

# We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

6,900

Open access books available

186,000

International authors and editors

200M

Downloads

Our authors are among the

154

Countries delivered to

TOP 1%

most cited scientists

12.2%

Contributors from top 500 universities



WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index  
in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?  
Contact [book.department@intechopen.com](mailto:book.department@intechopen.com)

Numbers displayed above are based on latest data collected.  
For more information visit [www.intechopen.com](http://www.intechopen.com)



---

# Quantum Dynamics, Entropy and Quantum Versions of Maxwell's Demon

---

Paul Bracken

Additional information is available at the end of the chapter

<http://dx.doi.org/10.5772/63563>

---

## Abstract

Several subjects which reside in the overlap area of quantum mechanics, statistical physics and thermodynamics are investigated in depth. This collection of subjects shares a common domain which is referred to as Maxwell's demon. The classical version of this idea is introduced, and then, the contribution made by Szilard to the subject is presented. Several demons are considered, and it is shown that to best understand this area, quantum mechanics and the role information plays in it must be appreciated deeply.

**Keywords:** quantum dynamics, entropy, wave function, information, density matrix, quantum measurement

---

## 1. Introduction

This is an introduction to the paradox referred to as Maxwell's demon from both the perspective of the second law of thermodynamics and its consequences for quantum dynamics and recent progress in resolving it [1–3]. The classical paradox of Maxwell's demon has been around for a century and a half and has had a strong influence on the study of the second law of thermodynamics and statistical mechanics in general in addition to the area of quantum dynamics and information theory. Many new ideas and paradigms have been introduced as a result of this paradox. Maxwell first introduced the idea in one of his books in 1871 as a way of discussing limitations of the second law of thermodynamics [4, 5]. Clausius's version of the second law states that, "It is impossible to devise an engine which, working in a cycle, will produce no effect other than the transfer of heat from a colder to a hotter body."

---

In brief, the classical Maxwell's demon has the capacity to separate hot particles, atoms or molecules from cold particles and therefore obtains work from a single heat bath, which seemed to violate the second law of thermodynamics [6, 7]. The classical paradox which arose well before quantum mechanics was developed and it will be introduced from the point of view of a physical model. The demon operates a tiny door in a partition that divides a box into two parts of equal volumes and contains a gas in thermal equilibrium, and hence, temperature is uniform over the box. The demon observes the molecules in the left side, and if a molecule is seen approaching the door with speed less than the average speed of the molecules, he opens the door and lets the molecules go right; if he sees one approaching with a speed greater than average, he opens the door to let it move into the left. Once a small temperature difference has been induced between the right and left sides, his action continues to transfer heat from a colder to a hotter region without exerting any work. This violates Clausius's form of the second law of thermodynamics. This process is referred to as temperature demon.

Another type of demon can be imagined which produces a difference in pressure. This is referred to as pressure demon. This demon runs a cycle by making the gas interact with a heat bath at constant temperature after generating a pressure inequality. This cycle converts heat transferred from the bath to work. This violates the second law in terms of the Kelvin form of the second law. Thus, in either case, for either type of demon, based on temperature or pressure, the role of the demon is to decrease the entropy of the whole system in a cyclic process.

It was Szilard who first made some progress subduing the demon [8]. Szilard had the idea of treating the demon's memory or intelligence, as a form of information that could be linked to physics, to thermodynamics in fact. Szilard took a gas consisting of a single molecule, and as a first step, a thin massless adiabatic partition is inserted into the chamber quickly which divides it into two parts of equal volume. The demon measures the position coordinate of the molecule on the left or right sides and records the result for the next step. A mass is attached to the partition on the side where the molecule is found. Using a heat bath to stabilize the temperature  $T$ , the demon lets the gas do work  $W$  by quasistatic isothermal expansion. The gas returns to its initial state and occupies the whole volume of the chamber. While this takes place, heat  $Q$  is extracted from the bath and so  $W = Q$ , as it is an isothermal process. The cycle is completed as the extracted heat  $Q$  is turned into an equal amount of mechanical work.

During isothermal expansion of the gas then, if  $k_B$  is Boltzmann's constant, the amount of extracted work is given by the following equation:

$$W = k_B T \int_{V/2}^V V^{-1} dV = k_B T \ln(2). \quad (1.1)$$

It may be asked whether it is reasonable to say the one-molecule gas is a normal ideal gas. Consider an ensemble of one-molecule gases, as it is done in statistical mechanics. By taking averages over the ensemble, calculations will be made as if it were an ideal gas composed of a large number of molecules. By considering the position of the molecule, one is led to its dual interpretation in terms of both thermodynamics and information theory. As a result of the

perfect conversion of heat  $Q$  into work  $W$ , the entropy of the heat bath is reduced by the following:

$$\frac{Q}{T} = \frac{W}{T} = k_B \ln(2). \quad (1.2)$$

The second law demands an entropy increase of at least the same amount somewhere in order to compensate for this decrease. Szilard attributed this increase to measurement. Although Szilard thought that the demon's memory was important in analyzing the engine, he failed to uncover its role in terms of the second law.

## 2. A classical Szilard engine

The first to state clearly that the paradox of Maxwell's demon could be solved by considering the increase in entropy due to memory erasure was Penrose in his well-known book on statistical mechanics [4]. It was later on that Landauer, and independently Bennett, arrived at a similar conclusion [9, 10]. Bennett realized that a major result from the thermodynamics of computation by Rolf Landauer could be used to show that a Maxwell's demon could not violate the second law. Information processing must be carried out by some sort of physical system, and thus, it follows that there should be a one-to-one correspondence between logical and physical states. Let us state that logical states can be described as an abstract set of variables on which the task of information processing will be carried out. A reversible process, which means an injective or one-to-one mapping for logical states, corresponds to a reversible physical process. If a correspondence between logical and physical entropies is assumed, it implies that a reversible logical process can be realized physically by a process which is isentropic. For our purposes, an isentropic process is an entropy-preserving process.

On the other hand, a logically irreversible process is a many-to-one mapping and thus noninjective. The mapping cannot be inverted and many initial states correspond to a single resulting state. Memory erasure is a logically irreversible process because many possible states of memory should be in one specific state in order not to carry any information. The specific state after erasure is called standard state. In terms of physical states, a logically irreversible process reduces degrees of freedom of a system, implying an entropy decrease. It was Landauer who realized that logical irreversibility must involve dissipation, and thus, erasure of information in a memory implies entropy increase in the environment. This result has been formulated into a statement that is now called Landauer's erasure principle. Alternatively, Landauer's principle states that although logically reversible computational processes can in principle be performed with arbitrarily little dissipation, erasure is a logically irreversible act that has a threshold entropy production. Landauer then states that for each erased bit, the entropy sent to the environment is at least  $k_B \ln(2)$ . A complete thermodynamic analysis of a demon's cyclic operations requires that its memory be brought back to its initial state. The entropy returned to the environment is just large enough to save the second law.

Bennett made another important contribution regarding the physics of information. Measurement can be carried out reversibly without any change in entropy, provided the measuring apparatus is in a standard state. This means that storing information in the memory does not involve the erasure of information previously stored in the same memory. Measurement will be regarded as a process that correlates the memory with the system, which can be achieved reversibly in principle. This process will be considered as one that copies the memory state to another system in a standard state [11].

Since measurement will be taken without energy use, it is dissipation due to erasure that compensates the entropy decrease induced by the demon in Szilard's model. The demon commits the result to memory by establishing the position in the box. The molecule is either on the left ( $L$ ) or right ( $R$ ) side, depending on the information it stores. The prescription for erasing the stored information is to remove the partition, insert a piston on the right when the standard memory state is ( $L$ ) and move it left isothermally at temperature  $T$  until the compressed volume is  $V/2$ . The resulting state ( $L$ ) is for both initial states and the information is erased. The erasing process should not depend on the initial state of the memory, and thus, erasure should be independent of the initial memory state. The work invested to compress the volume from  $V$  to  $V/2$  is  $W_{\text{erasure}} = k_B T \ln(2)$ . This is dissipated as heat into the environment, thereby increasing its entropy by  $k_B \ln(2)$ , in agreement with Landauer's principle.

