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Workshop "Thermodynamics, thermoelectrics and transport in quantum devices, September 19-21, 2018

Optimal protocols for a Maxwell Demon device with errors





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Plan

- Maxwell's demon (MD): Reminder
- The Szilard engine: Realization with a single electron
- Optimal protocol for a given extracted power
- Role of measurement errors:
 - Thermodynamics
 - ✓ Results
 - ✓ Sketch of calculations
- Summary & Outlook



J. C. Maxwell (1831-1879)

Maxwell's demon is a thought experiment created by James Clerk Maxwell in which he suggested how the Second Law of Thermodynamics might hypothetically be violated. The Demon and the friction-free trap door

System with Lower Entropy (in violation of the Second Law)

Maxwell's demon (1867-)

 1.6×10^{5} hits 0.65×10^{5} hits

Reminder

MD extracts heat from a thermal reservoir by observing a thermodynamic system to make a spontaneous, thermally-induced, transition into a state with larger-than-average free energy and using the feedback to collect this extra free energy as work.

Szilard demonstrated that by obtaining a single bit of information as a measurement result of the state of the system, one could collect up to $T \ln 2$ useful work.

The unavoidable thermodynamic costs of conversion of heat into work by a reversible MD is the creation of information about the state of the measured system.

<u>Landauer principle</u>: erasure of this information generates at least the extracted amount of heat, $T \ln 2$ per bit \longrightarrow The agreement with the second law.









The Szilard engine: Realization with a single electron

Differences with original Szilard engine:

- The charge configuration (excess electron) is manipulated
- The manipulation is performed by changing the potential difference between the electron gases in the two islands





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Double-dot MD: Protocol for work extracting

Double-dot Szilard engine



The pair of the dots contains only one excess electron, so each dot may contain either zero or one excess electron; the occupancy of each dot can be measured, say, by SET.

1. Begin in equilibrium with V(t) = 0, so that the probability of finding the extra electron is equal for the two islands.

2. Perform a measurement, and if the extra electron is found on one island, quickly raise the potential of the other island to some value $V_0 \equiv V(0^+)$.

3. Reduce the potential of the raised island according to some protocol V(t) until time $t = \tau$.

There is a probability that the electron will tunnel between the two islands, and whenever the electron occupies the island where the potential is being decreased, heat is extracted from the environment and converted to work.

4. Then we perform measurement. After finding of an electron at a given dot we quickly raise the potential of the "empty" dot up to V_0 , and shift potential of the occupied dot to 0, and in this way we continue the cycle.

Protocol for work extracting: Animation



If the electron tunnels "uphill" during slow decrease of the potential, then the energy is extracted from the thermal bath. the "idle" dot up to V_0 , and shift potential of the occupied dot to 0.

In this way we continue the cycle.

Q1: Which V(t) and τ correspond to minimum entropy production?

A: $\tau \to \infty$ and any V(t) with $V(0) \to \infty \ (\gg T)$

This is true only for vanishing power of heat extraction!

Q2: What is the optimal regime for a finite power of heat extraction from the environment?



<u>Results</u> Fully optimized - J. Bergli, Y. M. Galperin and N. B. Kopnin, Phys. Rev. E **88**, 062139 (2013) Partly optimized: - D. Averin & J. Pekola, Phys. Status Solidi B **254**, 1600677 (2017).

Role of measurement errors



If no errors, the cycle can be done fully reversible.

Measurement
error:reduces the information →
reduces the entropy decreaseErasure still gives increase in entropy,
the total process becomes irreversible

<u>Another consequence</u>: a bad feedback is applied, which further increases the entropy production if the proper protocol adapted to the expected error rate is not applied.

We consider the effect of measurement error on a realistic single-electron box Szilard engine, and find the optimal protocol for the cycle as a function of the desired power P and error ε .

If there is a chance that the measurement result is wrong \rightarrow the correlation between the state of the system and the state of measurement device is not perfect.

That is, the mutual information, *I*, between the two is less than the full information of the logical states of the measurement device.

Lower bound for the total work expended [Sagawa & Ueda, PRL 102, 250602 (2009)]:

$$W_{ ext{measure}} + W_{ ext{erase}} \geq TI$$
 Heat, extract utilizing the

Heat, extracted by utilizing the information

Although measurement errors will give a reduced mutual information, it is impossible to reach equality in this case.

