Szilard's Engine

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1 Introduction

One manifestation of the *second law of thermodynamics,* is the fact that heat engines cannot work on a single heat bath. In 1871 Maxwell devised the idea of the demon to show the probabilistic nature of the second law: an intelligent being capable of measuring the position and momentum of the particles in a gas could in principle violate this law, for example by inducing a flow of heat from a cold source to a hot one.
The Szilard engine was a thought experiment, devised by Leo Szilard in 1929. It was a refinement on some of the Maxwell's Demon models of the time. The engine demonstrates how a possession of information might have thermodynamic consequences, and in principle constitutes a single heat bath engine.

2 Classical Szilard's Engine (CSE)

The original model of the engine consists of a a single particle prepared in a box. The cycle consists of 4 main steps as shown in figure (1):

1. In the first step we insert the piston in the middle of the box, trapping the particle on one side or the other. The work necessary to insert the piston can be made zero (by taking the piston arbitrarily thin):

$$W_{ins} = 0 \tag{1}$$

2. A measurement device (our *demon*) in contact with a heat bath at temperature T_{demon}, performs a measurement to determine on which side the particle is trapped. According to the outcome, a load is attached to the piston. The work required will be some function of the temperature and other parameters:

$$W_{demon} = f(T_{demon}, X_1, X_2, X_3, ..) \tag{2}$$

3. The system is put in contact with a heat bath at temperature $T_{bath} > T_{demon}$, while the particle performs an isothermal quasi-static expansion until the piston reaches the end of the box. In this stage we see the importance of the *demon,* which allows us to extract positive work by controlling on which side of the piston the load is attached. The work at this stage is given by the ideal gas equation (for a single particle):

$$W_{exp} = \int_{V/2}^{V} pdV = T_{bath} \int_{V/2}^{V} \frac{dV}{V} = T_{bath} ln2 \tag{3}$$

4. The final step, deals with operation for completing the cycle and returning the system to its initial configuration. Meaning, the removal of the piston and detaching the load. Again the work for this can be zero:

$$W_{rem} = 0 \tag{4}$$

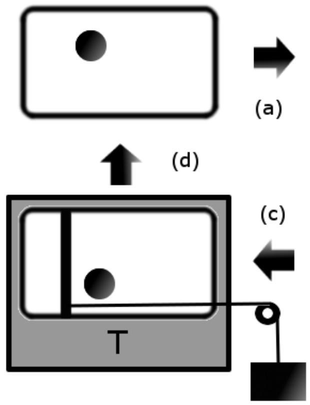

Figure 1: A description of the CSE cycle. (a) The box with the prepared particle, is inserted with the piston. (b) The particle's position is determined. (c) An isothermal quasi-static expansion in temperature T. (d) The piston with the load are removed and the system returnes to the initial state.

Although the demon requires some work, we neglect it in our analysis and concentrate only on the mechanical work of the engine. So the total work for a cycle is:

$$W_{tot} = W_{ins} + W_{exp} + W_{rem} = T_{bath} ln2 \tag{5}$$

3 Quantum Szilard's Engine (QSE)

In contrast with the CSE, in which the work for removal or insertion of the piston could be neglected. In the QSE these operations change the boundary conditions which effects the particles eigenvalues and states.

The system's model

The system is modeled using a hamiltonian for N particles in a box of size L as in figure (2) $\mathcal{H}(\mathbf{r}, \mathbf{p}; X, \alpha)$ which depends on two control parameters:
X - the position of the piston.
α - the height of the potential barrier which constitutes the piston.
The box is divided by the piston, in which case we can write:

$$Z_{n,N-n}(X) \equiv Z_n(X) Z_{N-n}(L-X) \tag{6}$$

this describes the situation of n particles to the left of the piston and $N-n$ to the right, in a thermal equilibrium. Although (6) formally depends on α and X, we usually omit α in the calculations.
The processes are all quasi-static isothermal, so we can use (6) in all stages of the cycle. Assuming such a process, we can use the *maximum work principle* to calculate the work between two equilibrium states:

$$W = -\Delta F = T \int_{X_1}^{X_2} \frac{\partial lnZ(X)}{\partial X} dX = T[lnZ(X_2) - lnZ(X_1)] \tag{7}$$

As in the classical case, the QSE consists of 3 mechanical processes:

Insertion

The state before the insertion is just that of an L length box with N particles, could be thought of as a state where the piston is just to the right of the box:

$$Z(L) \equiv Z_N(X = L) \tag{8}$$

A piston is inserted isothermally at $X = l$. Because the insertion divides the system into a random number of particles on each side, we define $N + 1$ different configurations according to the number of particles to the left of the piston. when the piston is inserted the measurement is not performed yet, so we cannot know in which specific configuration the system is in. Thus the total partition function after the insertion:

$$Z(l) \equiv \sum_{n=0}^{N} Z_{n,N-n}(l) = \sum_{n=0}^{N} Z_n(l) Z_{N-n}(L - l) \tag{9}$$

According to (7), the work for insertion is:

$$W_{ins} = T[lnZ(l) - lnZ(L)] = Tln\left(\frac{Z(l)}{Z(L)}\right) \tag{10}$$

Expansion

In each n'th configuration the piston will undergo an isothermal quasi-static expansion until it reaches the equilibrium position - l_n, different for each n, which satisfies the force balance condition:

$$\left\langle \frac{\partial \mathcal{H}}{\partial X}\bigg|_{X=l_n} \right\rangle = 0 \tag{11}$$

The work obtained by expansion for each n is:

$$W_{exp}^{(n)} = T[lnZ_{n,N-n}(l_n) - lnZ_{n,N-n}(l)] = Tln\left(\frac{Z_{n,N-n}(l_n)}{Z_{n,N-n}(l)}\right) \tag{12}$$

This will not give us much useful information, because the engine performs many cycles, each with a different configuration. But we can take the average to calculate the expansion work:

$$W_{exp} \equiv \sum_{n=0}^{N} p_n W_{exp}^{(n)} = T \sum_{n=0}^{N} p_n Tln\left(\frac{Z_{n,N-n}(l_n)}{Z_{n,N-n}(l)}\right) \tag{13}$$

where

$$p_n = \frac{Z_{n,N-n}(l)}{\sum_{n'} Z_{n',N-n'}(l)} \tag{14}$$

is the probability of measuring n particles to the left of the piston.
In reality the piston is not impenetrable, and has a finite potential height, α_∞, which is assumed to be high enough to satisfy $\tau_{tun} \gg \tau$. Meaning, the tunneling time τ_{tun} is much larger than any thermodynamic process time τ. This insures that the particles distribution p_n is well defined.

Removal

We start with the piston at $X = l_n$. The removal process is divided into two sub-processes:

1. We start the removal while the piston still satisfies the no-tunneling condition $\tau_{tun} > \tau$, until it reaches a certain height α_0 where $\tau_{tun} \approx \tau$. In this case for a quasi-static process $\tau \to \infty$ we get:

$$\alpha_0, \alpha_\infty \to \infty \tag{15}$$

or equivalently

$$(\alpha_\infty - \alpha_0) \to 0 \tag{16}$$

in this stage the work vanishes:

$$\int_{\alpha_\infty}^{\alpha_0} \frac{\partial ln Z_{n,N-n}(l_n)}{\partial \alpha} d\alpha = 0 \tag{17}$$

2. The second sub-process starts where the piston at height α_0. At this point, due to tunneling every eigenstate is delocalized over both sides. In this case there is no definite value of n particles on the left side. To find the partition function we need to sum over all possible configurations of particles for a specific equilibrium position of the piston:

$$Z(l_n) \equiv \sum_{n'=0}^{N} Z_{n',N-n'}(l_n) \tag{18}$$

   Notice the summation is over the number of particles to the left, because we want to include all the possibilities of particle distribution due to tunneling.

from (7) and (17) we get (for each n):

$$W_{rem}^{(n)} = T \int_{\alpha_\infty}^{\alpha_0} \frac{\partial ln Z_{n,N-n}(l_n)}{\partial \alpha} d\alpha + T \int_{\alpha_0}^{0} \frac{\partial ln Z(l_n)}{\partial \alpha} d\alpha = T ln \left(\frac{Z(L)}{Z(l_n)} \right) \tag{19}$$

and the average is:

$$W_{rem} \equiv T \sum_{n=0}^{N} p_n ln \left(\frac{Z(L)}{Z(l_n)} \right) \tag{20}$$