It is shown that the erasure work is proportional to the amount of information stored, that is,  $W_{\text{erasure}} = k_B T \ln(2) H(p)$ , where  $p$  is the probability for the molecule to be in state  $L$  and  $H(p)$  is the binary Shannon entropy. In other words, suppose a tendency in the frequency of appearance of a particular memory state exists, can we ask what the erasure work is. An unbalanced tendency between  $L$  and  $R$  can be expressed by the numbers of molecules in each region. Consider only an ideal gas, so removing the partition at the beginning allows the gas an undesired irreversible adiabatic expansion or compression. Let the gases in both parts expand or contract isothermally by making the partition free to move without friction. The gases generate work toward the outside. Let  $P_L$ ,  $P_R$  and  $V_L$  denote the pressures in the left and right sides and volume on the left of the partition, respectively. The work done by the gases is given as follows:

$$\begin{aligned} W &= \int_{V/2}^{pV} (P_L - P_R) dV_L = Nk_B T \int_{V/2}^{pV} \left( \frac{p}{V_L} - \frac{1-p}{V-V_L} \right) dV_L \\ &= Nk_B T [\ln(2) + p \ln(p) + (1-p) \ln(1-p)]. \end{aligned} \quad (2.1)$$

This work can be expressed in terms of the Shannon entropy which is defined to be

$$H(p) = -p \log_2 p - (1-p) \log_2 (1-p). \quad (2.2)$$

To do so, transform  $\ln(x)$  to  $\log_2(x)$  by means of the base change formula  $\log_2(x) = \ln(x)/\ln(2)$  to obtain

$$W = Nk_B T \ln(2)[1 + p \log_2 p + (1 - p) \log_2 (1 - p)] = Nk_B T \cdot \ln(2) \cdot [1 - H(p)]. \quad (2.3)$$

Since the pressures in the left and right are equal, this returns us to the configuration with the partition in the middle. Hence, at least  $Nk_B T \ln(2)$  of work needs to be consumed to set the memory to the standard state. In total, after dividing out  $N$ , an amount

$$W_{\text{erasure}} = k_B T \ln(2) - W = k_B T \ln(2) H(p) \quad (2.4)$$

of work per molecule is invested. Supposing the memory is in the standard state to begin with,  $W_{\text{erasure}}$  gives a measure of the additional energy required to erase the memory due to its information content. Without violating the second law, the state of the whole system consisting of the heat engine and demon is restored after completing a thermodynamic cycle.

### 3. The von Neumann entropy as the quantum entropy

Entropy is not an observable property, and thus, there does not exist an operator with the property that its expectation value in some state would give the entropy. Entropy is a state function. In order to study entropy in the context of quantum systems, it is necessary to give a precise definition of the concept before proceeding [7].

To provide some motivation for this, it may be supposed that the ground state of a quantum system is described by its density matrix  $\rho$ . If  $\mathbf{A}$  is an observable which pertains to the system characterized by  $\rho$ , the spectral theorem permits the spectral decomposition of  $\mathbf{A}$  as  $\mathbf{A} = \sum_i a_i \mathbf{P}_i$ , where  $\mathbf{P}_i$  is a projection operator onto the state with eigenvalue  $a_i$ . The probability of obtaining  $a_j$  in a measurement is given by  $p_j = \text{Tr}(\rho \mathbf{P}_j) = \text{Tr}(\mathbf{P}_j \rho)$ . The uncertainty in a given observable can be expressed by means of the  $P_i$  through the Shannon entropy,  $S(\mathbf{p})$ , not to confuse it with von Neumann entropy  $S_N(\mathbf{A})$ .

**Definition 3.1.** The uncertainty in a collection of possible classical states  $\{a_i\}$  with corresponding probability distribution  $\mathbf{p} = p(a_i)$  is given by its entropy, the Shannon entropy

$$S(\mathbf{p}) = - \sum_i p(a_i) \log_2(p(a_i)), \quad (3.1)$$

The Shannon information is a good indicator of how much two given observables are correlated. This quantity is inherently classical, as it describes the correlations between single observables. The quantity that is related to the correlations in the overall state as a whole is the von Neumann entropy or mutual information. It is assigned to a state as a whole, so naturally it depends on the density matrix.

**Definition 3.2.** The von Neumann entropy of a quantum system described by the density matrix  $\rho$  is defined to be

$$S_N(\rho) = -\text{Tr}(\rho \ln(\rho)). \quad (3.2)$$

The von Neumann entropy can also be defined in terms of the base two logarithms. Defined in this way, Eq. (3.2) implies that if  $\lambda_i$  are the eigenvalues of  $\rho$ , the von Neumann entropy can be expressed in Shannon form as  $S_N(\rho) = -\sum_i \lambda_i \log_2(\lambda_i) = S(\lambda(\rho))$ . There have been several studies recently of quantum operations that preserve the von Neumann entropy of quantum states. The Shannon entropy  $S(\mathbf{p})$  is equal to the von Neumann entropy only when it describes the uncertainties in the values of observables that commute with the density matrix and  $S(\mathbf{p}) \geq S_N(\mathbf{A})$  otherwise. Here,  $\mathbf{A}$  is any observable of a system described by the density matrix  $\rho$ . There are two important properties of the entropy in Eq. (3.2) which should be noted.

(a) additivity

$$S_N(\rho_A \otimes \rho_B) = S_N(\rho_A) + S_N(\rho_B). \quad (3.3)$$

(b) concavity

$$S_N\left(\sum_i \lambda_i \rho_i\right) \geq \sum_i \lambda_i S_N(\rho_i). \quad (3.4)$$

As in the classical instance, property (a) states that entropies add up. The concavity property (b) simply reflects the fact that mixing increases uncertainty. The von Neumann mutual information refers to the correlation between whole subsystems rather than that relating only two variables and it is introduced as follows.

**Definition 3.3.** The von Neumann mutual information between two subsystems  $\rho_U$  and  $\rho_V$  of a joint state  $\rho_{UV}$  is defined as follows:

$$I_N(\rho_U : \rho_V : \rho_{UV}) = S_N(\rho_U) + S_N(\rho_V) - S_N(\rho_{UV}). \quad (3.5)$$

This quantity can be interpreted as a distance between two quantum states.

**Definition 3.4.** The von Neumann relative entropy between two states  $\sigma$  and  $\rho$  is defined as follows:

$$S_N(\sigma \parallel \rho) = \text{Tr} \sigma (\ln \sigma - \ln \rho). \quad (3.6)$$

The relative entropy expresses how difficult it is to distinguish the state  $\sigma$  from the state  $\rho$ .

#### 4. A quasi-classical erasure process

An example of an erasure process that can be studied in detail is a way to erase classical information encoded in quantum states [6]. It straddles the classical-quantum interface and can be accomplished by thermal randomization. Thermal randomization makes use of the randomness of states in a heat bath, which is in thermal equilibrium. If a heat bath at temperature  $T$  and a state, which could represent a message, are brought into contact, the state will approach equilibrium with the heat bath. A message state  $\rho_i$  changes gradually after an interaction with the heat bath. A sufficient number of collisions make the state indistinguishable from that of the heat bath. In this way, the information that was carried by  $\rho_i$  is lost irreversibly. The entropy of the whole system necessarily increases.