Simple model

A total system (memory + system) with a phase space \mathcal{P} , which we divide in the subspaces corresponding to the logical states \mathcal{P}_i .

Both the device and the memory are Szilard engines \rightarrow 4 logical states for 2 particles

The phase space of each molecule is reduced to one dimension by only considering the movement of the molecule in the direction that the volume of the compartments expands/contracts and ignoring the momentum, as all processes will be isothermal and therefore the momentum distribution is independent of the protocol. Therefore a constant contribution to the internal entropy is omitted.

The relevant part of the total phase space is then 2-dimensional, and we represent the position of the molecule in the system on the horizontal axis, and in the memory on the vertical axis.

Simple model: Entropies

A total system (memory + system) with a phase space x, which we divide in the subspaces corresponding to the logical states, x – point in the phase space.

Both the device and the memory are Szilard engines \rightarrow 4 logical states for 2 particles

Probability distribution of the logical states (1 bit): $P_L(i) = \sum_{x \in \mathcal{P}_i} P(x), \quad i = 0 \lor 1$ Conditional probability: $P(x|i) = P(x)/P_L(i)$.

Total entropy:	$S = -\sum_{x} P(x) \ln P(x),$
Logical entropy (information):	$H = -\sum_i P_L(i) \ln P_L(i),$
Conditional entropy:	$S(\mathcal{P}_i i) = -\sum_{x \in \mathcal{P}_i} P(x i) \ln P(x i).$

The conditional entropy can be thought of as the internal physical entropy of the distribution for each of the logical states i. The average conditional (as we call, internal) entropy is $S_{in} = \sum_{i} P_L(i) S(\mathcal{P}_i | i) \longrightarrow S = H + S_{in}$

Simplified version of the derivation by Sagawa & Ueda, NJP (2013)

Illustration for ideal gas in 3d box

$$\begin{array}{ll} \mbox{Free energy:} & F(T,V,N) = -NT \ln \left[\frac{Ve}{N} \left(\frac{mT}{2\pi\hbar^2} \right)^{3/2} \right] & \mbox{Landau \& Lifshitz book} \\ \mbox{Entropy:} & S = - \left(\frac{\partial F}{\partial T} \right)_{V,N} = N \left[\frac{3}{2} + \ln \left(\frac{V}{NV_q} \right) \right] & \mbox{} \\ \mbox{} & V_q(T) \equiv \frac{4}{e\sqrt{2}} \left(\frac{\pi\hbar^2}{mT} \right)^{3/2} \\ \mbox{Single particle, $V \gg NV_q$:} & S = \frac{3}{2} + \ln \left(\frac{V}{V_q} \right). \end{array}$$

Double-dot system



4 boxes \rightarrow 4 logical states (i = 00, 01, 10, 11), 2 particles

Internal entropy for a logical state *i*:

$$\begin{split} S_{\rm in}(i) &= S_0 + \ln\left(\frac{x_S x_M}{L^2}\right), \quad S_0 \equiv 3 + 2\ln\left(\frac{V}{V_q}\right) \gg 1. \end{split} \\ \\ & \text{Probability of logical state} \end{split}$$

In the following we omit large constant S_0 .

Entropy production and measurement errors: Szilard engine

Both the system and the memory of the measurement device is a single molecule of ideal gas in a container with a dividing barrier.

The position of the gas molecule in the system is represented on the horizontal axis and the position of the molecule in the memory on the vertical axis.



 $\frac{1}{2}$ $\frac{1}{2}$

The initial state is such that the system has an equal probability of the particle being on the left or right, and the measurement not yet performed, so that the memory is reset to the left half

$$H = -2 \cdot \frac{1}{2} \ln \frac{1}{2} = \ln 2$$
$$S_{in} = 2 \cdot \frac{1}{2} \ln \frac{1}{4} = -2 \ln 2$$
$$S = -\ln 2$$



We make a measurement of the state and store the result in the memory. Assuming that the measurement has a probability of $1-\varepsilon$ of giving the true result and a probability ε of giving the wrong result we get:

$$H = -2 \cdot \frac{\epsilon}{2} \ln \frac{\epsilon}{2} - 2 \cdot \frac{1-\epsilon}{2} \ln \frac{1-\epsilon}{2} = \ln 2 + S_{\epsilon}$$
$$S_{in} = 2 \cdot \frac{\epsilon}{2} \ln \frac{1}{4} + 2 \cdot \frac{1-\epsilon}{2} \ln \frac{1}{4} = -2 \ln 2$$
$$S = -\ln 2 + S_{\epsilon}$$
$$S_{\epsilon} = -\epsilon \ln \epsilon - (1-\epsilon) \ln(1-\epsilon)$$

We assume that the measurement does not affect the state of the system.



