Quantum Szilard Engines

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Abstract

In this essay, I shall discuss the thermodynamic thought-experiment regarding a device known as the *Szilard Engine*. In the context of Maxwell's Demon and the perceived violation of the second law of thermodynamics, I will describe the classical operation of such an engine, and how its physical solution is related to information theory. I will then motivate a quantum mechanical treatment and discuss the common pitfalls and differences from the classical device, before more thoroughly examining the arising issues of quantum measurements and particle statistics.

1 Classical thermodynamics

The steam engine, particularly as it was developed by Newcomen and Savey (with later improvements by Watt) had a massive impact on 18$^{\text{th}}$ century society, providing the power source required to produce consumer goods on a scale never previously realised, and later a means of locomotive transport with the advent of the railway[1]. The changes effected by such an invention were so great that the period is often referred to as the *Industrial Revolution*. It was only natural that interest should blossom in the science behind such devices, and thus emerged the field of *thermodynamics*.

Of particular interest to physicists is the *second law*: that no physical device exists which has the sole effect of converting heat to work- or equivalently, global entropy can never decrease[2]. This law rules out *perpetual motion* machines of the second kind, which could be used as an endless power source from a single thermal bath[3].

1.1 Maxwell's demon

A thought experiment known as *Maxwell's demon* has proved to be a thorn in the side of the second law of thermodynamics since the late nineteenth century (see [4–7] and references therein). It was first postulated by James Maxwell in 1867, and publicly presented in his 1870 book[8][1].

The scenario consists of a thermally isolated box of gas with a partition in the centre, impenetrable except for a single well-oiled trapdoor, which is freely opened and closed by an intelligent being- the demon (see Figure 1). Initially, the gas on both sides of the partition is at the same temperature, with a range of velocities. By choosing only to open the trapdoor when fast-moving particles approach from the left, and slow moving particles approach from the right (otherwise allowing the particles to bounce off the closed door), the demon will eventually separate the gas such that the two sides of the partition are at different temperatures. This appears at odds with Clausius' statement of the second law: that no process exists where the sole effect is to move heat from a cold bath to a hot one.

[1] The term "Maxwell's demon" itself was coined several years later by William Thomson/Lord Kelvin[9].

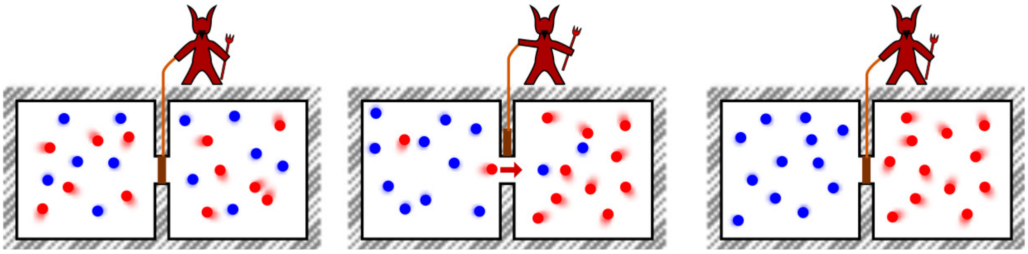

Figure 1: Maxwell's demon– *Through cunning choice of when to open the trapdoor, a gas initially at equal temperature on both sides can be separated into a hot side and a cool side.*

Particularly pathological to the second law, one could consider using a demon with negligibly small energy input to create a gradient in temperatures to form the hot and cold reservoirs used to drive a heat engine– a perpetual motion device of the second kind.

1.2 The Szilard Engine

In his 1929 paper[10], Szilard reformulated the problem in a manner easier for thermodynamic analysis by considering a single particle variant of Maxwell's demon. The Szilard Engine is a box divided into two volumes by a removable partition. Before the insertion of the partition, a single classical particle is in the box, moving freely between the two sides. The partition is inserted and is free to expand like a piston. An observer notes which side of the partition the particle is and chooses to connect gears or pulleys such that as the gas expands, it raises a weight. Once the partition has reached the edge, it is be removed, and the gas molecule is once more free to move around the box. The entire process may be repeated in a cycle to generate work (see Figure 2).

