do* have outcomes is in itself, therefore, an observable consequence of the existence of this process.

do this would be to interpret the density matrix as applying to individual systems, and this leads us into a similar dilemma as with the quantum measurement problem ⁷.

We can now consider an obvious resolution to both problems: if the density matrix can be a description of an individual system, rather than an ensemble, can we construct a Bohm trajectory model for it, and will this resolve the problem in [AA98]’s approach? By explicitly developing a simple and tentative model of Bohm trajectories for a density matrix, we will find the answer appears to be, yes.

Firstly we must understand how we can construct a Bohm trajectory model for a density matrix. This will not be the statistical mechanics suggested by [BH96a], which constructs statistical ensembles in the manner of ρ above. Instead we will apply the formalism recently developed by Brown and Hiley[BH00], who develop the use of the Bohm approach within a purely algebraic framework.

10.3.1 The Algebraic Approach

In [BH00], it is suggested that Bohm approach can be generalised to the coupled algebraic equations ⁸:

$$\frac{\partial \varrho}{\partial t} = \imath [\varrho, H]_i \tag{10.1}$$

$$\varrho \frac{\partial \hat{S}}{\partial t} = -\frac{1}{2} [\varrho, H]_+ \tag{10.2}$$

Equation 10.1 is simply the quantum Liouville equation, which represents the conservation of probability, and reduces to the familiar form of

$$\frac{\partial R(x)^2}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

where \mathbf{j} is the probability current

$$\mathbf{j} = R(x)^2 \frac{\nabla S(x)}{m}$$

in the case where the system is in a pure state $\varrho = |\psi\rangle \langle\psi|$ and $\langle x | \psi \rangle = R(x)e^{\imath S(x)}$

The second equation is the algebraic generalisation of the quantum Hamilton-Jacobi, which reduces to Equation 3.1 for pure states. The operator \hat{S} is a phase operator, and this equation can be taken to represent the energy of the quantum system. The application of this to the Aharonov-Bohm, Aharonov-Casher and Berry phase effects is demonstrated in [BH00].

[BH00] are concerned with the problem of symplectic symmetry, so their paper deals mainly with constructing momentum representations of the Bohm trajectories, for pure states, and does

⁷Although there is no equivalent to interference effects or Bell Inequality violations.

⁸

$$[A, B]_- = AB - BA$$

$$[A, B]_+ = AB + BA$$

not address the issue of when the density matrix is a mixed state. Here we will be concentrating entirely upon the mixed state properties of the density matrix, and so we will leave aside the questions of symplectic symmetry and the interpretation of Equation 10.2. Instead we will assume the Bohm trajectories are defined using a position 'hidden variable' or 'beable', and will concentrate on Equation 10.1.

The Brown-Hiley method, for our purposes, can be summarised by the use of algebraic probability currents

$$\begin{aligned} J_X &= \nabla_P (\varrho H) \\ J_P &= \nabla_X (\varrho H) \end{aligned}$$

for which

$$i \frac{\partial \varrho}{\partial t} + [J_X, P]_i - [J_P, X]_i = 0$$

To calculate trajectories in the position representation (which Brown and Hiley refer to as constructing a 'shadow phase space') from this we must project out the specific location x , in the same manner as we project out the wavefunction from the Dirac ket $\psi(x) = \langle x | \psi \rangle$

$$i \frac{\partial \langle x | \varrho | x \rangle}{\partial t} + \langle x | [J_X, P]_i | x \rangle - \langle x | [J_P, X]_i | x \rangle = 0$$

The second commutator vanishes and the first commutator is equivalent to the divergence of a probability current

$$\nabla_{\mathbf{x}} \cdot \mathbf{J}(\mathbf{x}) = \langle x | [J_X, P]_i | x \rangle$$

leading to the conservation of probability equation

$$\frac{\partial P(x)}{\partial t} + \nabla_{\mathbf{x}} \cdot \mathbf{J}(\mathbf{x}) = 0$$

To see the general solution to this, we will note that the density matrix of a system will always have a diagonal basis $|\phi_a\rangle$ (even if this basis is not the energy eigenstates), for which

$$\varrho = \sum_a w_a |\phi_a\rangle \langle \phi_a|$$

Note, the w_a are *not* interpreted here as statistical weights in an ensemble. There are physical properties of the state ϱ , with a similar status to the probability amplitudes in a superposition of states.

We can put each of the basis states into the polar form

$$R_a(x) e^{iS_a(x)} = \langle x | \phi_a \rangle$$

so the probability density is just

$$P(x) = \sum_a w_a R_a(x)^2$$

The probability current now takes the more complex form

$$\mathbf{J}(x) = \sum_a w_a R_a(x)^2 \nabla S_a(x)$$

So far we have not left standard quantum theory⁹. We may do this by now constructing trajectory solutions $X(t)$, in the manner of the Bohm approach, by integrating along the flow lines of this probability current[BH93, Hol93, BH00]. This leads to

$$m \frac{\partial \mathbf{X}(t)}{\partial t} = \frac{\mathbf{J}(X(t))}{P(X(t))} = \frac{\sum_a w_a R_a(X(t))^2 \nabla S_a(X(t))}{\sum_a w_a R_a(X(t))^2} \quad (10.3)$$

Notice the important fact that, when the density matrix represents a pure state, this reduces to *exactly* the Bohm interpretation in Chapter 3.

The most notable feature of Equation 10.3 is that the constructed particle velocity is *not* the statistical average of the velocities $\langle V(t) \rangle$, that would have been calculated from the interpretation of $\rho = \sum_a w_a |\phi_a\rangle \langle \phi_a|$ as an ensemble:

$$\langle \mathbf{V}(t) \rangle = \sum_a w_a \nabla S_a(X(t))$$

This should not be too surprising however. We are interpreting the density matrix as providing the activity of information necessary to guide the particle motion. *All* the elements of the density matrix are physically present, for a particle at $X(t)$, and each state $|\phi_a\rangle$ contributes a 'degree of activity', given by $R_a(x)^2$ to the motion of the trajectory, in addition to the weighting w_a . If a particular state has a probability amplitude that is very low, in a given location, then even if its weight w_a is large, it may make very little contribution to the active information when the trajectory passes through that location.

Let us consider this with the simple example of a system which has two states $|\phi_a\rangle$ and $|\phi_b\rangle$. The probability equations are

$$\begin{aligned} P(x) &= w_a R_a(x)^2 + w_b R_b(x)^2 \\ \mathbf{J}(x) &= w_a R_a(x)^2 \nabla S_a(x) + w_b R_b(x)^2 \nabla S_b(x) \end{aligned}$$

Let us suppose that the two states $|\phi_a\rangle$ and $|\phi_b\rangle$ are superorthogonal. This implies $\phi_a(X)\phi_b(X) \approx 0$ for all X . This must also hold for the probability amplitudes $R_a(X)R_b(X) \approx 0$. If the particle trajectory $X(t)$ is located in an area where $R_a(X)$ is non-zero, then now the value of $R_b(X) \approx 0$. The probability equations become

$$\begin{aligned} P(X) &\approx w_a R_a(X)^2 \\ \mathbf{J}(X) &\approx w_a R_a(X)^2 \nabla S_a(X) \end{aligned}$$

and so the particle trajectory

$$m \frac{\partial \mathbf{X}(t)}{\partial t} \approx \nabla S_a(X(t))$$

follows the path it would have taken if system was in the pure state $|\phi_a\rangle$. In this situation, where there is no overlap between the states, then the Bohm trajectories behave in exactly the same manner as if the system had, in fact, been in a statistical ensemble.

⁹The probability current is a standard part of quantum theory, as it's very existence is necessary to ensure the conservation of probability.

Now, if we make the assumption necessary to the Bohm interpretation, that the initial coordinate of the particle trajectory occurs at position $X(0)$, with a probability given by $P(X(0))$, it is apparent that the trajectories, at time t will be distributed at positions $X(t)$ with probability $P(X(t))$. We have therefore consistently extended the Bohm approach to treat density matrices (and therefore thermal states) as a fundamental property of individual systems, rather than statistical ensembles. As we know that the statistics of the outcomes of experiments can be expressed (

We see, exactly as in the pure state situation, that the evolution of one particle trajectory is dependant upon the instantaneous location of the second particle, and vice versa.

The first special case to consider is when the density matrices are uncorrelated

$$\varrho_{1,2} = \varrho_1 \otimes \varrho_2$$

The probability equations reduce to the form

$$P(x_1, x_2) = P(x_1)P(x_2) = \sum_a w_a R_a(x_1)^2 \sum_b w_b R_b(x_2)^2$$

$$\mathbf{J}(x_1, x_2) = P(x_2)\mathbf{J}_1(x_1) + P(x_1)\mathbf{J}_2(x_2)$$

where

$$\mathbf{J}_1(x_1) = \sum_a w_a R_a(x_1)^2 \nabla_{\mathbf{x}_1} S_a(x_1)$$

$$\mathbf{J}_2(x_2) = \sum_b w_b R_b(x_2)^2 \nabla_{\mathbf{x}_2} S_b(x_2)$$

The resulting trajectories

$$m \frac{\partial \mathbf{X}_1(t)}{\partial t} = \frac{\mathbf{J}_1(X_1(t))}{P(X_1(t))}$$

$$m \frac{\partial \mathbf{X}_2(t)}{\partial t} = \frac{\mathbf{J}_2(X_2(t))}{P(X_2(t))}$$

show the behaviour of the two systems are completely independant.

Now let us consider a correlated density matrix

$$\varrho_{1,2} = \frac{1}{2} (|\phi_a \chi_a\rangle \langle \phi_a \chi_a| + |\phi_b \chi_b\rangle \langle \phi_b \chi_b|)$$

where the $|\phi\rangle$ states are for system 1 and the $|\chi\rangle$ states are for system 2. The polar decompositions

$$R_a(x_1)R_a(x_2)e^{iS_a(x_1)+S_a(x_2)} = \langle x_1, x_2 | \phi_a \chi_a \rangle$$

$$R_b(x_1)R_b(x_2)e^{iS_b(x_1)+S_b(x_2)} = \langle x_1, x_2 | \phi_b \chi_b \rangle$$

lead to probability equations

$$P(x_1, x_2) = \frac{1}{2} (R_a(x_1)^2 R_a(x_2)^2 + R_b(x_1)^2 R_b(x_2)^2)$$

$$\mathbf{J}(x_1, x_2) = \frac{1}{2} (R_a(x_1)^2 R_a(x_2)^2 (\nabla_{\mathbf{x}_1} S_a(x_1) + \nabla_{\mathbf{x}_2} S_b(x_2))$$

$$+ R_b(x_1)^2 R_b(x_2)^2 (\nabla_{\mathbf{x}_1} S_b(x_1) + \nabla_{\mathbf{x}_2} S_a(x_2)))$$

The trajectories, $X(t)$, are then given by

$$m \frac{\partial \mathbf{X}_1(t)}{\partial t} = \frac{R_a(X_1(t))^2 R_a(X_2(t))^2 \nabla_{\mathbf{x}_1} S_a(X_1(t)) + R_b(X_1(t))^2 R_b(X_2(t))^2 \nabla_{\mathbf{x}_1} S_b(X_1(t))}{R_a(X_1(t))^2 R_a(X_2(t))^2 + R_b(X_1(t))^2 R_b(X_2(t))^2}$$

$$m \frac{\partial \mathbf{X}_2(t)}{\partial t} = \frac{R_a(X_1(t))^2 R_a(X_2(t))^2 \nabla_{\mathbf{x}_2} S_a(X_2(t)) + R_b(X_1(t))^2 R_b(X_2(t))^2 \nabla_{\mathbf{x}_2} S_b(X_2(t))}{R_a(X_1(t))^2 R_a(X_2(t))^2 + R_b(X_1(t))^2 R_b(X_2(t))^2}$$

Now in general this will lead to a complex coupled behaviour. However, if *either* of the states $|\phi\rangle$ or $|\chi\rangle$ are superorthogonal, then relevant co-ordinate, X_1 or X_2 respectively, will be active for only one of the R_a or R_b states. For example, suppose the $|\chi\rangle$ states are superorthogonal

$$R_a(X_2)R_b(X_2) \approx 0$$

For a given location of X_2 , only one of these probability densities will be non-zero. If we suppose this is the $|\chi_a\rangle$ wavepacket, then $R_b(X_2)^2 \approx 0$. The trajectory equations become

$$\begin{aligned} m \frac{\partial \mathbf{X}_1(t)}{\partial t} &= \frac{R_a(X_1(t))^2 R_a(X_2(t))^2 \nabla_{\mathbf{X}_1} S_a(X_1(t))}{R_a(X_1(t))^2 R_a(X_2(t))^2} \\ &= \nabla_{\mathbf{X}_1} S_a(X_1(t)) \\ m \frac{\partial \mathbf{X}_2(t)}{\partial t} &= \frac{R_a(X_1(t))^2 R_a(X_2(t))^2 \nabla_{\mathbf{X}_2} S_a(X_2(t))}{R_a(X_1(t))^2 R_a(X_2(t))^2} \\ &= \nabla_{\mathbf{X}_2} S_a(X_2(t)) \end{aligned}$$

Both trajectories behave as if the system was in the pure state $|\phi_a \chi_a\rangle$. If the location of X_2 had been within the $|\chi_b\rangle$ wavepacket, then the trajectories would behave exactly as if the system were in the pure state $|\phi_b \chi_b\rangle$. The trajectories, as a whole, behave as if the system was in a statistical mixture of states, as long as at least one of the subsystems has superorthogonal states.

The Bohm approach, by adding the trajectories to the quantum description, is able to avoid the new measurement problem of the density matrix above, by exactly the same method as it avoids the old measurement problem of quantum theory. The loss of phase coherence does not play a fundamental role in the Bohm theory of measurement. It is the superorthogonality that is important, and the principles of active and passive information implied by this. These principles carry directly over into the density matrix description. It is a simple matter to generalise the above arguments to a general N-body system, or to consider states where the diagonalised density matrix involves entangled states.

We will now briefly apply the analysis above to the Interferometer considered in Chapter 3 and the Szilard Engine in Chapters 4 to 8.

Interferometer

The experimental arrangement we will now be considering is not, strictly speaking, the interferometer in Figure 3.1. In that arrangement we send a pure states into a beam splitter, creating a superposition in the arms of the interferometer, and an interference pattern emerges in the region R . Instead we will be considering situations where the atomic state entering the arms of the interferometer is the mixed state

$$\frac{1}{2} (|\phi_u(x, t_1)\rangle \langle \phi_u(x, t_1)| + |\phi_v(x, t_1)\rangle \langle \phi_v(x, t_1)|)$$

No interference effects are expected in the region R .

We will describe the Bohm trajectories for this in the cases where:

1. The mixed state is a physically real density matrix ρ ;

2. The mixed state is a statistical mixture ρ ;
3. The mixed state is a physically real density matrix, and a measurement of the atomic location is performed while the atom is in the interferometer.

Physically real density matrix While the atom is in the arms of the interferometer, the wavepacket corresponding to $|\phi_u\rangle\langle\phi_u|$ and that corresponding to $|\phi_d\rangle\langle\phi_d|$ are superorthogonal. The trajectories in the arms of the interferometer are much as we would expect. However, when the atomic trajectory enters the region R the previously passive information from the other arm of the interferometer becomes active again.

No interference fringes occur in the region R , and if phase shifters are placed in the arms of the interferometer, their settings have no effect upon the trajectories¹⁰. However, the trajectories do change in R . The symmetry of the arrangement, and the 'no-crossing principle' for the flow lines in a probability current, ensures that no actual trajectories can cross the center of the region R . The Bohm trajectories follow the 'surrealistic' paths similar to those in Figure 3.4, even in the absence of phase coherence between the two arms of the interferometer.

Statistical Ensemble We have seen that, even in the absence of phase coherence, the Bohm trajectories for the density matrix show the surrealistic behaviour. Does this represent an unacceptable flaw in the model? To answer this, we now consider the situation where the density matrix is a statistical ensemble of pure states. This situation should more properly be described, for the point of view of the Bohm approach, as an assembly.