Irreversible transition to configuration D:





Reversible transition:



See also Sagawa & Ueda, NJP (2013)

If the correlation is not perfect, $I < H \rightarrow W_{measure} < 0$, we should be able to reach this state while extracting work if we can do it reversibly.



 Expand isothermally the memory (work W is performed by the system and heat Q = W is taken from the reservoir.):

$$\Delta S = \ln 2$$
$$\frac{W}{T} = \frac{Q}{T} = \Delta S = \ln 2$$



2. Measure the system, and insert the divider according to the result.

There is no error in the measurement, and the correlation between the position of the divider and position (left/right) of the gas molecule of the system is perfect. $\boldsymbol{\varepsilon}$ is just a parameter describing at which point we insert the divider. No entropy change





3. Compress isothermally the memory. We arrive at the same final state as when there was a measurement with error. On the way, we have extracted work from the thermal bath, and the reduction of the environment entropy is exactly the same as the increase of the system entropy, so that the total entropy is constant and the whole process reversible.

$$\Delta S = \ln 2 - S_{\epsilon}$$
$$\frac{W}{T} = S_{\epsilon} - \ln 2$$

Energy balance:
$$W_{\text{measure}} = -TS_{\epsilon} < 0, \ W_{\text{erase}} = T\ln 2$$

 $\rightarrow W_{\text{measure}} + W_{\text{erase}} = T\ln 2 - TS_{\epsilon} = TI^{D}$

Lower bound for the total work expended [Sagawa & Ueda, PRL 102, 250602 (2009)]:

 $W_{\text{measure}} + W_{\text{erase}} \ge TI$

The equality is saturated by a reversible process.

What happens when an irreversible measurement with errors takes place?





A complex structure of the accessible phase space becomes indistinguishable and replaced by a uniform distribution. This step is irreversible; the total entropy increases by S_{ϵ}

Just after the measurement: Most of the initial states in the phase space are mapped to the correct final region, but a small fraction gets mapped to a different region, which corresponds to "wrong" results. For an isolated system the mapping A to B is deterministic and entropy is the same. We can imagine that after the time B no further changes of the logical states will occur - the phase point will never again cross the lines separating the different logical states. In a short time the phase space region where the system can be found will develop into some complicated shape. For a closed system the entropy will still be the same.

Results for the optimal protocol with errors

The total entropy produced in a cycle:



when varying the driving protocol V(t) and the time τ , at which we perform the next measurement and repeat the cycle, for given extracted power, P, and error probability ε .

The results will be presented in the dimensionless units:

$$\Gamma t \to t, \quad V(t)/T \to V(t), \quad P \to P/\Gamma T$$



<u>Main</u>: the optimal period, τ , as a function of the power *P* for selected values of the error ε .

There is a maximal amount of power one can extract, $P^{\max}(\varepsilon)$, as τ approaches 0.

<u>Inset</u>: the scaled form of the same data, with τ as a function of P/P^{\max} .

As *P* approaches its maximum value the period approaches 0 linearly:

 $\tau \propto (P^{\max} - P)$

To a very good approximation, $P^{\max}(\varepsilon) = \frac{\varepsilon - 1/2}{\phi} \sinh \left[\phi(\varepsilon - 1/2)\right],$ where $\phi = 1.618$ is the golden ratio.

When the power P goes towards zero, the optimal period τ diverges to infinity. In other words, when we approach reversibility by performing the process in an infinite amount of time the power we can extract is zero.

In the limit of low power we find that $au = (\ln 2 - S_{arepsilon}) \, / P o Q_s(arepsilon) = \ln 2 - S_{arepsilon} = I$



Optimal protocol for $\varepsilon = 0.1$ and various *P*



For comparison: Error-free case

To extract maximum power one has to balance:

(i) the amount of energy gained per tunneling event,

(ii) the probability that tunneling occurs, and

(iii) the probability of back-tunneling while reducing the potential difference.

These results tells us the maximum power is reached with rapid measurements, favoring low probability high energy tunneling events, and a steeply sloped V(t).