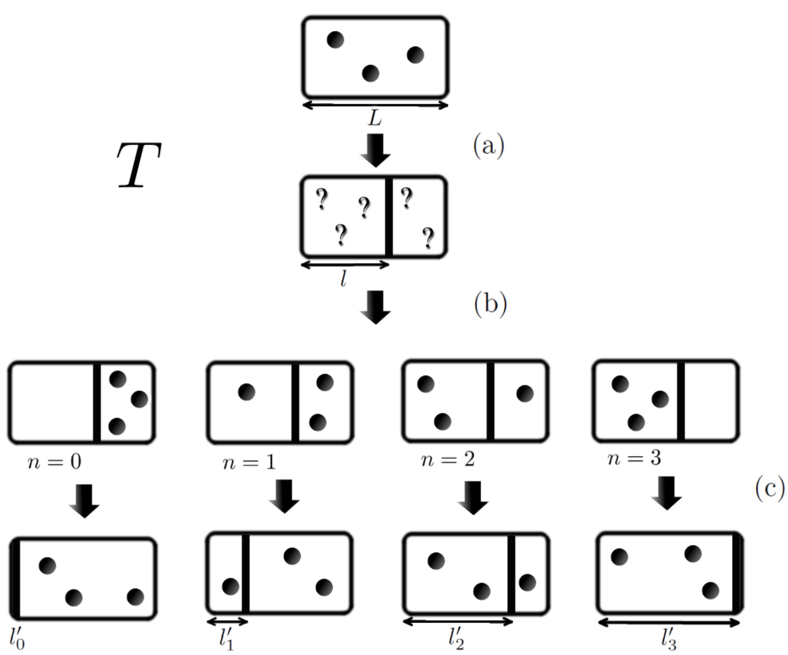

Figure 2: An example of a QSE cycle for 3 particles. (a) The prepared system is inserted with the piston, and (b) the number of particles on one of the sides is measured, which creates a specific configuration. (c) The isothermal quasi-static expansion continues until it reaches the equilibrium position.

The total work

Combining all the contributions, the work performed by the engine in one cycle is:

$$W_{tot} = W_{inc} + W_{exp} + W_{rem} = -T \sum_{n=0}^{N} p_n ln\left(\frac{p_n}{f_n}\right) \tag{21}$$

where

$$f_n \equiv \frac{Z_{n,N-n}(l_n)}{\sum_{n'} Z_{n',N-n'}(l_n)} \tag{22}$$

4 Some Particle Models

The one particle case

Consider a particle with mass M in a box of size L, the piston is inserted at $l = L/2$. Obviously $p_0 = p_1 = 1/2$. During the removal we have two possibilities:

1. If the particle was measured to the right $l_0 = 0$, meaning no particles to the left will be found: $f_0 = 1$.
2. If the particle was measured to the left $l_1 = L$, meaning there will absolutely be a particle to the left: $f_1 = 1$.

this can also be seen from the fact that $Z(l_n) = Z_{n,N-n}(l_n)$. Inserting these values into (21) we get $W_{tot} = Tln2$, the same as the classical result!
The difference arises when each stage is analyzed separately. The energy $E_r(X) = \frac{\pi^2 r^2}{2MX^2}$, and the partition function for one particle is $Z_1(X) = \sum_{r=1}^{\infty} e^{-\beta E_r(X)}$:

1. The work for Insertion:

$$\begin{aligned} W_{ins} &= T[lnZ(L/2) - lnZ(L)] && (23)\\ &= T[ln(2Z_1(L/2)) - lnZ_1(L)] && (24)\\ &= Tln2 - \varepsilon && (25) \end{aligned}$$

   where $\varepsilon \equiv Tln[\frac{Z_1(L)}{Z_1(L/2)}]$.

2. After averaging the cases $n = 0, 1$ we get: $W_{exp} = \varepsilon$.
3. The work for removal is obviously zero, the piston is at the edges and doesn't effect the eigenstates: $W_{rem} = 0$.

In the end, only the difference between the work gained during expansion and the work needed for insertion, gives us the net result.

The two particles case

In the same setting as before we put two identical particles. $f_0 = f_2 = 1$, in these two cases both of the particles are are on the same side, therefore the piston after expansion is at the edge.
For $n = 1$ the piston does not move $l = l_1$, which means that $p_1 = f_1$:

$$W_{tot} = -Tp_0lnp_0 - Tp_1lnp_1 = -2Tp_0lnp_0 \tag{26}$$

to get some insight we look at two limiting cases:

In the low temperature limit only the ground state is occupied, this works for bosons but for fermions which cannot occupy the same state (ignoring the spin) the work vanishes (The probability values taken from [1]):

$$W_{tot}^{(bosons)} = \frac{2}{3}Tln3, \qquad W_{tot}^{(fermions)} = 0 \tag{27}$$

However, in the high temperature limit the particles lose their indistinguishability (can be distinguished by their state):

$$W_{tot}^{(bosons)} = Tln2, \qquad W_{tot}^{(fermions)} = Tln2 \tag{28}$$

similar to the one particle classical case.