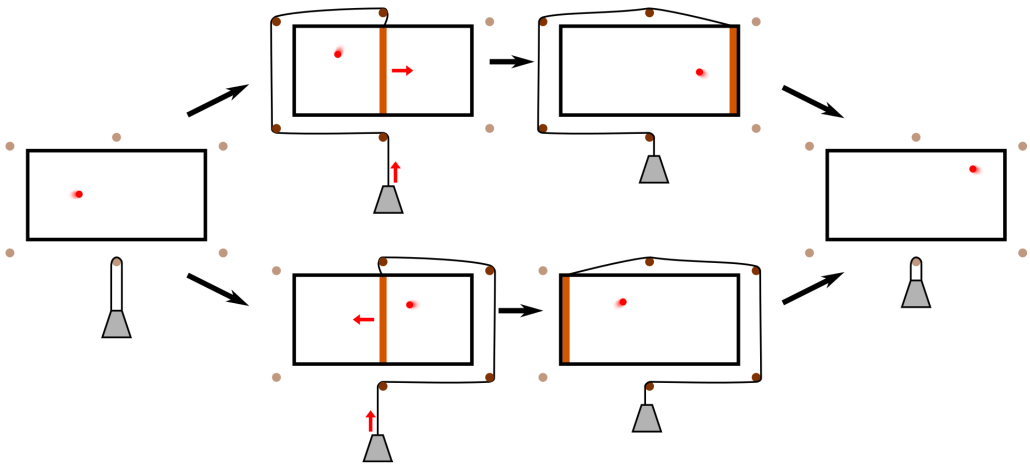

Figure 2: The Szilard Engine– *A barrier is inserted to bisect a box with a single particle in it. Depending on which side of the box the particle is on, a pulley system is attached such that when the barrier moves to expand like a piston, this will result in a weight being lifted. After the expansion is complete, the barrier is removed, and the whole process may be repeated.*

If one assumes that the box is in thermal contact with a large bath at temperature T so that the gas expands isothermally, and that the partition is always placed in the center, such that the expansion is from volume V to $2V$, it can be shown by elementary thermodynamics[2] that the work done by the expanding piston is given $W = k_B T \ln(2)$, where k_B is Boltzmann's constant.

Of instant striking note is that the amount of work done is independent of the volume of the box V, and depends instead on the ratio of how the box was partitioned. This hints strongly that the resolution to the paradox of the missing entropy lies in the realm of *information theory*.

From this, Szilard deduced that in order to preserve the second law of thermodynamics the assumption that an intelligent agent is costless must be incorrect, and so concluded that there must be an entropic cost associated with each measurement in order to offset the real reduction of entropy seen in the system. This was shown to not be entirely correct by Landauer in 1961, who argued that the entropic cost is actually associated with the irreversible process of erasing the measurement data[11].

2 Quantum Szilard Engines

2.1 Criticisms of the Classical Szilard Engine

By its very nature, the Szilard Engine is a particle in a box– the quintessential quantum system! This leads to very natural methods of interpreting the system in a quantum manner. Indeed, due to the very small nature of system, when treated purely classically, there are several inconsistencies which raise concerns about the validity of the assumptions made by Szilard, and hence undermine the conclusions drawn.

2.1.1 Subjectivity

One such inconsistency was illustrated in particularly critical analysis in 1972 by Jauch and Báron[12]: the instantaneous insertion of the partition violates the Gay-Lussac law[2], as the decrease in volume is allowed to occur as a *free action* without the expenditure of energy. In this stage of the cycle, Szilard treats the gas as a single localised particle, unaffected by the insertion of a barrier inserted at another disjoint region of space. However, when the barrier is connected to the weight, such that the enclosed volume acts like a piston, then the system is treated as a delocalised thermodynamic gas, once more subject to the usual governing equations. Jaunch and Báron hence conclude that the idealisations made by Szilard are "inadmissible in their actual context." In particular, if the gas is treated dynamically, when the barrier is placed, it should act as if the volume has not changed.

Zurek, in his seminal 1984 paper[13] considers this criticism, and highlights the "suspicious feature" to be that of *subjectivity*: that even before the measurement, there is still the ability to drive a piston and generate work; and that the ability to do work should depend on the objective state of the gas. He then resolves this problem by considering a quantum variation of the system. In this scenario, after the barrier is inserted but before measurement, the particle is in a superposition of being on the left and the right hand side - a state allowable in quantum mechanics, but not classically possible. He shows that it is only after measurement, where the wave-function will collapse into one side or the other, that the expansion can take place. Thus, the link between performing the measurement and ability to extract work from the system is strengthened. A similar argument is also presented by Biedenharn and Solem in their 1995 paper[14].