Entropy production

As $P \to P^{\max}$, the entropy production diverges as $\dot{S}_{tot} \propto (P^{\max} - P)^{-1}$.

As
$$P o 0$$
 , $\Delta S_{
m tot} = c_0 + c_1 P$

For perfect measurements $c_0 = 0$, since there is no entropy production during reversible operation. Since $\tau = I/P \rightarrow \dot{S}_{\rm tot} = \Delta S_{\rm tot}/\tau \propto P^2$

If there are errors, the measurement entropy $S_{arepsilon}$ exists even for a reversible operation. As a result $c_0=S_arepsilon o \dot{S}_{
m tot}=(S_arepsilon/I)P+c_1^*P^2$



Up to the second order in P,

$$\dot{S}_{\rm tot}/P = c_1(\varepsilon) + c_2(\varepsilon)P$$

Plots of c_1 and c_2 are shown in the inset.

$$c_1 = S_{\varepsilon} (\ln 2 - S_{\varepsilon})^{-1}.$$

Role of measurement error: Plots of S_{ϵ}/S_{tot}

For $P \rightarrow 0$, we approach reversible operation $(\Delta S = 0)$ and all of the total entropy production is due to the measurement error.

When $P \rightarrow P^{\max}$ the measurement entropy dominates again since the there is no time for heat transfer from the environment when $\tau \rightarrow 0$.

When the error is extremely small its effect is only noticeable at the boundary values of *P*, but even for minor measurement errors a significant portion of the entropy production is due to the measurement error, for all *P*.





Non-analytical behavior versus **E**

If we make an error in a measurement, there is an associated net entropy production.
 For a symmetric binary measurement where the probability of error is ε, the entropy increases by the amount S_ε.

- This entropy increase can be understood either from a course graining of the phase space (for a closed system) or the dynamical evolutions (for an open system).
- We have investigated the consequences of a finite error probability on the optimal performance of a realistic Szilard engine at a finite (given) power.
- We found the existence of a maximal power P^{max} which is finite for error-free measurements, and which decreases with increasing error probability. The entropy production rate diverges as the maximal power is approached.
- For small power, the entropy production rate is quadratic in P in the absence of errors, but changes to linear when errors are present.
- > We have also found the time τ between measurements and the driving protocol V (t) minimizing the entropy production.

New detailed experiments are desirable.

Summary of the results



Sketch of calculations

Master equation:

$$\dot{p}_1 = -\Gamma_{12}p_1 + \Gamma_{21}p_2 = -\Gamma p_1 + \Gamma_{21}, \quad \Gamma \equiv \Gamma_{12} + \Gamma_{21} \\ \dot{p}_2 = \Gamma_{12}p_1 - \Gamma_{21}p_2 = -\Gamma p_2 + \Gamma_{12}$$

 $\frac{\text{Simple model:}}{\Gamma = \text{constant}(t)}$

Energies of the states:

Extracted work per cycle:

Change of internal energy:

Heat transfer:

$$E_{1}(t) \equiv 0, \ E_{2}(t) \equiv V(t)$$

$$W_{ex} = -\sum_{i=1}^{2} \int_{0}^{\tau} dt \, p_{i} \dot{E}_{i},$$

$$\Delta U = \sum_{i=1}^{2} \left[p_{i}(\tau) E_{i}(\tau) - p_{i}(0) E_{i}(0) \right]$$

$$Q = \Delta U + W_{ex} = \sum_{i=1}^{2} \int_{0}^{\tau} dt \, \dot{p}_{i} E_{i}(t)$$

$$H = -\sum_{i=1}^{2} p_{i} \ln p_{i}$$

Entropy production per cycle

$$\dot{H} = -\sum_{i=1}^{2} \dot{p}_i \ln p_i$$

Change in information entropy per cycle: $\Delta H = -\sum_{i=1}^{2} \int_{0}^{\tau} dt \, \dot{p}_{i} \ln p_{i}$

$$\frac{\Delta H}{\tau} = -\frac{1}{\tau} \int_0^\tau dt \ \dot{p} \ln\left(\frac{p}{1-p}\right), \quad p \equiv p_2 = 1-p_1$$

Master equation: $\dot{p} = -p + rac{1}{e^V + 1}$ Time is measured in 1/ Γ ; V -> in units of T

Power:

Power:
$$P = \frac{Q}{\tau} = \frac{1}{\tau} \int_0^{\tau} dt \ \dot{p}V = \frac{1}{\tau} \int_0^{\tau} dt \ \dot{p} \ln\left(\frac{1}{p+\dot{p}} - 1\right)$$