Suppose each external 'message' state is in a pure state. Before erasure, the whole message consists of an ensemble  $\{p_i, |\phi_i\rangle\}$ . Thus, its average state is described by a density operator of the form  $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$ . The process of thermalization brings all states  $|\phi_i\rangle$  to the same state,  $\varphi$  in thermal equilibrium at temperature  $T$ . Consequently, the density matrix is as follows:

$$\varphi = \frac{1}{Z} e^{-\beta \hat{H}} = \sum_j q_j |e_j\rangle\langle e_j|, \quad (4.1)$$

where  $\hat{H} = \sum_i e_i |e_i\rangle\langle e_i|$  is the Hamiltonian operator of the message state in terms of energy eigenstates  $|e_i\rangle$ , and  $Z = \text{Tr}(e^{-\beta \hat{H}})$  is the partition function. It follows from Eq. (4.1) that  $\text{Tr}\varphi = 1$ .

The total entropy  $\Delta S_{\text{erasure}}$  is the sum of the entropy change of the message or reference system and of the heat bath:  $\Delta S_{\text{erasure}} = \Delta S_{\text{system}} + \Delta S_{\text{bath}}$ . Since the state before erasure is pure and its state after erasure is the same as the heat bath, the minimum entropy change in the reference state is given by the following equation:

$$\Delta S_{\text{system}} = k_B \ln(2) S(\varphi), \quad (4.2)$$

where  $S(\varphi) = -\text{Tr}(\varphi \ln(\varphi))$  is the von Neumann entropy of state  $\varphi$ .

The entropy change in the heat bath is equal to the average heat transfer from the bath to the reference system divided by temperature  $T$ ,

$$\Delta S_{\text{bath}} = \frac{1}{T} \Delta Q_{\text{bath}}. \quad (4.3)$$

The heat change in the heat bath must agree with that of the system, but with an opposite sign,  $\Delta Q_{\text{bath}} = -\Delta Q_{\text{system}}$ . When heat transfer is done quasistatically, the mechanical work required for the state change is arbitrarily close to zero. Moreover, energy conservation requires  $\Delta Q_{\text{system}}$

be equal to the change of internal energy of the system,  $\Delta U_{system}$ . This can be computed as the change of average values of the Hamiltonian  $\hat{H}$  before and after the erasure process,

$$\Delta S_{bath} = -\frac{1}{T} \Delta Q_{system} = -\frac{1}{T} \Delta U_{system} = -\frac{1}{T} [Tr(\varphi \hat{H}) - Tr(\rho \hat{H})] = -\frac{1}{T} Tr[(\varphi - \rho) \hat{H}]. \quad (4.4)$$

The Hamiltonian  $\hat{H}$  can be expressed using Eq. (4.1) as  $\hat{H} = -k_B T \ln(Z\varphi)$ . As  $Z$  is a trace, it follows from the properties of the trace, converting the natural logarithm to base two that the following result holds

$$\Delta S_{bath} = k_B Tr[(\varphi - \rho) \ln(Z\varphi)] = k_B Tr[(\varphi - \rho) \ln(\varphi)] = -k_B \ln(2) [S(\varphi) + Tr(\rho \log_2 \varphi)]. \quad (4.5)$$

Therefore, the required total energy change is given by the following equation:

$$\Delta S_{erasure} = \Delta S_{system} + \Delta S_{bath} = -k_B \ln(2) Tr(\rho \log_2 \varphi). \quad (4.6)$$

Since the quantum relative entropy satisfies the following inequality

$$S(\rho \parallel \varphi) = -S_N(\rho) - Tr(\rho \log_2 \varphi) \geq 0, \quad (4.7)$$

the minimum of the entropy change  $\Delta S_{erasure}$  can be obtained,

$$\Delta S_{erasure} = -k_B \ln(2) Tr(\rho \log_2 \varphi) \geq S_N(\rho). \quad (4.8)$$

The minimum corresponding to equality in Eq. (4.8) is achieved by choosing the temperature of the bath and  $\{p_i, |\phi_i\rangle\}$  such that  $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i|$  is the same as the thermal equilibrium state.

Consequently, the minimum entropy increase required for erasure of the classical information which is encoded in quantum states is given by the von Neumann entropy  $S_N(\rho)$ , where  $\rho$  is the average state of the system, in place of the Shannon entropy,  $H(\rho)$ , in the case of information erasure of classical states.

## 5. Quantum entanglement and Maxwell's demon

Formally, entanglement is defined as a form of quantum correlation that is not present in any separable states and represents a true type of quantum behavior [12, 13]. Entanglement can be approached from the point of view of Maxwell's demon. Let  $\mathcal{H}^A$  and  $\mathcal{H}^P$  be the Hilbert spaces for two spatially separated or noninteracting subsystems, called  $A$  and  $P$ , and define the entire

Hilbert space  $\mathcal{H}^{AP} = \mathcal{H}^A \otimes \mathcal{H}^P$ . Let  $\mathcal{S}(\mathcal{H})$  denote the state space that consists of a set of density operators acting in  $\mathcal{H}$ . The case studied here is that of bipartite entanglement.

A state of a bipartite system is said to be separable or classically correlated if its density operator can be expressed as a convex sum of products of density operators

$$\rho = \sum_{i=1}^n p_i \rho_i^A \otimes \rho_i^P, \quad (5.1)$$

where all the  $p_i$  are nonnegative and  $\sum_i p_i = 1$ . Any state that cannot be written in the form of Eq. (5.1) is called entangled. Let  $\mathcal{S}_{sep}$  denote the subspace that contains all separable states.

It is natural to ask whether or not a given state  $\rho \in \mathcal{S}(\mathcal{H}^{AP})$  is separable considering how important the subject of entanglement is in quantum mechanics. This can usually be expressed in terms of an operator or function. In general, it is very hard to obtain a good separability criterion, that is, something that is efficient and singles out as many entangled states as possible. The separable subspace formed by all separable states is convex and is the main reason for the difficulty of the problem.

Another question pertains to the amount of entanglement a pair or set of quantum objects contains. The amount plays a major role when it comes to characterization or manipulation of entanglement. This topic might be approached by trying to quantify entanglement by means of a thermodynamic quantity.

In a chamber such as the one encountered in Szilard's engine, it can be thought of as a general information-storage apparatus, that is, physical states are distinguishable by measurement, and therefore, stored information will be extracted. Information could be transferred from a different system to the memory of a Szilard engine, if the initial state of the engine is in a standard state.

Now that the memory has been identified with the one molecule gas of Szilard's engine, consider the following picture. From an ensemble of memories, each of which stores the value of an  $n$ -bit random variable  $\eta$ , mechanical work can be extracted whose average amount per single memory register is

$$W_c = n - H(\eta), \quad (5.2)$$

where  $H(\eta)$  is the Shannon entropy of  $\eta$ , in units such that  $k_B \ln 2 = 1$ . The extractable work is the work done by the gas, so it is  $W = Nk_B T \ln(2)[1 - H(\eta)]$  when  $n = 1$ . To understand Eq. (5.2) more completely, suppose there are  $N$  memory registers. If all  $N$  registers are measured, the remaining uncertainty in the memory is zero, hence  $Nn$  bits of work can be obtained. However, the information due to the measurement on memory is kept, and this must be erased in order to consider the amount of extractable work. The least energy consumption needed to erase information is  $NH(\eta)$  bits, according to the erasure principle. The maximum total extractable

work is  $N[\eta - H(\eta)]$ . Also, from the thermodynamic point of view Eq. (5.2) follows, as the work done by the gas in an isothermal process is equal to the entropy change multiplied by the temperature.

This argument can be applied to the case of work extraction from quantum bits. Let  $\rho$  be the density operator for the state in a given ensemble. The qubits are in a known pure state after measurements, which is essentially classical in terms of information. Information stored in this set of pure states can be copied to the Szilard memory, and each register gives one bit of work. After erasing the information acquired by measurement, the net maximum amount of work we obtain becomes  $1 - S_N(\rho)$  bits of work.