First consider the assembly

$$\rho_1 = \Pi_i |\phi_{a_i}\rangle \langle\phi_{a_i}|$$

where $a_i = u$ or d with a probability of one-half. As the assembly consists entirely of product states, the behaviour in each case is independent of the other cases.

If the state is $|\phi_u\rangle\langle\phi_u|$, then the trajectories pass down the u-branch, and go through the interference region without deflection. Similarly, systems in the $|\phi_d\rangle\langle\phi_d|$ state pass down the d-branch and are undeflected at R . These trajectories are what we would expect from an incoherent mixture.

However, now let us consider the assembly

$$\rho_2 = \Pi_i |\phi_{b_i}\rangle \langle\phi_{b_i}|$$

where $b_i = +$ or $-$ occur with equal probability and

$$\begin{aligned} |\phi_+\rangle &= \frac{1}{\sqrt{2}} (|\phi_u\rangle + |\phi_d\rangle) \\ |\phi_-\rangle &= \frac{1}{\sqrt{2}} (|\phi_u\rangle - |\phi_d\rangle) \end{aligned}$$

¹⁰To observe interference fringes we would need a density matrix that diagonalises in a basis that includes non-isotropic superpositions of $|\phi_u\rangle$ and $|\phi_d\rangle$.

This forms exactly the same statistical ensemble. Now, however, in each individual case there will be interference effects within the region R , it is just that the combination of these effects will cancel out over the ensemble. If we were to measure the state in the $(+, -)$ basis, then we would be able to correlate the measurements of this to the location of the atom on the screen and exhibit the interference fringes. The Bohm trajectories for the assembly ρ_2 all reflect in the region R and display the supposed 'surrealistic' behaviour.

There are no observable consequences of the choice of the different assemblies to construct the statistical ensemble¹¹. Consequently, if we are only given the density matrix of a statistical ensemble, we are unable to say which assembly it is constructed from and cannot simply assume that the underlying Bohm trajectories will follow the pattern in Figure 3.2. It is only legitimate to assume the trajectories will pass through the interference region undeflected if we know we have an assembly of $|\phi_u\rangle$ and $|\phi_d\rangle$ states, in which case the Bohm trajectories agree. Thus we conclude the behaviour of the trajectories for the physically real density matrix cannot be ruled out as unacceptable on these grounds.

Measuring the path Finally, we consider what happens when we have the physically real density matrix

$$\varrho = \frac{1}{2} (|\phi_u(x, t_1)\rangle \langle\phi_u(x, t_1)| + |\phi_d(x, t_1)\rangle \langle\phi_d(x, t_1)|)$$

and we include a conventional measuring device in the u-path. The measuring device starts in the state $|\xi_0\rangle$. If the atom is in the state $|\phi_u\rangle$, the measuring device moves into the state $|\xi_1\rangle$. The states $|\xi_0\rangle$ and $|\xi_1\rangle$ are superorthogonal.

If we now apply the interaction to the initial state

$$\varrho \otimes |\xi_0\rangle \langle\xi_0|$$

the system becomes the correlated density matrix

$$\frac{1}{2} (|\phi_u\xi_1\rangle \langle\phi_u\xi_1| + |\phi_u\xi_0\rangle \langle\phi_u\xi_0|)$$

As we saw above, as the measuring device states are superorthogonal, the system behaves exactly as if it were the statistical ensemble. This is true even when the atomic states enter the region R . The Bohm trajectories of the atom pass undeflected through in the manner of Figure 3.2.

We conclude that the Bohm trajectories for the density matrix cannot be considered any more or less acceptable than the trajectories for the pure states.

The Szilard Box

We saw in Section 10.2 that the atom in the Szilard Box can be represented by the physically real density matrix

$$\varrho_{G0} = \frac{1}{Z_{G0}} \sum_n e^{i \frac{\epsilon_n^2}{kT_G}} |\psi_n\rangle \langle\psi_n|$$

¹¹It is interesting to note that if we were to measure the assembly ρ_1 in the $(+, -)$ basis we would still obtain interference fringes!

The probability density calculated from this is

$$P_{G0}(x) = \frac{1}{Z_{G0}} \sum_n e^{i \frac{\epsilon n^2}{\hbar T_G}} R_n(x)^2$$

However, the probability current is zero, ($\mathbf{J}_{G0}(x) = 0$). As a result, the Bohm trajectories for the atom in the box represent it as stationary. This should not be considered too surprising. A similar result occurs for pure states, when the system is in an energy eigenstate. The state ϱ_{G0} is an equilibrium state. While we have a classical picture of such a state as a fluctuating system, in the quantum case we see the equilibrium state is simply stationary!

In reality, of course, the box will be weakly interacting with the environment. This weak interaction will perturb the states of the joint system, and joint density matrix will not be diagonalised exactly in the basis of the joint Hamiltonian. The result will be a complicated correlation of movements of the atom and the environmental degrees of freedom that, in the long run, may produce an equivalent effect to the classical picture of dynamic fluctuations.

However, we will ignore this potential for environmentally induced fluctuation. The potential barrier is inserted into the box and the density matrix divides into

$$\varrho_{G2} = \frac{1}{2} (\varrho_{G2}^\lambda + \varrho_{G2}^\rho)$$

Now the atomic trajectory is actually located on one side or the other of the potential barrier. The information in the other half of the thermal state is rendered passive.

When we insert the moveable piston into the box, the joint density matrix moves into the correlated state

$$\varrho_3(Y) = \frac{1}{2} (\varrho_{G6}^\lambda(Y) \otimes |\Phi(Y)\rangle \langle \Phi(Y)| + \varrho_{G6}^\rho(-Y) \otimes |\Phi(-Y)\rangle \langle \Phi(-Y)|)$$

The changing boundary conditions and the interaction between the piston and gas ensures that the $\varrho_{G6} \otimes |\Phi\rangle \langle \Phi|$ states are not diagonalised in eigenstates of the joint Hamiltonian (we considered this in Section 5.3), so now the Bohm trajectories can move. If the atomic trajectory was located on the left of the partition, then only the lefthand branch of the state is active. The piston trajectory moves to the right, and the atomic trajectory also moves to the right, as the Bohm trajectories of the atom spread out to fill the expanding space.

As the piston states move, the ϱ_{G6}^λ and ϱ_{G6}^ρ states start to overlap. However, this can only happen once the piston states have become superorthogonal. The information in the passive atomic state does not become active again.

So the Bohm trajectories for the thermal states, in this case, confirm the naive classical picture of the Szilard Box. The atom is indeed located on one side of the partition, and the piston can move in the opposite direction, extracting heat from the expansion of the gas. However, as we have seen, the Engine cannot violate the second law of thermodynamics. We explained this in Chapter 8 from the unitarity of the evolution. The unitary operator must be defined upon the entire Hilbert space. This so constrains the evolution that the Engine cannot operate without either error or an input of work from outside (as a heat pump).

From the point of view of the Bohm theory, the need to define the unitary operation upon the entire Hilbert space is not an abstract issue. The portion of the Hilbert space that is not active is not empty anymore. It is filled with the physically real, but passive, alternate state. The passive information in this state cannot be abandoned, anymore than the passive information from the second arm of the interferometer can be abandoned. Attempting to reset the piston at the end of the cycle fails because the previously passive information, representing the piston state that moved to the left in our example above, is still physically present, and will combine with the active state containing the actual piston trajectory.

What of the Szilard paradox? If the atom and piston have physically real trajectories, does the correlation reduce the entropy? The answer is that the entropy, as defined for the complete density matrix, does not decrease. On the other hand, the entropy of the active part of the density matrix *can* go down, and does when a correlated measurement takes place. This does not represent a conceptual problem, however, as the passive part of the density matrix no longer represents a fictitious possibility that did not occur. Instead it represents the physically real thermal state, which just happens to be passive at this point in time.

10.4 Conclusion

The classical conception of information, given by the Shannon measure, represents the ignorance about an actually existing property of a system. As measurements are performed, the state of the observer becomes correlated to the state of the observed system. The correlation, or mutual information, represents the increase in knowledge the observer has about the actual state of the system. With sufficiently refined measurements the observer can gain a perfect knowledge of the exact state of the system and over an ensemble of systems, can discover the ensemble probability distribution.

In classical statistical mechanics, the Gibbs entropy shares the same functional form as the Shannon information measure. This can lead to the argument that entropy *is* simply the lack of information about the system. Such an argument, however, directly implies that, by performing a measurement upon the system, its entropy can be reduced. The flaw in this argument is that it fails to include the observer as an active participant in the system. This inclusion is necessary to understand why the second law of thermodynamics cannot be broken by Maxwell's Demon. However, this inclusion now makes it hard to interpret entropy as a lack of information. Originally, we described the entropy of the system as the lack of information possessed by the observer. However, as we now have to include the entropy of the observer in the system, it is unclear whose lack of information we are supposed to attribute this to. It can no longer be the observer, who is fully aware of which state he is in.

With quantum theory, the situation becomes more complex. The Schumacher information measure shares the same form as the von Neumann entropy. However, except in the case of

communication, where a receiver is in possession of a priori knowledge of which signal states are being sent, it is no longer clear what the 'information' is referring to. It cannot be simply assumed that the measurement reveals a pre-existing property of the measured system. A given density matrix may be formed from many different combinations of signal states, and there is no measurement procedure that is able to uncover which is the correct one. When the system is in a superposition of states, such as in the interferometer, the information gathering measurement plays an active role in the creation of the phenomena it is intended to measure.

It has been suggested that the 'wavefunction collapse' involved in the measurement process is a necessary part of understanding the problem of Maxwell's Demon. However, we have shown that the linearity of quantum mechanics proves the opposite: wavefunction collapse plays no role in Szilard's Engine. The demon, in fact, need perform no information processing at all and still fulfil it's function as an auxiliary system. Nevertheless, the conceptual problem remains, that the thermodynamic properties are possessed only by the fictitious ensemble and not by the actual physical system.

We now turn to the concept of active information in quantum theory. This suggests that, in addition to the wavefunction, there is a particle trajectory, or center of activity. The Hamiltonian encodes the information about the system into the evolution of the wavefunction, and this information guides the particle trajectory. When a measurement occurs, the information in the unobserved outcomes is no longer active, through the non-local correlation between the system and the measuring device. The information considered here is not simply a static correlation between two systems, but is a dynamic principle, actively organising the behaviour of the system.

By extending the Bohm interpretation to cover density matrices, we showed it was possible to consistently treat the density matrix as a property, not of an ensemble, but of an individual system. The temperature and entropy of thermal systems can then be regarded as physically real attributes. Again, when a measurement occurs, the information in unobserved outcome is passive, but still physically real. Although the entropy of the active branch of the system may be reduced, the total entropy is constant.

It is interesting to note that it is only because the Bohm interpretation is a no-collapse interpretation that this is possible. Suppose we assumed the density matrix was physically real, rather than an ensemble, and applied a wavefunction collapse interpretation. As we performed our measurements, the density matrix would rapidly become converted into a statistical ensemble again. We would be forced to say that the physical entropy of the system was decreasing. The total entropy would again become a property only of the statistical ensemble.

In both statistical mechanics and quantum measurement it is necessary to include the observer as an active participant in the system if we are to avoid apparent paradoxes. The Bohm interpretation and activity of information provides a unified framework for understanding both.

Appendix A

Quantum State Teleportation

Quantum state teleportation¹ has focused attention on the role of quantum information. Here we examine quantum teleportation through the Bohm interpretation. This interpretation introduced the notion of active information and we show that it is this information that is exchanged during teleportation. We discuss the relation between our notion of active information and the notion of quantum information introduced by Schumacher.

A.1 Introduction

The recent discovery of quantum state teleportation [BBC⁺93] has re-focused attention on the nature of quantum information and the role of quantum non-locality in the transfer of information. Developments in this area have involved state interchange teleportation [Mou97], as well as multi-particle entanglement swapping [BKV97], and position/momentum state teleportation [Vai94]. Although these effects arise from a straight forward application of the formalism, the nature of the quantum information and its transfer still presents difficulties. Attempts to address the issue from the perspective of information theory [HH96, AC95] and without invoking wave function collapse [Bra96] have clarified certain aspects of this process but problems still remain.

In order to obtain a different perspective on these phenomena we first review the salient features of the Bohm interpretation that are of direct relevance to these situations [Boh52a, Boh52b, BH93, Hol93, Bel87], before applying its techniques to the specific example of spin teleportation. One of the advantages of using this approach in the present context is that to account for quantum processes it is necessary to introduce the notion of ‘active’ information. This notion was introduced by Bohm & Hiley [BH93] to account for the properties of the quantum potential which cannot be consistently regarded as a *mechanical potential* for reasons explained in Bohm & Hiley [BH93]. There is also the added advantage that the approach gives a clear physical picture of the process at all times, and, therefore provides an unambiguous description of where and how the

¹The material in this Appendix originally appeared in [HM99] as a joint paper with B J Hiley.

‘quantum information’ is manifested. In this paper we will discuss how the three notions of active, passive and inactive information are of relevance to the teleportation problem.

A.2 Quantum Teleportation

The basic structure of quantum teleportation can be expressed using three spin- $\frac{1}{2}$ particles, with particles 2 and 3 initially in a maximally entangled EPRB state, and particle 1, in an unknown superposition:

$$\Psi_1 = (a|\uparrow\rangle_1 + b|\downarrow\rangle_1)(|\uparrow\rangle_2|\downarrow\rangle_3 - |\downarrow\rangle_2|\uparrow\rangle_3)/\sqrt{2}$$

By introducing the ‘Bell states’

$$\begin{aligned} \beta_1^{(ij)} &= (|\uparrow\rangle_i|\uparrow\rangle_j + |\downarrow\rangle_i|\downarrow\rangle_j)/\sqrt{2} & \beta_2^{(ij)} &= (|\uparrow\rangle_i|\uparrow\rangle_j - |\downarrow\rangle_i|\downarrow\rangle_j)/\sqrt{2} \\ \beta_3^{(ij)} &= (|\uparrow\rangle_i|\downarrow\rangle_j + |\downarrow\rangle_i|\uparrow\rangle_j)/\sqrt{2} & \beta_4^{(ij)} &= (|\uparrow\rangle_i|\downarrow\rangle_j - |\downarrow\rangle_i|\uparrow\rangle_j)/\sqrt{2} \end{aligned}$$

we can re-write Ψ_1 as

$$\begin{aligned} \Psi_2 &= (\beta_1^{(12)} [-b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \beta_2^{(12)} [+b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \\ &\quad \beta_3^{(12)} [-a|\uparrow\rangle_3 + b|\downarrow\rangle_3] + \beta_4^{(12)} [-a|\uparrow\rangle_3 - b|\downarrow\rangle_3])/2 \end{aligned}$$

If we now measure the Bell state of particles 1 and 2, and communicate the result to the recipient of particle 3 who will, using that information, then perform one of the local unitary operations on particle 3 given below

$$\begin{aligned} U_1 &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, & U_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ U_3 &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, & U_4 &= \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}. \end{aligned}$$

In this way we have disentangled particle 3 from particle 2 and produced the state $(a|\uparrow\rangle_3 + b|\downarrow\rangle_3)$ on particle 3. Thus the information represented by [a,b] has been perfectly ‘teleported’ from particle 1 to particle 3, without our having measured a or b directly. Furthermore, during the transfer process we have only passed 2 classical bits of information (corresponding only to the choice of U) between the remote particles. Note that as ‘a’ and ‘b’ are continuous parameters, it would require an infinite number of classical bits to perfectly specify the [a,b] state. This ability to teleport accurately has been shown to be critically dependant upon the degree of entanglement of particles 2 and 3 [HH96, Pop94].

We may note that in the Bell state expansion, the information signified by the coefficients [a,b] appears on the particle 3 spin states before any actual measurement has taken place (although this information is encoded in a different way for each Bell state). What are we to make of this?