Entropy production:
$$\frac{\Delta S_{\text{tot}}}{\tau} = \frac{\Delta H}{\tau} + \frac{S_{\epsilon}}{\tau} - P$$

It is sufficient to minimize only

$$\begin{split} \mathcal{I} &= \frac{\Delta H}{\tau} + \lambda P = \frac{1}{\tau} \int_0^\tau dt \ L(p, \dot{p}, \lambda) \\ \text{Lagrangian:} \qquad L(p, \dot{p}, \lambda) = \left[-\ln\left(\frac{p}{1-p}\right) + \lambda \ln\left(\frac{1}{\dot{p}+p} - 1\right) \right] \dot{p} \end{split}$$

$$\frac{\partial L}{\partial p} = \frac{d}{dt} \frac{\partial L}{\partial \dot{p}} \longrightarrow \ddot{p} = \frac{\dot{p}^2 (\dot{p} + p - 1/2)}{p(\dot{p} + p - 1) + \dot{p}/2}, \qquad p(0) = \epsilon \qquad \bigstar$$

Power constraint: $G(\tau, p, \dot{p}) \equiv P - \frac{1}{\tau} \int_0^{\tau} dt \ \dot{p} \ln \left(\frac{1}{p + \dot{p}} - 1 \right) = 0$

Boundary condition, p(au) : From $(\partial L/\partial \dot{p})_{t= au}=0$, or

$$F_1(\lambda,\tau,p) \equiv \lambda \left[\ln \left(\frac{1}{p+\dot{p}} - 1 \right) + \frac{\dot{p}}{(\dot{p}+p-1)(\dot{p}+p)} \right] - \ln \left(\frac{p_\tau}{1-p_\tau} \right) = 0$$

Final constraint:
$$\frac{\partial \Delta S_{\text{tot}}/\tau}{\partial \tau} = 0 \text{ , or}$$
$$\frac{\partial \Delta S_{\text{tot}}}{\partial \tau} = \lambda \frac{\partial P}{\partial \tau} - \frac{1}{\tau^2} \left(\Delta H + S_\epsilon \right) + \frac{1}{\tau} \frac{\partial S_\tau}{\partial \tau} = 0 \quad \square$$
$$F_2(\lambda, \tau, p) \equiv \left[\ln \left(\frac{1 - p_\tau}{p_\tau} \right) + \lambda \dot{p}_\tau \ln \left(\frac{1}{p_\tau + \dot{p}_\tau} - 1 \right) \right] - \lambda P - \frac{1}{\tau} \left[\Delta H + S_\epsilon \right] = 0$$

We use Euler's method to solve the second order differential equation for p(t).

We find the values of τ and V_0 by using Newton's method.

In this way we determine $\, p(t) \,$ for given extracted power, $\, P \,$, and measurement error, $\, \epsilon \,$

Following the master equation we find that the optimal protocol, V(t) , of the Maxwell's demon is related to $\ p(t)$ as

$$V = \ln\left(\frac{1}{p+\dot{p}} - 1\right)$$

More realistic model - NIS junction,
$$\Delta \gg V(t), k_B T$$
:
 $\Gamma = 2\Gamma_m \cosh^2(V/2), \qquad \Gamma_m = \frac{\sqrt{2\pi\Delta k_B T}}{R_T e^2} e^{-\Delta/k_B T}$
 $\longrightarrow \dot{p} = 2\Gamma_m \cosh^2(V/2) \left[\frac{1}{1+e^V} - p\right]$

J. P. Pekola, O.-P. Saira, V. F. Maisi, A. Kemppinen, M. Möttönen, Y. A. Pashkin, and D. V. Averin, Rev. Mod. Phys. **85**, 1421 (2013). More realistic model - NIS junction, $\Delta \gg V(t)$, k_BT :

$$\Gamma = 2\Gamma_m \cosh^2(V/2), \qquad \Gamma_m = \frac{\sqrt{2\pi\Delta k_B T}}{R_T e^2} e^{-\Delta/k_B T}$$

The tunneling rate becomes time-dependent through V(t).

It results in effective increase of the tunneling rate and, consequently, increase of the extracted power.

This increase is limited by the condition $\Delta \gg k_B T$.



THANK YOU FOR YOUR ATTENTION !