However, it could be argued that after the insertion of the barrier, Zurek has replaced the *mixture* of left and right in the classical case, with a *coherent superposition* in the quantum case- and argued that whilst the former leads to problems of subjectivity, the

[2]That is, it does not act as an *ideal gas* should.

latter does not. This is a dangerous ground to tread, as one could easily step into the long-debated and still contentious issue of quantum realism (see e.g [15–19]).

2.1.2 Fluctuations

As a single particle in a box, the Szilard engine is far from the thermodynamic limit used in its derivation. This is simply resolved by taking a large ensemble of identical engines, still remaining in the classical world, such that fluctuations smoothed out on average[13]. However, this raises the concern of whether entropy, a quantity usually defined in the thermodynamic limit, is a sensible measure to use on such a small scale- particularly if the event from which work is drawn can only occur once.

2.2 Definition of heat and work

Of critical importance to discuss a quantum mechanical system in thermodynamic terms is to form a quantum concept of *heat* and *work*. As a general concept, work may be viewed as "useful energy". For our purposes, a more rigorous definition must be used, such as that applied to the analysis of quantum heat engines by Kieu[20], and later specifically Quantum Szilard Engines by Kim et al.[21]:

For system with probability p_i of being in energy level E_i, we note that the average internal energy U is given by $U = \sum_i p_i E_i$, and so we see for infinitesimal changes:

$$dU = \sum_i (E_i dp_i + p_i dE_i).$$

By comparison with the first law, $dU = dW + dQ$, we can identify the change in work,

$$dW = \sum_i p_i dE_i, \tag{1}$$

and the change in heat,

$$dQ = \sum_i E_i dp_i. \tag{2}$$

This association of work with a change in the values of the energy levels reflects the assertion that any work done on or by the system will necessarily result in a change of the generalised co-ordinates of the system[22].

Such a classification is not always appropriate, as discussed in a 2008 letter by Weimer et al.[23], particularly in the internal interactions between small quantum systems. In their discussion, they argue for a definition that identifies changes in energy that do not affect the local von Neumann entropy as work, and changes that do as heat, so that the amount of work or heat will depend on the choice of measurement basis in the system.

An alternative definition of work in the context of quantum mechanical engines is put forth by Brunner et al. in their 2011 paper[24], where they state "producing work and generating population inversion are one and the same thing". In this paper (and others related[25, 26]), the idea of work in a quantum mechanical sense is likened to Carnot's definition of equivalence with raising a weight- the very example of the work done by the Szilard engine. Here, by analogy they consider a quantum system which can occupy one of many energy levels, and classify the action of exciting the system from one level to a higher one as a process of doing work. When this process of raising states is done systematically, it is known as *population inversion*[3]. Here, the adjustment of the relative populations of energy levels is thought of as work, rather than as heat, as would be suggested by Equation 2.

[3] A concept very well-known in the context of laser physics.

2.3 Insertion of the dividing barrier

As discussed in Section 2.1.1, under classical dynamics, inserting the dividing barrier is a *free action*: as the barrier is inserted at a different location in space from the particle, this should not affect the energy of the system.

Zurek assumes that the post-insertion state is in a superposition[13], and in 2005, Bender, Brody and Meister examine the implications of this in more detail[27]. In their paper, inspired by Zurek's formulation, they more precisely probe how the wavefunction would change as a result of the insertion of the barrier, with particular consideration to the energy.

For a quantum particle of mass m in a 1D infinite well with steep walls at $x = 0$ and $x = L$, they note that the energy eigenstates, E_n, and stationary wavefunctions ϕ_n are given by the familiar results:

$$\phi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \qquad E_n = \frac{\pi^2 \hbar^2 n^2}{2mL^2} \tag{3}$$

In this context, the insertion of an infinitely high barrier at a point $x = d$ will fall into one of two cases: the first where d is a node of the wave-function, and the second where before the insertion, the wavefunction is non-zero at d.

2.3.1 Insertion at a node

Bender first remarks that the insertion an infinite barrier at $x = d$ when d is a stationary node[4] of the wavefunction, as in Zurek's treatment, has no associated work cost.

The pre-insertion wavefunction can be expressed entirely in terms of the post-insertion wavefunctions on the left-hand and right-hand side of the barrier. As the barrier is infinite, the energy eigenstates are exactly those of two infinite wells, governed by equations similar to those in Equation 3, but taking into account the narrower width of the two wells. As the barrier has been inserted at a node, the wavefunction before insertion is zero at this point, and being at the extremal edges of the the two post-insertion wells, all energy eigenstate wavefunctions from both sides are also zero at this point. Thus, the boundary condition at the barrier can be trivially satisfied by some finite combination of wavefunctions.