It would seem absurd to assume that the information described by a and b was already attached to particle 3 as, at this stage, particle 1 could be any other particle in the universe. Indeed all

that has happened is that Ψ_1 has been re-written in a different basis to give Ψ_2 . Clearly this cannot be regarded as an actual physical effect.

Following Heisenberg [Hei58] and Bohm [Boh51], we can regard the wave function as describing potentialities. At this stage Ψ_2 describes the potentiality that particle 3 could carry the [a,b] information that would be actualised during the measurement. However, here we have a problem as Braunstein [Bra96] has shown that a collapse of the wavefunction (the usual mechanism by which such potentialities become actualised) is unnecessary to the description of quantum teleportation, by including the Bell state measuring device within the quantum formalism. Using this description, we find that the attachment of the [a,b] information to particle 3, *after* the Bell state interaction, is the same as in the Ψ_2 expansion *prior* to the interaction. While this is clearly necessary to maintain the no-signalling theorem, it leaves ambiguous the question of whether the [a,b] information has been transferred to particle 3, at this stage, or not.

To resolve these issues, we need to give a clearer meaning to the nature of the information contained in [a,b] and to understand how and when this information becomes manifested at particle 3. We now turn to the Bohm interpretation (Chapter 3) to provide some new insights into these questions.

A.3 Quantum State Teleportation and Active Information

In order to examine how the idea of active and passive information can be used in quantum teleportation, we must explain how spin is discussed in the Bohm interpretation. There have been several different approaches to spin [BH93, Hol88, Alb92], but this ambiguity need not concern us here as we are trying to clarify the principles involved. Thus for the purpose of this article we will adopt the simplest model that was introduced by Bohm, Schiller and Tiomno [BST55, DHK87]. We start by rewriting the polar decomposition of the wave function as $\Psi = R e^{iS} \Phi$ where Φ is a spinor with unit magnitude and zero average phase. If we write:

$$\Phi = \begin{pmatrix} r_1 e^{i s_1} \\ r_2 e^{i s_2} \\ \vdots \\ r_n e^{i s_n} \end{pmatrix}$$

where n is the dimension of the spinor space, then $\sum_i s_i = 0$ and $\sum_i (r_i)^2 = 1$. The many-body Pauli equation then leads to a modified quantum Hamilton-Jacobi equation given by:

$$\frac{\partial S}{\partial t} - i \Phi^\mathcal{Y} \frac{\partial \Phi}{\partial t} = - \sum_i \left(\frac{p_i^2}{2m} + Q_i + 2\mu_i \mathbf{B} \cdot \mathbf{s}_i \right)$$

with a momentum $p_i = \nabla_i S + \Phi^\mathcal{Y} \nabla_i \Phi$, a quantum potential $Q_i = \frac{1}{2m} (-\nabla_i^2 R + \nabla_i \Phi^\mathcal{Y} \nabla_i \Phi + (\Phi^\mathcal{Y} \nabla_i \Phi)^2)$. \mathbf{B} is the magnetic field and μ_i is the magnetic dipole moment associated with particle i . We can, in addition, attribute a real physical angular momentum to each particle i given by $\mathbf{s}_i = \frac{1}{2} \Psi^\mathcal{Y} \sigma_i \Psi$, where σ_i are the Pauli matrices operating solely in the spinor subspace of particle i .

The information contained in the spinor wave function is again encoded in the quantum potential, so that the trajectory of the particle is guided by the evolution of the spinor states, in addition to the classical interaction of the \mathbf{B} field with the magnetic dipole moment of the particle. Contracting the Pauli equation with $\Psi^\mathcal{Y}\sigma_i$ leads the equation of motion for the particle i spin vector:

$$\frac{d\mathbf{s}_i}{dt} = \mathbf{T}_i + 2\mu_i\mathbf{B} \times \mathbf{s}_i$$

where \mathbf{T}_i is a quantum torque. The k components of the torque are given by

$$[T_i]_k = \sum_j \frac{1}{2\rho m_j} \epsilon_{klm} \{ [s_i]_l [\nabla_j]_n (\rho [\nabla_j]_n [s_i]_m) + s_{lr} [\nabla_j]_n (\rho [\nabla_j]_n s_{mr}) \}$$

where $\rho = R^2$ and s_{ij} is the non-local spin correlation tensor formed from $\Psi^\mathcal{Y}\sigma_i\sigma_j\Psi$. Equations of motion for these tensors can be derived by contracting the Pauli equation with $\Psi^\mathcal{Y}\sigma_i\sigma_j$, and similarly for higher dimension correlation tensors. Detailed application of these ideas to the entangled spin state problem has been demonstrated in Dewdney et al. [DHK87].

To complete the description of the particles, we must attach position wave functions to each of the particles. We do this by assuming that each particle can be represented by a localised wavepacket. Thus, for the teleportation problem:

$$\begin{aligned} \Psi &= (a|\uparrow\rangle_1 + b|\downarrow\rangle_1)(|\uparrow\rangle_2|\downarrow\rangle_3 - |\downarrow\rangle_2|\uparrow\rangle_3)\rho(x_1)\phi(x_2)\xi(x_3)/\sqrt{2} \\ &= \{\beta_1^{(12)}[-b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \beta_2^{(12)}[+b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \\ &\quad \beta_3^{(12)}[-a|\uparrow\rangle_3 + b|\downarrow\rangle_3] + \beta_4^{(12)}[-a|\uparrow\rangle_3 - b|\downarrow\rangle_3]\}\rho_j \end{aligned}$$

subsequent measurement of the spin of particle 3, would divide $\xi(x_3)$ into two, but particle 3 would always enter the wavepacket on the same branch of the superposition as particle 2 had entered earlier, as only the information in that branch is active. This has been beautifully illustrated by Dewdney et al. [DHK87]

As the particle 1 is in a separable state for both spin and position, no local interactions on particle 2 or 3 will have any effect on the trajectory and spin of particle 1. Neither will any measurement on particle 1 produce any effect on particles 2 and 3. The behaviour of the spins of particles 2 and 3 will be determined by the pool of information common to them both, while only the behaviour of particle 1 is determined by the [a,b] information, regardless of the basis in which the spin states are expanded.

Now let us return to the main theme of this paper and consider the measurement that produces teleportation. Here we need to introduce a Bell state measurement. Let the instrument needed for this measurement be described by the wavepacket $\eta(x_0)$ where x_0 is a variable (or a set of variables) characterising the state of this apparatus. The measurement is achieved via an interaction Hamiltonian that can be written in the form $H = \mathbf{O}^{(12)}\nabla_0$.

The interaction operator $\mathbf{O}^{(12)} = \lambda O_\lambda^{(12)}$ couples the x_0 co-ordinate to the Bell state of particles 1 and 2 through the Bell state projection operators $O_\lambda = \beta_\lambda \beta_\lambda^y$. This creates the state

$$\begin{aligned} \Psi_f = & \{ \eta_1(x_0)\beta_1^{(12)}[-b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \eta_2(x_0)\beta_2^{(12)}[+b|\uparrow\rangle_3 + a|\downarrow\rangle_3] + \\ & \eta_3(x_0)\beta_3^{(12)}[-a|\uparrow\rangle_3 + b|\downarrow\rangle_3] + \eta_4(x_0)\beta_4^{(12)}[-a|\uparrow\rangle_3 - b|\downarrow\rangle_3] \} \\ & \rho(x_1)\phi(x_2)\xi(x_3)/2 \end{aligned}$$

where $\eta_1(x_0)$, $\eta_2(x_0)$, $\eta_3(x_0)$ and $\eta_4(x_0)$ are the wavepackets of the four non-overlapping position states corresponding to the four outcomes of the Bell state measuring instrument. Initially all four systems become entangled and their behaviour will be determined by the new common pool of information. This includes the [a,b] information that was initially associated *only* with particle 1.

As the position variable x_0 of the measuring device enters one of the non-overlapping wavepackets $\eta_i(x_0)$, only one of the branches of the superposition remains active, and the information in the other branches will become passive. As this happens, particle 3 will develop a non-zero particle spin \mathbf{s}_3 , through the action of the quantum torque. The explicit non-locality of this allows the affects of the Bell state measurement to instantaneously have an effect upon the behaviour of particle 3. The significance of the Ψ_2 Bell state expansion is now revealed as simply the appropriate basis for which the [a,b] information will be transferred entirely onto the behaviour of particle 3, if only a single branch of the superposition were to remain active. The interaction with the Bell state measuring device is required to bring about this change from active to passive information in the other branches (and thereby actualising the potentiality of the remaining branch).

However, no meaningful information on [a,b] may yet be uncovered at particle 3 until it is known which branch is active, as the average over all branches, occurring in an ensemble, will be statistically indistinguishable from no Bell state measurement having taken place. Simply by noting the actual position (x_0) of the measuring device, the observer, near particles 1 and

2, immediately knows which wavepacket x_0 has entered, and therefore which state is active for particle 3. The observer then sends this classical information to the observer at 3 who will then apply the appropriate unitary transformation $U_1 \cdots U_4$ so that the initial spin state of particle 1 can be recovered at particle 3.

A.4 Conclusion

In the approach we have adopted here, the notion of active information introduced by Bohm and Hiley [BH93] has been applied to the phenomenon of state teleportation. This gives rise to a different perspective on this phenomenon and provides further insight into the notion of quantum information. To see more clearly how teleportation arises in this approach let us re-examine the above spin example in more general terms. The essential features can be seen by examining the general structure of the quantum potential. Using the initial wave function, Ψ_i given above, the quantum potential takes the form

$$Q(x_1, x_2, x_3) = Q_1(x_1, a, b)Q_{23}(x_2, x_3)$$

Here the coefficients a and b characterise the quantum potential acting only on particle 1. This means that initially the information carried by the pair $[a, b]$ actively operates on particle 1 alone. At this stage the behaviour of particle 3 is independent of a and b , as we would expect.

To perform a Bell State measurement we must couple particle 1 to particle 2 by introducing the interaction Hamiltonian given above. During this process, a quantum potential will be generated that will couple all three particles with the measuring apparatus. When the interaction is over, the final wave function becomes Ψ_f . This will produce a quantum potential that can be written in the form

$$Q(x_1, x_2, x_3, x_0) = Q_{12}(x_1, x_2, x_0)Q_3(x_3, x_0, a, b)$$

Thus after the measurement has been completed, the information contained in a and b has now been encoded in Q_3 which provides the active information for particle 3. Thus we see that the information that was active on particle 1 has been transferred to particle 3. In turn this particle has been decoupled from particle 2. Thus the subsequent spin behaviour of particle 3 will be different after the measurement.

What we see clearly emerging here is that it is *active information* that has been transferred from particle 1 to particle 3 and that this transfer has been mediated by the non-local quantum potential. Let us stress once again that this information is in-formation for the particle and, at this stage has nothing to do with ‘information for us’.

Previous discussions involving quantum information have been in terms of its relation to Shannon information theory [Sch95]. In classical information theory, the expression $H(A) = -\sum p_a \log_2 p_a$ is regarded as the entropy of the source. Here p_a is the probability that the message source produces the message a . This can be understood to provide a measure of the mean

number of bits, per signal, necessary to encode the output of a source. It can also be thought of as a capacity of the source to carry potential information. The interest here is in the transfer of ‘information for us’.

Schumacher[Sch95] extended Shannon’s ideas to the quantum domain by introducing the notion of a ‘qbit’ (the number of qbits per quantum system is $\log_2(H)$, where H is the dimension of the system Hilbert space). A spin state with two eigenvalues, say 0 and 1, can be used to encode 1 bit of information. To relate this to Shannon’s source entropy, Schumacher represents the signal source by a source density operator

$$\rho = \sum_a p(a)\pi_a$$

where $\pi_a = |a_i\rangle\langle a_i|$ is the set of orthogonal operators relevant to the measurements that will be performed and $p(a)$ is the probability of a given eigenvalue being found. The von Neumann information $S(\rho) = \text{Tr}(\rho \log_2 \rho)$ corresponds to the mean number of qbits, per signal, necessary for

Appendix B

Consistent histories and the Bohm approach

In a recent paper Griffiths¹ claims that the consistent histories interpretation of quantum mechanics gives rise to results that contradict those obtained from the Bohm interpretation. This is in spite of the fact that both claim to provide a realist interpretation of the formalism without the need to add any new *mathematical* content and both always produce exactly the same probability predictions of the outcome of experiments. In contrasting the differences Griffiths argues that the consistent histories interpretation provides a more physically reasonable account of quantum phenomena. We examine this claim and show that the consistent histories approach is not without its difficulties.

B.1 Introduction

It is well known that realist interpretations of the quantum formalism are known to be notoriously difficult to sustain and it is only natural that the two competing approaches, the consistent history interpretation (CH) [Gri84] [Gri96] and the Bohm interpretation (BI)[BH87, BH93], should be carefully compared and contrasted. Griffiths [Gri99] is right to explore how the two approaches apply to interferometers of the type shown in Figure B.1.

Although the predictions of experimental outcomes expressed in terms of probabilities are identical, Griffiths argues that, nevertheless, the two approaches actually give very different accounts of how a particle is supposed to pass through such an interferometer. After a detailed analysis of experiments based on Figure B.1, he concludes that the CH approach gives a behaviour that is ‘physically acceptable’, whereas the Bohm trajectories behave in a way that appears counter-intuitive and therefore ‘unacceptable’. This behaviour has even been called ‘surrealistic’ by some authors². Griffiths concludes that a particle is unlikely to actually behave in such a way so that one

¹The material in this Appendix originally appeared on the Los Alamos e-print archive[HM00] as a joint paper with B J Hiley.

²This original criticism was made by Englert et al. [ESSW92]. An extensive discussion of this position has been

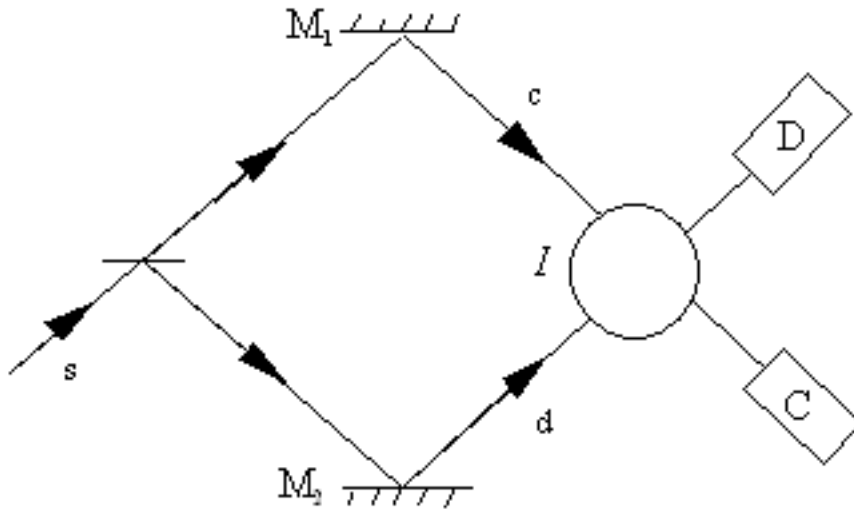


Figure B.1: Simple interferometer

can conclude that the CH interpretation gives a ‘more acceptable’ account of quantum phenomena. Notice that these claims are being made in spite of the fact no new mathematical structure whatsoever is added to the quantum formalism in either CH or BI, and in consequence all the experimental predictions of both CH and BI are identical to those obtained from standard quantum mechanics. Clearly there is a problem here and the purpose of our paper is to explore how this difference arises. We will show that CH is not without its difficulties.

We should remark here in passing that these difficulties have already been brought out by Bassi and Ghirardi [BG99a, BG99b, BG99c] and an answer has been given by Griffiths [Gri00]. At this stage we will not take sides in this general debate. Instead we will examine carefully how the analysis of the particle behaviour in CH when applied to the interferometer shown in Figure B.1 leads to difficulties similar to those highlighted by Bassi and Ghirardi [BG99b].

