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Thank you for the invitation!

Nonequilibrium Thermodynamics and Fluctuations in Small Systems

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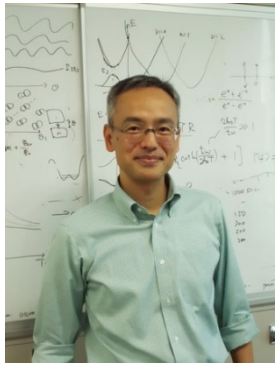

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Plan:

1. Thermodynamics: Reminder from textbooks
   - Large and small systems, averages and fluctuations
   - Equilibrium and non-equilibrium states
   - Small fluctuations from equilibrium state: Gaussian distributions

2. Fluctuation theorems (FTs) and Jarzynski relation
   - Formulation
   - Physical meaning: Particle in a box (deterministic motion)
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   - Optimal protocol for a given extracted power
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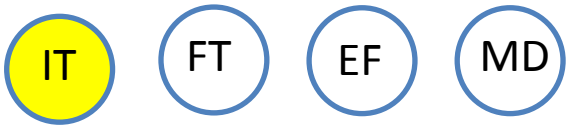
Introductory part. Block # 1

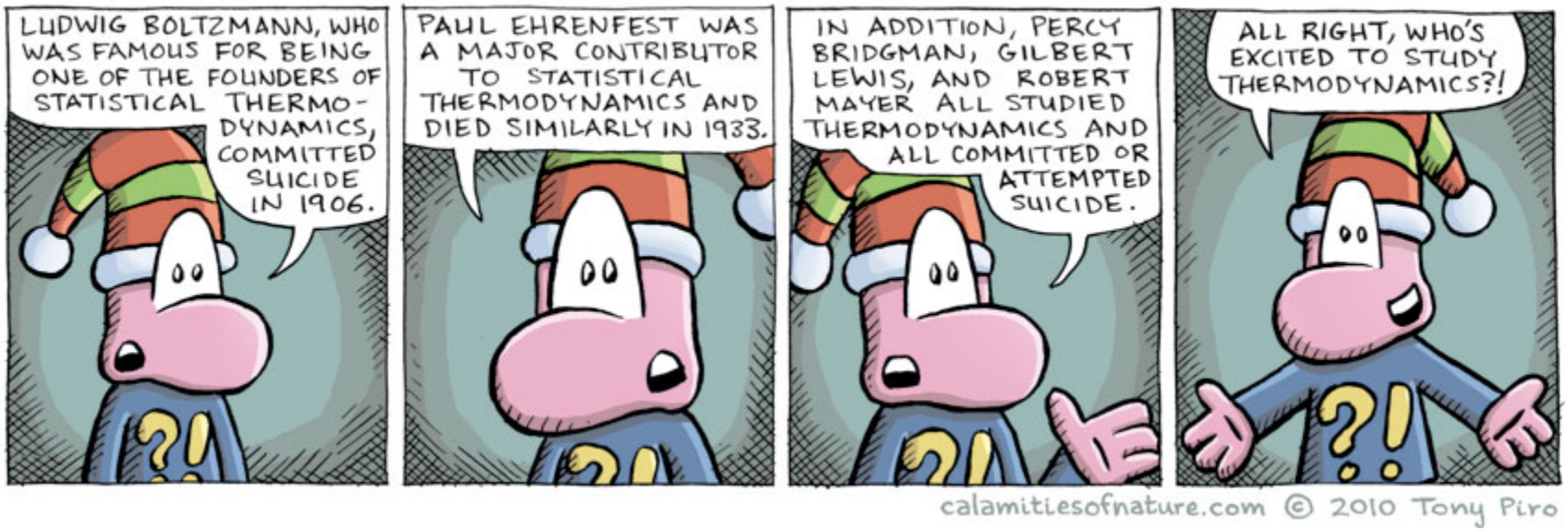


1. Thermodynamics: Reminder from textbooks
   - Large and small systems, averages and fluctuations
   - Equilibrium and non-equilibrium states
   - Small fluctuations from equilibrium state: Gaussian distributions

Thermodynamics is a discipline built in order to explain and interpret energetic processes occurring in macroscopic systems made out of a large number of particles.

Its full applicability is found in equilibrium systems where it can make quantitative predictions just based on a few laws.

The subsequent development of statistical mechanics has provided a solid probabilistic basis for thermodynamics and increased its predictive power at the same time.



What are small systems?

In large (classical) systems, the thermodynamic parameters are characterized by averages, the relative fluctuations are of the order $\sqrt{N}$, where N is number of particles.

Small systems are those in which the energy exchanged with the environment is a few times $k_B T$ and energy fluctuations are observable.

At the same time, a molecular system may not be considered as small if the transferred energy is measured over long times compared to the characteristic heat diffusion time.

Conversely, a macroscopic system operating at short time scales could deliver a tiny amount of energy to the environment, small enough for fluctuations to be observable and the system being effectively small.

We will deal with the situations when fluctuations are important.

The interest of the scientific community on small systems has been boosted by the recent advent of nanotechnologies. These provide adequate scientific instruments that can measure tiny energies in physical systems under nonequilibrium conditions.

Equilibrium and non-equilibrium states

State variables are those that, once determined, uniquely specify the thermodynamic state of the system.

Examples: temperature, pressure, volume, and mass of the different components .

To specify the state variables of the system it is common to put it in contact with a bath. The bath is any set of sources (of energy, volume, mass, etc.) large enough to remain unaffected by the interaction with the system under study.

The bath ensures that a system can reach a given temperature, pressure, volume, and mass concentration of the different components when put in thermal contact with the bath.

Equilibrium states are then generated by putting the system in contact with a bath and waiting until the system properties relax to the equilibrium values.

Under such conditions the system properties do not change with time and the average heat/work/mass exchanged between the system and the bath is zero.

Nonequilibrium states can be produced either by continuously changing the parameters of the bath or by preparing the system in an initial nonequilibrium state that slowly relaxes toward equilibrium.

In general, the net heat/work/mass exchanged by the system and the bath is nonzero.

Small fluctuations in an equilibrium state: The Gaussian distribution

Consider a closed system, some physical quantity x describing the system. Assume $\bar{x} = 0$.

Probability distribution: $w(x) \propto e^{S(x)}$ (A. Einstein 1907)

Entropy

Maximum at $x = \bar{x} = 0 \quad \rightarrow \quad \left.\frac{\partial S}{\partial x}\right|_{x=0} = 0\,, \quad \left.\frac{\partial^2 S}{\partial x^2}\right|_{x=0} < 0$

Expanding in small x, $S(x) = S(0) - \gamma\frac{x^2}{2}$, we obtain:

$$w(x)\,dx = \sqrt{\frac{\gamma}{2\pi}}e^{-\gamma x^2/2}\,dx, \quad \langle x^2\rangle = \gamma^{-1}$$

Gaussian

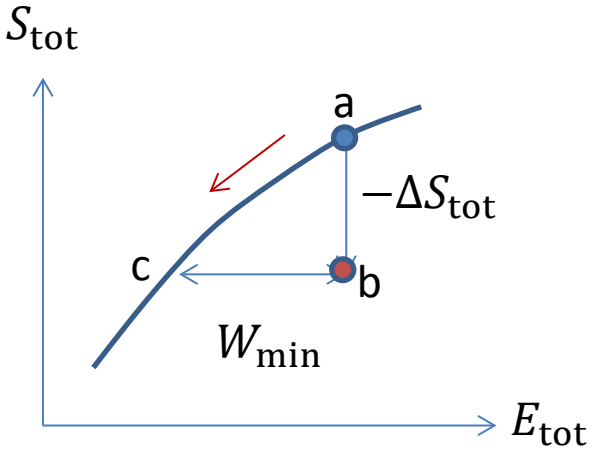
For an arbitrary quantity, $\langle(\Delta\phi)^2\rangle = \left[\frac{d^2\phi}{dx^2}\right]_{x=0}\langle x^2\rangle$

We assume that x behaves classically

Minimum work

Consider total entropy of a system + bath. In the equilibrium, $S_{\rm tot}(E_{\rm tot})$.

Out of equilibrium, $S = S_{\rm tot}(E_{\rm tot}) + \Delta S_{\rm tot}$, $\quad \Delta S_{\rm tot} < 0$.



$$\Delta S_{\rm tot} = -\frac{dS_{\rm tot}}{dE_{\rm tot}} W_{\rm min} = -\frac{W_{\rm min}}{T_0}$$
$$= -\frac{\Delta E - T_0 \Delta S + P_0 \Delta V}{T_0}$$

The Gaussian distributions are obtained by expansion of the above expression up to the second order in the fluctuating quantities.

Example: if P and S are independent variables,

$$w \propto \exp\left[\frac{1}{2T}\left(\frac{\partial V}{\partial P}\right)_S (\Delta P)^2 - \frac{1}{2C_p}(\Delta S)^2\right]$$

Multiple variables

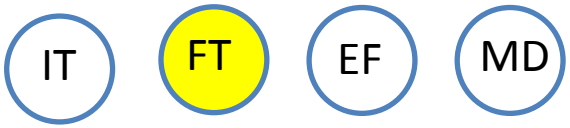
The above expression has a straightforward generalization to the probability distribution $w(x_1, x_2, \ldots, x_n)dx_1 dx_2 \ldots dx_n$:

$$w = \prod_{i,j=1\ldots n} \frac{1}{(2\pi)^{n/2}\sqrt{\langle x_i x_j \rangle}} \exp\left(-\frac{x_i x_j}{2\langle x_i x_j \rangle}\right),$$

where $\langle x_i x_j \rangle$ is the mean value of $x_i x_j$.[4]

Averages $\langle x_i x_j \rangle$ of thermodynamic fluctuations. Temperature is in energy units (divide by Boltzmann's constant k_B to get degrees). C_P is the heat capacity at constant pressure; C_V is the heat capacity at constant volume.[4]

	ΔT	ΔV	ΔS	ΔP
ΔT	$\frac{T^2}{C_V}$	0	T	$\frac{T^2}{C_V}\left(\frac{\partial P}{\partial T}\right)_V$
ΔV	0	$-T\left(\frac{\partial V}{\partial P}\right)_T$	$T\left(\frac{\partial V}{\partial T}\right)_P$	$-T$
ΔS	T	$T\left(\frac{\partial V}{\partial T}\right)_P$	C_P	0
ΔP	$\frac{T^2}{C_v}\left(\frac{\partial P}{\partial T}\right)_V$	$-T$	0	$-T\left(\frac{\partial P}{\partial V}\right)_S$



2. Fluctuation theorems and Jarzynski relation
   - Formulation
   - Physical meaning: Particle in a box (deterministic motion)
   - Particle in a box : Stochastic motion

Non-equilibrium processes: Fluctuation theorems

Fluctuation theorems (FTs) make statements about energy exchanges that take place between a system and its surroundings under general nonequilibrium conditions. Discovered in the mid 90's.

FTs provide a fresh look to our understanding of old questions such as the origin of irreversibility and the second law in statistical mechanics.

In addition, FTs provide statements about energy fluctuations in small systems which, under generic conditions, should be experimentally observable.

FTs are related to the so-called nonequilibrium work relations introduced by Jarzynski.

The **Jarzynski equality** (JE) is an equation that relates free energy differences between two *equilibrium* states and *non-equilibrium* processes. It is named after Christopher Jarzynski (then at Los Alamos National Laboratory) who derived it in 1997.

PRL 78, 2690 (1997) – 1788 citations

Jarzynski energy relation

Suppose we have an arbitrary system and let us consider two states of this system specified by parameters, say A_{initial} and A_{final} (volumes, magnetic fields, etc).

If the initial state is equilibrium, it has (Helmholtz) free energy $F(A_{\text{initial}}) \equiv F_{\text{initial}}$. Similarly, if the final state is equilibrium, then $F(A_{\text{final}}) \equiv F_{\text{final}}$. The difference is

$$\Delta F = F_{\text{final}} - F_{\text{initial}}$$

$-W$ is the work, performed *on the system*

Jarzynski equality (JE):

$$\langle e^{W/k_B T} \rangle = e^{-\Delta F/k_B T}$$

For cyclic processes:

$$\langle e^{W/k_B T} \rangle = 1$$

The average is calculated over all non-equilibrium "trajectories" in the phase space connecting the initial state and the final one, both being equilibrium at the same temperature.

Extensive literature

[1] Jarzynski C 1997 Nonequilibrium equality for free energy differences *Phys. Rev. Lett.* **78** 2690

[2] Jarzynski C 1997 Equilibrium free-energy differences from nonequilibrium measurements: a master-equation approach *Phys. Rev.* E **56** 5018–35

[3] Crooks G E 1999 Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences *Phys. Rev.* E **60** 2721

[4] Imparato A and Peliti L 2005 Work-probability distribution in systems driven out of equilibrium *Phys. Rev.* E **72** 046114

[5] Kawai R, Parrondo J M R and Van den Broeck C 2007 Dissipation: the phase–space perspective *Phys. Rev. Lett.* **98** 080602

[6] Adib A B 2005 Entropy and density of states from isoenergetic nonequilibrium processes *Phys. Rev.* E **71** 056128

[7] Hendrix D A and Jarzynski C 2001 A 'fast growth' method of computing free energy differences *J. Chem. Phys.* **114** 5974–81

[8] Ytreberg F M, Swendsen R H and Zuckerman D M 2006 Comparison of free energy methods for molecular systems *J. Chem. Phys.* **125** 184114

[9] Híjar H, Quintana-H J and Sutmann G 2008 Probability distributions of Hamiltonian changes in linear magnetic systems under discontinuous perturbations *J. Stat. Mech.* P05009

[10] Liphardt J, Dumont S, Smith S B, Tinoco I Jr and Bustamante C 2002 Equilibrium information from nonequilibrium measurements in an experimental test of Jarzynski's equality *Science* **296** 1832–5

[11] Harris N C, Song Y and Kiang C-H 2007 Experimental free energy surface reconstruction from single-molecule force spectroscopy using Jarzynski's equality *Phys. Rev. Lett.* **99** 068101

[12] Vilar J M G and Rubi J M 2008 Failure of the work-Hamiltonian connection for free-energy calculations *Phys. Rev. Lett.* **100** 020601

[13] Horowitz J and Jarzynski C 2008 Comment on 'Failure of the work-Hamiltonian connection for free-energy calculations' *Phys. Rev. Lett.* **101** 098901

[14] Lua R C and Grosberg A Y 2005 Practical applicability of the Jarzynski relation in statistical mechanics: a pedagogical example *J. Phys. Chem. B* **109** 6805–11

[15] Crooks G E and Jarzynski C 2007 Work distribution for the adiabatic compression of a dilute and interacting classical gas *Phys. Rev.* E **75** 021116

[16] di Liberto F 2007 Entropy production and lost work for some irreversible processes *Phil. Mag* **87** 569–79

[17] Cuendet M A 2006 Statistical mechanical derivation of Jarzynski's identity for thermostated non-Hamiltonian dynamics *Phys. Rev. Lett.* **96** 120602

[18] Bena I, van den Broeck C and Kawai R 2005 Jarzynski equality for the Jepsen gas *Europhys. Lett.* **71** 879–85

[19] Jarzynski C 2007 Comparison of far-from-equilibrium work relations *C. R. Phys.* **8** 495–506

Equivalent formulation:

$$\frac{P(A \to B)}{P(A \leftarrow B)} = e^{-\beta(W_{A\to B}+\Delta F)}$$

Crooks fluctuation theorem

Jarzynski's and related non-equilibrium work theorems have found many practical applications in research.