The total energy of the system is the same after the insertion as it was before. The energy of the particle is not trivially distributed through the whole system as measuring which side of the box the particle is on will cause the energy to localise entirely on one side. This will happen even if the systems are completely detached and moved far apart. It is this phenomenon that is asserted by Bender to be the energy conservation equivalent of the Einstein-Podolsky-Rosen thought experiment[15], more familiarly expressed in terms of (angular) momentum or polarisation[28, 29].

2.3.2 Insertion elsewhere

Only being able to insert the barrier at a node is a very stringent requirement, insufficient even to describe a system in the ground state mode ($n = 1$) which has no stationary nodes. Thus, Bender et al. turn their attention to the situation where the infinite barrier is inserted infinitely quickly at a point with a non-zero wavefunction. They note that a naïve attempt to express the system as a sum of eigenstates from each sub-chamber will lead to

[4] The qualifier *stationary* is used as the wavefunction of the system is time-dependent, so there may be points which at some given time have a value of zero, but in general are not; for example, the wavefunction $\psi(x, 0) = \frac{1}{\sqrt{2}} (\phi_3(x) + \phi_6(x))$ has nodes at $\frac{x}{L} = 0, \frac{2}{9}, \frac{1}{3}, \frac{4}{9}, \frac{2}{3}, \frac{8}{9}, 1$, but only the nodes at $\frac{x}{L} = 0, \frac{1}{3}, \frac{2}{3}, 1$ are nodes of $\psi(x, t)$ for all times t.

a divergent expression for the energy, as the old wavefunction, when expressed as a Fourier series composed of the new function, will exhibit the Gibbs phenomenon[5]- the Fourier series will converge non-uniformly on the endpoint at the barrier. A renormalisation trick on the expression of the initial state overcomes this difficulty, but with interesting consequences, such as fractal wavefunctions.

Although beyond the context of a physically realisable Szilard engine, this discussion draws attention to the subtlety required in handling the insertion of the barrier- in particular, that if the cost of barrier insertion is not taken into account, even for a finite barrier, the reduction of entropy in the system can not be totally accounted for by the entropic cost of the measurement. A rigorous analysis of these energy costs and considerations has recently (August 2012) been discussed by Li et al.[31].

2.4 Quantum measurement

In the original classical scenario, the method by which the particle's position is determined is not well-defined, and of little consequence to the result. However, in Zurek's paper[13], the interaction between the (quantum) engine and the measuring device is explicitly probed: both in the context of a classical measurement device and a quantum system. In the classical case, this is done by measuring the observable of the form

$$\Pi = \lambda \left(|L\rangle\langle L| - |R\rangle\langle R| \right), \tag{4}$$

where $|L\rangle\langle L|$ ($|R\rangle\langle R|$) is the projector onto states on the left (right) of the barrier, and λ is some constant.

After measurement is made and recorded, the density matrix of the system updates depending on the outcome, but *regardless* of the outcome the free energy of the system increases by $kT \ln 2$, the precise amount of work done when the piston expands. Thus Zurek concludes that Szilard's suspicion was correct: that the measurement is the part of the process which facilitates the ability to do work.

Zurek then formulates a coupling Hamiltonian between the quantum system and some prepared measurement device state. Using a temperature scaled variant of the von Neumann entropy for a density matrix ρ, $S(\rho) = -kT\ \mathrm{Tr}(\rho \ln \rho))$, he shows that after measurement, the entropy of the system stays the same from the view of an external observer, but that of the measurement device will have increased- in a Schrödinger's cat-like paradox: beforehand the state of system was uncertain, but after measurement, if the device doesn't reveal its results to the external observer, it is now also uncertain! However, the combined entropy of the entire system, as it is considered in isolation, should not have increased. Zurek explains this discrepancy by the establishment of mutual information between measurement device and the engine, and so states the formula relating change of information (ΔI) and entropy (ΔS) at the heart of Szilard's engine,

$$\Delta I = \Delta S / k, \tag{5}$$

or in words, *information is entropy.*

2.4.1 Measure and forget

In contrast to Zurek's coherent superposition, in the work of Plesch et al.[32], after the barrier is inserted the gas is asserted to be in a mixed state. The rationale is that the

[5]This is a familiar cause of *ringing* in signal processing that occurs when a discontinuity is expressed by a Fourier series- where for even large numbers of terms, the overshoot of the Fourier series compared to the actual height of the discontinuity is significant. The series may pointwise converge, but it does not uniformly converge. See Appendix V of [30].

thermalising interaction with the walls of the chamber will implicitly measure the number of particles on each side of the barrier, such that even if after insertion the system is in a quantum state, it is soon projected into the "which side of the barrier" basis. The result of this measurement is not known to the engine's operator, and so it is a *measure and forget* operation.