B.2 Histories and trajectories

The first problem we face in comparing the two approaches is that BI uses a mathematically well defined concept of a trajectory, whereas CH does not use such a notion, defining a more general notion of a history.

Let us first deal with the Bohm trajectory, which arises in the following way. If the particle satisfies the Schrödinger equation then the trajectories are identified with the one-parameter solutions of the real part of the Schrödinger equation obtained under polar decomposition of the wave function [BH93]. Clearly these one-parameter curves are mathematically well defined and unambiguous.

CH does not use the notion of a trajectory. It uses instead the concept of a history, which, again, is mathematically well defined to be a series of projection operators linked by Schrödinger evolution presented by Hiley, Callaghan and Maroney [CHM00].

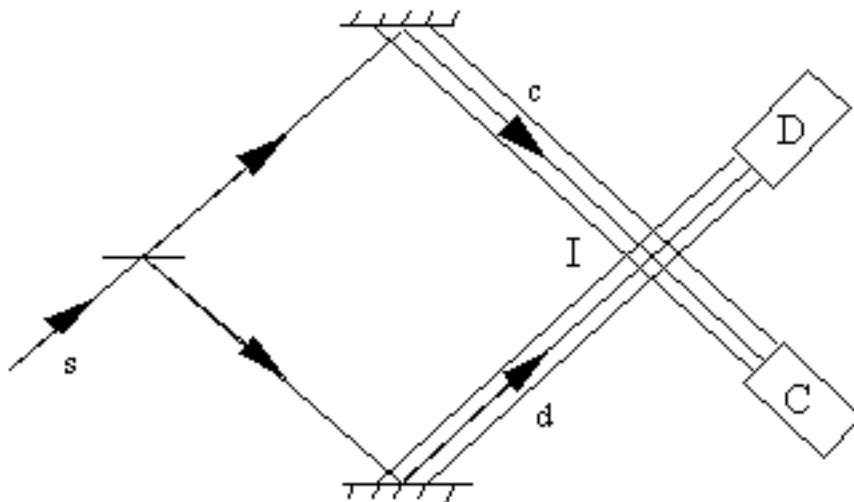


Figure B.2: The CH ‘trajectories’.

evolution and satisfying a certainty consistency condition [Gri84]. Although in general a history is not a trajectory, in the particular example considered by Griffiths, certain histories can be considered to provide approximate trajectories. For example, when particles are described by narrow wave packets, the history can be regarded as defining a kind of broad ‘trajectory’ or ‘channel’. It is assumed that in the experiment shown in figure 1, this channel is narrow enough to allow comparison with the Bohm trajectories.

To bring out the apparent difference in the predictions of the two approaches, consider the interferometer shown in Figure B.1. According to CH if we choose the correct framework, we can say that if *C* fires, the particle must have travelled along the path *c* to the detector and any other path is regarded as “dynamically impossible” because it violates the consistency conditions. The type of trajectories that would be acceptable from this point of view are sketched in Figure B.2. In contrast a pair of typical Bohm trajectories³ are shown in Figure B.3. Such trajectories are clearly not what we would expect from our experience in the classical world. Furthermore there appears, at least at first sight, to be no visible structure present that would ‘cause’ the trajectories to be ‘reflected’ in the region *I*, although in this region interference between the two beams is taking place. In the Bohm approach, an additional potential, the quantum potential, appears in the region of interference and it is this potential that has a structure which ‘reflects’ the trajectories as shown in Figure B.3. (See Hiley et al. [CHM00] for more details). In this short note we will show that the conclusions reached by Griffiths [Gri99] cannot be sustained and that it is not possible to conclude that the Bohm ‘trajectories’ must be ‘unreliable’ or ‘wrong’. We will show that CH cannot be used in this way and the conclusions drawn by Griffiths are not sound.

³Detailed examples of these trajectories will be found in Hiley, Callaghan and Maroney [CHM00].

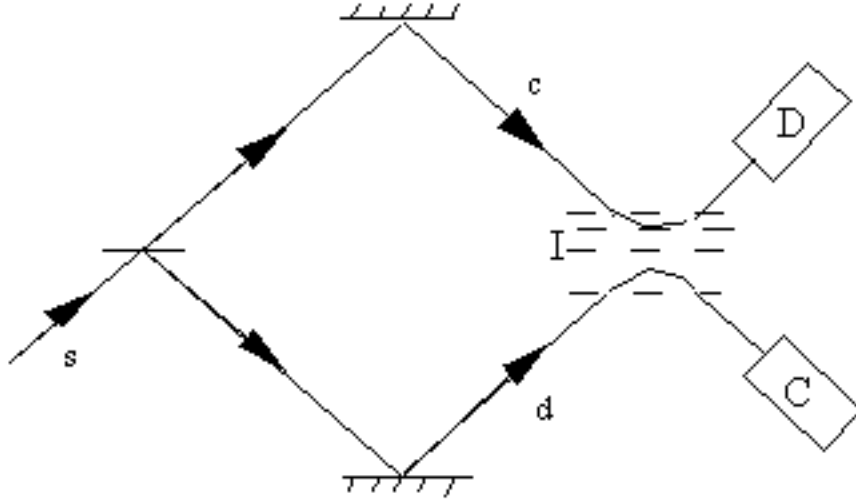


Figure B.3: The Bohm trajectories.

B.3 The interference experiment

Let us analyse the experimental situation shown in figure 1 from the point of view of CH. A unitary transformation $U(t_{j+1}, t_j)$ is used to connect set of projection operators at various times. The times of interest in this example will be t_0, t_1 , and t_2 . t_0 is a time before the particle enters the beam splitter, t_2 is the time at which a response occurs in one of the detectors C or D and t_1 is some intermediary time when the particle is in the interferometer before the region I is reached by the wave packets.

The transformation for $t_0 \rightarrow t_1$ is

$$|\psi_0\rangle = |sCD\rangle_0 \rightarrow \frac{1}{\sqrt{2}}[|cC^{\sigma}D\rangle_1 + |dCD^{\sigma}\rangle_1] \quad (\text{B.1})$$

The transformation for $t_1 \rightarrow t_2$ is, according to Griffiths [Gri93, Gri99]

$$|cCD\rangle_1 \rightarrow |C^{\sigma}D\rangle_2, \quad \text{and} \quad |dCD\rangle_1 \rightarrow |CD^{\sigma}\rangle_2 \quad (\text{B.2})$$

These lead to the histories

$$\psi_0 \otimes c_1 \otimes C_2^{\sigma}, \quad \text{and} \quad \psi_0 \otimes d_1 \otimes D_2^{\sigma} \quad (\text{B.3})$$

Here ψ_0 is short hand for the projection operator $|\psi\rangle\langle\psi|$ at time t_0 etc.

These are not the only possible consistent histories but only these two histories are used by Griffiths to make judgements about the Bohm trajectories. The two other possible histories

$$\psi_0 \otimes d_1 \otimes C_2^{\sigma}, \quad \text{and} \quad \psi_0 \otimes c_1 \otimes D_2^{\sigma} \quad (\text{B.4})$$

have zero weight and are therefore deemed to be *dynamically impossible*.

The significance of the histories described by equation B.3 is that they give rise to new conditional probabilities that *cannot* be obtained from the Born probability rule [Gri98]. These conditional probabilities are

$$Pr(c_1|\psi_0 \wedge C_2^{\sigma}) = 1, \quad Pr(d_1|\psi_0 \wedge D_2^{\sigma}) = 1. \quad (\text{B.5})$$

Starting from a given initial state, ψ_0 , these probabilities are interpreted as asserting that when the detector C is triggered at t_2 , one can be certain that, at the time t_1 , the particle was in the channel c and not in the channel d . In other words when C fires we know that the triggering particle must have travelled down path c with certainty.

This is the key new result from which the difference between the predictions of CH and the Bohm approach arises. Furthermore it must be stressed that this result cannot be obtained from the Born probability rule and is claimed by Griffiths [Gri98] to be a new result that does not appear in standard quantum theory⁴.

Looking again at Figure B.1, we notice that there is a region I where the wave packets travelling down c and d overlap. Here interference can and does take place. In fact fringes will appear along any vertical plane in this region as can be easily demonstrated. Indeed this interference is exactly the same as that produced in a two-slit experiment. The only change is that the two slits have been replaced by two mirrors. Once this is realised alarm-bells should ring because the probabilities in B.5 imply that we know with certainty through which slit the particle passed. Indeed equation B.5 shows that the particles passing through the lower slit will arrive in the upper region of the fringe pattern, while those passing through the upper slit will arrive in the lower half⁵.

Recall that Griffiths claims CH provides a clear and consistent account of standard quantum mechanics, but the standard theory denies the possibility of knowing which path the particle took when interference is present. Thus the interpretation of equation B.5 leads to a result that is not part of the standard quantum theory and in fact contradicts it. Nevertheless CH uses the authority of the standard approach to strengthen its case against the Bohm approach. Surely this cannot be correct.

Indeed Griffiths has already discussed the two-slit experiment in an earlier paper [Gri94]. Here he argues that CH does not allow us to infer through which slit the particle passes. He writes; -

Given this choice at t_3 [whether C or D fires], it is inconsistent to specify a decomposition at time t_2 [our t_1] which specifies which slit the particle has passed through, i.e., by including the projector corresponding to the particle being in the region of space just behind the A slit [our c], and in another region just behind the B slit [our d]. That is (15) [the consistency condition] will not be satisfied if projectors of this type at time t_2 [our t_1] are used along with those mentioned earlier for time t_3 .

The only essential difference between the two-slit experiment and the interferometer described by equation B.3 above is in the position of the detectors. But according to CH measurement merely reveals what is already there, so that the position of the detector in the region I or beyond should not affect anything. Thus there appears to be a contradiction here.

⁴It should be noted that the converse of B.5 must also hold. Namely, if C does not fire then we can conclude that at t_2 the particle was in channel c . That is, if C does not fire then we can conclude that at t_2 the particle was in channel c . That is, if C does not fire then we can conclude that at t_2 the particle was in channel c .

To emphasise this difficulty we will spell out the contradiction again. The interferometer in Figure B.1 requires the amplitude of the incident beam to be split into two before the beams are brought back together again to overlap in the region I . This is exactly the same process occurring in the two-slit experiment. Yet in the two-slit experiment we are not allowed to infer through which slit the particle passed while retaining interference, whereas according to Griffiths we are allowed to talk about which mirror the particle is reflected off, presumably without also destroying the interference in the region I . We will return to this specific point again later.

One way of avoiding this contradiction is to assume the following: -

1. If we place our detectors in the arms c and d before the interference region I is reached then we have the consistent histories described in equation B.3. Particles travelling down c will fire C , while those travelling down d will fire D . In this case we have an exact agreement with the Bohm trajectories.

2. If we place our detectors in the region of interference I then, according to Griffiths [Gri94], the histories described by equation B.3 are no longer consistent. In this case CH can say nothing about trajectories.

3. If we place our detectors in the positions shown in Figure B.1, then, according to Griffiths [Gri99], the consistent histories are described by equation B.3 again. Here the conditional probabilities imply that all the particles travelling down c will always fire C . Bohm trajectories contradict this result and show that some of these particles will cause D to fire. These trajectories are shown in Figure B.3.

It could be argued that this patchwork would violate the *one-framework rule*. Namely that one must either use the consistent histories described by equation B.3 or use a set of consistent histories that do not allow us to infer off which mirror the particle was reflected. This latter would allow us to account for the interference effects that must appear in the region I .

A typical set of consistent histories that do not allow us to infer through which slit the particle passed can be constructed in the following way.

Introduce a new set of projection operators $|(c+d)\rangle\langle(c+d)|$ at t_3 where $t_1 < t_3 < t_2$. Then we have the following possible histories

$$\psi_0 \otimes (c+d)_3 \otimes C_2^\alpha, \quad \text{and} \quad \psi_0 \otimes (c+d)_3 \otimes D_2^\alpha \quad (\text{B.6})$$

Clearly from this set of histories we cannot infer any generalised notion of a trajectory so that we cannot say from which mirror the particle is reflected. What this means then is that if we want to talk about trajectories we must, according to CH, use the histories described by equation (3) to cover the whole region as, in fact, Griffiths [Gri99] actually does. But then surely the nodes in the interference pattern at I will cause a problem.

To bring out this problem let us first forget about theory and consider what actually happens experimentally as we move the detector C along a straight line towards the mirror M_1 . The detection rate will be constant as we move it towards the region I . Once it enters this region, we

will find that its counting rate varies and will go through several zeros corresponding to the nodes in the interference pattern. Here we will assume that the detector is small enough to register these nodes.

Let us examine what happens to the conditional probabilities as the detector crosses the interference region. Initially according to B.5, the first history gives the conditional probability $Pr(c_1|\psi_0 \wedge C_3^a) = 1$. However, at the nodes this conditional probability cannot even be defined as $Pr(C_3^a) = 0$. Let us start again with the closely related conditional probability, derived from the same history $Pr(C_3^a|\psi_0 \wedge c_1) = 1$. Now this probability clearly cannot be continued across the interference region because $Pr(C_3^a) = 0$ at the nodes, while $Pr(\psi_0 \wedge c_1) = 0.5$ regardless of where the detector is placed. In fact, there is no consistent history that includes both c_1 and C_3^a , when the detector is in the interference region. We are thus forced to consider different consistent histories in different regions as we discussed above.

If we follow this prescription then when the detector C is placed on the mirror side of path c , before the beams cross at I , we can talk about trajectories and as stated above these trajectories agree with the corresponding Bohm trajectories. When C is moved right through and beyond the region I , we can again talk about trajectories. However in the intermediate region CH does not allow us to talk about trajectories. This means that we have no continuity across the region of interference and this lack of continuity means that it is not possible to conclude that any ‘trajectory’ defined by $\psi_0 \otimes c_1 \otimes C^a$ before C reaches the interference region is the same ‘trajectory’ defined by the same expression after C has passed through the interference region. In other words we cannot conclude that any particle travelling down c will continue to travel in the same direction through the region of interference and emerge still travelling in the same direction to trigger detector C .

What this means is that CH cannot be used to draw any conclusions on the validity or otherwise of the Bohm trajectories. These latter trajectories are continuous throughout *all* regions. They are straight lines from the mirror until they reach the region I . They continue into the region of interference, but no longer travel in straight lines parallel to the initial their paths. They show ‘kinks’ that are characteristic of interference-type bunching that is needed to account for the interference [DHP79]. This bunching has the effect of changing the direction of the paths in such a way that some of them eventually end up travelling in straight lines towards detector D and not C as Griffiths would like them to do.

Indeed it is clear that the existence of the interference pattern means that any theory giving relevance to particle trajectories must give trajectories that do not move in straight lines directly through the region I . The particles must avoid the nodes in the interference pattern. CH offers us no reason why the trajectories on the mirror side of I should continue in the same general direction towards C on the other side of I . In order to match up trajectories we have to make some assumption of how the particles cross the region of interference. One cannot simply use classical intuition to help us through this region because classical intuition will not give interference fringes. Therefore we cannot conclude that the particles following the trajectories before they enter the

region I are the same particles that follow the trajectories after they have emerged from that region. This requires a knowledge of how the particles cross the region I , a knowledge that is not supplied by CH.

Where the consistent histories B.3 could provide a complete description is when the coherence between the two paths is destroyed. This could happen if a measurement involving some irreversible process was made in one of the beams. This would ensure that there was no interference occurring in the region I . In this case the trajectories would go straight through. This would mean that the conditional probabilities given in equation B.5 would always be satisfied.

But in such a situation the Bohm trajectories would also go straight through. The particles coming from Mirror M_1 would trigger the detector C no matter where it was placed. The reason for this behaviour in this case is because the wave function is no longer $\psi_c + \psi_d$, but we have two incoherent beams, one described by ψ_c and the other by ψ_d . This gives rise to a different quantum potential which does not cause the particles to be ‘reflected’ in the region I . So here there is no disagreements with CH.