The work deficit is a difference between the globally and locally extractable work within the context of local operations, or at least when  $\rho$  is a system with spatially separated subsystems. Suppose there is an  $n$ -qubit state  $\rho_{AP}$  shared by  $A$  and  $P$ , then the optimal extractable work is given by

$$W_{global} = n - S_N(\rho^{AP}), \quad (5.3)$$

If the entire system can be accessed globally. On the other hand, letting  $W_{local}$  be the largest amount of work that  $A$  and  $P$  can locally extract from the same system under local operations and classical communication. Define the deficit to be  $\Delta = W_{global} - W_{local}$ . In order to understand this, the deficits for a classically correlated state

$$\rho_{cl}^{AP} = \frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|), \quad (5.4)$$

and a maximally entangled state

$$|\Phi^{AP}\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \quad (5.5)$$

will be calculated.

The globally extractable work  $W_{global}^{cl}$  from  $\rho_{cl}^{AP}$  is simply one bit. The locally extractable work  $W_{local}^{cl}$  is also one bit. The strategy is as follows: observer  $A$  will measure its bit in the basis  $\{|0\rangle, |1\rangle\}$  and will send the result to observer  $P$ , who obtains one bit of work from it. Although  $A$  can extract one bit of work from  $A$ 's own bit, using  $A$ 's measurement result,  $A$  needs to consume all this energy to erase the information stored in the memory used to communicate with observer  $P$ . Thus, the deficit for state  $\rho_{cl}^{AP}$  is  $\Delta_{cl} = 1 - 1 = 0$ . The locally extractable work is the same, one bit, even if the state is maximally entangled as in Eq. (5.5). However, as this state is globally pure, it must be  $W_{global} = 2 - S_N(|\Phi^{AP}\rangle\langle\Phi^{AP}|) = 2$ , and therefore,  $\Delta_{entangled} = 2 - 1 = 1$ .

It can be shown that the deficit is bounded from below as follows:  $\Delta \geq \max\{S_N(\rho^A), S_N(\rho^B)\} - S_N(\rho)$ , where  $\rho^A$  and  $\rho^B$  are given by  $\rho^A = \text{Tr}_P(\rho)$  and  $\rho^B = \text{Tr}_A\rho$ . The bound can be achieved when the state is pure and turns out to be equal to the entanglement measure for pure states. This is simply due to the fact that a pure state can be expressed as  $|\psi\rangle = \sum_i \alpha_i |e_i\rangle |f_i\rangle$  in the Schmidt decomposition, then  $\Delta = S_N(\rho^A) = E(\psi)$ , where  $\rho^A = \text{Tr}_P |\psi\rangle\langle\psi|$  and  $E$  is the entanglement measure for pure states.

## 6. A nuclear magnetic resonance demon

A very sophisticated model of a demon which is based on a type of nuclear magnetic resonance experiment to introduced. The model studied here is close to the one originally proposed by Lloyd [14] in 1997. It is worth discussing the model though as it may be possible to realize it experimentally. It permits a detailed discussion on several levels and unites several subjects. This gives a nontrivial, fully quantum mechanical model that unlike semiclassical models allows the thermodynamics of the demon's entire cycle of operation to be treated within a unified quantum picture. In this section, the abbreviation  $\beta_i = 1/k_B T_i$  will be used.

A spin is immersed in a magnetic field  $B$ . If the spin has the same direction as  $B$ , it has energy  $-\mu B$ , where  $\mu$  is the spin's magnetic dipole moment,  $B$  is the magnitude of the field. In the opposite direction, the spin has energy  $+\mu B$ . The spin can be flipped from one energy to another by applying a  $\pi$  pulse at the spin's precession frequency,  $\omega = 2\mu B/\hbar$ . When the spin flips, it exchanges energy with the oscillatory field. When it absorbs one photon of energy  $\hbar\omega$  from the field, it goes from lower to higher energy, and proceeding the other way, it coherently emits a photon of energy  $\hbar\omega$  to the field. When the field is in a coherent state, as with fields which are normally produced by lasers or masers, the energy exchange involves no information exchange, entropy increase or loss of quantum coherence and so the oscillating field may be treated as if it were classical.

A device that acquires information about such a spin could use the information to make the spin do work. Suppose a device can measure whether the spin is in the low-energy quantum state  $|\downarrow\rangle$  or the high-energy state  $|\uparrow\rangle$ . If it is in the high-energy state, a  $\pi$  pulse is sent to extract its energy. This device waits for the spin to come to equilibrium at  $T_1 > 2\mu B/k_B$  and repeats the operation. Each time, it converts an average of  $\mu B$  of heat into work. It is Landauer's principle which prevents such a device from violating the second law of thermodynamics. To proceed in a cyclic fashion, the device must erase the information that it has gained about the state of the spin. At erasure, entropy  $S_{out} \geq k_B \ln(2)$  is forced into the environment, which compensates for the entropy  $S_{spin} = k_B \ln(2)$  in the spin originally. If the environment is a heat bath at  $T_2$  different from the temperature of the spin heat bath  $T_1$ , heat  $k_B T_2 \ln(2)$  flows to the heat bath along with entropy, decreasing the energy available to convert into work. To account for energy and entropy in the cycle, the heat in is  $Q_{in} = T_1 S_{in}$ , and the heat out is  $Q_{out} = T_2 S_{out}$ . Thus, the work out is  $W_{out} = Q_{in} - Q_{out}$ , and the efficiency  $\epsilon$

satisfies  $\epsilon = W_{out}/Q_{in} \leq 1 - T_2/T_1 = \epsilon_C$ , where  $\epsilon_C$  is the Carnot efficiency. Landauer's principle implies that instead of violating the second law, the device operates as a heat engine, pumping heat from a high-temperature reservoir to one at low-temperature and doing work in the process.

It can be shown that such a device operates as a heat engine that undergoes a cycle analogous to a Carnot cycle. Thus, a quantum device that interacts with a thermal environment can get information and use it to do useful work, but not by violating the second law of thermodynamics. A detailed picture of the erasure model agrees with Landauer's principle. Two sets of modes of the electromagnetic field constitute the environment for the spins. The first will be a set of modes at  $T_1$  with average frequency  $\omega_1$  and frequency spread greater than the coupling constant  $|\kappa|$  between the spins but less than  $\omega_1 - \omega_2$ . The second will be a set of modes at temperature  $T_2$  with average frequency  $\omega_2$  and the same frequency spread. This can be achieved by immersing the spins in incoherent radiation with the given frequencies and temperatures. This should provide separate heat reservoirs for spin 1 and 2. This means spin 1 interacts strongly with the on-resonance radiation at frequency  $\omega_1$ , and weakly with the off-resonance radiation at  $\omega_2$ , with the reverse for spin 2. Spin 1 can be regarded as interacting only with mode 1, and spin 2 as interacting only with mode 2.