This treatment is sufficient for the points raised raised in Plesch's paper (discussed in Section 2.5.2)- and does not lead to any inconsistencies; the scenario is treated quantumly throughout, in the manner of the classical measuring device of Zurek[13].

One might worry that this has reintroduced subjectivity to the concept of work; two agents with differing knowledge of the system will be able to leverage a different amount of work from the system. It could be that the entire "subjectivity paradox" is generated by attempting to treat the possible work as an objective property of the system, when in fact the definition of work is not so clear (see Section 2.2).

2.5 Particle statistics

One extension to the basic (quantum) Szilard engine is to place more than one particle inside the chamber. The information theoretic properties of the scenario are instantly more complicated, as the total system is no longer (qu)binary- the particles could be distributed in some complex manner.

As both sides of the divided chamber could have particles, when left to expand the piston will not necessarily reach the edges, as the gas with fewer particles when compressed will push back until the system is in equilibrium. In an extreme case, for a completely even distribution of particles, the piston will not move at all. In the thermodynamic limit $N \to \infty$, by the law of large numbers, one finds that approximately the same number of particles will be on either side of the barrier and so the potential to extract work is limited.

The important statistic about a particle is which side of the barrier it's on. Even though there may be 2^N configurations for N particles, when indistinguishability is taken into account, there are only $N+1$ different states for the purpose of calculating how much work will be done - and significantly fewer bits than $\log_2(N+1)$ will be required to store this information, as the outcomes close to Np particles on the left (where p is the chance a single particle being on the left) are significantly more likely[6]. Finally, the decision as to which side of the barrier should the pulleys be attached depends on a single binary question: "does the left hand side have more particles than the right?"

This line of thinking could lead to the fallacious conclusion that only one bit of information is required to leverage a significant amount of work, thus violating the second law. This is not true, as pointed out by Egloff[33] (discussed in Section 2.6) as leveraging more work than expected also leads to the generation of heat. To use his example, when you lift a stone into a water reservoir, if it is raised above the necessary height, it will splash down and transfer the unnecessary energy into random kinetic motion (heat!) in the water.

2.5.1 Fermions and Bosons

The treatment of a group of particles differs depending on whether the particles are distinguishable or indistinguishable. Furthermore in the quantum treatment, due to spin-statistics there are two indistinguishable cases: bosons and fermions.

In 2011, Kim et al.[21] presented an analysis in which they consider bosons, fermions and distinguishable particles at low temperatures. They make the simplifying assump-

[6]Using a binomial distribution assuming each particle is independently equally likely to be on the left or right, for large N, the Shannon entropy is approximately $H \approx \frac{1}{2}\log_2\left(\frac{\pi e N}{2}\right)$

tion to ignore each particle's different spin states, and explicitly consider the case where $N = 2$. In this scenario, at temperature $T = 0$, there are 4 possible arrangements for the distinguishable particles, 3 for the bosons and just 1 for the fermions as the Pauli exclusion principle ensures they are always on opposite sides when the barrier is inserted (see Figure 3).

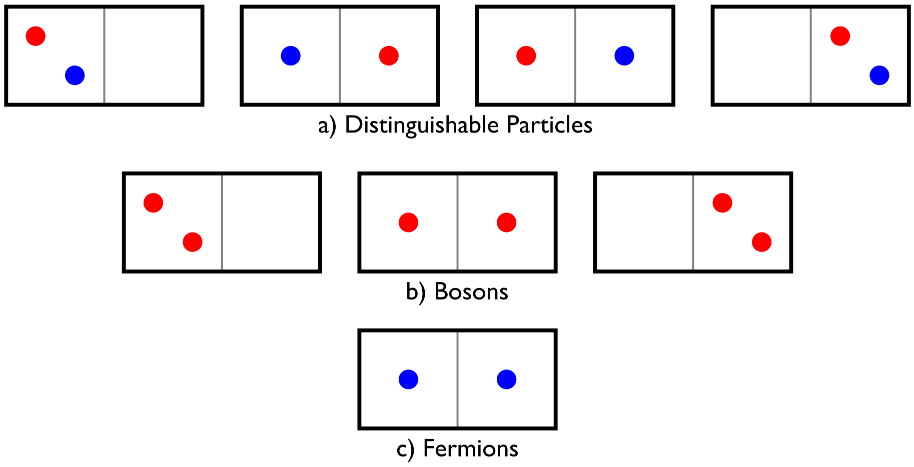

Figure 3: *Configurations for a two-particle system when the particles are: a) distinguishable, b) bosons, c) fermions.*