Originally, Jarzynski proposed his result as a simple and computationally advantageous way of calculating free energies in molecular simulations, and indeed it was successfully employed with this aim [7].

More recently, for instance, non-equilibrium work theorems have been used to computationally estimate free energy differences in a solution of charged particles in water [8], or the surface tension of magnetic domains in the Ising model [9].

Another important is single-molecule experiments. This application was originally done in [10] for the open and the close state of an RNA hairpin.

Recent applications to biophysics are discussed in the review by Felix Ritort, Advances in Chemical Physics, **137** (2008).

Still there are some discussions regarding definition of thermodynamic work, especially in quantum systems.

Conventional thermodynamics:

if we drive the system from initial to final state by a reversible process, such that the system remains at equilibrium at every stage, then we have to perform work, -*W*, which is equal the free energy change:

$$-W = \Delta F$$

If the process is not reversible, then the second law of thermodynamics tells us that

$$\langle -W \rangle \geq \Delta F$$

The difference $W_{\mathrm{diss}} \equiv \langle -W \rangle - \Delta F$ is just the dissipated work associated with the increase of entropy during an irreversible process.

Therefore, along conventional thermodynamics, for *non-equilibrium processes* one cannot formulate a general relationship between the average work and variation in the free energy.

All happy families are alike; every unhappy family is unhappy in its own way.

Leo Tolstoy, “Anna Karenina”, part 1.

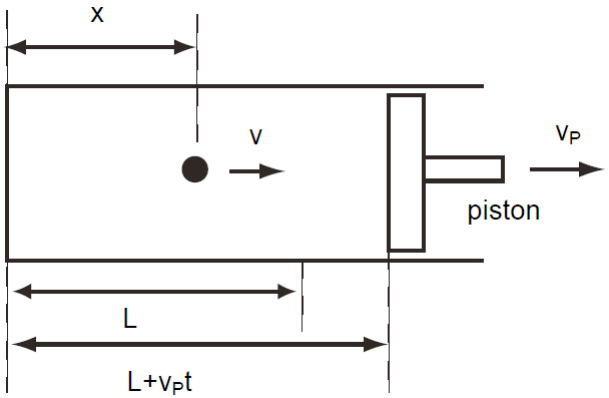
The 2nd law of thermodynamics is of a statistical nature, and, therefore, from time to time, very infrequently, the fluctuations occur in which $-W < \Delta F$

These fluctuations might be very rare, but with large *W* (strongly negative -*W*) their contribution to the average of $\left\langle e^{W/k_BT} \right\rangle$ might be significant. This is the essence of the JE.

`transient/temporary violations of the second law of thermodynamics'

Proper exploration of a representative set of fluctuations.

Simple classical model



We move a piston to the right with constant velocity v_p during time τ.

The gas inside the cylinder is ideal:

$$\left(\left\langle e^{W_1/k_BT}\right\rangle\right)^N = \left(e^{-\Delta F_1/k_BT}\right)^N$$

Therefore we consider only 1 molecule.

For brevity, we put $k_BT = 1,\ m = 1,\ \text{time interval } \tau = 1\,.$

Rhonald C. Lua, Alexander Y. Grosberg , *J. Phys. Chem. B* **2005,** *109,* 6805-6811

To make it simple:

massless piston moving without any friction, while the piston is moving, the system is considered to be disconnected from the thermostat, etc.

Initially, the piston is at some distance L from the bottom of the vessel and the gas temperature is T. Then we move the piston by some distance ΔL and stop it again, thus preparing the final state.

When the wall movement ends, the system is not in equilibrium, the thermostat has to be reconnected and some energy has to be exchanged between the system and the thermostat to regain equilibrium at the same initial temperature T.

But the energy exchanged in this re-equilibration step does not modify our results, because from a thermodynamic point of view it has to be considered as heat, as long as the final position of the wall is not modified.

Seeming paradox: suppose that we move the piston at a very high speed, so no molecules can hit the piston when it is moving. Therefore,

$$W = 0,\ \left\langle e^{\beta W} \right\rangle = 1,\ \text{but}\ \Delta F \neq 0\,.$$

Solution: There are always particles at the tail of the Maxwell distribution.

Jarzynski identity has to do with the tails of the relevant distributions.

Kinematics

$v > 0$

Time of the 1st reflection:

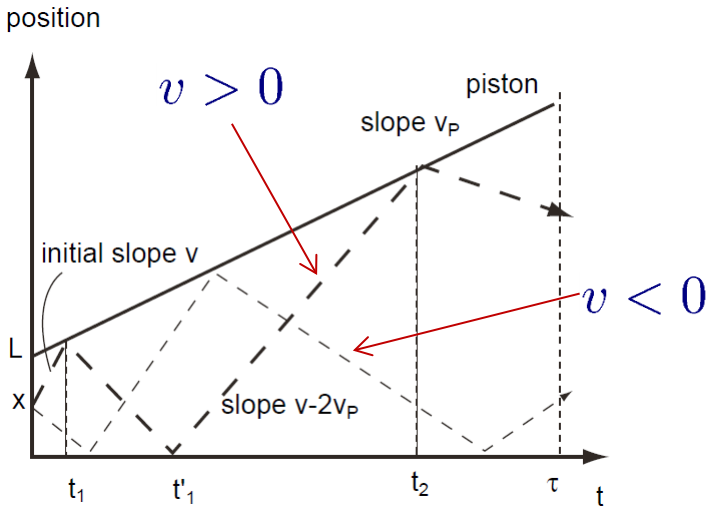
$$t_1 = \frac{L - x}{v - v_p}$$

After 1st reflection:

$$v_p \to v - 2v_p$$

Time of the 2nd reflection:

$$t_2 = \frac{3L - x}{v - 3v_p}$$



Time of the nth reflection:

$$t_n^+ = \frac{(2n-1)L - x}{v - (2n-1)v_p} \qquad t_n^- = \frac{(2n-1)L + x}{v - (2n-1)v_p}$$

Dynamics

Work done by piston on the molecule:

$$-w_1 = (-(v - 2v_p) - v)v_p = -2(v - v_p)v_p$$

$$-w_n = -2vv_p n + 2v_p^2 n^2$$

Change in kinetic energy

Average

$$\langle e^W \rangle = \frac{\int_0^L dx \int_{-\infty}^{\infty} dv e^{-v^2/2} e^{w_\tau(x,v)}}{\int_0^L dx \int_{-\infty}^{\infty} dv e^{-v^2/2}}$$

Don't be confused with dimensionality: to simplify writing it is assumed that the temperature is such that $k_B T = 1$, the mass of the molecule is $m = 1$, and the piston is moving during the time interval $\tau = 1.$.

It is convenient to divide the interval of integration into pieces corresponding to exactly *n* collisions

$$(2n-1)(L+v_p) - x < |v| < (2n+1)(L+v_p) - x$$

$$(2n-1)(L+v_p) + x < |v| < (2n+1)(L+v_p) + x$$

After cumbersome calculation the result can be cast in the form

$$\langle e^W \rangle = \frac{\int_0^{L+v_p} dx \int_{-\infty}^{\infty} dv e^{-v^2/2}}{\int_0^L dx \int_{-\infty}^{\infty} dv e^{-v^2/2}} = \frac{L + v_p \tau}{L} = \frac{Z(L + v_p\tau, T)}{Z(L,T)} = e^{-\Delta F / k_B T}$$

The Jarzynski equality is met!

Probability distribution

$$P(W) = \frac{1}{\sqrt{2\pi}L} \int_0^L dx \int_{-\infty}^{\infty} dv e^{-v^2/2} \delta\left[W - w_\tau(x,v)\right] \ .$$

Method:

Splitting integration over x into the intervals with exact number of collisions with the piston

$$(2n-1)(L+v_p) - x < |v| < (2n+1)(L+v_p) - x$$
$$(2n-1)(L+v_p) + x < |v| < (2n+1)(L+v_p) + x$$

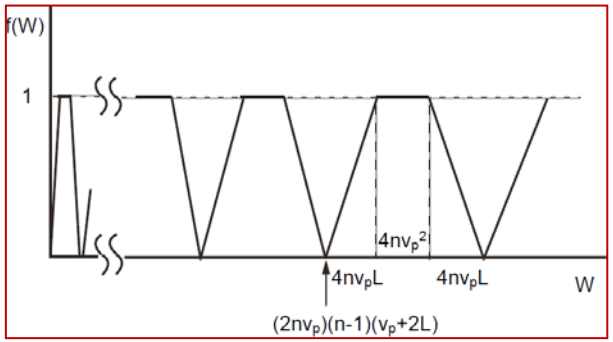
and subsequent relating *n* to the work *W*

$$n = \text{int}\left[\frac{1}{2}\left(1 + \sqrt{1 + \frac{2W}{v_p(2L+v_p)}}\right)\right]$$

Result

$$P(W) = \delta(W)P_0 + \frac{e^{-\frac{1}{2}\left(nv_p + \frac{W}{2nv_p}\right)^2}}{\sqrt{2\pi}nv_p} f(W)$$

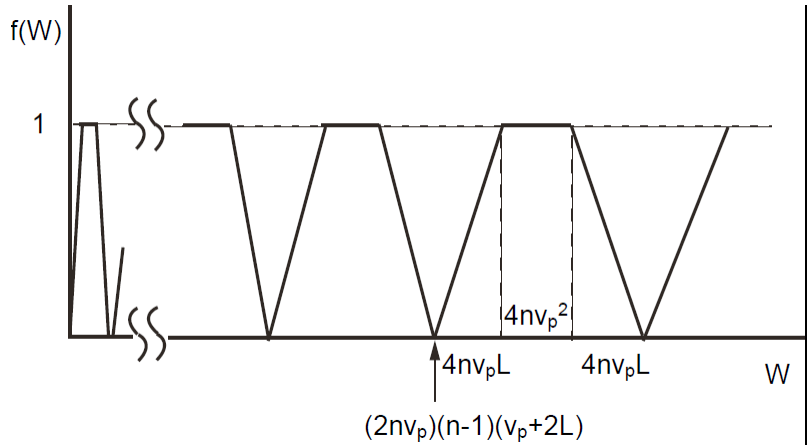
Probability for 0 collisions



$$P(W) = \delta(W)P_0 + \frac{e^{-\frac{1}{2}\left(nv_p + \frac{W}{2nv_p}\right)^2}}{\sqrt{2\pi}nv_p} f(W)$$

$$P_0 = \frac{1}{\sqrt{2\pi}L}\int_0^L dx \int_{-(L+v_p)}^{(L+v_p)} dv e^{-(v-x)^2/2} \qquad n = \text{int}\left[\frac{1}{2}\left(1 + \sqrt{1 + \frac{2W}{v_p(2L+v_p)}}\right)\right]$$

$$f(W) = \begin{cases} -(n-1)\left(\frac{v_p}{2L}+1\right) + \frac{W}{4nv_pL} & \text{when} \quad (n-1)(v_p+2L) < \frac{W}{2nv_p} \le (n-1)(v_p+2L)+2L \\ 1 & \text{when} \quad (n-1)(v_p+2L)+2L < \frac{W}{2nv_p} \le (n-1)(v_p+2L)+2L+2v_p \\ (n+1)\left(\frac{v_p}{2L}+1\right) - \frac{W}{4nv_pL} & \text{when} \quad (n-1)(v_p+2L)+2L+2v_p < \frac{W}{2nv_p} \le (n+1)(v_p+2L) \end{cases}$$



Simulations:

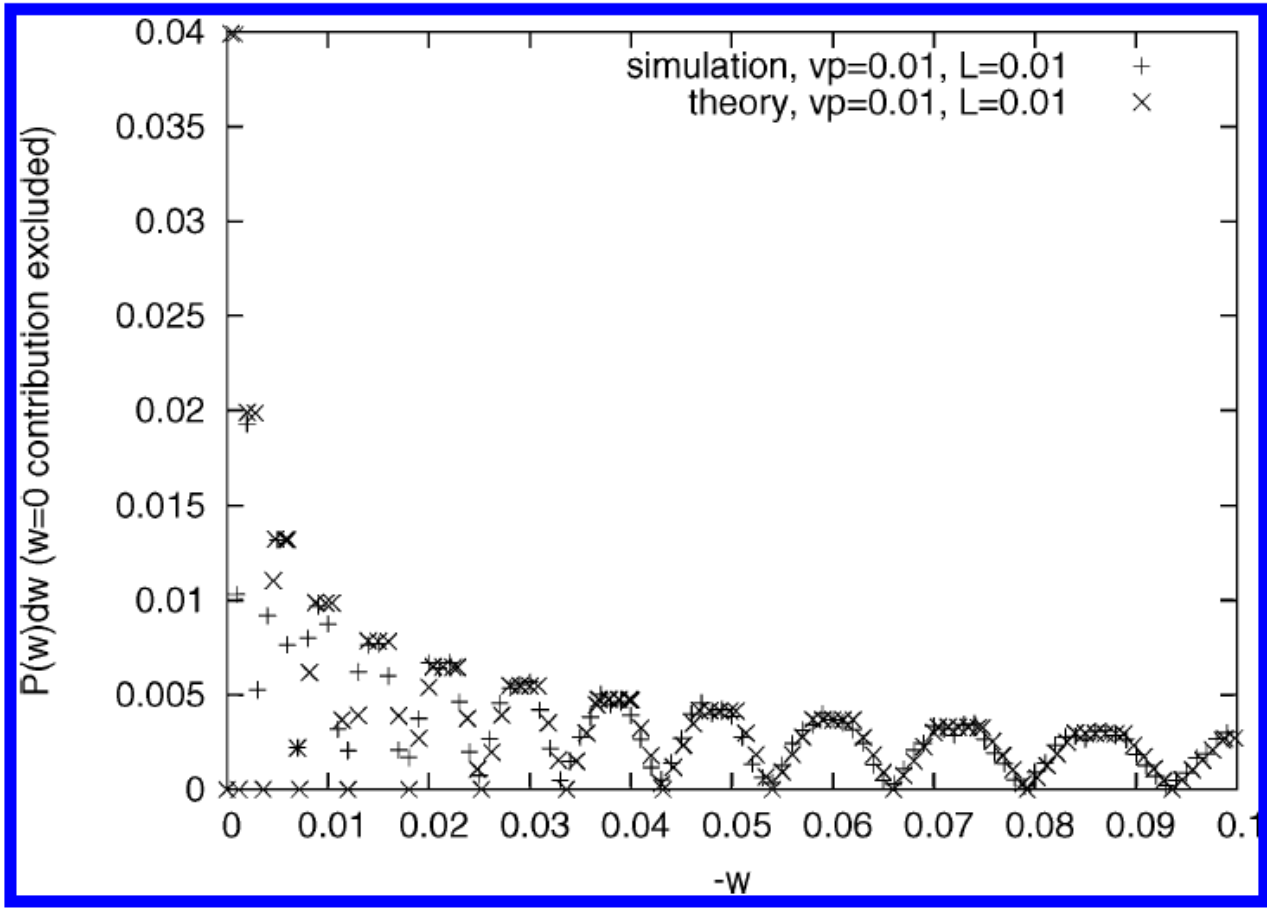


Figure 3. Simulation results (denoted by pluses, +) together with theoretical calculation (expression (13); denoted by crosses, ×) for the work distribution. For each trial run, the cylinder volume was doubled ($v_p = 0.01$, $\tau = 1$, $L = 0.01$). The bin width used was $\Delta w = k_B T/1000 = 1/1000$. The average number of collisions between molecule and piston was about 20.