With respect to this approximation, the initial probabilities for the state of the  $j$ -th spin are

$$p_{\uparrow,j} = \frac{1}{Z_j} e^{-\mu_j B \beta}, \quad p_{\downarrow,j} = \frac{1}{Z_j} e^{\mu_j B \beta}, \quad \beta = \frac{1}{k_B T}. \quad (6.1)$$

Using Eq. (6.1), the energy can be calculated to be the following:

$$E_j = -\mu_j B p_{\uparrow,j} + \mu_j B p_{\downarrow,j} = -\mu_j B \tanh(\mu_j B \beta). \quad (6.2)$$

The entropy is given by

$$S_j = -k_B \sum_{i=\uparrow,\downarrow} p_{(i),j} \ln(p_{(i),j}) = \frac{1}{T} E_j + k_B \ln(Z_j), \quad (6.3)$$

where  $Z_j = e^{-\mu_j B \beta} + e^{\mu_j B \beta} = 2 \cosh(\mu_j B \beta)$ . Spin 2 can acquire information about spin 1, and this information can be exploited to perform work. Therefore, the spins can function as a heat engine by passing through the following cycle:

First, using spin coherence double resonance, flip spin 2 if spin 1 is in state  $|\uparrow\rangle_1$ . This causes spin 2 to acquire information  $(\tilde{S}_2 - S_2)/k_B \ln(2)$  about spin 1 at the cost of  $W_1 = p_{1,1} 2\mu_2 B \tanh(\mu_2 B \beta)$  of work supplied by the oscillating field, where  $\tilde{S}_2 = -k_B \sum_{i=1,2} \tilde{p}_{(i),2} \ln(p_{(i),2})$ , such that

$\tilde{p}_{1,2} = p_{1,1}p_{1,2} + p_{1,1}p_{1,2}$  and  $\tilde{p}_{1,2} = p_{1,1}p_{1,2} + p_{1,1}p_{1,2}$  are the two probabilities for the states of spin 2 after the conditional spin flip.

Second, flip spin 1 if spin 2 is in the state  $|\uparrow\rangle_1$ . This step permits spin 2 to take the amount  $(S_2 - S_1)/k_B \ln(2)$  of the information it has acquired, and in the process carry out work  $-\mu_1 B [\tanh(\mu_1 B \beta_1) - \tanh(\mu_2 B \beta_2)]$  back on the field.

Third, spin 2 still has information in the amount  $(\tilde{S}_2 - S_1)/k_B \ln(2)$  about spin 1, which can be converted into work by flipping spin 2 if spin 1 is in state  $|\uparrow\rangle_1$ , thereby carrying out work in the amount  $p_{1,2} 2\mu_2 B \tanh(\mu_1 B \beta_2)$  on the field.

The set of pulses has finally exchanged the information associated in 1 with the information in 2. Next, after the three conditional spin flips, spin 1 has probabilities  $p'_{(i),1} = p_{(i),2}$ , while 2 has probabilities  $p'_{(i),2} = p_{(i),1}$ . Consequently,  $S'_1 = S_2$  and  $S'_2 = S_1$  and the new energies of the spins are given by the following equation:

$$E'_1 = -\mu_1 B \tanh(\mu_2 B \beta_2), \quad E'_2 = -\mu_2 B \tanh(\mu_1 B \beta_1). \quad (6.4)$$

Thus, the total amount of work done by the spins on the field is given as follows:

$$W = -(E'_1 + E'_2 - E_1 - E_2) = -(\mu_1 - \mu_2) B [\tanh(\mu_1 B \beta_1) - \tanh(\mu_2 B \beta_2)] \quad (6.5)$$

When the temperatures satisfy the inequalities  $T_i \gg \mu_i B / k_B$ , then work  $W$  simplifies to the form

$$W = -(\mu_1 - \mu_2) \left( \frac{\mu_1}{T_1} - \frac{\mu_2}{T_2} \right) \frac{B^2}{k_B}. \quad (6.6)$$

These results for work done are a function of only conservation of energy and not the pulse. If  $T_1 = T_2$ , Eq. (6.6) implies  $W$  is zero or negative, no work can be extracted from the spins at equilibrium. The cycle can be completed by allowing the spins to re-equilibrate with their reservoirs. The following two steps then can be included to allow the spins to re-equilibrate isentropically.

Return spin 1 to its original state: take the spin out of contact with its reservoir by varying the frequency of the reservoir modes; next vary the field according to  $B \rightarrow \tilde{B} = B T_\lambda / T_2$  adiabatically, with no heat flowing between spin and reservoir; thirdly, slowly change  $\tilde{B} \rightarrow B$ , keeping the spin in contact with the reservoir at temperature  $T_1$ , so that heat flows isentropically between the spin and reservoir. Entropy  $S_1 - S_2$  moves from the spin to the reservoir while the spin does work of  $E_1 - E'_1 - T_1(S_2 - S_1)$  on the field.

Spin 2 returns to its original state by the same steps. The total work done by the spins on the electromagnetic field throughout the cycle is  $W_C = (T_1 - T_2)(S_1 - S_2)$ .

Consider a simple model in which spin 1 is initially in the state

$$|\rightarrow\rangle_1 = \frac{1}{\sqrt{2}}(|\uparrow\rangle_1 + |\downarrow\rangle_1). \quad (6.7)$$

This state has nonminimum free energy available for conversion into work. Apply a  $\pi/2$  pulse to rotate spin 1 into state  $|\downarrow\rangle_1$ , thereby adding energy  $\mu_1 B$  to the field. Suppose the demon operates in a mode whereby, instead of taking the energy directly, it uses magnetic resonance to correlate the state of 2 with the state of 1. Suppose 2 is in state  $|\downarrow\rangle_2$  initially; coherently flipping 2 if 1 is in state  $|\uparrow\rangle_1$  results in the state

$$\frac{1}{\sqrt{2}}[|\uparrow\rangle_1 |\uparrow\rangle_2 + |\downarrow\rangle_1 |\downarrow\rangle_2]. \quad (6.8)$$

This represents an entangled state in which the state 2 is perfectly correlated with the state of 1. Energy extraction can be continued by flipping spin 1 if spin 2 is in state  $|\uparrow\rangle_2$  which allows energy of  $(\mu_1 - \mu_2)B$  to be taken from the spin. The resulting state of the spins is  $\frac{1}{\sqrt{2}}|\downarrow\rangle_1 |\rightarrow\rangle_2$ . No extra thermodynamic cost has been incurred up till now. Since the conditional spin flipping occurs coherently, the process may be reversed by repeating the steps in reverse order to return to the original state  $|\rightarrow\rangle_1$ , with a total energy and entropy change of zero.

In the original cycle, decoherence occurs when 2 is placed in contact with the reservoir to erase it. The energy exchange between spin and reservoir is an incoherent process such that the pure state  $|\rightarrow\rangle_2 = 1/\sqrt{2}(|\uparrow\rangle_2 + |\downarrow\rangle_2)$  transforms into the mixed state which has density matrix  $\tilde{\rho} = 1/\sqrt{2}(|\uparrow\rangle_2 \langle\uparrow| + |\downarrow\rangle_2 \langle\downarrow|)$ . This is significant since interaction of the spin with the reservoir turns the process by which 2 coherently picks up quantum information about 1 into a decoherent measurement process and creates one bit of information. The bit corresponds to an entropy increase in  $k_B \ln(2)$ . In agreement with Landauer's principle, erasure results in the transfer of entropy from spin 2 to the low-temperature reservoir.