B.4 Conclusion

When coherence between the two beams is destroyed it is possible to make meaningful inferences about trajectories in CH. These trajectories imply that any particle reflected from the mirror M_1 must end up in detector C . In the Bohm approach exactly the same conclusion is reached so that where the two approaches can be compared they predict exactly the same results.

When the coherence between the two beams is preserved then CH must use the consistent histories described by equation B.6. These histories do not allow any inferences about trajectories to be drawn. Although the consistent histories described by equation B.3 enable us to make inferences about particle trajectories because, as we have shown they lead to disagreement with experiment. Unlike the situation in CH the Bohm approach can define the notion of a trajectory which is calculated from the real part of the Schrödinger equation under polar decomposition. These trajectories are well defined and continuous throughout the experiment including the region of interference. Since CH cannot make any meaningful statements about trajectories in this case it cannot be used to draw any significant conclusions concerning the validity or otherwise of the Bohm trajectories. Thus the claim by Griffiths [Gri99], namely, that the CH gives a more reasonable account of the behaviour of particle trajectories interference experiment shown in Figure B.1 than that provided by the Bohm approach cannot be sustained.

Appendix C

Unitary Evolution Operators

The time evolution of a quantum system is usually calculated by starting with a Hamiltonian energy operator H and the Schrödinger equation. When the Hamiltonian is time independent this leads to the evolution, in the Schrödinger picture, of a quantum state $|\phi\rangle$

$$|\phi(t)\rangle = e^{iHt} |\phi(0)\rangle$$

The operator $U = e^{iHt}$ is referred to as the unitary evolution operator. When the Hamiltonian is not time independent, the evolution of the system is still described by a unitary evolution operator, but now U is the solution to the more complex operator Schrödinger equation

$$i\hbar \frac{\partial U}{\partial t} = HU \tag{C.1}$$

U is unitary if H is hermitian and the integration constant is such that at some given $t = t_0$, then $U(t_0) = I$, the unit matrix. (We will assume $t_0 = 0$).

It would be normal practice to proceed by analysing the classical interaction of a one-atom gas in a box, with a moveable partition, replace the terms in the classical Hamiltonian with canonically quantized operators, and then solve the operator Schrödinger equation. However, this would tie our analysis to examining the properties of a particular Hamiltonian. This is precisely the criticism that was made of Brillouin and Gabor, that they generalised to a conclusion from a specific form of interaction.

In order to avoid this, we will not attempt to start from a specific Hamiltonian operator. Instead we will proceed by constructing unitary time evolution operators, and assume that an appropriate Hamiltonian can be defined by:

$$H(t) = i\hbar \frac{\partial U(t)}{\partial t} U^\dagger(t)$$

This Hamiltonian will be hermitian, if $U(t)$ is unitary¹.

¹We shall, nevertheless, present arguments as to the plausibility of the existence of the necessary Hamiltonians,

The problem is therefore simplified to that of determining how the evolution of the Szilard Engine is constrained by the requirement of ensuring the evolution operator remains unitary. If the appropriate transformations of the state of the Szilard Engine can be expressed with a unitary time evolution operator, then there is nothing, in principle, to prevent some physical system of being constructed with an appropriate Hamiltonian. Such a system would then perform all the necessary operations of the Szilard Engine without needing an external 'demon' to make measurements or process information about the system.

A unitary operator is defined by the conditions

$$U^\dagger U = U U^\dagger = I$$

$$U(\alpha|a\rangle + \beta|b\rangle) = \alpha U(|a\rangle) + \beta U(|b\rangle)$$

It can easily be shown that this is equivalent to the statement that the unitary operator can be written in the form:

$$U = \sum_n |\phi_n\rangle \langle \psi_n|$$

where the $|\phi_n\rangle$ and $|\psi_n\rangle$ are two (usually different) sets of orthonormal basis for the Hilbert space. If the instantaneous eigenstates of the unitary operator at time t are given by the basis $|\varphi_n(t)\rangle$, then the unitary operator will have eigenvalues $e^{i\theta_n(t)}$ and the form

$$U(t) = \sum_n e^{i\theta_n(t)} |\varphi_n(t)\rangle \langle \varphi_n(t)|$$

The associated Hamiltonian is given by

$$H(t) = \sum_n \hbar \frac{d\theta_n(t)}{dt} |\varphi_n(t)\rangle \langle \varphi_n(t)|$$

$$+ \sum_{m,n} e^{i(\theta_m(t) - \theta_n(t))} |\varphi_m(t)\rangle \langle \varphi_n(t)| \frac{d(|\varphi_n(t)\rangle \langle \varphi_n(t)|)}{dt}$$

For the Hamiltonian to be time independent, the eigenstates must to be constant in time, and the eigenvalues must be of the form:

$$\theta_n(t) = \frac{E_n}{\hbar} t$$

An alternative formulation of this requirement is that the unitary operator has the form

$$U(t)U(t^\theta) = U(t + t^\theta)$$

Instantaneous eigenstates of the time evolution operator are only eigenstates of the Hamiltonian if they are also constant in time. There are two special cases of the general time dependent where it seems appropriate to do so. According to the theory of quantum computation [Deu85, Deu89] any unitary operation can, in principle, be efficiently simulated on a universal quantum computer. This strongly suggests that any condition more restrictive than unitarity would be too restrictive not to risk coming under threat from developments in quantum computing.

Hamiltonian: rapid transition and adiabatic transition [Mes62, Chapter 17]. These correspond to very fast and very slow changes in the Hamiltonian, or alternatively, to the change in the Hamiltonian taking place over a very short or very long period τ . In the first case (rapid transition) the asymptotic evolution is given by:

$$\lim_{\tau \rightarrow 0} U(\tau) = 1$$

while in the second case (adiabatic transition)

$$\lim_{\tau \rightarrow \infty} U(\tau) = \sum_n e^{i \int_0^\tau E_n(t) dt} |n(\tau)\rangle \langle n(0)|$$

where the $|n(t)\rangle$ are the instantaneous eigenstates of the Hamiltonian, and $E_n(t)$ are their instantaneous energy levels.

Time dependant Hamiltonians correspond to evolutions that do not conserve the internal energy of a system. These will require energy to be drawn from, and deposited in, a work reservoir - corresponding to work done upon or extracted from the system - through varying boundary conditions (or 'switching on' potentials). Unitarity requires only that the variation in the boundary condition (or potential) does not have any dependance upon the specific internal state of the system². Instead, to analyse the energy drawn from, or deposited in, the work reservoir it is necessary to calculate the change in the energy of the system once the boundary conditions become fixed again (or the potential is 'switched off') compared to the energy of the system beforehand.

A more detailed approach separates the Hamiltonian into a time-indepedant parts H_i , that refers to specific subsystems i , and into a time-dependant part $V_{ij}(t)$, that refers to the interaction between subsystems ij or with the changing external conditions.

$$H(t) = \sum_{ij} (H_i + V_{ij}(t))$$

If V_{ij} does not commute with all the H_i , then the eigenstates of $H(t)$ will involve superpositions of the eigenstates of the H_i . Strictly speaking, this means there will not be well-defined energies to the individual subsystems. Nevertheless, it is usual practice to regard the change of internal energy of subsystem i as the expectation value of the internal, time-independant Hamiltonian $\langle H_i \rangle$, while the complete system evolves under the influence of the full Hamiltonian $H(t)$. When the time-dependant part is "small" this can be treated by perturbation theory, but it is still meaningful when the time-dependant part is "large", as $\langle H_i \rangle_t$ is still the expectation value of measuring the internal energy of subsystem i at time t .

The Hamiltonian H_i is also relevant as an internal energy where a particular subsystem i is in contact with a heat bath. The interaction with a heat bath generally causes a subsystem density matrix to diagonalise along the eigenstates of the subsystems Hamiltonian H_i (see Section 6.1).

²The use of work reservoirs and their connection to time dependant Hamiltonians is essential to the standard definition of a number of thermodynamic entities, such as free energy.

Appendix D

Potential Barrier Solutions

This Appendix contains a detailed analysis of the eigenstates of the particle in a box, with a potential barrier of height V and width $2d$ raised in the centre of the box. We start with the Hamiltonian given in Equation 5.7

$$H\Psi = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi$$

with

$$V(x) = \left\{ \begin{array}{ll} \infty & (x < -L) \\ 0 & (-L < x < -d) \\ V & (-d < x < d) \\ 0 & (d < x < L) \\ \infty & (L < x) \end{array} \right\}$$

and substitute

$$\begin{aligned} X &= \frac{x}{L} \\ K_{al} &= \frac{L\sqrt{2mE_l}}{\hbar} \\ K_{bl} &= \frac{L\sqrt{2m(E_l - V)}}{\hbar} \\ K_{cl} &= \frac{L\sqrt{2m(V - E_l)}}{\hbar} \\ p &= \frac{d}{L} \\ \epsilon &= \frac{\hbar^2 \pi^2}{8mL^2} \end{aligned}$$

The solution is divided into three regions:

$$\begin{aligned} \Psi_1(X) & \quad -1 < X < -p \\ \Psi_2(X) & \quad -p < X < p \\ \Psi_3(X) & \quad p < X < 1 \end{aligned}$$

As the Hamiltonian is symmetric in X , then the solutions must be of odd or even symmetry, imposing the additional conditions

$$\begin{array}{ll} ODD & \Psi_1(X) = -\Psi_3(-X) \\ & \Psi_2(X) = -\Psi_2(-X) \\ EVEN & \Psi_1(X) = \Psi_3(-X) \\ & \Psi_2(X) = \Psi_2(-X) \end{array}$$

Boundary conditions and continuity requires:

$$\begin{aligned} \Psi_1(-1) &= \Psi_3(1) = 0 \\ \Psi_1(-p) &= \Psi_2(-p) \\ \Psi_3(p) &= \Psi_2(p) \\ \frac{\partial \Psi_1(X)}{\partial X} \Big|_{X=-p} &= \frac{\partial \Psi_2(X)}{\partial X} \Big|_{X=-p} \\ \frac{\partial \Psi_2(X)}{\partial X} \Big|_{X=p} &= \frac{\partial \Psi_3(X)}{\partial X} \Big|_{X=p} \end{aligned}$$

The energy of the eigenstates are given by

$$E_l = \frac{4\epsilon}{\pi^2} (K_{al})^2$$

Outside Barrier

The l^{th} odd or even eigenstates have $\Psi_{1l}(X)$ and $\Psi_{3l}(X)$ as sine functions of the form

$$\begin{aligned} \Psi_{1l}(X) &= A_l \sin(K_{al}(1+X)) \\ \Psi_{3l}(X) &= \pm A_l \sin(K_{al}(1-X)) \end{aligned}$$

with \pm depending upon the odd or even symmetry.

Within Barrier

The form of $\Psi_{2l}(x)$ depends upon the height of the barrier, V relative to the energy of the eigenstate E_l . For $E_l > V$, $\Psi_{2l}(x)$ is a sine (odd symmetry) or cosine (even symmetry) function, with wavenumber K_{bl} . When the barrier height is higher than the energy, $E_l < V$, the wavefunction becomes a hyperbolic function (sinh for odd symmetry, cosh for even symmetry) of wavenumber K_{cl} . When the barrier height $V = E$, the Hamiltonian in the barrier region leads to:

$$\frac{\partial^2}{\partial X^2} \Psi = 0$$

which has solutions

$$\Psi_l = B_l X + C_l$$

For odd functions, $C_l = 0$, while for even functions, $B_l = 0$.

Two approximations will be made consistently: $p \ll 1$, and when, for any a, b

$$\begin{aligned} \tan(a) &= b \ll 1 \\ a + l\pi &\approx b \end{aligned}$$

with $l = 1, 2, 3 \dots$. In addition, two further approximations will be made, in the limit of a narrow, and a high potential barrier.

Narrow Barrier Approximation (NBA)

The NBA is used whenever

$$K_{bl}p < K_{al}p \ll 1$$

The first inequality always holds when $E_l \geq V$, and the second effectively states that the wavelength of the eigenstate is much larger than the width of the potential barrier. Obviously for very high quantum numbers this cannot be true. It will be justified by the fact that we will later be using a thermal wavefunction, and there will be exponentially little contribution from high quantum number wavefunctions.

The NBA will also be used for $E < V$ if the energy eigenvalue is only slightly lower than the barrier so that

$$K_{cl}p < K_{al}p \ll 1$$

High Barrier Approximation (HBA)

HBA can only be used where $V \gg E$, which approaches the limit of an infinitely high potential. In this case we assume:

$$K_{cl}p \gg 1 \gg K_{al}p$$

where the second inequality is again assuming that very high quantum numbers are thermodynamically suppressed. The main approximations are:

$$\begin{aligned} \tanh(K_{cl}p) &\approx 1 - 2e^{-2K_{cl}p} \\ \sinh(K_{cl}p) &\approx \frac{1}{2}e^{K_{cl}p} \\ \cosh(K_{cl}p) &\approx \frac{1}{2}e^{K_{cl}p} \end{aligned}$$

D.1 Odd symmetry

D.1.1 $E > V$

$$\Psi_l = \begin{aligned} &A_l \sin(K_{al}(X + 1)) && -1 < X < -p \\ &B_l \sin(K_{bl}X) && -p < X < p \\ &A_l \sin(K_{al}(X - 1)) && p < X < 1 \end{aligned}$$

Continuity conditions lead to:

$$\begin{aligned} A_l &= B_l \frac{\sin(K_{bl}p)}{\sin(K_{al}(p-1))} \\ \frac{\tan(K_{bl}p)}{K_{bl}} &= \frac{\tan(K_{al}(p-1))}{K_{al}} \end{aligned}$$

and normalisation gives:

$$|A_l|^2 = \frac{2K_{al}K_{bl}\sin^2(K_{bl}p)}{L \left(\begin{aligned} &K_{al}\sin^2(K_{al}(1-p))(2K_{bl}p - \sin(2K_{bl}p)) \\ &+ K_{bl}\sin^2(K_{bl}p)(2K_{al}(1-p) - \sin(2K_{al}(1-p))) \end{aligned} \right)}$$

NBA

Applying the NBA to K_{bl} in the second continuity equation leads to

$$\begin{aligned} \tan(K_{al}(p-1)) &\approx K_{al}p \\ (K_{al}(p-1)) + l\pi &\approx K_{al}p \\ K_{al} &\approx l\pi \\ E_l &\approx \epsilon(2l)^2 \end{aligned}$$

This corresponds to the energy of the $n = 2l$ (symmetry odd) solutions of the unperturbed wavefunction. For normalisation we use

$$\begin{aligned} \sin(K_{al}(p-1)) &\approx \sin(K_{al}p - l\pi) = (-1)^l \sin(K_{al}p) \\ &\approx (-1)^l K_{al}p \\ \sin(2K_{al}(p-1)) &\approx \sin(2K_{al}p - l2\pi) = \sin(2K_{al}p) \\ &\approx 2K_{al}p \end{aligned}$$

to give

$$\begin{aligned} A_l &\approx \frac{1}{\sqrt{L}} \\ B_l &\approx (-1)^l \frac{K_{al}}{K_{bl}} \frac{1}{\sqrt{L}} \end{aligned}$$

The wavefunction in the region of the barrier approximates

$$\begin{aligned} \Psi_l &= B_l \sin(K_{bl}X) \approx B_l K_{bl}X \\ &\approx (-1)^l \frac{K_{al}}{\sqrt{L}} \end{aligned}$$

D.1.2 $E = V$

$$\Psi_l = \begin{aligned} &A_l \sin(K_{al}(X+1)) && -1 < X < -p \\ &B_l X && -p < X < p \\ &A_l \sin(K_{al}(X-1)) && p < X < 1 \end{aligned}$$

Continuity:

$$\begin{aligned} A_l &= B_l \frac{p}{\sin(K_{al}(p-1))} \\ \tan(K_{al}(p-1)) &= K_{al}p \end{aligned}$$

Normalisation:

$$|A_l|^2 = \frac{6K_{al}}{L(4K_{al}p \sin^2(K_{al}(1-p)) + 6K_{al}(1-p) - 3 \sin(2K_{al}(1-p)))}$$

NBA

$$\begin{aligned} (K_{al}(p-1)) + l\pi &\approx K_{al}p \\ K_{al} &\approx l\pi \\ E_l &\approx \epsilon(2l)^2 \\ A_l &\approx \frac{1}{\sqrt{L}} \left(\frac{1}{1 + \frac{8}{3}K_{al}p^2} \right) \approx \frac{1}{\sqrt{L}} \\ B_l &\approx (-1)^l K_{al} \frac{1}{\sqrt{L}} \end{aligned}$$

D.1.3 $E < V$

$$\begin{aligned} \Psi_l &= \begin{aligned} &A_l \sin(K_{al}(X+1)) & -1 < X < -p \\ &B_l \sinh(K_{cl}X) & -p < X < p \\ &A_l \sin(K_{al}(X-1)) & p < X < 1 \end{aligned} \end{aligned}$$

Continuity:

$$\begin{aligned} A_l &= B_l \frac{\sinh(K_{cl}p)}{\sin(K_{al}(p-1))} \\ \frac{\tanh(K_{cl}p)}{K_{cl}} &= \frac{\tan(K_{al}(p-1))}{K_{al}} \end{aligned}$$

Normalisation:

$$|A_l|^2 = \frac{2K_{al}K_{cl} \sinh^2(K_{cl}p)}{L \left(\begin{aligned} &K_{cl} \sinh^2(K_{cl}p)(2K_{al}(1-p) - \sin(2K_{al}(1-p))) \\ &+ K_{al} \sin^2(K_{al}(1-p))(\sinh(2K_{al}p) + 2K_{al}p) \end{aligned} \right)}$$

NBA

When E is only slightly larger than V (ie. $K_{cl}p \ll 1$), then the approximations for \sinh and \tanh match those made for the NBA with $E < V$ and lead to the same approximate solutions.