Discussion

Q: Is the JE useful?

A1: Very useful: one does not have to equilibrate the system and by doing purely non-equilibrium measurements, one nevertheless recovers the equilibrium free energy.

A2: There are complications on this way. To do equilibrium measurements, one has to proceed very slowly, to keep the system close to equilibrium all the time; for this, τ has to be larger than the system relaxation time, which grows with the system size L.

But, on the other hand, if one proceeds very rapidly, then one has to perform exponentially many experiments in order to catch the exponentially rare but decisively important fluctuations.

There might be some optimal strategy. For the ideal gas model, such optimal strategy is most likely the (classical) slow `equilibrium' experiment, because the time for such an experiment grows only linearly with $L$, while the time for a `fast' experiment is exponential.

For other systems, the optimal strategy might be intermediate between one very slow experiment and very many rapid ones.

Rapid non-equilibrium measurements are not automatically advantageous.

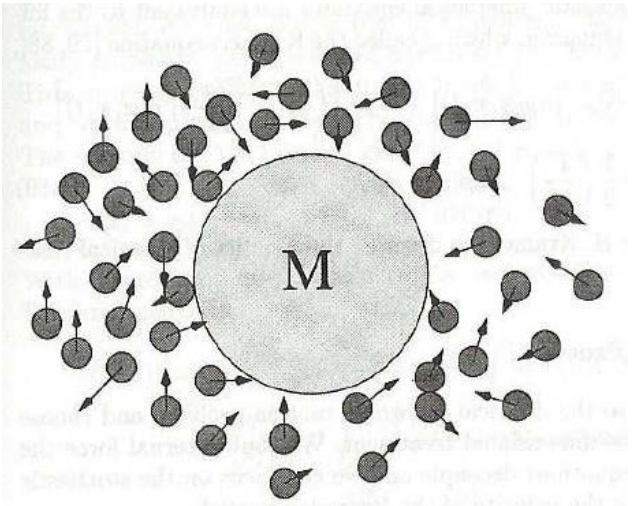
Stochastic motion: Langevin approach (1908)

The theory of Brownian motion is perhaps the simplest approximate way to treat the dynamics of nonequilibrium systems.

The fundamental equation is called the Langevin equation; it contain both frictional forces and random forces.

The fluctuation-dissipation theorem relates these forces to each other.

Consider a large particle (the Brownian particle) immersed in a fluid of much smaller particles.



Three characteristic time scales, which are very different:

$$\tau_s \ll \tau_B = m/\gamma \ll \tau_D = a^2/D$$

As a result, random instantaneous forces $\xi(t)$ can be introduced to the Newtonian equation of motion:

$$m\dot{v} = -m\gamma v + \xi(t)$$

Viscous friction: $m\gamma = 6\pi\mu a$

Random force: $\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = g\delta(t-t')$

$D = k_B T/\gamma$ – diffusion constant

Neglecting random forces one would get $v(t) = v(0)\, e^{-\gamma t}$ that is obviously wrong since in the equilibrium one should get the equipartition: $m\langle v^2(t)\rangle_{\rm eq} = k_B T$

Including random forces one obtains:

$$v(t) = e^{-\gamma t} v(0) + \frac{1}{m}\int_0^t ds\, e^{-\gamma(t-s)}\xi(s)$$

At $t_1, t_2 \gg \gamma^{-1}$ $\quad v(t_1)v(t_2) \to \frac{1}{m^2}\int_0^{t_1} ds \int_0^{t_2} dk\, e^{-\gamma(t_1+t_2)} e^{\gamma(s+k)}\xi(s)\xi(k)$

$$\langle v(t_1)v(t_2)\rangle_\xi \to \frac{g}{m^2}\int_0^{t_1} ds \int_0^{t_2} dk\, e^{-\gamma(t_1+t_2)} e^{\gamma(s+k)}\delta(s-k) \to \frac{g}{2m\gamma} e^{-\gamma|t_1-t_2|}$$

To get the equipartition one has to require $g = 2\gamma k_B T$

Particle in a box: Stochastic motion

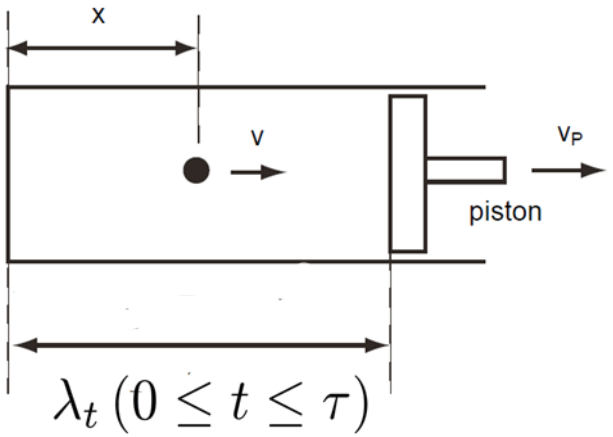
Previous consideration was *purely deterministic*. What happens if dynamics is *stochastic*?

PRL **117,** 180603 (2016) PHYSICAL REVIEW LETTERS week ending 28 OCTOBER 2016

Stochastic Thermodynamics of a Particle in a Box

Zongping Gong,[1,2] Yueheng Lan,[3,4,*] and H. T. Quan[1,4,†]

Brownian Szilard engine



Brownian particle:

$$\dot{x} = \frac{p}{m} \quad , \quad \dot{p} = -\gamma \frac{p}{m} + \sqrt{\frac{2\gamma}{\beta}}\eta_t + I_c,$$

$(x, p) \equiv \Gamma$ viscosity $1/T$ collisions

η_t - standard Wiener process: $\langle \eta_t \eta_{t'} \rangle = \delta(t - t'),\ \eta_t dt \sim N(0, dt)$ - normal distribution with mean zero and variance *dt*

I_c suddenly changes *p* into $2m\dot{\lambda}_t - p\ (\text{or}\ -p)$ once a collision at the right (or left) boundary occurs at time *t*.

Work along the trajectory: $W[\Gamma_t] = -\sum_{t \in C[x_t]} 2\dot{\lambda}_t (p_{t-} - m\dot{\lambda}_t)$ New definition of work!

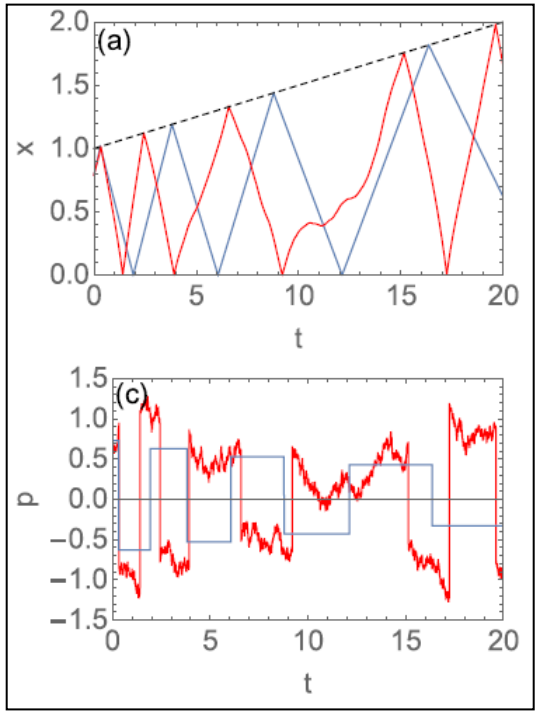
Collisions are assumed to be elastic; $C[x_t] \equiv \{t : x_t = \lambda_t, 0 \le t \le \tau\}$ - set of collision time points for a trajectory x_t in real space; p_{t-} is the momentum value at the time point immediately prior to *t*.

Initial distributions of *x* and *p* are respectively $U(0, \lambda_0)$ (uniform distribution) and $N(0, m/\beta)$ (normal distribution). So we are in the canonical ensemble.

During the course the right boundary is driven according to an arbitrary protocol λ_t and ends at $\lambda_\tau = 2\lambda_0$.

Coordinate transformation: $(-)^{\lfloor \xi \rfloor + 1} h(\xi) \equiv \frac{x}{\lambda_t}$, $\mathcal{P} \equiv (-)^{\lfloor \xi \rfloor} p + m\dot{\lambda}_t h(\xi)$

$h(\xi) \equiv 2\lfloor (\xi + 1)/2 \rfloor - \xi$ where $\lfloor ... \rfloor$ is the Gauss floor function



After coordinate transformation

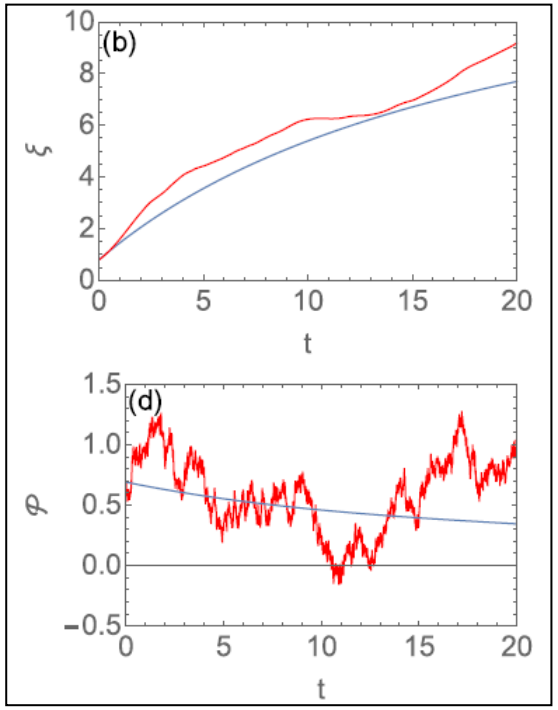
The expansion protocol is the linear one, i.e.,

$$\lambda_t = \lambda_0(1 + t/\tau)$$

Where $\lambda_0 = 1$ and $\tau = 20$, black dashed line in (a).

All the blue curves correspond to the adiabatic process $(\gamma = 0)$, while the red ones correspond to the isothermal process with

$$\gamma = 0.05, \ \beta = 1$$

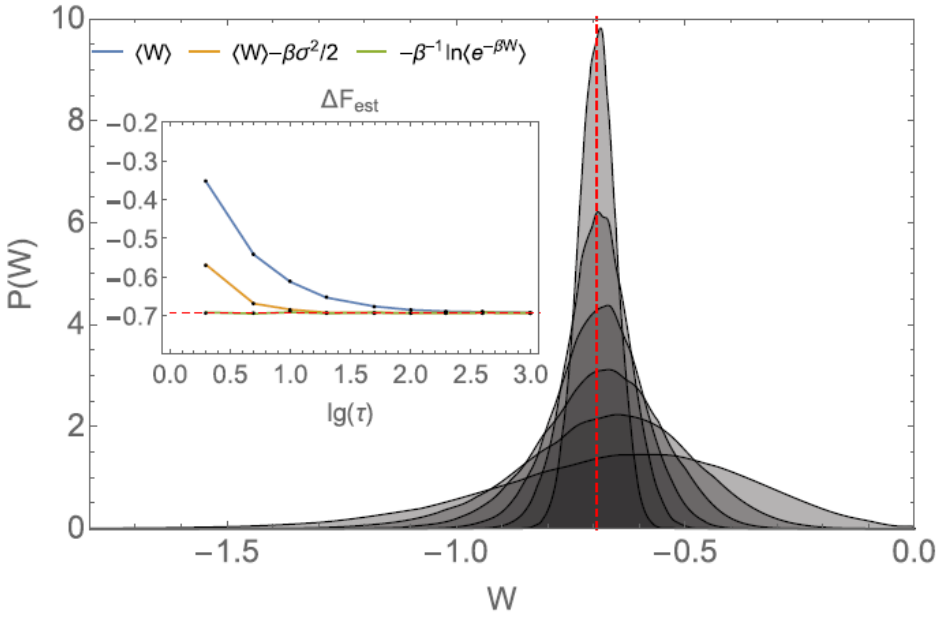


Continuous variables -> collision-free equation of motion

$$\dot{\xi} = \frac{\mathcal{P}}{m\lambda_t},$$

$$\dot{\mathcal{P}} = \left(\gamma\dot{\lambda}_t + m\ddot{\lambda}_t\right) h(\xi) - \left(\frac{\gamma}{m} + \frac{\dot{\lambda}_t}{\lambda_t}\right)\mathcal{P} + \sqrt{\frac{2\gamma}{\beta}}\eta_t.$$

Work: $W[\widetilde{\Gamma}_t] = -\int_0^\tau dt \frac{\mathcal{P}_t^2\dot{\lambda}_t}{m\lambda_t}\left[h'(\xi_t) + 1\right]$ where $h'(\xi) + 1 \equiv 2\sum_{k\in\mathbb{Z}}\delta(\xi - 2k - 1)$



Work distribution functions for the uniform expansion protocol with τ = 20, 50, 100, 200, 400, 1000 obtained from stochastic simulations, where the *P(W)* curve with sharper peak corresponds to larger τ.