The amount of inefficiency generated by decohering 2 to measure spin 1 increasing the entropy may be measured by means of a Carnot cycle model. A general state for the 1 spin would have density matrix

$$\rho = p_1(|\uparrow_\vartheta\rangle_1 \langle\uparrow_\vartheta| + p_1(|\downarrow_\vartheta\rangle_1 \langle\downarrow_\vartheta|) \quad (6.9)$$

where the basis  $\{|\uparrow_\vartheta\rangle, |\downarrow_\vartheta\rangle\}$  is made up of spin states along an axis making an angle  $\vartheta$  with the z-axis. Let temperature  $T_1$  and field  $B$  be chosen so that

$$p_1(\uparrow_{\vartheta}) = \frac{1}{Z_1} e^{-\mu_1 B \beta_1}, \quad p_1(\downarrow_{\vartheta}) = \frac{1}{Z_1} e^{\mu_1 B \beta_1}. \quad (6.10)$$

Eq. (6.9) is not an equilibrium state and has free energy that may be extracted by applying a tipping pulse that rotates the spin by  $\vartheta$  and carries out the mapping  $|\uparrow_{\vartheta}\rangle \rightarrow |\uparrow\rangle$  and  $|\downarrow_{\vartheta}\rangle \rightarrow |\downarrow\rangle$ . The amount of extracted work is

$$W^* = E_1^* - E_1 = \mu_1 B [p_1^*(\uparrow) - p_1^*(\downarrow)] - \mu_1 B [p_1(\uparrow) - p_1(\downarrow)], \quad (6.11)$$

with  $p_1^*(\uparrow) = p_1(\uparrow) \cos^2 \vartheta + p_1(\downarrow) \sin^2 \vartheta$  and  $p_1^*(\downarrow) = p_1(\downarrow) \cos^2 \vartheta + p_1(\uparrow) \sin^2 \vartheta$ . Undergoing a Carnot cycle through the five steps just presented above extracts work of  $(T_1 - T_2)(S_1 - S_2)$  and energy is extracted isentropically with no entropy increase. By performing measurements with respect to which the density matrix is diagonal, the upper limit  $\epsilon_Q = \epsilon_C$  can be attained. If the tipping pulse is used at first to remove the free energy from 1, the demon is carrying out measurements such that the density matrix possesses off-diagonal elements. As a result, the measurement introduces information and the efficiency satisfies the inequality  $\epsilon_Q < \epsilon_C$ .

The steps can be summarized in this way: three conditional spin flips swap the states of 1 and 2 so that spin 1 is in state  $\rho_2$  and 2 is in state  $\rho'_2 = \rho'_1$ . Interaction with the heat reservoir decoheres 2 and destroys the off-diagonal elements in the density matrix so that

$$\rho'_2 \rightarrow p_1^*(\uparrow) |\uparrow\rangle\langle\uparrow| + p_1^*(\downarrow) |\downarrow\rangle\langle\downarrow|, \quad (6.12)$$

which has entropy

$$S_1^* = -k_B \sum_{i=\uparrow,\downarrow} p_1^*(i) \ln(p_1^*(i)), \quad (6.13)$$

with  $\Delta S_0 = S_1^* - S_1$  as the extra entropy introduced by quantum decoherence. The entropy  $S_1^* - S_2$  that flows out to reservoir 2 is then greater than the entropy  $S_{in} = S_1 - S_2$  that flowed in from 1. The total amount of work done is then  $T_1(S_1 - S_2) - T_2(S_1^* - S_2) + W^*$  and less than  $(T_1 - T_2)(S_1 - S_2) + W^*$ , which is done by simply undoing the tipping pulse and running the engine as before.

## 7. Conceptual systems for future speculation and conclusions: quantum Szilard engines

The preceding model showed how a quantum system that obtains information about another quantum system can function in the capacity of a Maxwell's demon using information to

perform work. It would be interesting if progress could be made on the experimental front in this area. At some point, nucleon-nucleon double resonance methods could be used to construct a demon in the form of a maser that functions as a demon and carries out a net amplification of pulses that causes spins to flip. Two different species of nucleons must start the cycle at different temperatures, which could be achieved by preparing one of them in a low temperature state using electron-nucleon double resonance as in the Pound-Overhauser effect.

Three final systems are presented to provide a summary and conclusion, both illustrate what has been achieved and provide work for the future. These are more conceptual in nature and are given in summary form. The processes in the first two examples are likely to be difficult to realize in practice. The first shows that there is a close relationship between dynamical evolutions, which violate some fundamental principle of quantum theory and those forbidden by the second law of thermodynamics. Thermodynamics does impose severe constraints on the choice of the fundamental axioms of quantum theory. This relies on the equivalence of the von Neumann entropy to ordinary entropy appearing in thermodynamics. Perhaps some of these physical situations would end up providing a test of this. The von Neumann entropy is essential in the second model, which represents a true quantum version of a Szilard engine, and it appears in the analysis of two cycles. The last system that involves a molecule in a variable double well may be closer to realization experimentally. A solvable model is proposed and used to describe it here. The conclusion to be drawn is that if the integrity of the axiomatic structure of quantum theory is not strictly respected, then every aspect of the theory must be examined.

(1) The first model to be studied is due to Peres and is a conceptual experiment based on the distinguishability of quantum states [12, 13]. Peres showed that if it were possible to distinguish nonorthogonal quantum states perfectly, then the second law of thermodynamics would necessarily be violated. Consider an elementary work extraction process that uses a collection of pure orthogonal states. A chamber is partitioned into two sections with volumes  $p_1 V$  and  $p_2 V$  such that  $p_1 + p_2 = 1$ . The chamber contains a gas of molecules whose quantum internal degree of freedom is a spin; as a first example before the more novel case of Peres, consider a gas with spin up  $|\uparrow\rangle$  on the left and spin down  $|\downarrow\rangle$  on the right. Similar experiments could also be imagined using polarized photons as well. The existence of semipermeable membranes is essential to all of this formalism. In this event, introduce two membranes  $M_\uparrow$  and  $M_\downarrow$  which distinguish the orthogonal states. The convention is that the membrane  $M_\uparrow$  is completely transparent to the  $|\downarrow\rangle$  spin gas and opaque to the  $|\uparrow\rangle$  spin gas. The membrane  $M_\downarrow$  has exactly the opposite properties. If the membranes replace the partition so that  $M_\uparrow$  and  $M_\downarrow$  face the  $|\downarrow\rangle$  and  $|\uparrow\rangle$  gases, respectively, the gases give work expanding isothermally by contact with a heat bath at temperature  $T$ . The total extractable work is then  $W = -p_1 \log_2 p_1 - p_2 \log_2 p_2$ .

The cycle imagined by Peres is related to this example; however, the key to its impact is the use of nonorthogonal states. The volume of the chamber is  $2V$  and in the initial state, the gas of volume  $V$  is divided into two equal volumes  $V/2$  and separated by an impenetrable wall. On the left side, the gas molecules are in the state  $|\uparrow\rangle$  but on the right side, they are in the linear combination state

$$|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle). \quad (7.1)$$

Both sections contain the same number of gas molecules  $N/2$  and hence the same pressure.

The first step of the cycle is to let the gas expand isothermally at temperature  $T$ , so the entire chamber is finally occupied. During the expansion, the gases exert work equal to  $Nk_B T \ln(2)$  toward the outside and absorbing the same amount of heat from the bath.

In the second step, conceptual membranes are introduced, which have the ability to distinguish nonorthogonal states. The partition at the center has to be replaced by these membranes. Next, insert an impenetrable piston on the right side of the vessel. The membrane  $M_+$  transparent to  $|\rightarrow\rangle$ , but opaque to  $|\uparrow\rangle$ , is fixed at the center, while the other membrane  $M_-$  of opposite transparency to  $M_+$  can move in the left-hand region. As the piston is inserted on the right,  $M_-$  is forced to the left at the same speed so that the volume and pressure of the spin  $|\rightarrow$  gas in between the piston and membrane  $M_-$  will remain constant. Due to the nature of the membranes, this process can be done without friction or resistance, and consequently, there is no work consumption or heat transfer required.