At this limit, a pairs of fermions can not do any work, consistent with the fact that the system's state is always certain- no new information needs to be recorded in order to describe the state of the system. Conversely, the extra possibility for the distinguishable particles over the bosonic case does not offer any additional useful information, as regardless of which particle is on each side, when the system is in an equally distributed state, it has no capacity to do work. This means at low temperatures, the bosonic case can leverage slightly more work per cycle out of the system than the distinguishable case as (assuming an even distribution in state space) it only has a $\frac{1}{3}$ chance of being in a useless state after the barrier is inserted, as opposed to $\frac{1}{2}$.

Distinguishability re-establishes itself as the temperature increases as the particles are likely to occupy different states as they have access to a large spread of higher energy levels. Thus, as $T \to \infty$, both the bosonic and fermionic cases tend to the same result as the distinguishable case.

2.5.2 The importance of the measurement

In response to Kim, Plesch et al. "clarify the role of particle statistics" by stressing the importance of the initial measurement[32]. They derive a unifying expression for the work extractable, W given:

$$W = kT \ln (M) , \tag{6}$$

where M is the number of different equiprobable measurement outcomes in the initial state. The role played by particle statistics is solely to determine the amount of memory required to encode the measurement results– returning the scenario to its information theoretical roots.

They also consider how much work can be leveraged from a coarse-grain measurement, where some of the measurement outcomes are grouped together and only the coarse groups are recorded. Here, labelling the M coarse-grain probabilities as $\{p_i\}$ they write the work performable as $W = TS$, where

$$S = -k \sum_{m=1}^{M} p_m \ln p_m, \tag{7}$$

which is the Shannon entropy (in nats) of the measurement, with a constant factor of k, similar to the Gibbs entropy, expressed in terms of outcomes rather than microstates. The maximum entropy, and hence maximum work, occurs for a distribution where all outcomes are equiprobable ($S = -k \ln \left(\frac{1}{M}\right)$ as in Equation 6)[7].

Through this analysis, Plesch also concludes that bosons can do more work than an equivalent ensemble of distinguishable particles, noting that whereas for bosons every outcome is equiprobable, in the distinguishable case (as discussed in 2.5) some number states will be far more likely than others, and so the overall information is reduced, such that in the limit $N \to \infty$, the work performable by a bosonic gas is twice that of a distinguishable one.

2.6 Single-shot statistics

As discussed in Section 2.1.2, it is not obvious whether thermodynamics should be applicable to a system as small as a single Szilard engine. This question pertains to statistical mechanics and probabilities. Dahlsten et al.[35], taking inspiration from single-shot information theory (particularly the Smooth Entropy approach of Renner[36]), foray into a field they call "single shot statistical mechanics". They relate the amount of work that might be produced with a quantifiable risk of failure that the agent is willing to take given uncertain knowledge about the system, thus allowing a more meaningful quantity for single events than the averaged expectation value[8]. The "work extraction game" they use is based around the Szilard engine. Later work with Egloff[33], extends the result to arrive at a more general formulation of thermodynamics, describing a stricter version of the second law, governing whether or not a thermal process is possible.

3 Conclusion and outlook

Despite the additional technical considerations required to describe a particle quantumly, we see that under quantum analysis, we obtain a more consistent description of the Szilard engine. Thus, the quantum analysis of the Szilard engine clarifies rather than confuses the core principle of equivalence between entropy and information.

Through cunning formulation (such as Seth Lloyd's[37]), it is possible to consider experimentally testable scenarios (e.g. [38, 39]) analogous to the Szilard engine. It seems to me that the next step in theory would be to attempt to formulate the scenario in the language of pure quantum information, rather than complicate it with implementation-specific ideas of wave-functions. This would allow new settings to be considered, whilst truly laying bare the heart of the matter. I would also give consideration to constructing similar work-extraction scenarios in the language of *generalised probabilistic theories* (along the lines of Hänggi and Wehner[40]).

[7]This can be shown by a method of Lagrange multipliers (see e.g. [34])

[8]Provided, of course, one believes probability, typically defined as a ratio of frequency of events, has physical meaning for a one-off event.

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