HBA

$$\tan(K_{al}(p-1)) \approx \frac{K_{al}}{K_{cl}} (1 - 2e^{i 2K_{cl}p}) \ll 1$$

$$\begin{aligned}
K_{al}(p-1) + l\pi &\approx \frac{K_{al}}{K_{cl}} (1 - 2e^{i 2K_{cl}p}) \\
K_{al} &\approx \frac{l\pi}{(1-p)} \left(1 + \frac{(1 - 2e^{i 2K_{cl}p})}{K_{cl}(1-p)}\right)^{i-1} \\
&\approx \frac{l\pi}{(1-p)} \left(1 - \frac{(1 - 2e^{i 2K_{cl}p})}{K_{cl}(1-p)}\right) \\
E_l &\approx \epsilon \left(\frac{2l}{(1-p)}\right)^2 \left(1 - 2\frac{(1 - 2e^{i 2K_{cl}p})}{K_{cl}(1-p)}\right)
\end{aligned}$$

which approaches $E_l \approx \epsilon \left(\frac{2l}{(1-p)}\right)^2$.

Normalisation of the wavefunction is more complex, but dropping terms of order $e^{i 2K_{cl}p}$ we get

$$\begin{aligned}
K_{al}(p-1) + l\pi &\approx \frac{K_{al}}{K_{cl}} \\
\sin(K_{al}(p-1)) &\approx (-)^l \sin\left(\frac{K_{al}}{K_{cl}}\right) \approx (-)^l \left(\frac{K_{al}}{K_{cl}}\right) \\
\sin(2K_{al}(1-p)) &\approx -2\frac{K_{al}}{K_{cl}} \\
A_l &\approx \frac{1}{\sqrt{L(1-p)}} \\
B_l &\approx 2(-)^l \left(\frac{K_{al}}{K_{cl}}\right) \frac{e^{i K_{cl}p}}{\sqrt{L(1-p)}}
\end{aligned}$$

The wavefunction in the region of the barrier ($|X| < p$) is then:

$$\Psi_l = B_l \sinh(K_{cl}X) \approx \frac{(-)^l}{\sqrt{L}} \left(\frac{K_{al}}{K_{cl}}\right) \frac{e^{i K_{cl}(p+X)} - e^{i K_{cl}(p-X)}}{\sqrt{(1-p)}}$$

For large K_{cl} this is non-negligible at the very edges of the barrier ($|X| \approx p$).

D.1.4 Summary

The wavefunction and eigenvalues undergo negligible perturbation until $E > V$. As the potential barrier becomes large, the wavefunction becomes zero inside the barrier and the wavenumber increases by a factor of $\frac{1}{1-p}$, causing a minor increase in the energy levels.

D.2 Even symmetry

D.2.1 $E > V$

$$\Psi_l = \begin{cases} A_l \sin(K_{al}(1+X)) & -1 < X < -p \\ C_l \cos(K_{bl}X) & -p < X < p \\ A_l \sin(K_{al}(1-X)) & p < X < 1 \end{cases}$$

Continuity:

$$\begin{aligned}
A_l &= C_1 \frac{\cos(K_{bl}p)}{\sin(K_{al}(1-p))} \\
\frac{1}{K_{bl} \tan(K_{bl}p)} &= \frac{\tan(K_{al}(1-p))}{K_{al}}
\end{aligned}$$

Normalisation:

$$|A|^2 = \frac{2K_{al}K_{bl} \cos^2(K_{bl}p)}{L \left(\begin{array}{l} K_{al} \sin^2(K_{al}(1-p))(2K_{bl}p + \sin(2K_{bl}p)) \\ + K_{bl} \cos^2(K_{bl}p)(2K_{al}(1-p) - \sin(2K_{al}(1-p))) \end{array} \right)}$$

NBA

$$\begin{aligned} \cot(K_{al}(1-p)) &\approx K_{bl}p \frac{K_{bl}}{K_{al}} \ll 1 \\ -(K_{al}(1-p)) + \frac{(2l-1)}{2}\pi &\approx K_{bl}p \frac{K_{bl}}{K_{al}} \end{aligned}$$

If we assume the barrier is low ($K_{al} \approx K_{bl}$)

$$\begin{aligned} K_{al} &\approx \frac{(2l-1)}{2}\pi \\ E_l &\approx \epsilon(2l-1)^2 \end{aligned}$$

which gives the $n = (2l-1)$ unperturbed energies.

When the barrier rises to $V = E$, then K_{bl} becomes small enough to be negligible, and

$$\begin{aligned} K_{al} &\approx \frac{(2l-1)}{2(1-p)}\pi \\ E_l &= \epsilon \left(\frac{2l-1}{1-p} \right)^2 \end{aligned}$$

corresponding to a slightly perturbed ($p \ll 1$) energy of the $n = (2l-1)$ solutions. For normalisation

$$\begin{aligned} \sin(K_{al}(1-p)) &\approx -(-1)^l \\ \sin(2K_{al}(1-p)) &\approx 2K_{bl}p \frac{K_{bl}}{K_{al}} \\ |A_l|^2 &\approx \frac{1}{L} \left(\frac{1}{1+p \left(1 - \left(\frac{K_{bl}}{K_{al}} \right)^2 \right)} \right) \\ C_l &\approx -(-1)^l A_l \end{aligned}$$

which gives the unperturbed values when $K_{bl} \approx K_{al}$. When $K_{bl} \ll K_{al}$ it leads to

$$|A_l|^2 \approx \frac{1}{L} \left(\frac{1}{1+p} \right)$$

The wavefunction in the region of the barrier approximates:

$$\Psi = C_l \cos(K_{bl}X) \approx C_l$$

D.2.2 $E = V$

$$\begin{aligned} \Psi_l &= \begin{array}{ll} A_l \sin(K_{al}(1+X)) & -1 < X < -p \\ C_l & -p < X < p \\ A_l \sin(K_{al}(1-X)) & p < X < 1 \end{array} \end{aligned}$$

Continuity :

$$\begin{aligned} A_l &= \frac{C_l}{\sin(K_{al}(1-p))} \\ A_l K_{al} \cos(K_{al}(1-p)) &= 0 \end{aligned}$$

This has *exact* solutions

$$\begin{aligned} (K_{al}(1-p)) &= \frac{(2l-1)\pi}{2} \\ K_{al} &= \frac{(2l-1)}{2(1-p)}\pi \\ E_l &= \epsilon \left(\frac{2l-1}{1-p} \right)^2 \end{aligned}$$

Normalisation uses $\sin(K_{al}(1-p)) = -(-1)^l$ and $\sin(2K_{al}(1-p)) = 0$

$$\begin{aligned} A_l &= \frac{1}{\sqrt{L(1+p)}} \\ C_l &= \frac{-(-1)^l}{\sqrt{(1+p)}} \end{aligned}$$

D.2.3 $E < V$

$$\Psi = \begin{cases} A_l \sin(K_{al}(1+X)) & -1 < X < -p \\ C_l \cosh(K_{cl}X) & -p < X < p \\ A_1 \sin(K_{al}(1-X)) & p < X < 1 \end{cases}$$

Continuity:

$$\begin{aligned} A_l &= C_l \frac{\cosh(K_{cl}p)}{\sin(K_{al}(1-p))} \\ \frac{1}{K_{cl} \tanh(K_{cl}p)} &= -\frac{\tan(K_{al}(1-p))}{K_{al}} \end{aligned}$$

Normalisation:

$$|A_l|^2 = \frac{2K_{al}K_{cl} \cosh^2(K_{cl}p)}{L \left(\begin{aligned} &K_{cl} \cosh^2(K_{cl}p)(2K_{al}(1-p) - \sin(2K_{al}(1-p))) \\ &+ K_{al} \sin^2(K_{al}(1-p))(2K_{al}p - \sinh(2K_{al}p)) \end{aligned} \right)}$$

NBA

When E is only slightly higher than V , these results approximate to the same results as the approximation for NBA with $E > V$. These approximations match the exact solutions for $E = V$.

HBA

$$\begin{aligned} \tan(K_{al}(1-p)) &\approx -\frac{K_{al}}{K_{cl}} (1 + 2e^{2K_{cl}p}) \ll 1 \\ K_{al}(1-p) - l\pi &\approx -\frac{K_{al}}{K_{cl}} (1 + 2e^{2K_{cl}p}) \end{aligned}$$

$$\begin{aligned}
K_{al} &\approx \frac{l\pi}{(1-p)} \left(1 + \frac{(1+2e^{i2K_{cl}p})}{K_{cl}(1-p)}\right)^{i-1} \\
&\approx \frac{l\pi}{(1-p)} \left(1 - \frac{(1+2e^{i2K_{cl}p})}{K_{cl}(1-p)}\right) \\
E_l &\approx \epsilon \left(\frac{2l}{(1-p)}\right)^2 \left(1 - 2\frac{(1+2e^{i2K_{cl}p})}{K_{cl}(1-p)}\right)
\end{aligned}$$

which approaches $E_l \approx \epsilon \left(\frac{2l}{(1-p)}\right)^2$. For normalisation, we drop terms involving $e^{i2K_{cl}p}$ and get

$$\begin{aligned}
K_{al}(p-1) + l\pi &\approx \frac{K_{al}}{K_{cl}} \\
\sin(K_{al}(p-1)) &\approx (-)^l \sin\left(\frac{K_{al}}{K_{cl}}\right) \\
&\approx (-)^l \left(\frac{K_{al}}{K_{cl}}\right) \\
\sin(2K_{al}(1-p)) &\approx 2\frac{K_{al}}{K_{cl}} \\
A_l &\approx \frac{1}{\sqrt{L}} \frac{1}{\sqrt{1-p}} \\
C_l &\approx \frac{2(-)^l}{\sqrt{L}} \left(\frac{K_{al}}{K_{cl}}\right) \frac{e^{iK_{cl}p}}{\sqrt{1-p}}
\end{aligned}$$

The wavefunction in the region of the barrier ($|X| < p$) is then:

$$\begin{aligned}
\Psi_l &= C_l \cosh(K_{cl}X) \\
&\approx \frac{(-)^l}{\sqrt{L}} \left(\frac{K_{al}}{K_{cl}}\right) \frac{e^{iK_{cl}(p-X)} + e^{iK_{cl}(p+X)}}{\sqrt{1-p}}
\end{aligned}$$

For large K_{cl} this is non-negligible at the very edges of the barrier ($|X| \approx p$)

D.2.4 Summary

The even symmetry wavefunctions undergo a minor perturbation, of order p , as the barrier rises to $V = E$. As the barrier rises above the energy eigenvalue, the initial peak at $X = 0$ becomes a node, as the wavefunction is expelled from the potential barrier region. The energy of the l^{th} even eigenstate increases from the unperturbed value $E_l = \epsilon(2l-1)^2$ to $E_l = \epsilon \left(\frac{2l}{1-p}\right)^2$. The final energy level, in the limit of an infinitely high barrier, becomes degenerate with the l^{th} odd symmetry eigenstate.

D.3 Numerical Solutions to Energy Eigenvalues

Given the dependancies of K_{al} , K_{bl} and K_{cl} on E_l and V , each of the second of the continuity equations can be rewritten in the form $f(E_n, V) = 0$, which defines a discrete set of eigenstates for a given V . These eigenstates can be evaluated by numerically solving the differential equation

$$\frac{dE_l}{dV} = - \left(\frac{\partial f}{\partial V}\right) / \left(\frac{\partial f}{\partial E_l}\right)$$

with initial values given by solutions to E_l for the unperturbed eigenstates of $V = 0$ given in Section 5.1. The solutions for E_l can then be used to calculate K_{al} and so plot the wavefunction itself. Numerical solutions to these equations were evaluated using the MATLAB[MAT] analysis

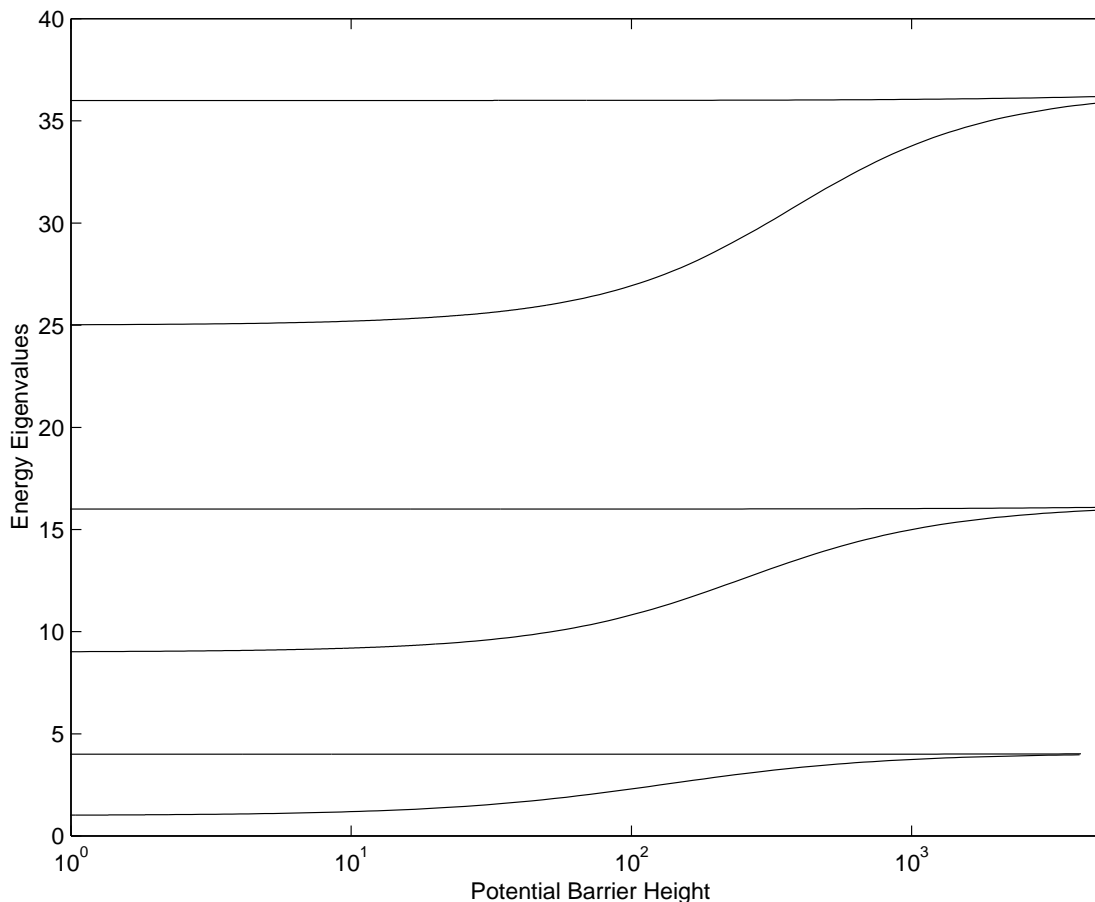


Figure D.1: First six energy eigenvalues with potential barrier

package, and setting $\epsilon = L = 1$, $p = 0.01$ The results are shown in Figures D.1,D.2 and D.3.