The work distribution for τ = 20 is clearly non-Gaussian, and thus beyond the linear response regime.

The vertical red dashed line marks the position of $\Delta F = \beta^{-1} \ln 2$. Inserted figure shows the numerical estimation of the free energy difference ΔF_{est} based respectively on the mean work <W> (blue line), the linear response correction $\langle W \rangle - \beta\sigma^2/2$ (orange line) and the JE $-\beta^{-1} \ln\langle e^{-\beta W} \rangle$ for nine different uniform expansion processes, with τ = 2, 5, 10, 20, 50,100, 200, 400, 1000.

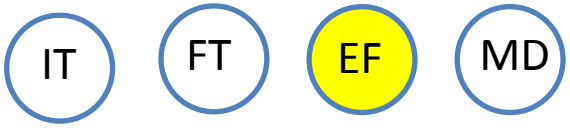
The horizontal red dashed line is the theoretical free energy difference while the dots are the simulation results. Here, $\lambda_0 = 1$, $\beta = 1$, and $\gamma = 1$ are all fixed

Where we are?

We have considered examples of classical systems with deterministic and stochastic dynamics. The result of our analysis is compatible with the Jarzynski work relations.

What about quantum systems?

Block # 3

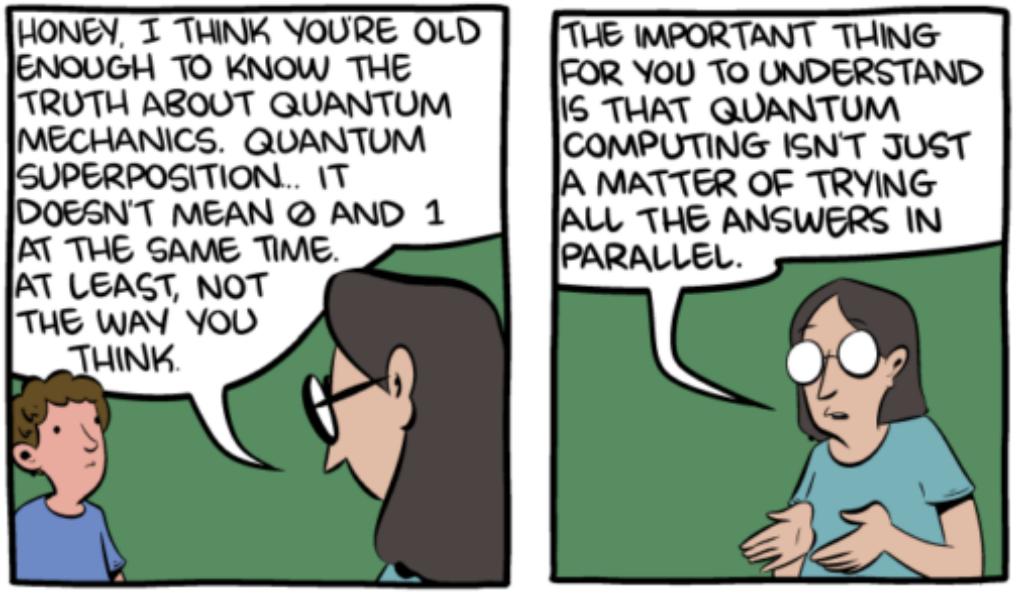


3. Energy fluctuations in generic quantum devices
   - Qubit as an instrument for studies of energy fluctuations
   - Quantum jumps
   - Two-measurement protocol: Relationship between the energy fluctuations and decoherence.

We have considered fluctuations of work of a classical small system, both for deterministic and stochastic dynamics.

To illustrate some features of quantum systems let us consider a generic quantum device – two-level system (Qubit)

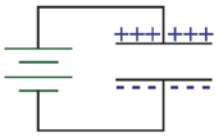
Qubit as an instrument



In this part we will discuss a device for quantum computation – qubit – as an instrument for studies of thermodynamics of simple quantum systems

Devices for quantum computation: Brief introduction

Classical bit



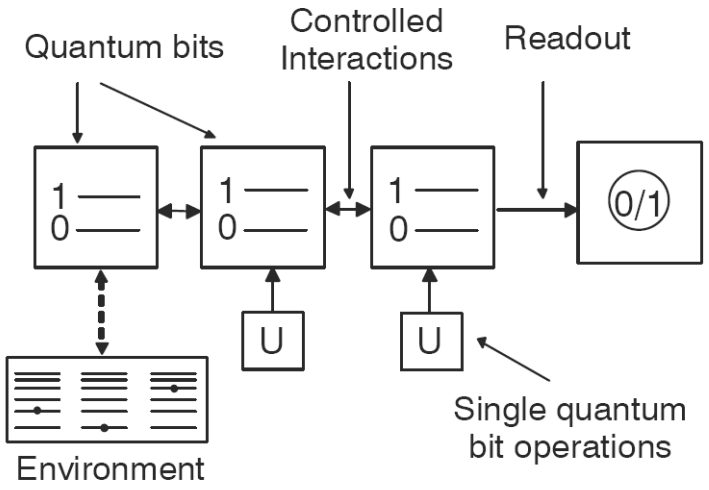
values 0 or 1

Quantum bit (or "qubit")

Information as state of a two-level quantum system

values $|0\rangle$, $|1\rangle$ ***or***

superposition: $\alpha|0\rangle + \beta|1\rangle$



A quantum processor consists of a collection of interacting quantum bits which can be independently manipulated and measured.

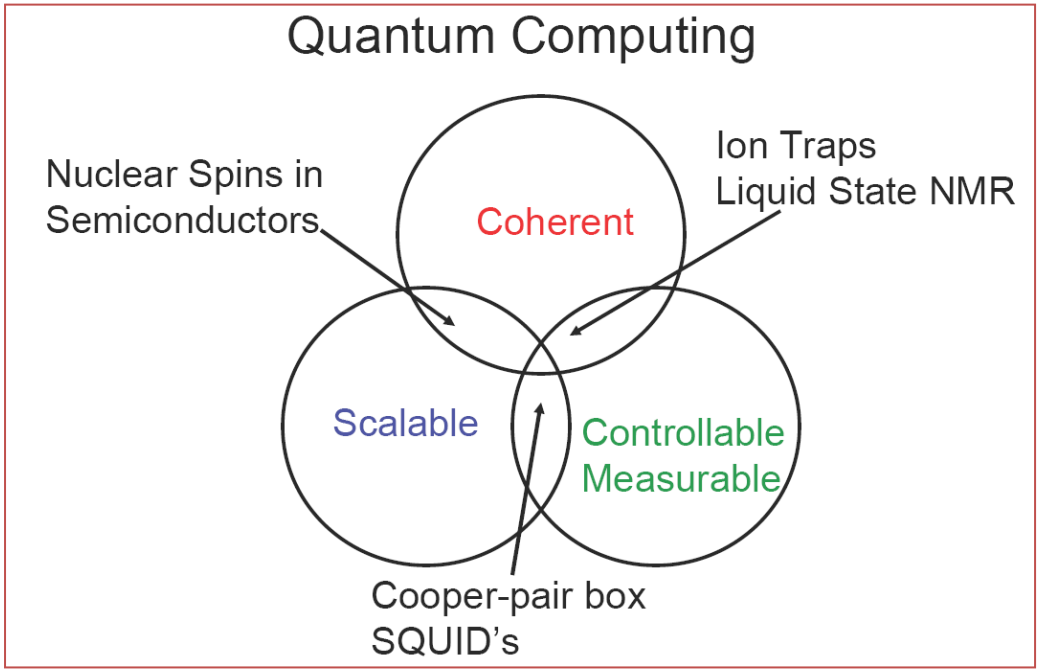
The coupling to the environment should be kept low enough to maintain quantum coherence.

What do we need to make it working?

DiVinchenzo criteria (1997)

1. A scalable physical system with well characterized qubits
2. The ability to initialize the state of the qubits
3. Long relevant decoherence times, much longer than the gate operation times (by factor of about 10^4)
4. A universal set of quantum gates, i. e., logical operations involving two or more qubits
5. The ability to measure specific single qubits

Today qubits are also used as tools for investigation of quantum systems.



Hardware:

Atomic systems:

- atoms in an ion trap,
- atoms in an optical lattice,
- ensemble of nuclear spins in a liquid

Solid-state systems:

- spins of electrons in semiconductor quantum dots,
- nuclear spins of donor atoms in a semiconductor,
- superconducting microcircuits containing Josephson junctions

Scalable, allow to preserve coherence

What is a qubit?

A typical quantum two-level system equivalent to ½ spin:

$$H_{\mathrm{ctrl}} = -\frac{1}{2}B_z\hat{\sigma}_z - \frac{1}{2}B_x\hat{\sigma}_x$$

B_i are tunable to perform single-qubit operations

To maintain coherence people use macroscopically-coherent systems – superconductors – with two-component order parameter:

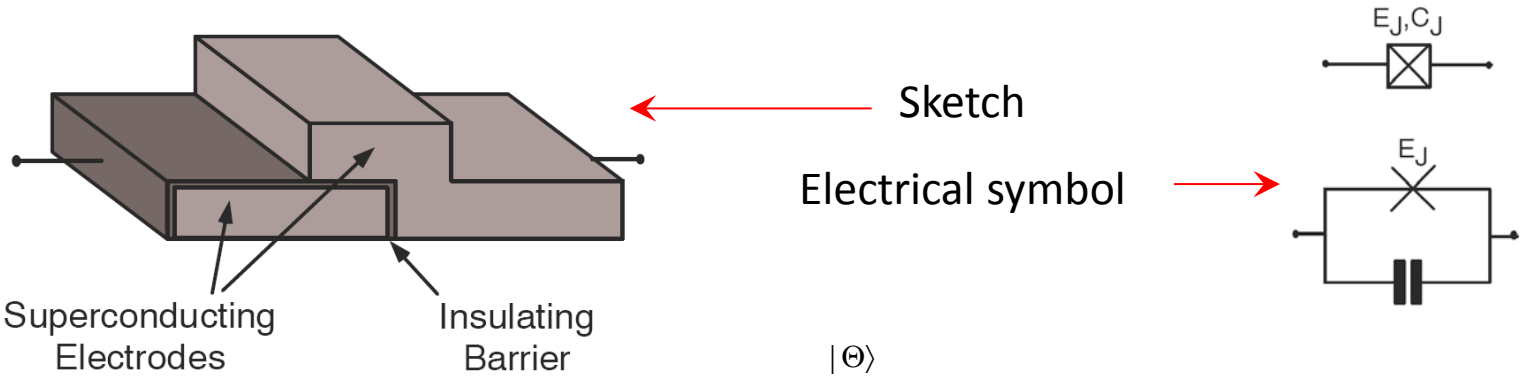
$$\Psi = |\Psi|e^{i\chi(\vec{r},t)}$$

Since it can be considered as wave function for the Cooper pairs condensate, assuming spatially uniform $|\Psi|$ we get for the current

$$\vec{j} = e|\Psi|^2\vec{v}_s, \quad \vec{v}_s = \frac{\hbar}{2m}\nabla\chi$$

In the presence of current a phase difference $\Theta = \chi_1 - \chi_1$ across the superconductor is created.

Josephson junction



Non-dissipative current → Phase difference entering an effective Hamiltonian.
In the phase representation

$$\hat{H}_J = -E_J \cos\Theta$$

According to quantum mechanics, the phase should be considered as an operator with eigenstates, $|\Theta\rangle$:

$$\hat{\Theta}|\Theta\rangle = \Theta|\Theta\rangle$$

The phase variable resembles the coordinate operator for a quantum particle.

What is the conjugate operator similar to the momentum operator?

$$|N\rangle = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} d\Theta\, e^{-iN\Theta} |\Theta\rangle \;\rightarrow\; |\Theta\rangle = \frac{1}{\sqrt{2\pi}} \sum_N e^{iN\Theta} |N\rangle$$

We have preserved the periodicity in the phase!

We can introduce operator $\hat{N}$, which is diagonal in the $|N\rangle$ -basis: $\hat{N}|N\rangle = N|N\rangle$.

Note that eigenvalues of the operator $\hat{N}$ are discrete! This operator has a meaning of the number of Cooper pairs

Quantum mechanics: Conjugated operators → $[\hat{\Theta}, \hat{N}] = i.$

In the N-representation

$$\hat{H}_J = -\frac{E_J}{2} \sum_N \left(|N\rangle\langle N+1| + |N+1\rangle\langle N| \right)$$

N has a meaning of the number of CPs passed through the junction.

Josephson effect is a coherent transfer of Cooper pairs!

In the phase representation $\hat{N} = -i\partial/\partial\Theta$

Single Cooper pair box: Parity Effect

How much we pay to transfer *N* electrons to the box?