At this point, the vessel is a mixture of two spin states. In terms of the basis  $\{|\uparrow\rangle, |\downarrow\rangle\}$ , the density matrix for the mixture using Eq. (7.1) is

$$\rho = \frac{1}{2} |\uparrow\rangle\langle\uparrow| + \frac{1}{4} (|\uparrow\rangle + |\downarrow\rangle)(\langle\uparrow| + \langle\downarrow|). \quad (7.2)$$

This  $\rho$  can be mapped to a matrix representation given as follows:

$$\rho = \begin{pmatrix} \frac{3}{4} & \frac{1}{4} \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix} \quad (7.3)$$

The eigenvalues of matrix Eq. (7.3) are found to be

$$\lambda_1 = \frac{1}{2} \left(1 + \frac{1}{\sqrt{2}}\right), \quad \lambda_2 = \frac{1}{2} \left(1 - \frac{1}{\sqrt{2}}\right), \quad (7.4)$$

and the corresponding eigenvectors in terms of the  $\{|\uparrow\rangle, |\downarrow\rangle\}$  bases have the form,

$$|\phi_1\rangle = \cos\left(\frac{\pi}{8}\right)|\downarrow\rangle + \sin\left(\frac{\pi}{8}\right)|\uparrow\rangle, \quad |\phi_2\rangle = \cos\left(\frac{3\pi}{8}\right)|\downarrow\rangle - \sin\left(\frac{3\pi}{8}\right)|\uparrow\rangle. \quad (7.5)$$

If the membranes  $M_+$ ,  $M_-$  are replaced by two new membranes that distinguish between the two orthogonal states  $|\phi_i\rangle$  in Eq. (7.5), which we call  $M_{|\phi_i\rangle}$  the reverse process separates the states  $|\phi_1\rangle$  and  $|\phi_2\rangle$ . After replacing the semipermeable membrane by an impenetrable wall, the gases on the left and right segments are compressed isothermally until the total volume and pressure of the gases become equal to the initial ones. This compression requires work of  $-\lambda_1 \log_2 \lambda_1 - \lambda_2 \log_2 \lambda_2 = 0.6$  upon using Eq. (7.4), which is dissipated into the heat bath.

Finally, an opaque wall is inserted into the vessel which divides the volume  $V$  occupied by the gases in two. Next rotate the state  $|\phi_1\rangle \rightarrow |\uparrow\rangle$  in the first region on the left  $|\phi_1\rangle \rightarrow |\rightarrow\rangle$  in the center and  $|\phi_2\rangle \rightarrow |\rightarrow\rangle$  on the right, along with a trivial spatial shift restores the initial state. Rotations are unitary transformations and an isentropic process, so any energy that has to be supplied can be reversibly recaptured. Hence work expenditure need not be considered in principle when the process is isentropic.

Throughout this cycle, the network gained is  $1.0 - 0.6 = 0.4$  bits. Therefore, it is concluded that Peres's system can complete a cycle that can withdraw heat from a heat bath and converts it into mechanical work without leaving any other effect on the environment. This model actually implies that the second law itself sets a strict barrier to quantum state discrimination.

(2) Quantum variants of the basic Szilard engine have seen renewed interest recently [15–17], partly because of their overlap with statistical mechanics and also due to links with quantum information theory and computation. Zurek [18, 19] examined the Szilard one-particle gas obeying Boltzmann statistics quantum mechanically. He begins by noting that a one-molecule gas is a microscopic system and it may be wondered whether conclusions of Szilard's classical analysis remain valid in the quantum domain. Following Jauch and Baron [20], it may be argued that Szilard's analysis is inconsistent because it employs two different, incompatible classical idealizations of the one-molecule gas, dynamical and thermodynamical. Zurek shows that the apparent inconsistency pointed out by Jauch and Baron is removed by a quantum treatment. Thermodynamic entropy is incompatible with classical mechanics, as it becomes infinite in the limit  $\hbar \rightarrow 0$ . Thus, he views partitioning as a slow, reversible process that creates a potential barrier of some height which is large relative to  $k_B T$ . The system's energy levels are then modified.

In the quantum Szilard engine, the appearance of a wall is signaled by the increase in height of a potential barrier, which becomes infinite when it is impermeable. This is crucial since the energy levels in the box vary with potential height and boundary conditions. The energy levels contribute to the quantum thermodynamic work and internal energy of the device. The position of the barrier and the rate of its appearance influence the level shifts. The faster the height of the barrier increases, the greater the change of internal energy of the system. The energy becomes infinite when the height of the barrier approaches infinity instantaneously. If the system is initially in the ground state and the barrier appears in an adiabatic fashion with

the barrier off center, the particle will end up in the larger region of the box, and different from the classical situation. For isothermal insertion, the effect of energy level shifts is concealed by heat exchange. In order to show quantum effects of the quantum Szilard engine completely, it is necessary to consider adiabatic insertion. In this instance, a cycle of the quantum Szilard engine can be treated with fully quantum considerations.

Recently, such a model has been worked out in detail under the hypothesis that the von Neumann entropy determines the entropy of the quantum state. The model is based on a one-dimensional infinite square well, and the device is allowed to pass through two different cyclic processes. Here, the model will simply be introduced and then two distinct cycles will be outlined. It is too long to look at entirely. Consider a single particle of mass  $m$  which is confined to a one-dimensional infinite well of width  $a$ . The eigenvalues  $E_n$  and eigenstates  $|E_n\rangle$  depend on the dimension of the box and are given as follows:

$$E_n(a) = \frac{\hbar^2 \pi^2}{2ma^2} n^2, \quad |E_n(a)\rangle = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi(x-\frac{a}{2})}{a}\right), & n=2k, \\ \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi(x-\frac{a}{2})}{a}\right), & n=2k-1, \end{cases} \quad (7.6)$$

where  $k$  is a positive integer and  $0 \leq x \leq a$ .

Since the particle's state is determined by a wave function, crucial properties such as the number of nodes in the wave function are determined by the dimension of the box. These may vary during an expansion or contraction phase.

Assume that the system is initially in thermal equilibrium with a bath at temperature  $T$ . The density matrix  $\rho_0(a)$  takes the form

$$\rho_0(a) = \sum_n p_n(a) |E_n(a)\rangle \langle E_n(a)|, \quad p_n(a) = \frac{e^{-\beta E_n}}{Z(a)}, \quad (7.7)$$

and  $p_n(a)$  is the probability of the particle residing in the eigenstate  $|E_n\rangle$  and is normalized to unity. Also,  $Z(a)$  is the associated partition function given by the following:

$$Z(a) = \sum_{n=1}^{\infty} e^{-\beta E_n} \quad (7.8)$$

The internal energy of the internal energy  $U_0(a)$  and von Neumann entropy  $S_0$  are given in terms of Eqs. (7.6) and (7.7) as

$$U_0(a) = \sum_{n=0}^{\infty} p_n(a) E_n(a), \quad S_0 = -k_B \text{Tr}(\rho_0 \ln \rho_0) = -k_B \sum_{n=1}^{\infty} p_n(a) \ln(p_n(a)). \quad (7.9)$$

The model is capable of working over at least two different cycles. There is a cycle where the expansion is isothermal and a different cycle in which the expansion phase is adiabatic. Each of these cycles is composed of four segments. First, there is adiabatic insertion, measurement, expansion, and finally, there is extraction. The first two steps can usually be performed simultaneously and so can be regarded as one. Based on these cycles, the physics can be revealed by calculating the physical quantities, namely the internal energy, work, heat and entropy changes over each of the segments of the cycle being studied using the formulas for the basic physical quantities such as those in Eq. (7.9).

(3) Recently, Landauer's thought experiment has been realized by using a colloidal particle, which is trapped in a double-well potential that has been produced by two strongly focused laser beams. This could be regarded as an extension of the previous model above, but it is closer to realization experimentally. Such a system has two distinct states, that is, the particle may be in the right or left well of the double-well system. The particle is confined with equal probability to one of two optical potential wells and constitutes one bit of information. It may thus be thought to store one bit of information. The bit can be erased by means of the following procedure. First, the potential barrier between the two wells is lowered by varying or modulating the laser intensity. Next, the particle is pushed to the right by, in effect, inclining or tilting the trapping potential. Finally, the potential is restored to its original shape. The barrier places the particle in the right well, regardless of which well it started off in. Moreover, it will end up in the right well with probability close to one irrespective of the particle's initial position. The final configuration corresponds to zero bits of information. For a full erasure cycle, the average heat dissipated into the environment is equal to the average work needed to modulate the form of the double well potential. In the limit of long erasure cycles, the heat dissipated during the erasure process approaches, but does not drop below  $k_b T \ln(2)$ , in accord with Landauer's principle.