Figure D.1 shows the changes in the eigenvalues of the first three (odd and even symmetry) pairs of eigenstates as the barrier height increases. The eigenvalues pass continuously from the $V = 0$ values, through $V = E$, to the $V \gg E$ values, becoming degenerate only in the limit of the infinitely high barrier. Figure D.2 shows the changes in the wavefunction of the first and third even symmetry eigenstates, with barrier heights starting at twice the energy eigenvalue. The eigenstates clearly develop a node in the center, shortening their wavelengths, until they reach the same wavelength as the corresponding odd symmetry state. Finally, in the limit of the infinite potential barrier the odd and even symmetry states differ only by a change of sign at they pass through the origin, shown in Figure D.3

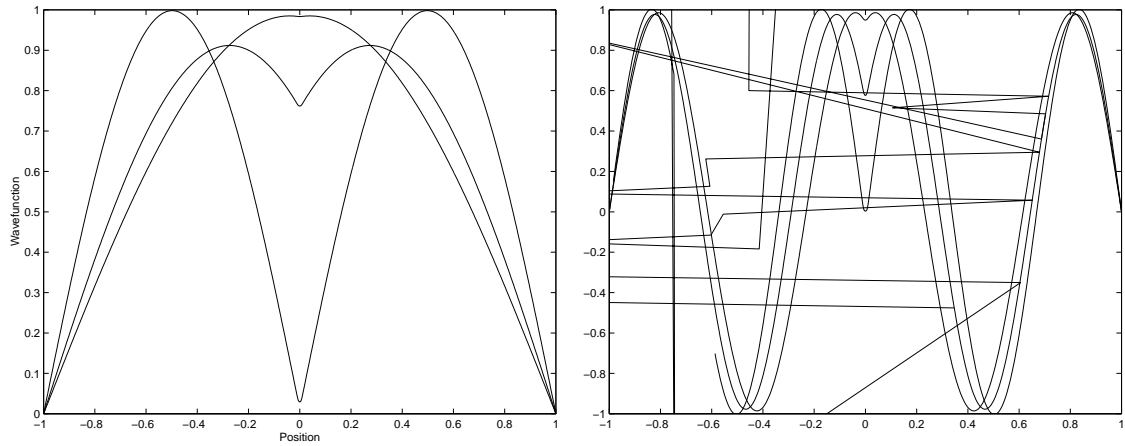


Figure D.2: Perturbation of Even Symmetry Eigenstates

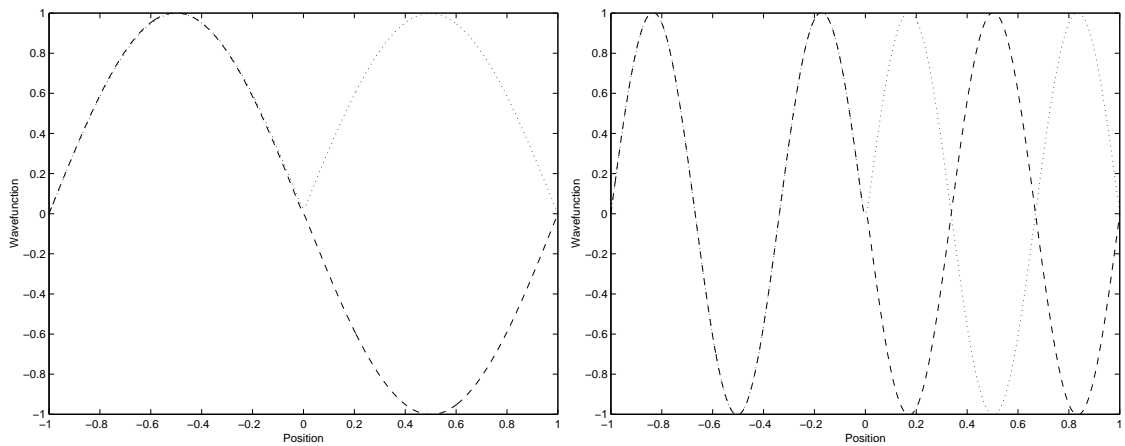


Figure D.3: Degeneracy of Even and Odd Symmetry Eigenstates

Appendix E

Energy of Perturbed Airy Functions

The insertion of shelves at height h into the wavefunction of a quantum weight will cause a perturbation of the energy eigenvalues. Due to the nature of the Airy functions, it is not possible to calculate the effect of this perturbation exactly. However, it can be estimated for two extremes, and be shown to involve negligible energy changes for high quantum numbers. It is argued that it is reasonable to assume that there is also negligible energy changes between the two extremes.

This is based upon calculations in [NIS] for the quantum state of a particle in a linear potential between two barriers. We will calculate the effect of inserting a potential barrier for high quantum numbers n , where the shelf height is large and small in comparison with the characteristic height of the wavefunction $-a_n H$. The unperturbed energy of the state is $E_n = -a_n M g H$. We will always use the asymptotic approximation $a_n = -\left(\frac{3\pi n}{2}\right)^{2/3}$.

Large Shelf Height

If the shelf is inserted at a height $h \gg -a_n H$ then there is negligible perturbation of the wavefunction, as the potential changes only in a region where the wavefunction is negligibly small. The final energy is therefore approximately the same as the unperturbed energy:

$$E_n^{(1)} = \left(\frac{3\pi n}{2}\right)^{2/3} M g H$$

Small Shelf Height

If the shelf is inserted at a height $h \ll -a_n H$, the wavefunction is split into two, above and below the shelf. We will start by assuming that the shelf is inserted at a node, and that m nodes are above the shelf height (see Figure 5.5). The number of nodes below the shelf height is given by $k = n - m$, and the shelf height is $h = (a_m - a_n)H$.

The low shelf height is equivalent to the assumption that $k \ll n$. There are two subcases, depending upon whether k itself is large or small.

If k is small, then $m \approx n$ and there is negligible probability of the weight being located below the shelf, and we only need to consider the wavefunction above. This is the same as an unperturbed wavefunction with m nodes, raised by a height h , and so will have an energy

$$\begin{aligned} E_m^{(2)} &= -a_m MgH + Mgh \\ &= -a_n MgH \\ &= E_n \end{aligned}$$

If $1 \ll k \ll n$ we need to estimate the energy of the wavefunction above and below the barrier. Above the barrier, we again have a wavefunction with energy $E_m^{(2)} =$

of the potential barrier will then have negligible effect upon the energy levels of the high quantum number states.

Appendix F

Energy Fluctuations

We suppose that the expansion of the gas, described in Section 6.2 takes places in n steps, and after each step the gas is allowed to thermalise through interactions with an environment. This thermalisation randomises the individual state of the gas from step to step.

The energy transferred by the i^{th} state, on the m^{th} step is denoted by δE_{im} and the probability of the gas being in the i^{th} state, on the m^{th} step is p_{im} . Clearly $\sum_i p_{im} = 1$. The randomisation of the state between steps means that the probabilities at different steps can be treated as statistically independent.

We describe the ordered set of states that the system passes through on a given expansion by the array $\alpha = (ijk\dots)$, which means the system is in the i^{th} state on the first step, j^{th} state on the second step, etc. We also write this as $\alpha_1 = i$, $\alpha_2 = j$ or $\alpha = (\alpha_1\alpha_2\dots)$. The probability of α occurring is given by

$$P_\alpha = \prod_{m=1,n} p_{\alpha_m m}$$

$$\sum_\alpha P_\alpha = \sum_{\alpha_1, \alpha_2, \dots} \left(\prod_{m=1,n} p_{\alpha_m m} \right) = 1$$

and the energy transferred on such an expansion is

$$E_\alpha = \sum_m \delta E_{\alpha_m m}$$

We also need to note the following identities

$$\sum_{\alpha_1, \alpha_2, \dots} \left(\prod_{m=1,n} p_{\alpha_m m} f(\alpha_k) \right) = \sum_{\alpha_k} p_{\alpha_k k} f(\alpha_k)$$

$$\sum_{\alpha_1, \alpha_2, \dots} \left(\prod_{m=1,n} p_{\alpha_m m} f(\alpha_k, \alpha_l) \right) = \sum_{\alpha_k, \alpha_l} p_{\alpha_k k} p_{\alpha_l l} f(\alpha_k, \alpha_l)$$

etc.

We can now write the following results

Mean energy transfer and fluctuation on m^{th} step:

$$\begin{aligned}\langle \delta E_m \rangle &= \sum_i p_{im} \delta E_{im} \\ \langle \delta E_m^2 \rangle &= \sum_i p_{im} (\delta E_{im})^2\end{aligned}$$

Mean energy transfer and fluctuation of the overall expansion is:

$$\begin{aligned}\langle E \rangle &= \sum_{\alpha} \left(\prod_{l=1,n} p_{\alpha_l l} \right) \left(\sum_m \delta E_{\alpha_m m} \right) = \sum_m \left(\sum_{\alpha_m} p_{\alpha_m m} \delta E_{\alpha_m m} \right) \\ &= \sum_{m=1,n} \langle \delta E_m \rangle \\ \langle E \rangle^2 &= \sum_m \langle \delta E_m \rangle^2 + 2 \sum_{l < m} \langle \delta E_l \rangle \langle \delta E_m \rangle \\ \langle E^2 \rangle &= \sum_{\alpha} \left(\prod_{l=1,n} p_{\alpha_l l} \right) \left(\sum_m \delta E_{\alpha_m m} \right)^2 = \sum_{\alpha} \left(\prod_{k=1,n} p_{\alpha_k k} \right) \left(\sum_{l,m} \delta E_{\alpha_l l} \delta E_{\alpha_m m} \right) \\ &= \sum_m \left(\sum_{\alpha_m} p_{\alpha_m m} (\delta E_{\alpha_m m})^2 \right) + 2 \sum_{l < m} \sum_{\alpha_m, \alpha_l} p_{\alpha_m m} p_{\alpha_l l} \delta E_{\alpha_m m} \delta E_{\alpha_l l} \\ &= \sum_m \langle \delta E_m^2 \rangle + 2 \sum_{l < m} \langle \delta E_l \rangle \langle \delta E_m \rangle \\ \langle E^2 \rangle - \langle E \rangle^2 &= \sum_{m=1,n} \left(\langle \delta E_m^2 \rangle - \langle \delta E_m \rangle^2 \right)\end{aligned}$$

For the expansions in Section 6.2, we have $\langle \delta E_m^2 \rangle - \langle \delta E_m \rangle^2 = 2 \langle \delta E_m \rangle^2$. We may therefore introduce the following inequalities:

$$\begin{aligned}\langle E^2 \rangle - \langle E \rangle^2 &\leq 2n \langle \delta E_{\text{max}} \rangle^2 \\ \langle E \rangle^2 &\geq (n \langle \delta E_{\text{min}} \rangle)^2\end{aligned}$$

and prove our required result that

$$\frac{\langle E^2 \rangle - \langle E \rangle^2}{\langle E \rangle^2} \leq \frac{2}{n} \left(\frac{\langle \delta E_{\text{max}} \rangle}{\langle \delta E_{\text{min}} \rangle} \right)^2$$

The ratio $\frac{\hbar \delta E_{\text{max}}/j}{\hbar \delta E_{\text{min}}/j}$ approaches $\frac{P_{\text{max}}}{P_{\text{min}}}$, where $P_m = \frac{\partial E_m}{\partial X}$ is the generalised pressure, as the size of the step reduces, and so becomes independant of n . As $n = t/\tau_{\theta}$, where τ_{θ} is a characteristic thermal relaxation time, and t is the length of time of the expansion, the size of fluctuations in the total energy transfer can be made negligible if the expansion takes place sufficiently slowly with respect to τ_{θ} .

It should be clear that the result obtained here is not the same as, although it is similar to, the usual fluctuation formula. The usual formula refers to the deviation from the mean value of the thermodynamic variable at a given time, and is reciprocally related to the number of constituents of the system. The formula here refers to potentially large fluctuations at any particular moment,

for systems which may have only a few constituents, but which, when integrated over a significant period of time, still leads to negligible long term fluctuations.

Appendix G

Free Energy and Temperature

The free energy, F is only one of a number of thermodynamics potentials that may be associated with a system. For example, we can also use the energy E , Gibbs function G or enthalpy H , defined by

$$E$$

$$F = E - TS$$

$$G = E - TS + PV$$

$$H = E + PV$$

to describe the behaviour of a system. These terms can then be generalised even further, when the number of particles is allowed to vary. The choice of which thermodynamic potential to use entirely is a question of which constraints are acting upon the system, or which pair of the variables S , T , P and V are controlled.

In Section 7.1, the significance of F and from that S was derived from the work that can be extracted from an isothermal expansion of a system. In terms of classical thermodynamics potentials, this is derived from the infinitesimal relationships

$$dF = dE - TdS - SdT$$

and the general relationship for heat and work acting upon a system

$$dE = TdS - PdV$$

which is equivalent to the statistical mechanical relationship

$$dE = \sum_i E_i dp_i + \sum_i p_i dE_i$$

This gives

$$dF = -SdT - PdV$$

and clearly, if the temperature is held fixed

$$dF = -PdV$$

so the change in free energy is equal to the negative of the work extracted from the system, $dW = PdV$.

Now, if the temperature is not held fixed, then we clearly have

$$dF + dW = -SdT$$

If we can interpret the work as being the gain in free energy of a second system (which has no change in entropy), such as a raised weight, we can express this equation as being a net gain in free energy $\Delta F = dF + dW$, of a closed system, when a quantity of entropy S is taken through a temperature difference $\Delta T = dT$. We will express this as

$$\Delta F = -S\Delta T \tag{G.1}$$

and refer to this as the characteristic equation for free energy in the presence of a temperature differences.

Adiabatic expansion The derivation above is essentially based upon the adiabatic (essentially isolated) expansion of a gas. If we take a gas in essential isolation, and extract work from it's expansion, the free energy before and after is given by

$$\begin{aligned} F_1 &= E_1 - T_1 S_1 \\ F_2 &= E_2 - T_2 S_2 \end{aligned}$$

As the expansion is reversible but thermally isolated we have $\Delta W = E_1 - E_2$ and $S_2 = S_1 = S$. This gives

$$\begin{aligned} \Delta F &= F_2 - F_1 \\ &= -\Delta W - (T_2 - T_1)S \\ \Delta F + \Delta W &= -S\Delta T \end{aligned}$$

Carnot Cycle The Carnot heat engine operates by drawing energy in the form of heat Q_1 from a heat bath at temperature T_1 , extracting W as work, and depositing Q_2 in a heat bath at temperature T_2 . The usual means of achieving this would be to have gas initially in contact with the heat bath T_1 . This is isothermally expanded, drawing the Q_1 out as work. The gas is then removed from contact with the heat bath, and adiabatically expanded, again extracting work, until it's temperature falls to T_2 . It is then placed in contact with the T_2 heat bath, isothermally

compressed, depositing the Q_2 heat, and is then isolated again, and adiabatically compressed further until it returns to its initial volume, at which point, on a reversible cycle, it will have risen back to temperature T_2 .