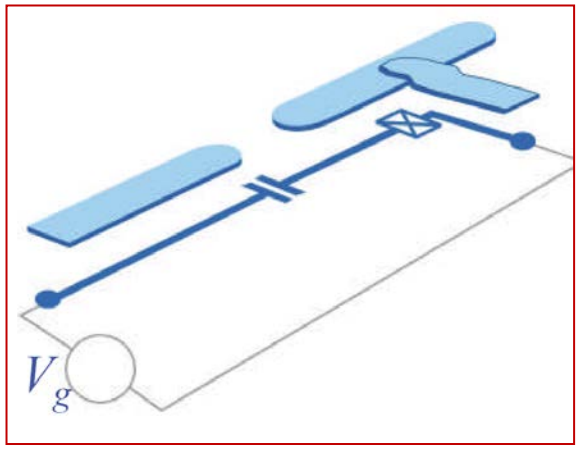
Coulomb energy: $E = \frac{Q^2}{2C} + QV_g, \quad Q = -eN$

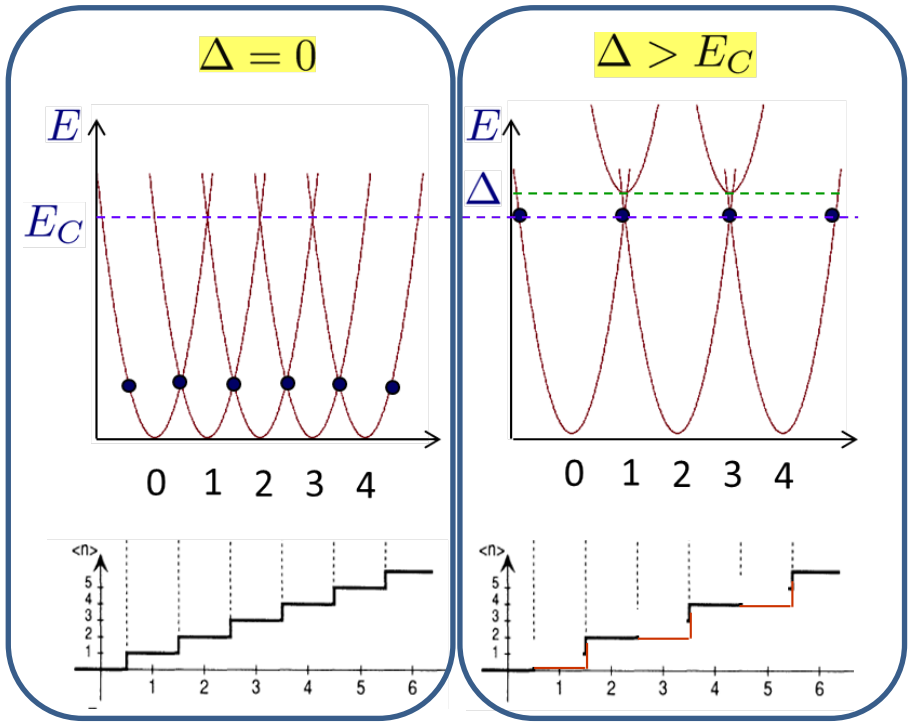
Parity effect:

$$E(N) = E_C(N - \alpha V_g)^2 + \Delta_N$$

$$\Delta_N = \begin{cases} 0, & N = 2n \\ \Delta, & N = 2n+1 \end{cases}$$

$$E_C = (2e)^2/2C, \ \Delta - \text{gap}$$





Coulomb blockage of electrons (SET)

Coulomb blockage of Cooper pairs Single-Cooper-Pair Box (SCPB)

At $\alpha V_g = (2n+1)$ ground state is degenerate with respect to addition of 1 CP.

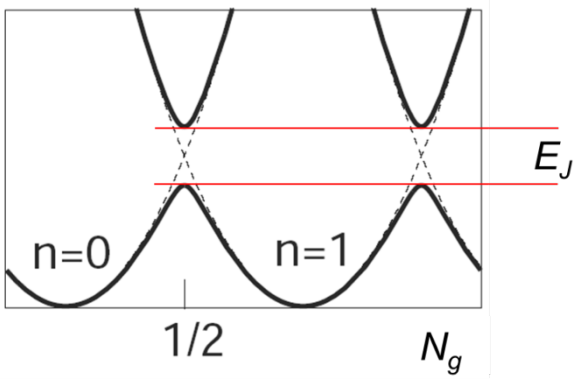
Classical Hamiltonian: $\mathcal{H} = E_C(N - N_g)^2 - E_J \cos\Theta, \quad N_g \equiv \alpha V_g$

Quantization: $N \to \hat{N} = -i\partial/\partial\Theta$

$$\mathcal{H} = E_C\left(-\frac{\partial}{\partial\Theta} - N_g\right)^2 - E_J\cos\Theta, \quad \Psi(\Theta) = \Psi(2\pi + \Theta)$$

Just like a Bloch electron in a periodic field! In general, its solution can be expressed through Mathieu functions.

Close to the degeneracy points, $|N_g - 1/2| \ll 1$, and $E_C \gg E_J$ we arrive at a two-level quantum systems behaving as an ½ quasi-spin.



Then the charge states *N=0* and *N=1* can be mapped on the spin states

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

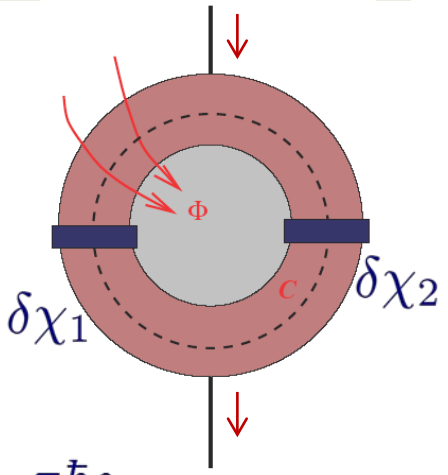
described by the effective Hamiltonian

$$H = -\frac{E_c}{2}(N - N_g)^2\,\hat{\sigma}_z - \frac{E_J}{2}\hat{\sigma}_x$$

At this stage we can control - by the gate voltage – only B_z, while B_x has a constant value set by the Josephson energy → No chance to realize quantum logics.

Solution: Josephson interferometer.

$$\vec{j} = e|\Psi|^2 \vec{v}_s, \quad \vec{v}_s = \frac{\hbar}{2m}\left(\nabla\chi - \frac{2e}{\hbar c}\vec{A}\right)$$ ← vector potential



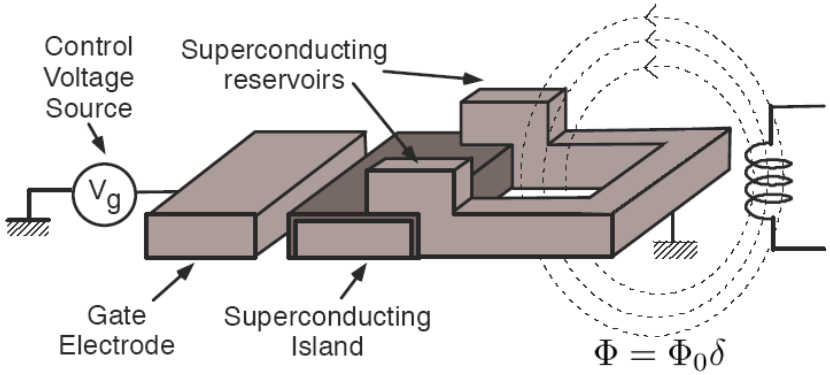
In the bulk: $\vec{j} = 0 \;\rightarrow\; 2\pi n - \frac{2e}{\hbar c}\oint \vec{A}\cdot d\vec{r} + \delta\chi_1 - \delta\chi_2 = 0$

$$\delta\chi_1 - \delta\chi_2 = -2\pi n + \pi\frac{\Phi}{\Phi_0}, \quad \Phi \equiv \oint \vec{A}\cdot d\vec{r}, \;\; \Phi_0 \equiv \frac{\pi\hbar c}{e}.$$

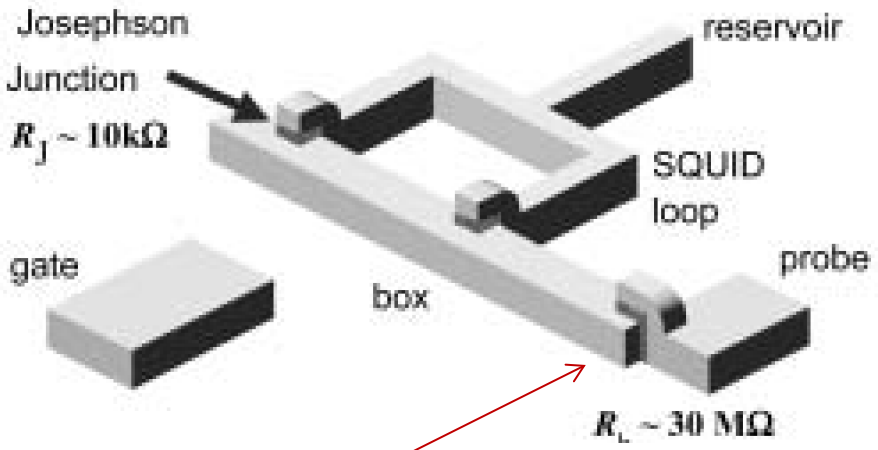
Total current: $$J = J_C \sin\delta\chi_1 + J_C \sin\delta\chi_2 = 2J_C \sin\frac{\delta\chi_1 - \delta\chi_1}{2}\cos\frac{\delta\chi_1 + \delta\chi_1}{2}$$

$$J_C^{\text{eff}} = 2E_J \cos\pi\frac{\Phi}{\Phi_0} \;\rightarrow\; E_J^{\text{eff}} = 2E_J\cos\pi\frac{\Phi}{\Phi_0}.$$

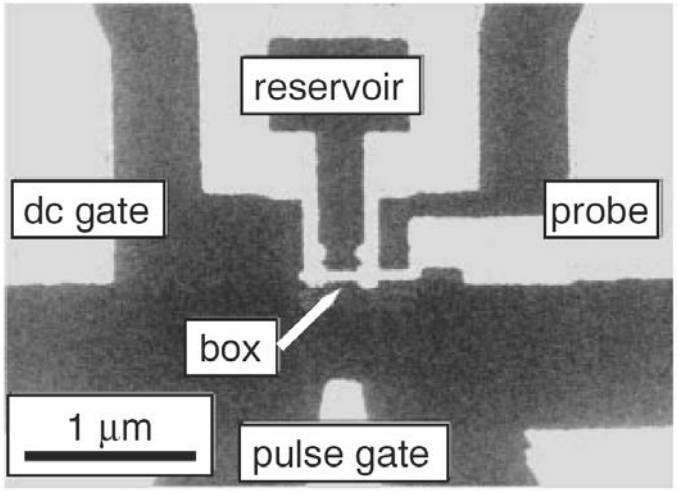
Realization: the split Cooper pair box



Charge qubit (prototype)



Experimental realization (Nakamura *et al.*, 1999)



SET electrometer measuring the state

The electrodes were fabricated by electron-beam lithography and shadow evaporation of Al on a SiN_x insulating layer (400-nm thick) above a gold ground plane (100-nm thick) on the oxidized Si substrate.

The `box' electrode is an Al strip containing 10^8 conduction electrons.

Since then qubits were substantially improved.

Optimizing qubit operation

Two crucial quantities: the anharmonicity and the charge dispersion of the energy levels.

Large anharmonicity is needed to prevent qubit operations from exciting other transitions in the system.

The charge dispersion describes the variation of the energy levels with respect to offset charge and gate voltage: the smaller the charge dispersion, the less the qubit frequency will change in response to gate charge fluctuations.

Both quantities are determined by the ratio E_J / E_C . Increasing this ratio reduces the energy level anharmonicity. However, it also decreases the overall charge dispersion and thus the sensitivity of the box to charge noise.

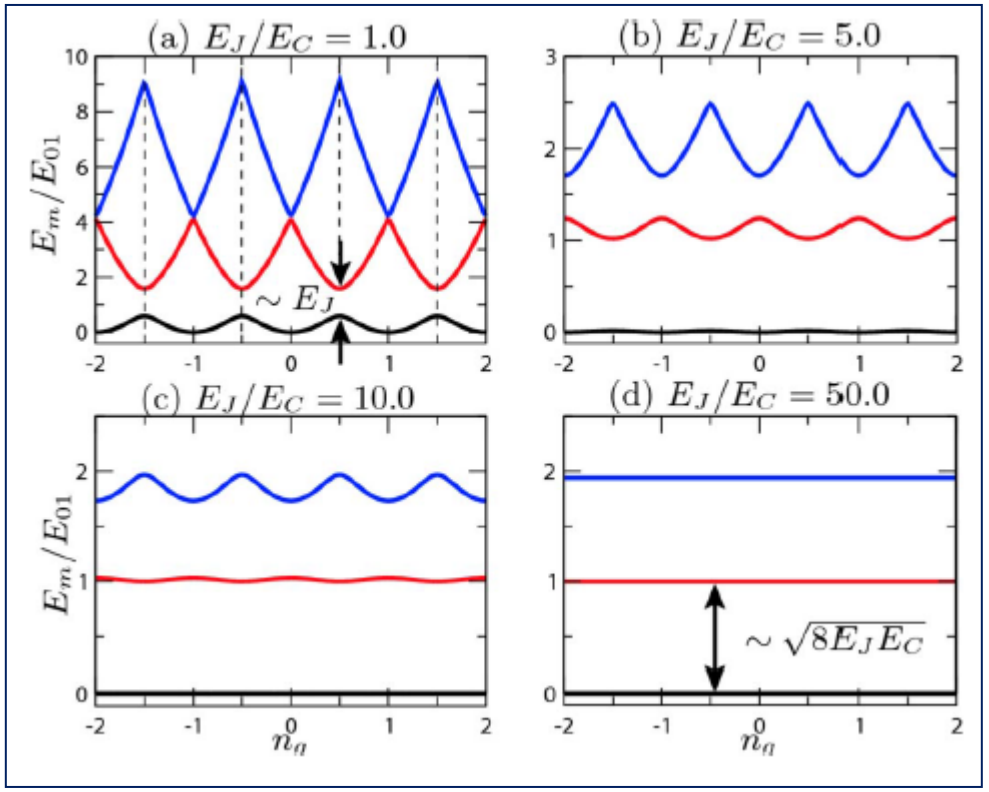
A trade-off is a “transmission-line shunted plasma oscillation qubit” (transmon) working at relatively large values of the ratio E_J / E_C (several tens up to several hundreds).

This eliminates the need for individual electrostatic gates and tuning to a charge sweet spot, and avoids the susceptibility to quasiparticle poisoning.

Transmon qubit: Adapted from PRA 76, 042319 (2007)

Main idea is to make the qubit insensitive to charge fluctuations by using the devices with large ratio E_J/E_C .

This is possible because the charge dispersion reduces *exponentially* in *this ratio*, while the anharmonicity only decreases *algebraically*.



$$\mathcal{H} = E_C \left(-\frac{\partial}{\partial \Theta} - N_g \right)^2 - E_J \cos \Theta$$

Eigenenergies first three levels, m =0,1,2 of the qubit Hamiltonian as a function of the effective offset charge for different ratios E_J/E_C.

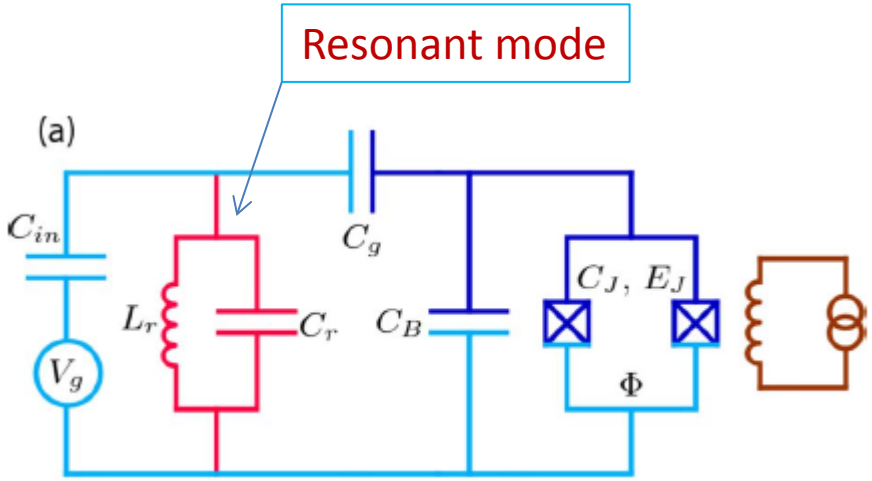
Energies are given in units of the transition energy E_{01}, evaluated at the degeneracy point. The zero point of energy is chosen as the bottom of the m=0 level.