It is worth mentioning that such a system could be modeled by a potential well model. The inclining of the potential could be modeled at a more sophisticated level by raising the level of the potential on the left half. A primitive version could be modeled as follows. The Schrödinger equation can be solved in each of the three potential regions of the well. The corresponding solutions are as follows:

$$\begin{aligned} \psi_1(x) &= A \sin(kx), \quad \psi_2(x) = B_1 e^{\omega x} + B_2 e^{-\omega x}, \quad a < x < a + b, \\ \psi_3(x) &= C \sin(k(2a + b - x)), \quad a + b < x < 2a + b, \end{aligned} \quad (7.10)$$

$$k = \sqrt{\frac{2mE}{\hbar}}, \quad \omega = \sqrt{\frac{2m(V_0 - E)}{\hbar}}. \quad (7.11)$$

It is required that the wave function and derivative remain continuous at  $x = a$  and  $x = a + b$ . Manipulating this system of equations, it can be realized in the following form:

$$A\left(\frac{\omega}{k} \tan(ka) + 1\right)e^{\omega b} - C\left(\frac{\omega}{k} \tan(ka) - 1\right) = 0, \quad A\left(\frac{\omega}{k} \tan(ka) - 1\right)e^{-\omega b} - C\left(\frac{\omega}{k} \tan(ka) + 1\right) = 0. \quad (7.12)$$

From the condition that the determinant of the coefficients of system Eq. (7.12) vanishes, it is found that

$$\tan(ka)(1 \mp e^{-\omega b}) = -\frac{k}{\omega} \mp \frac{k}{\omega} e^{-\omega b}. \quad (7.13)$$

By solving Eq. (7.13) in the form

$$\tan(ka) = \frac{k}{\omega} \left( \frac{-1 \mp e^{-\omega b}}{1 \mp e^{-\omega b}} \right), \quad (7.14)$$

from which the corresponding energies can be obtained at least numerically as in Eq. (7.6).

It has been observed that much progress has been made in this area. Similar to setup (3), Piechocinska verified Landauer's principle within the domains of both classical and quantum mechanics [21]. It is assumed that the particle is in a bistable potential well. Piechocinska assumes that the bit to be erased is in contact with a constant temperature reservoir. It is also assumed the reservoir begins in energy eigenstate  $|n\rangle_{res}$ . The external field is turned on and splits the degeneracy until the probability of the higher energy state being occupied is very small, so the lower energy state  $|1\rangle$  is occupied with high probability. This accomplishes erasure. The external field is removed, with the final reservoir and bit states being  $|m\rangle_{res}$  and  $|1\rangle$ .

Further work remains to be done, as the story is likely not finished. Armen Allahverdyan and Theo Nieuwenhuizen recently reported [22, 23] violations of Landauer's principle for two model systems. It concerns a Brownian particle in contact with a constant-temperature reservoir. Landauer's principle seems to break down in the extreme quantum domain. This is when the particle and reservoir are in an entangled quantum state. The total entropy cannot be written as a sum of system and reservoir entropies. The Clausius inequality and Landauer's principle both seem to be violated. Consequently, their work suggests that Landauer's principle is not a universal law. But this would be a subject for future work [24–27].

## Author details

Paul Bracken

Address all correspondence to: paul.bracken@utrgv.edu

Department of Mathematics, University of Texas, Edinburg, TX, USA

## References

- [1] Leff H S and Rex A F, editors, *Maxwell's Demon 2; Entropy, Classical and Quantum Information, Computing*, Bristol: Adam Hilger, 2003.
- [2] Wheeler J A and Zurek W H, editors, *Quantum Theory and Measurement*, Princeton: Princeton University Press, 1983.
- [3] Sheehan D P, editor, *Quantum Limits to the Second Law*, AIP Conference Proceedings, p. 643, New York: AIP Publishers, 2002.
- [4] Penrose O, *Foundations of Statistical Mechanics*, Oxford: Pergamon Press, 1970.
- [5] Planck M, *Treatise on Thermodynamics*, London: Longmans, Green and Co, 1997.
- [6] Marayama K, Nori F and Vedral V, *The physics of Maxwell's demon and information*, *Rev. Mod. Phys.*, 2009; 81, 1-23
- [7] Vedral V, *The role of relative entropy in quantum information theory*, *Rev. Mod. Phys.*, 2002; 74, 197–234.
- [8] Szilard L, *Thermodynamic system by the intervention*, *Z. f. Phys.*, 1929; 53, 840–856.
- [9] Bennett C H, *The thermodynamics of computation-a review*, *Int. J. Theor. Phys.*, 1982; 21, 905–940.
- [10] Landauer, *Irreversibility and heat generation in the computing process*, *IBM J. Res. Dev.*, 1961; 5, 183–191.
- [11] Sherchenko S N, Ashhab S and Nori F, *Landau-Zener-Stückelberg interferometry*, *Phys. Rep.*, 2010; 492, 1–30.
- [12] Raimond J M, Brune M and Haroche S, *Manipulating quantum entanglement with atoms and photons in a cavity*, *Rev. Mod. Phys.*, 2001; 73, 565–582.
- [13] Peres A, *Quantum Theory: Concepts and Methods*, Dordrecht: Kluwer Academic Publishers, 1995.
- [14] Lloyd S, *Quantum mechanical Maxwell's demon*, *Phys. Rev. A*, 1997; 56, 3374–3382.

- [15] Li H, Zou J, Li J-G, Shao B and Wu L-A, Revisiting the quantum Szilard engine with fully quantum considerations, *Ann. Phys.* 2012; 327, 2955–2971.
- [16] Bracken P, A quantum version of the classical Szilard engine, *Central Eur J. Phys.*, 2014; 12, 1–8.
- [17] Bracken P, A quantum Carnot engine in three-dimensions, *Adv. Stud. Theor. Phys.*, 2014; 8, 627–633.
- [18] Zurek W H, Algorithmic randomness, physical entropy, measurements, and the demon of choice. In: Hey J, editor. *Feynman and Computation: Exploring the Limits of Computers*. Reading: Perseus; 1999.
- [19] Zurek W H, Algorithmic randomness and physical entropy, *Phys. Rev. A*, 1989; 40, 4731–4751.
- [20] Jauch J M and Baron J G, Entropy, information and Szilard's paradox, *Helv. Phys. Acta*, 1972; 45, 220–232.
- [21] Piechocinska B, Information erasure, *Phys. Rev. A*, 2000; 61, 062314.
- [22] Allahverdyan A E and Nieuwenhuizen T M, Breakdown of the Landauer bound for information erasure in the quantum regime, *Phys. Rev. E*, 2001; 64, 056117.
- [23] Allahverdyan A E, Balian R and Nieuwenhuisen T M, Understanding quantum measurement from the solution of dynamical models, *Phys. Rep.*, 2013; 525, 1–166.
- [24] Landauer R, Information is a physical entity, *Physica A*, 1999; 263, 63.
- [25] Park J, Kim K-H, Sagawa T and Kim S W, Heat engine driven by purely quantum information, *Phys. Rev. Lett.*, 2011; 111, 230402.
- [26] Plenio M and Vitelli V, The physics of forgetting: Landauer's erasure principle and information theory, *Contemp. Phys.*, 2001; 42, 25–60.
- [27] Sagawa T and Ueda M, Minimal energy cost for thermodynamic information processing: measurement and information erasure, *Phys. Rev. Lett.* 2009; 102, 250602.