N particles classical ideal gas

We consider a one dimensional ideal gas of N particles, For convenience $l = L/2$ as before. The partition function for n particles in a box of width X is:

$$Z_n(X) = \frac{X^n}{\lambda_T n!} \tag{29}$$

The probability of finding n particles (after the measurement) to the left of the piston is given by

$$p_n = \frac{1}{2^N}\binom{N}{n} \tag{30}$$

this can be derived by substituting (29) into (14). We have only left to find the value of f_n:

$$\begin{aligned} f_n &= \frac{Z_{n,N-n}(l_n)}{\sum_{n'} Z_{n',N-n'}(l_n)} && (31)\\ &= \frac{Z_n(l_n)Z_{N-n}(L-l_n)}{\sum_{n'} Z_{n'}(l_n)Z_{N-n'}(L-l_n)} && (32)\\ &= \frac{\binom{N}{n}(l_n)^n(L-l_n)^{N-n}}{\sum_{n'}\binom{N}{n'}(l_n)^{n'}(L-l_n)^{N-n'}} && (33)\\ &= \binom{N}{n}\frac{(l_n)^n(L-l_n)^{N-n}}{L^N} && (34)\end{aligned}$$

from here we find the ratio in (21):

$$\frac{p_n}{f_n} = \frac{L^N}{(l_n)^n(L-l_n)^{N-n}} \tag{35}$$

and the total work is:

$$W_{tot} = \frac{T}{2^N}\sum_{n=0}^{N}\binom{N}{n} ln\left(\frac{2^N(l_n)^n(L-l_n)^{N-n}}{L^N}\right) \tag{36}$$

For an ideal gas the equilibrium position is $l_n = \frac{n}{N}L$ (can be found from the ideal gas equation), substituting into (36) we get:

$$W_{tot} = \frac{T}{2^N}\sum_{n=0}^{N}\binom{N}{n} ln\left(2^N\left(\frac{n}{N}\right)^n\left(1-\frac{n}{N}\right)^{N-n}\right) \tag{37}$$

With some numerical calculation we can observe the behavior of the gas, as shown in figure (3):

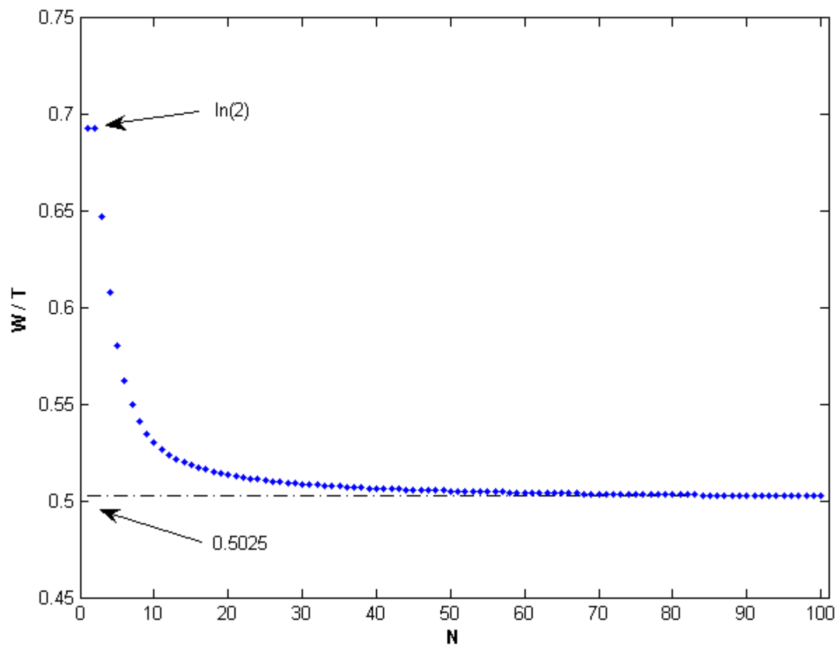

Figure 3: W/T as a function of N, the number of particles: We see that for $N = 1, 2$ we have $W = Tln2$. For a larger number the work decreases until it reaches an asymptotic value $W = 0.5025T$

References

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