Charge-insensitive qubit design derived from the Cooper pair box

Jens Koch,[1] Terri M. Yu,[1] Jay Gambetta,[1] A. A. Houck,[1] D. I. Schuster,[1] J. Majer,[1] Alexandre Blais,[2] M. H. Devoret,[1] S. M. Girvin,[1] and R. J. Schoelkopf[1]

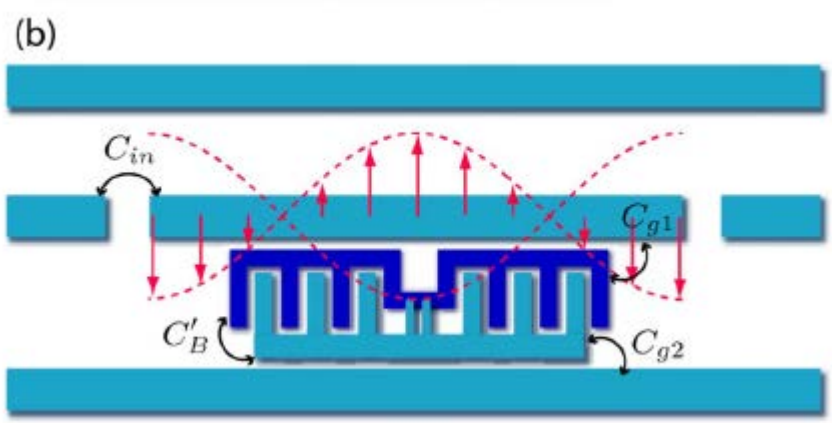
Main idea: Reduce charge noise sensitivity in the qubit while only sacrificing a small amount of anharmonicity.

Amazingly, the transmon can at the same time increase the strength of electrical coupling between qubits, or between a qubit and a transmission line cavity serving as a bus.



Effective circuit diagram of the transmon qubit.

The two Josephson junctions with capacitance and Josephson energy C_J and E_J are shunted by an additional large capacitance C_B, matched by a comparably large gate capacitance C_g.



Simplified schematic of the transmon device design not to scale.

It consists of a traditional split Cooper pair box, shunted by a short ($\lambda/20$)s ection of twin-lead transmission line, formed by extending the superconducting islands of the qubit. This short section of line can be well approximated as a lumped-element capacitor.

Qubit: $\hat{H} = E_C(-i\partial/\partial\Theta - N_g)^2 - E_J\cos\Theta, \quad E_C = \dfrac{e^2}{2(C_J + C_g + C_B)}$ To decrease E_C

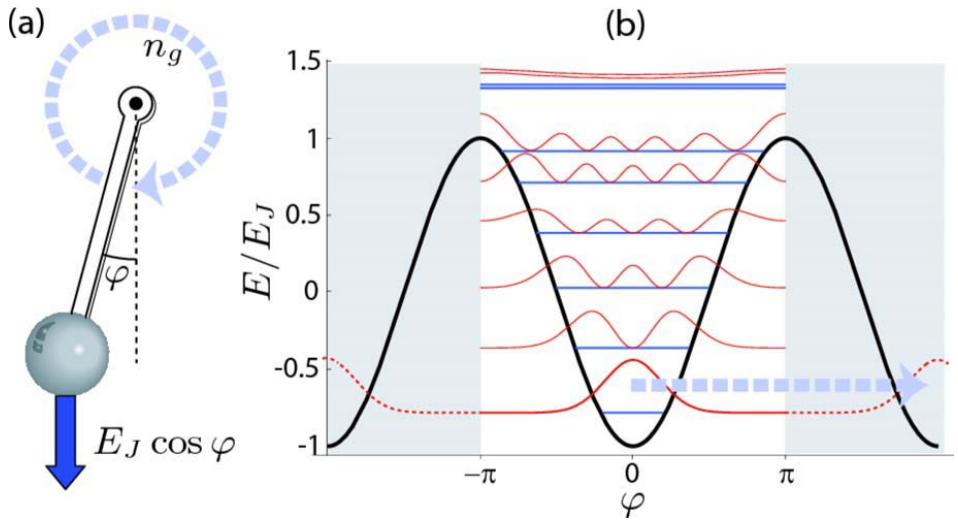
Exact solution in terms of Mathieu functions for 3 lowest levels are shown earlier.
Close to the degeneracy point

$$E_m(N_g) = E_m\left(\frac{1}{2}\right) - \frac{\epsilon_m}{2}\cos(\pi N_g), \quad \frac{\epsilon_m}{E_C} \sim \left(\frac{E_J}{2E_C}\right)^{m/2+3/2} e^{-\sqrt{8E_J/E_c}}$$

Rotor analogy for the transmon.

A charged quantum rotor in a constant magnetic field N_g. For large E_J/E_C there is a significant "gravitational" pull on the pendulum. Only tunneling events between adjacent cosine wells, i.e., a full 2π rotor movement will acquire an Aharonov-Bohm-type phase due to N_g.

The tunneling probability decreases exponentially with E_J/E_C, explaining the exponential decrease of the charge dispersion.



Cosine potential black solid line with corresponding eigenenergies and squared moduli of the eigenfunctions.

Rotor analogy for the transmon: Mapping

Cylindrical coordinates (r, φ, z) , motion in the plane $z = 0$.

Potential energy: $V = -mgl\cos\varphi$, kineti$\hat{L}_z^2/2ml^2 = -(\hbar^2/2ml^2)\,\partial^2/\partial\varphi^2$

$$\hat{H}_{\mathrm{rot}} = -\frac{\hbar^2}{2ml^2}\frac{\partial^2}{\partial\varphi^2} - mgl\cos\varphi$$

Mapping for $N_g = 0$: $\hat{n} \leftrightarrow \hat{L}_z/\hbar,\ E_J \leftrightarrow mgl,\ E_C \leftrightarrow \hbar^2/2ml^2$

Account of induced charge: magnetic field B_0 along z direction and electrical charge q of the tip.

$$\mathbf{p} \to q\mathbf{A} \Rightarrow L_z \to L_z - qB_0l^2/2$$

Thus the mapping is: $N_g \to qB_0l^2/2\hbar$

$\hat{n}$ has discrete eigenvalues, φ is a compact variable: $\psi(\varphi) = \psi(\varphi + 2\pi)$

At large E_J/E_C strong "gravitational" field favors small oscillations around $\varphi = 0$.
Perturbation theory leads to the Duffing oscillator.

Interestingly, the charge dispersion cannot be captured in a perturbative picture, since the presence of the "magnetic field" breaks the periodicity of the wave function in φ .

The effect of the offset charge N_g only enters through the rare event of a full 2π rotation, in which case the system picks up an Aharonov-Bohm-type phase.

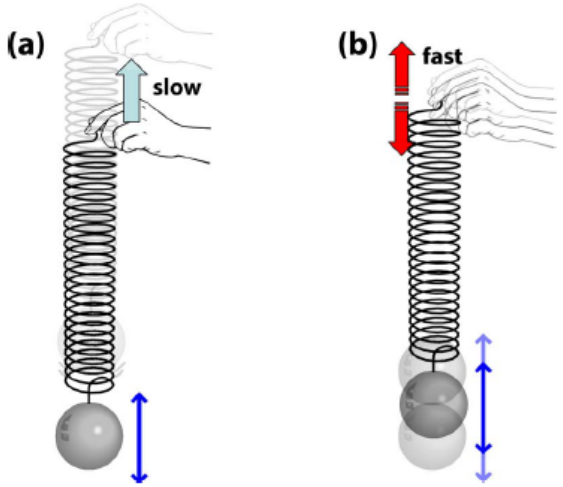
It is truly a nonperturbative quantum effect, which can be ascribed to the discreteness of charge or equivalently to the peculiar role of the vector potential in quantum mechanics leading to the Aharonov-Bohm effect.

How the transmon can be addressed?

Central message: Despite the exponentially decreasing charge dispersion for large E_J/E_C, the coupling between cavity and transmon, expressed by the coupling energies, does *not* become small but in fact even increases.

Even more: While the sensitivity of the transmon spectrum to the dc component of N_g *decreases* exponentially, the ac response to the oscillating cavity field *increases* in a power-law fashion.

For a slow adiabatic change in the suspension point of the almost harmonic oscillator, its mass is displaced but the frequency does not change.



For an ac drive at resonance, energy is forced into or extracted from the system.

Quantum mechanically, this leads to the coupling between the transmon and the cavity field.

Qubit operations are implemented by means of microwave pulses, readout corresponds to a measurement of the phase or amplitude of the transmitted radiation of a microwave drive field.

In fact, readout and control of the transmon work exactly the same way as for the CPB.

Circuit QED for the transmon

$$\beta \equiv C_g/C_\Sigma,\ V^0 \equiv \sqrt{\hbar\omega_r/C_r}$$

$$\hat{H} = 4E_c(\hat{n}-N_g)^2 - E_J\cos\hat{\varphi} + \hbar\omega_r\hat{a}^\dagger\hat{a} + 2\beta V^0\hat{n}(\hat{a}+\hat{a}^\dagger)$$

CPB basis:

$$\hbar g_{ij} = \hbar g_{ji}^* = 2\beta V^0\langle i|\hat{n}|j\rangle$$

$$\hat{H} = \hbar\sum_j \omega_j|j\rangle\langle j| + \hbar\omega_r\hat{a}^\dagger\hat{a} + \hbar\sum_{ij} g_{ij}|i\rangle\langle j|(\hat{a}+\hat{a}^\dagger)$$

Rotating wave approximation (eliminating terms describing the simultaneous excitation and de-excitation of both the transmon and the resonator) leads to essential simplification: $j = i+1$.

As a result one arrives at the effective Jaynes-Cummings Hamiltonian

$$\hat{H} = \hbar\sum_j \omega_j|j\rangle\langle j| + \hbar\omega_r\hat{a}^\dagger\hat{a} + \left(\hbar\sum_i g_{i,i+1}|i\rangle\langle i+1| + \text{h.c.}\right)$$

Dispersive limit: $\Delta_i \equiv |\omega_{i,i+1} - \omega_r| \gg g_{i,i+1}$

$$\hat{H} = \hbar \sum_j \omega_j |j\rangle\langle j| + \hbar\omega_r \hat{a}^\dagger \hat{a} + \left(\hbar \sum_i g_{i,i+1} |i\rangle\langle i+1| + \text{h.c.} \right)$$

allows analytical treatment.

Canonical transform:

$$\hat{H}_{\text{eff}} = \frac{\hbar\omega'_{01}}{2}\hat{\sigma}_z + (\hbar\omega'_r + \hbar\chi\hat{\sigma}_z)\hat{a}^\dagger\hat{a}$$

$$\omega_r \to \omega'_r = \omega_r - \chi_{12}/2, \qquad \chi \equiv \chi_{01} - \chi_{12}/2$$

$$\omega_{01} \to \omega'_{01} = \omega_{01} + \chi_{01} \qquad \chi_{ij} = g_{ij}^2/(\omega_{ij} - \omega_r)$$

Renormalized qubit frequency depends on the number of photons

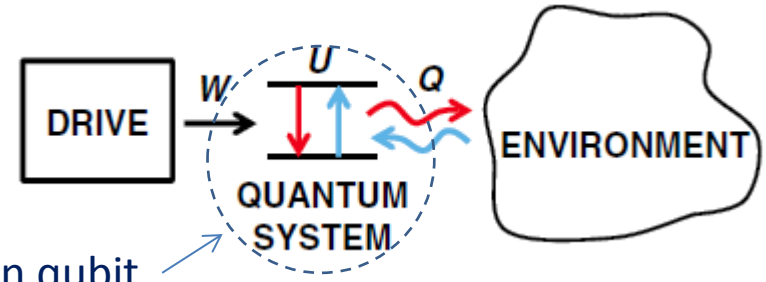
Since now we have prepared a coherent two-level system – one-half spin in controllable AC magnetic field –

$$\hat{H}(t) = -\frac{1}{2}B_z(t)\hat{\sigma}_z - \frac{1}{2}B_x(t)\hat{\sigma}_x$$

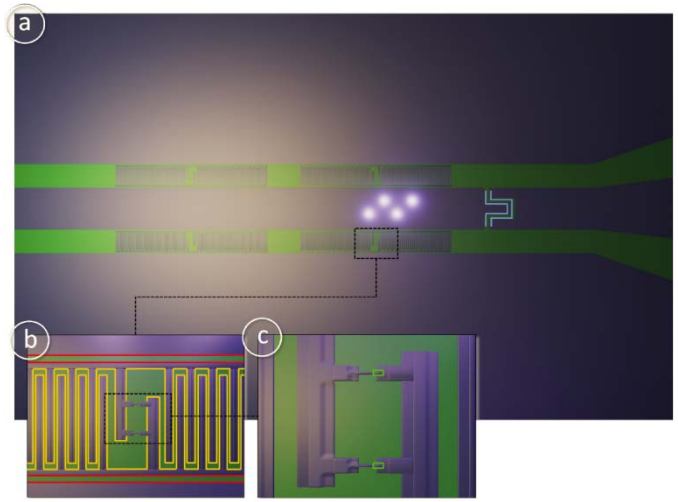
we return to our primary topic.

J. P. Pekola, Y. Masuyama, Y. Nakamura, J. Bergli, and YG, Phys. Rev. E**91**, 062109 (2015)

Driven quantum two-level system (TLS)



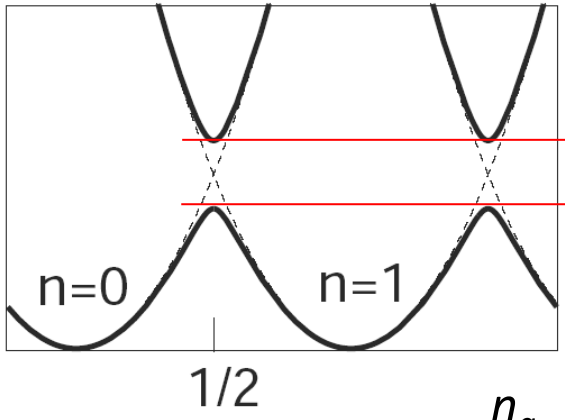
Transmon qubit



A **transmon** is a type of superconducting charge qubit that was designed to have reduced sensitivity to charge noise. Its name is an abbreviation of the term

transmission line shunted plasma oscillation qubit.