For a reversible process the entropy loss from the T_1 heat bath must match the gain from the T_2 heat bath, so

$$S = \frac{Q_1}{T_1} = \frac{Q_2}{T_2}$$

and conservation of energy is

$$Q_1 = Q_2 + W$$

This is usually rearranged to give the Carnot efficiency

$$\frac{W}{Q_1} = 1 - \frac{T_2}{T_1}$$

However, there is an alternative way of expressing this

$$W = -S(T_2 - T_1)$$

which is again the characteristic equation G.1 for free energy in the presence of two different temperatures.

Entropy Engine The two previous examples can be regarded as equations about the movement of energy between, or within, systems, rather than an equation about the gain in free energy from moving entropy between different temperatures. We will now demonstrate a system, based upon the Szilard Engine, and with some similarities to the heat engines described in Chapter 8, but which produces this characteristic equation without any energy changes taking place anywhere. This makes it very clear that the gain in free energy is actually a consequence of the transferral of entropy between temperatures.

First we start with two Szilard boxes, each containing a single atom, and initially of length L . The boxes are initially at temperatures T_1 and T_2 , but are thermally isolated. A partition is raised in the centre of the first box, dividing the one atom gas into left and right subensembles, and a piston is inserted between them.

Now, however, we modify the behaviour of the box, as shown in Figure G.1. The piston is constrained so that it cannot move to the right, even when the gas is located to the left. If the gas is on the right, the piston moves to the left, as before. However, regardless of the location of the gas, the right most wall of the box starts to move to the left, at the same rate as a left-moving piston would. When the wall of the box reaches the initial center, it stops. If the gas was initially located to the left of the partition, the right wall simply moves in through empty space on the right, until it comes against the piston, still in the center. If, on the other hand, the gas was initially located to the right, the piston and wall move leftwards together. As long as this movement is sufficiently slow, any work done upon the piston would be matched by work done by the wall. In effect, no work is done upon the gas at all, as the right subensemble keeps the same volume

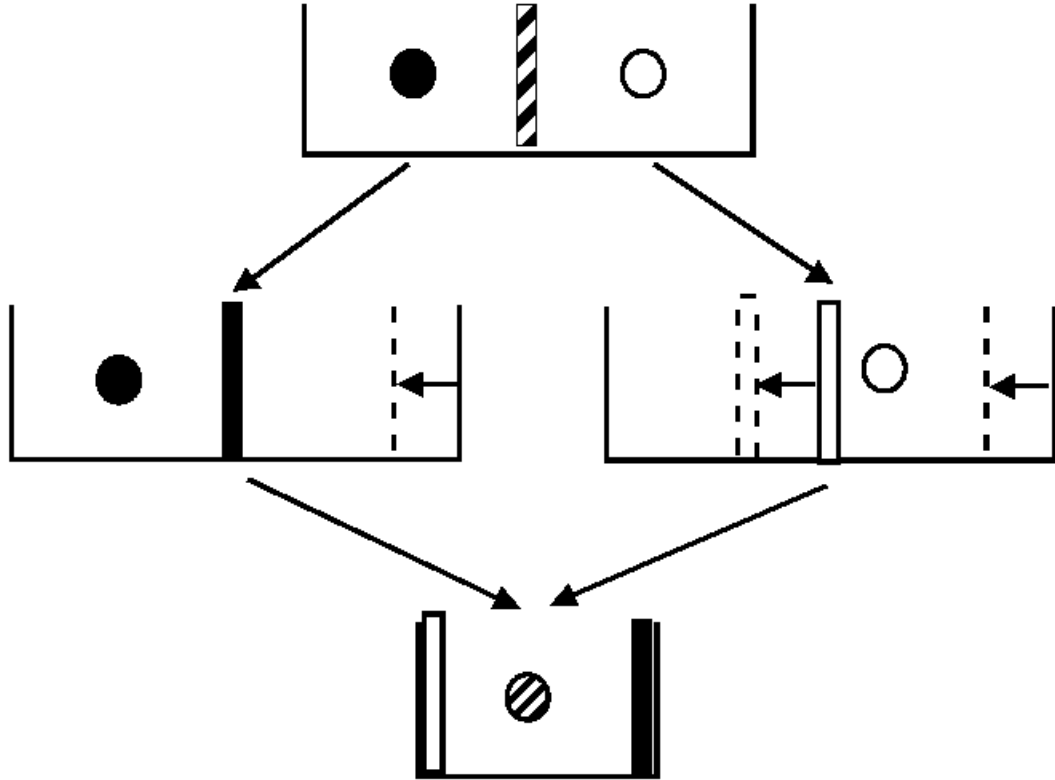


Figure G.1: The Entropy Engine

throughout. At the end of this process, the wall is in the initial center, and the piston is against the left wall. The initially left and right gas subensembles are now entirely overlapping.

The remarkable consequence of this is that we have compressed the gas to exactly half its volume, but without performing any work upon it, or changing its energy in any other way. We have succeeded in this by increasing the entropy of the piston, which is now in a mixture of being on the left or the right. This effect is possible only from statistical mechanics: there is no equivalent process in phenomenological thermodynamics by which such a compression can be achieved without any flow of energy.

We now remove the piston states from the ends of the first box and insert them in the corresponding ends of the second. We can now perform the same operation on the second Szilard box, in the reverse direction. The second gas expands to twice its volume, while the piston is restored to its initial state. Again, there is no contact with a heat bath, no work is extracted from the gas, and its internal energy is constant throughout.

It is clear that we can continue this process indefinitely, compressing the first gas to as small a fraction of its initial volume as we like, without ever performing any work upon it. However, the cost is that we must proportionately increase the volume occupied by the second. The only quantity that is transferred between the two systems is the mixing entropy of the piston, $S = k \ln 2$. However, by compressing the first gas we increase its free energy by $kT_1 \ln 2$, and by expanding

the second gas, reduce its free energy by $kT_2 \ln 2$. The net change in free energy is

$$\begin{aligned}\Delta F &= k \ln 2(T_1 - T_2) \\ &= -S\Delta T\end{aligned}$$

which corresponds to the entropy being transferred through the temperature difference $\Delta T = T_2 - T_1$. This provides an 'engine' by which the free energy of a system can be increased indefinitely, by reversibly moving entropy between parts of the system at different temperatures, yet without any energy flow taking place.

Of course, when we attempt to extract this free energy by, for example, isothermally restoring the system to its initial configuration, we simply recover the Carnot cycle efficiency. Although this process produces the characteristic equation G.1 for the free energy change in the presence of different temperatures, it should be clear that its physical basis is a purely statistical mechanical effect, and quite different to the more commonly encountered manifestation in the adiabatic expansion and Carnot Cycle.

Appendix H

Free Energy and Non-Equilibrium Systems

In Section 7.1 the free energy of a system in a canonical thermodynamical state $\rho = \frac{1}{Z} e^{i \frac{H}{kT}}$ was derived in terms of its partition function $Z = \text{Tr} \left[e^{i \frac{H}{kT}} \right] = \sum_i e^{i \frac{E_i}{kT}}$ as $F = -kT \ln Z$.

When the Hilbert space is split into subspaces with partition functions $Z_a = \sum_{i \in \mathcal{I}_a} e^{i \frac{E_i}{kT}}$, the equilibrium probability of the density matrix being in the subspace is

$$p_a = \sum_{i \in \mathcal{I}_a} p_i = \frac{\sum_{i \in \mathcal{I}_a} e^{i \frac{E_i}{kT}}}{\sum_i e^{i \frac{E_i}{kT}}} = \frac{Z_a}{Z}$$

From this we can express the free energy of a density matrix in equilibrium in the subspace by

$$F_a = F - kT \ln p_a$$

When the Hilbert space is divided into several orthogonal subspaces, so that $Z = \sum_\alpha Z_\alpha$, we have

$$\begin{aligned} F &= \sum_\alpha p_\alpha F_\alpha + kT \sum_\alpha p_\alpha \ln p_\alpha \\ &= -kT \ln \left(\sum_\alpha e^{i \frac{F_\alpha}{kT}} \right) \end{aligned}$$

and also

$$p_a = \frac{e^{i \frac{F_a}{kT}}}{\sum_\alpha e^{i \frac{F_\alpha}{kT}}}$$

The equilibrium density matrix may be expressed as

$$\begin{aligned} \rho &= \sum_\alpha p_\alpha \rho_\alpha \\ &= \frac{1}{Z} \sum_\alpha e^{i \frac{F_\alpha}{kT}} \rho_\alpha \end{aligned}$$

Note that this is expressed in terms of the free energies of the subensembles, rather than the energies of the microstates.

We now wish to consider what happens when a density matrix is composed of the same equilibrium subensembles ρ_α but for which the mixing probabilities p_α^θ are not in thermal equilibrium¹

$$\rho^\theta = \sum_{\alpha} p_{\alpha}^{\theta} \rho_{\alpha}$$

We know the entropy of this matrix from the mixing equation

$$S^\theta = \sum_{\alpha} p_{\alpha}^{\theta} S_{\alpha} - k \sum_{\alpha} p_{\alpha}^{\theta} \ln p_{\alpha}^{\theta}$$

However, it may seem unclear whether the free energy is at all meaningful in this situation. We cannot simply use F as the equations would not agree. At the same time, there is a well defined temperature associated with the system. We need to develop a well defined generalisation of the equilibrium equations above.

We are going to proceed by proposing a non-equilibrium version of the partition function

$$Z^\theta = \sum_{\alpha} D_{\alpha} e^{i \frac{F_{\alpha}}{kT}}$$

where the D_α are a set of factors which determine the extent to which the system is out of equilibrium. If all $D_\alpha = 1$ then the system is in equilibrium. We define the D_α from the constraint $\sum_{\alpha} p_{\alpha}^{\theta} \ln D_{\alpha} = 0$ to give

$$kT \ln D_{\alpha} = (F_{\alpha} + kT \ln p_{\alpha}^{\theta}) - \sum_{\alpha} p_{\alpha}^{\theta} (F_{\alpha} + kT \ln p_{\alpha}^{\theta})$$

which allows us to write

$$\begin{aligned} p_{\alpha}^{\theta} &= \frac{1}{Z^\theta} D_{\alpha} e^{i \frac{F_{\alpha}}{kT}} \\ \rho^\theta &= \frac{1}{Z^\theta} \sum_{\alpha} D_{\alpha} e^{i \frac{F_{\alpha}}{kT}} \rho_{\alpha} \end{aligned}$$

in analogy to our equilibrium equations.

We would now like to express the non-equilibrium free energy as just $F^\theta = -kT \ln Z^\theta$. Our primary justification for believing this is because the mean energy E , the non-equilibrium entropy S^θ and the subensemble temperature T can be shown to be related by

$$E - TS^\theta = -kT \ln Z^\theta$$

which is precisely the relationship we would like a free energy to fulfil. However, the operational definition free energy, that makes it a useful to use, is that it corresponds to the work required to

¹We may imagine that each of the subspaces corresponds to a separate 'box', between which transitions are inhibited. We can then easily prepare a system in which the 'boxes' are each in equilibrium with some heat bath, but the probabilities of the 'boxes' being occupied are not in an equilibrium. As long as the thermal relaxation time for transitions between boxes is very large, this will be stable.

put the system into some reference state, by an isothermal procedure. We must show the work required to change the state matches the change in F^θ . To be sure that this is valid, the final reference state should be one in which the subensembles occur with equilibrium probability.

Let us start with a particularly simple example, consisting of Szilard box and a piston system. It is the piston system that we are going to focus upon. The piston system is initially in one of two states, which have the same internal entropies S_p , energies E_p and are in equilibrium temperature T , which for simplicity will be the same temperature as the Szilard box. The 'internal' free energy of the piston states are therefore $F_p = E_p - TS_p$. In a 'thermal equilibrium' each of the piston states would be equally likely and in an equilibrium mixture of piston states, the free energy would be $F = F_p - kT \ln 2$.

If we placed two piston states in opposite ends of the Szilard box, and compress the gas until each piston state was found in the center of the box, the isothermal work required is just $kT \ln 2$. The piston is now no longer in the mixture, and has free energy F_p . When the piston is removed, the gas expands to refill the entire box. This allows us to isothermally put the equilibrium state into a reference state, with a work requirement of $kT \ln 2$. We could also reverse the procedure, and allow the piston reference state to expand into an *equilibrium* mixture, extracting $kT \ln 2$ work.

We now consider what happens if the initial piston states occur with the more general probabilities of p and $1 - p$. We will again place the two piston states at each end of the box, but now we compress the two sides by different amounts, so the piston ends up in some position Y , not necessarily the center. If the piston is on the left, with probability p , we allow it to compress the gas to the right of Y . This requires a work of $kT \ln \left(\frac{2}{1-Y} \right)$. If the piston is on the right, with probability $(1 - p)$, the gas is compressed to the left of Y , and the work required is $kT \ln \left(\frac{2}{1+Y} \right)$. The mean work requirement is therefore

$$\frac{W}{kT} = p \ln \left(\frac{2}{1-Y} \right) + (1-p) \ln \left(\frac{2}{1+Y} \right)$$

This has its smallest value when $p = \left(\frac{1+Y}{2} \right)$ and therefore

$$W = -kT (p \ln p + (1-p) \ln(1-p))$$

This leaves the piston at position $Y = (1 - 2p)$, with the one atom gas located to the left of the piston, with probability $\left(\frac{1+Y}{2} \right)$ and to the right with probability $\left(\frac{1-Y}{2} \right)$. Had we inserted a partition into the box at position Y , we would have precisely these probabilities for the location of the one atom gas. The piston can therefore be reversibly removed from the box. Had the compression of the gas left the piston at some other value of Y^θ , removing and reinserting the piston at Y^θ would lead to a rearrangement of the probabilities of the one atom gas. This would not be a reversible procedure. This demonstrates that the work requirement to reversibly put the non-equilibrium mixture of piston states into the reference state is exactly $-T\Delta S$, where ΔS is just the mixing entropy of the non-equilibrium state.

We consider this to be the required generalisation of isothermal compression. For the change in free energy to be equal to the work done, the initial free energy must be

$$F^\theta = F_p + kT(p \ln p + (1-p) \ln(1-p))$$

This can be readily generalised to a situation with many different subensembles and with different free energies in each subensemble, but with all subensembles at the same temperature² to yield

$$\begin{aligned} F^\theta &= \sum_{\alpha} p_{\alpha}^{\theta} (F_{\alpha} + kT \ln p_{\alpha}^{\theta}) \\ &= E - TS^{\theta} \\ &= -kT \ln Z^{\theta} \end{aligned}$$

which is the desired result, and justifies the form of the non-equilibrium partition function.

With regard to the other relationships involving the free energy, we find these generalise to

$$\begin{aligned} F^\theta &= -kT \ln \left(\sum_{\alpha} D_{\alpha} e^{i \frac{F_{\alpha}}{kT}} \right) \\ p_a^{\theta} &= \frac{D_a Z_a}{Z^{\theta}} \\ F_a &= F^{\theta} - kT \ln \left(\frac{p_a^{\theta}}{D_a} \right) \end{aligned}$$

These relations are less useful than they might appear. We have justified the existence of a free energy for situations where a system is in a stable, non-equilibrium state, but has a well defined temperature. However the dependance upon the values of D_{α} makes the non-equilibrium partition function of limited value when these are changeable (unless they can be constrained to be changeable in a well defined way eg. when the system is not isolated, the D_{α} will approach 1, typically with an exponential decay, and over a time period of the same order as the thermal relaxation time). It should be noted, however, that the non-equilibrium state will have a higher free energy than the equivalent equilibrium state. As the system approaches equilibrium this extra free energy will be lost in the process of thermalisation.

²If the internal states of the piston are assumed to be thermally isolated from the Szilard box, then the compression may take place at a different temperature. While this complicates the process, it will still be consistent with the free energy defined here, taking into account the results of Appendix G, where there is more than one temperature present.

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