The transmon achieves its reduced sensitivity to charge noise by significantly increasing the ratio of the Josephson energy to the charging energy. This is accomplished through the use of a large shunting capacitor (a transmission line).



$$'_{CB} = 4E_C \sum_{n=-\infty}^{\infty} (\hat{n} + n_g)^2 |n\rangle\langle n| - \frac{E_J}{2} \sum_{n=-\infty}^{\infty} [|n+1\rangle\langle n| + |n\rangle\langle n+1|]$$

ing the transformation $\hat{n} \rightarrow -i\frac{d}{d\phi}$ the Hamiltonian takes the form of a
um rotor in phase space

$$\hat{H}_{SCB} = 4E_C(-i\frac{d}{d\phi} + n_g)^2 - E_J \cos\phi$$

Total work: $W = U + Q$

$U = E_f - E_i$ - "useful" work

Q - heat dissipated into environment

According to the Jarzynski equality (JE) for a cycle procedure, $\langle \exp(-\beta W) \rangle = 1$

A proposal to study fluctuation theorems was put forward as the so-called two-measurement protocol (TMP), where the state of the system is measured first before the work is applied, and second after the application of this work. This yields the difference *U* in the internal energy.

J. Kurchan, e-print cond-mat/0007360.
P. Talkner, E. Lutz, and P. Hänggi, Phys. Rev. E **75**, 050102(R) (2007).

For a closed system, *Q=0* and *W=U*. Therefore, $\langle \exp(-\beta U) \rangle = \langle \exp(-\beta W) \rangle = 1$
This is not the case for an open system where a TMP does not yield the total work *W*.

Q: Can we extract a useful information from the average $\langle \exp(-\beta U) \rangle$ for an open system?

We will analyze this issue using the so-called quantum jumps (QJ) method and show that the difference $\langle \exp(-\beta U) \rangle - \langle \exp(-\beta W) \rangle$ depends on the measurement protocol and on the amount and mechanism of decoherence in the system.

What we would like to check?

Total work: $W = U + Q$

$U = E_f - E_i$ - "useful" work

Q - heat dissipated into environment

According to the Jarzynski equality (JE) for a cycle procedure, $\langle \exp(-\beta W) \rangle = 1$

Q: How one can check the fluctuation theorems in a quantum system?

One of the approaches is the so-called two-measurement protocol (TMP), where the state of the system is measured first before the work is applied, and second after the application of this work. This yields the difference *U* in the internal energy, and one can study statistics of *U*.

J. Kurchan, e-print cond-mat/0007360.
P. Talkner, E. Lutz, and P. Hänggi, Phys. Rev. E **75**, 050102(R) (2007).

For a closed system, $Q=0$ and $W=U$. Therefore, $\langle \exp(-\beta U) \rangle = \langle \exp(-\beta W) \rangle = 1$
This is not the case for an open system where a TMP does not yield the total work *W*.

Q: Can one extract useful information from the difference $\langle \exp(-\beta U) \rangle - 1$ in an open system?

We need to allow for quantum stochastic dynamics. For that we employ so-called quantum jump (QJ) approach.

VOLUME 68, NUMBER 5 PHYSICAL REVIEW LETTERS 3 FEBRUARY 1992

Wave-Function Approach to Dissipative Processes in Quantum Optics

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(Received 15 October 1991)

A novel treatment of dissipation of energy from a "small" quantum system to a reservoir is presented. We replace the usual master equation for the small-system density matrix by a wave function evolution including a stochastic element. This wave-function approach provides new insight and it allows calculations on problems which would otherwise be exceedingly complicated. The approach is applied here to a two- or three-level atom coupled to a laser field and to the vacuum modes of the quantized electromagnetic field.

Application to statistics of work in a driven TLS:

PRL 111, 093602 (2013) PHYSICAL REVIEW LETTERS week ending 30 AUGUST 2013

Quantum Jump Approach for Work and Dissipation in a Two-Level System

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(Received 22 May 2013; published 27 August 2013)

Qubit evolution

QJ method:

It is assumed that we are able to register the acts of photon (or phonon) emission or absorption. After that we know for sure in which state, ground |*g*> or excited |*e*>, the system is.

Even if there is no jump during some time interval, a possibility for such a jump must be taken into account. This is done constructing an effective non-Hermitian Hamiltonian, *H*.

It has been shown that during the small non-jump time interval Δt the wave function evolves according to the Schrödinger-like equation

Non-Hermitian

$$|\psi(t+\Delta t)\rangle = (1-p)^{-1/2}\left(1-\frac{i}{\hbar}H\Delta t\right)|\psi(t)\rangle$$

where $|\psi(t)\rangle = a(t)|g\rangle + b(t)|e\rangle,\ p = (\Gamma_\uparrow|a|^2 + \Gamma_\downarrow|b|^2)\Delta t,\ \Gamma_{\downarrow,\uparrow}$ are the relaxation (excitation) rates, $\Gamma_\uparrow = e^{-\beta\hbar\omega_0}\Gamma_\downarrow$, $\hbar\omega_0$ is the level spacing of the qubit.

These rates determine the probabilities of interrupting the evolution, $p_\uparrow = \Gamma_\uparrow|a|^2\Delta t$ and $p_\downarrow = \Gamma_\downarrow|b|^2\Delta t$ during the time Δt .

Hamiltonian:

$$H = H_0 + \delta H + V + N$$

$\delta\omega(t)$ - classical stochastic process.

$$H_0 = (\hbar\omega_0/2)(|e\rangle\langle e| - |g\rangle\langle g|) \quad \text{- TLS}$$

$$\delta H = (\hbar\delta\omega/2)(|e\rangle\langle e| - |g\rangle\langle g|) \quad \text{- Noise}$$

$$V = \lambda(t)(|g\rangle\langle e| + |e\rangle\langle g|) \quad \text{- Drive}$$

$$N = -(i\hbar/2)(\Gamma_\downarrow|e\rangle\langle e| + \Gamma_\uparrow|g\rangle\langle g|) \quad \text{- Non-Hermitian}$$

In the interaction picture, representing the wave function as $|\psi_I(t)\rangle = a|g\rangle + b|e\rangle$ we express the dissipative "Schrödinger equation" as a set of equations for the amplitudes

$$\dot{a} = -\frac{i}{\hbar}\lambda(t)e^{-i\omega_0 t}b + i\frac{\delta\omega}{2}a + \frac{\Delta\Gamma}{2}a|b|^2,$$

$$\dot{b} = -\frac{i}{\hbar}\lambda(t)e^{i\omega_0 t}a - i\frac{\delta\omega}{2}b - \frac{\Delta\Gamma}{2}|a|^2 b.$$

$$\Delta\Gamma \equiv \Gamma_\downarrow - \Gamma_\uparrow$$

A jump resets the TLS to its ground or excited state.

It has been shown that the above scheme (for $\Gamma\Delta t \ll 1$) is fully equivalent to the Bloch-Redfield equations for the density matrix of the system.

Thermodynamics

Long interval between measurements, $\Gamma_{\downarrow\uparrow}\tau \gg 1$:

$$\langle e^{-\beta U}\rangle = p_g^i\, p_{g|g}^f\, e^0 + p_g^i\, p_{e|g}^f\, e^{-\beta\hbar\omega_0} + p_e^i\, p_{g|e}^f\, e^{\beta\hbar\omega_0} + p_e^i\, p_{e|e}^f\, e^0.$$

Populations are thermally distributed:

$$p_g^i = 1 - p_e^i = p_{g|g,e}^f = 1 - p_{e|g,e}^f = (1 + e^{-\beta\hbar\omega_0})^{-1}$$

$$\downarrow$$

$$\langle e^{-\beta U}\rangle - \langle e^{-\beta W}\rangle = \tanh^2(\beta\hbar\omega_0/2)$$

- The difference does not depend on the decoherence and characteristics of the TLS.
- At low temperatures, dissipation into environment is important. This result holds for any driving protocol between the two measurements.

Our aim is to evaluate and compare the averages $\langle e^{-\beta W}\rangle$ and $\langle e^{-\beta U}\rangle$ for the case of weak dissipation, $\Gamma_{\downarrow\uparrow}\tau \ll 1$, where τ is the time between the measurements.

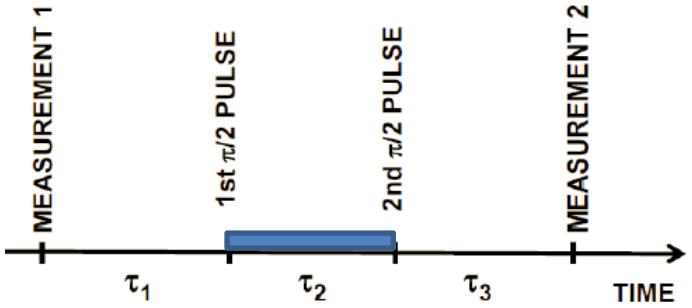
Small dissipation limit – at most one quantum jump (excitation or relaxation event) between measurements.

$$\langle e^{-\beta W}\rangle = P_0\langle e^{-\beta W}\rangle_0 + P_1\langle e^{-\beta W}\rangle_1$$

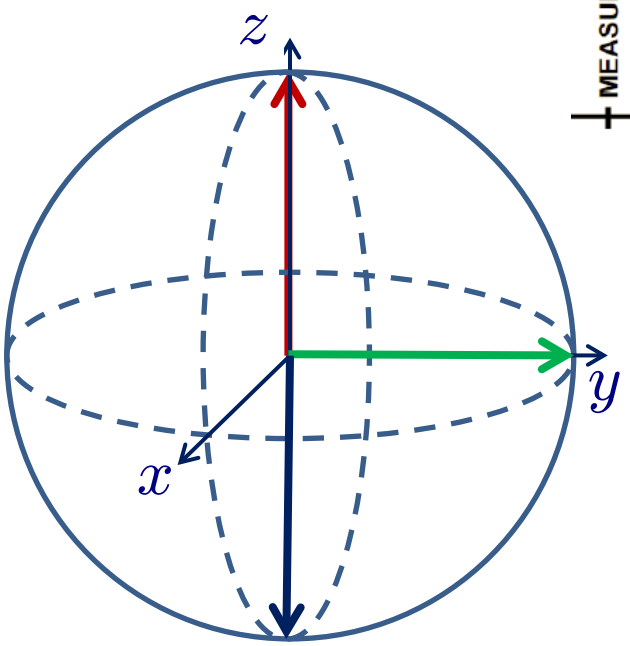
P_0, P_1 are the probabilities of zero- and one-photon processes, respectively

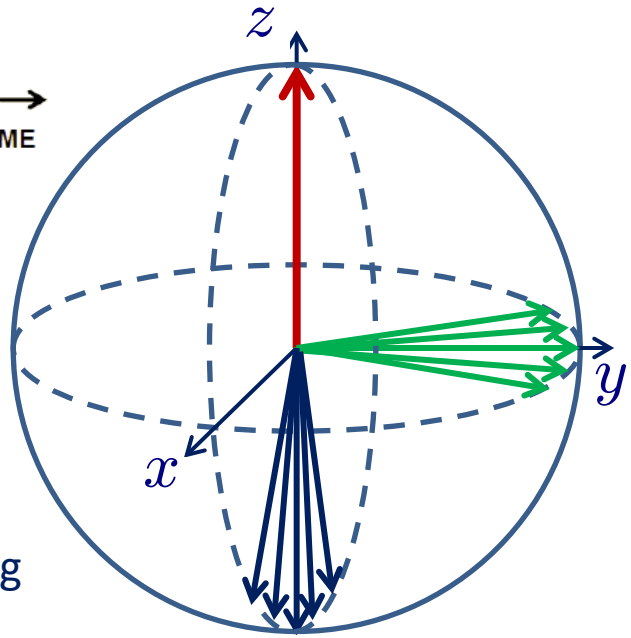
In a TMP we measure $\langle e^{-\beta U}\rangle = P_0\langle e^{-\beta U}\rangle_0 + P_1\langle e^{-\beta U}\rangle_1$ and for the zero-photon process $W=U$.

We choose the following protocol:



Dephasing



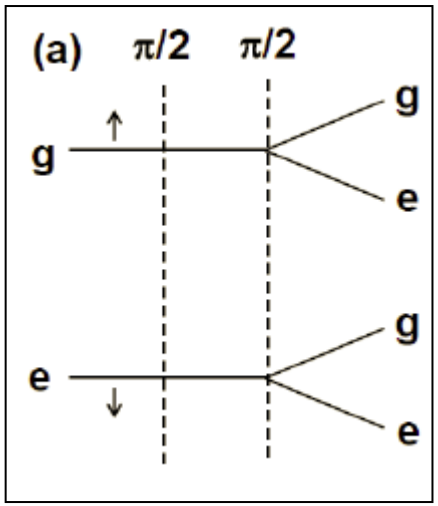


With dephasing

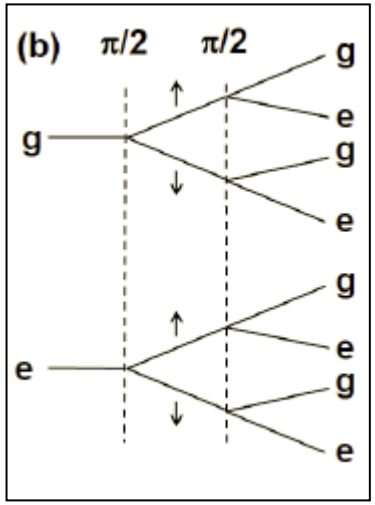
Sketch of derivation for low dissipation

For the selected protocol, we calculate evolution of amplitudes taking into account the trajectories involving 0 and 1 jumps.

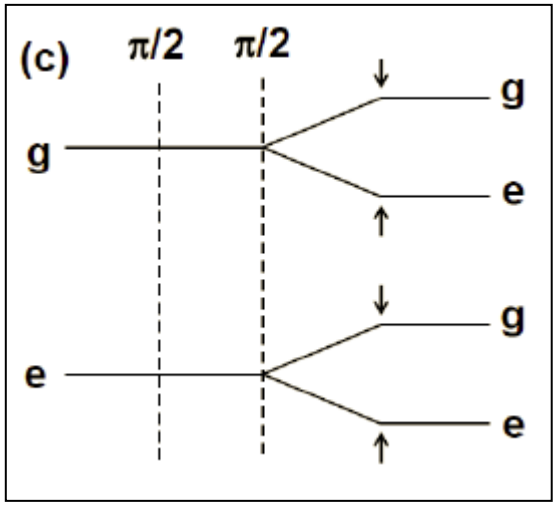
Single-jump configurations (contribute to $P_1 \langle \cdots \rangle_1$)



$0 < t_j < \tau_1$



$\tau_1 < t_j < \tau_1 + \tau_2$



$\tau_1 + \tau_2 < t < \tau_1 + \tau_2 + \tau_3$

Knowing the amplitudes we evaluate the probabilities of different trajectories and then calculate the thermal averages up to the first order in Γ's.

(Algebra is simple, but rather tedious)

Results:

(1) $$\langle e^{-\beta W}\rangle_{\delta\omega} \equiv P_0\langle e^{-\beta W}\rangle_0 + \sum_{i=a,b,c} P_{1,i}\langle e^{-\beta W}\rangle_{1,i} = 1$$

Sequences of pulses and jumps (diagram)

for a given realization of δω . That proves the JE is valid for any distribution of δω.

(2) $$\langle e^{-\beta U}\rangle_{\delta\omega} = 1 + [\tau_3 - \tau_1\cos(\delta\varphi_2)]\,\Gamma_\Sigma \coth^2(\beta\hbar\omega_0/2).$$

$$\delta\varphi_2 \equiv \int_{\tau_1}^{\tau_1+\tau_2} \delta\omega(t)\,dt \qquad \Gamma_\Sigma = \Gamma_\uparrow + \Gamma_\downarrow$$

Averaging over the stochastic processes $\delta\omega(t)$ we get:

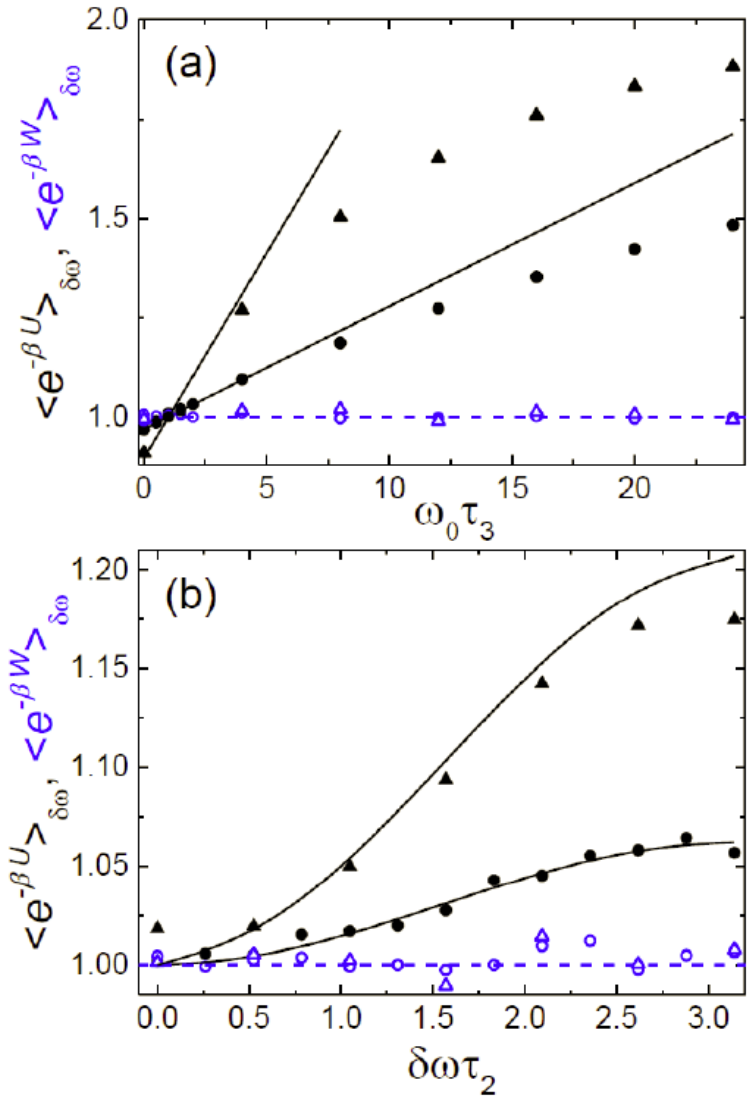
$$\langle e^{-\beta U}\rangle = 1 + [\tau_3 - \tau_1\langle\cos(\delta\varphi_2)\rangle]\,\Gamma_\Sigma \coth^2(\beta\hbar\omega_0/2).$$

Depends on the dephasing rate

$$\langle e^{-\beta U}\rangle - \langle e^{-\beta W}\rangle = [\tau_3 - \tau_1\langle\cos(\delta\varphi_2)\rangle]\,\Gamma_\Sigma \coth^2(\beta\hbar\omega_0/2)$$

Our central result

Analytic expressions compared to numerical results obtained by stochastic simulations



$$\beta\hbar\omega_0 = 5,\ \frac{\Gamma_\downarrow}{\hbar\omega_0} = \begin{cases} 0.03\ \text{(circles)} \\ 0.1\ \text{(triangles)} \end{cases}$$

(a) - $\omega_0\tau_1 = \omega_0\tau_2 = 1,\ \delta\omega = 0$

Open symbols refer to $\left\langle e^{-\beta W}\right\rangle_{\delta\omega}$, while the filled ones – to $\left\langle e^{-\beta U}\right\rangle_{\delta\omega}$. The solid lines represent the analytic predictions.

(b) - $\left\langle e^{-\beta U}\right\rangle_{\delta\omega}$ is plotted for

$$\omega_0\tau_1 = \omega_0\tau_2 = \omega_0\tau_3 = 1$$

versus $\delta\varphi_2 \equiv \delta\omega\tau_2$ (solid lines and filled symbols). The results for $\left\langle e^{-\beta W}\right\rangle_{\delta\omega}$ indicated by the corresponding open symbols, are again concentrated around unity.

In all cases we employed 10^7 repetitions of the protocol for each data point.

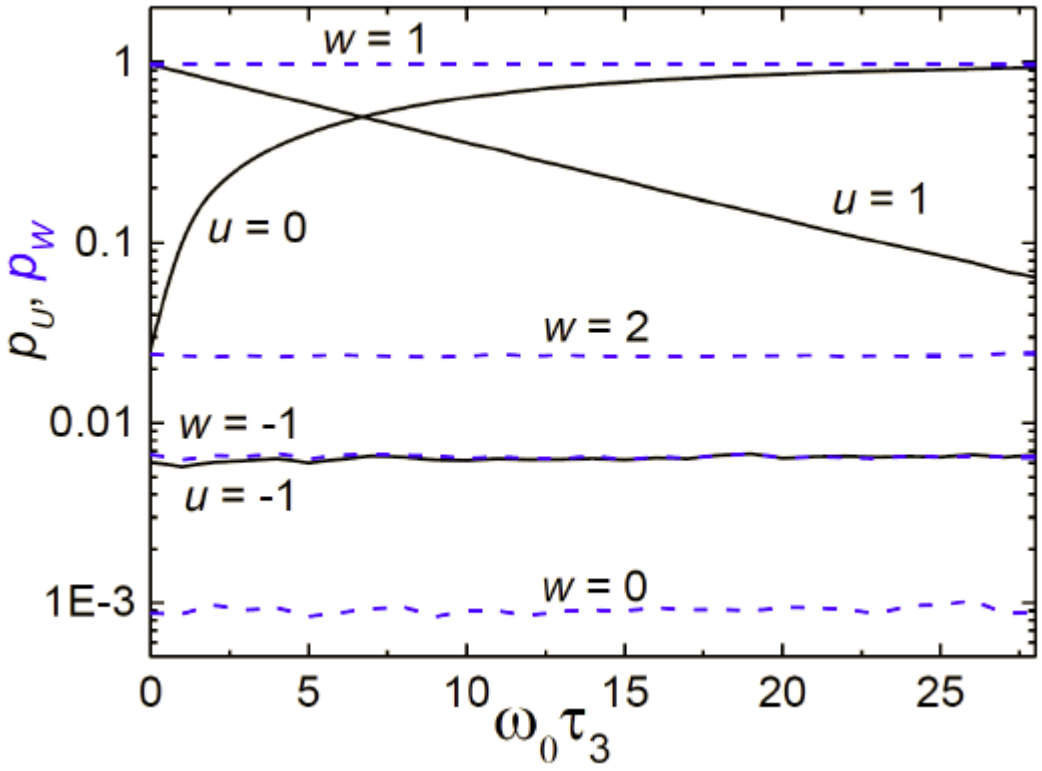


FIG. 3. Probabilities of different possible outcomes of $u \equiv U/\hbar\omega_0$ and $w \equiv W/\hbar\omega_0$. We assume the same protocol as before with $\beta\hbar\omega_0 = 5$, $\Gamma_\downarrow/\hbar\omega_0 = 0.1$, $\delta\omega = 0$, and $\omega_0\tau_1 = \omega_0\tau_2 = 1$. We vary the delay time of the second measurement, τ_3. The solid lines refer to U and the dashed ones to W. We employed $3{\cdot}10^5$ repetitions of the protocol for each data point.

Discussion & Explanations

Firstly, the probabilities $p_U(U)$ relax with time $\tau_3$since *U* measures the internal energy which changes after the non-equilibrium driving.

On the contrary, the waiting period τ_3 does not influence $p_W(W)$ since there is no work done after the second rotation pulse.

These dependences are consistent with our basic expectations.

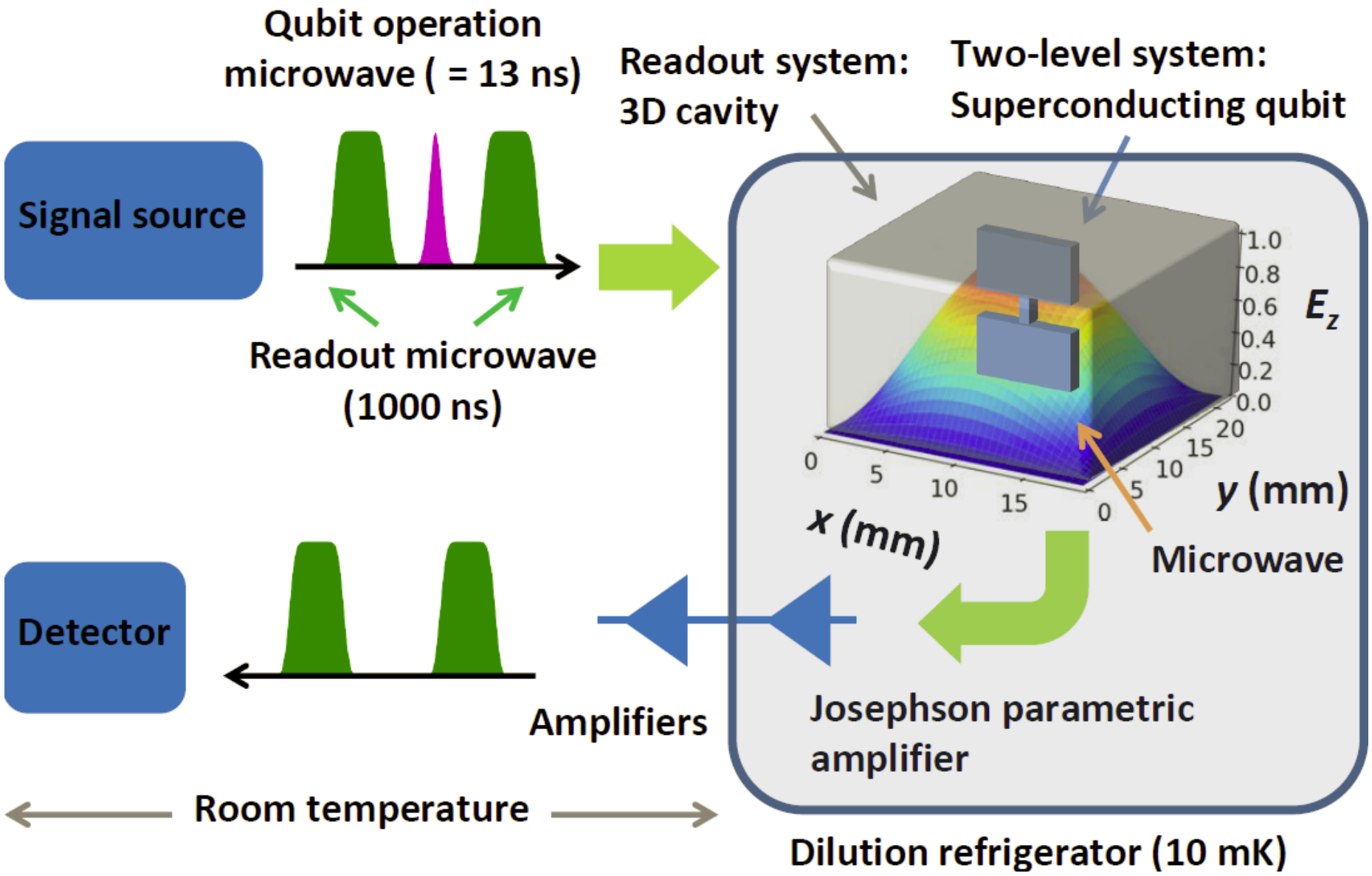
Finally, we also recover the important Crooks fluctuation relation for work in the form

$$\frac{p_W(W)}{p_W(-W)} = e^{\beta W}$$

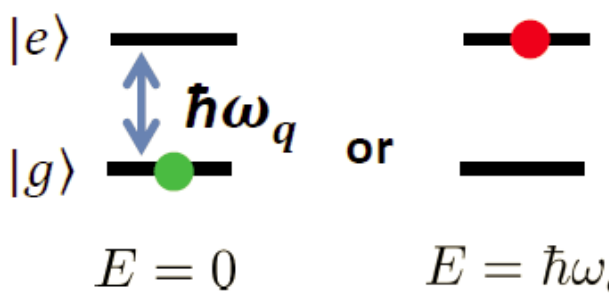
for those values of work that are within the reach in this situation (for $W/\hbar\omega_0 = \pm 1$).

On the contrary, the ratio $p_U(U)/p_U(-U)$ is not constant in τ_3 and thus does not satisfy a fluctuation relation.

Experiment (Y. Nakamura and Y. Masuyama, in progress)



Two level system: superconducting qubit



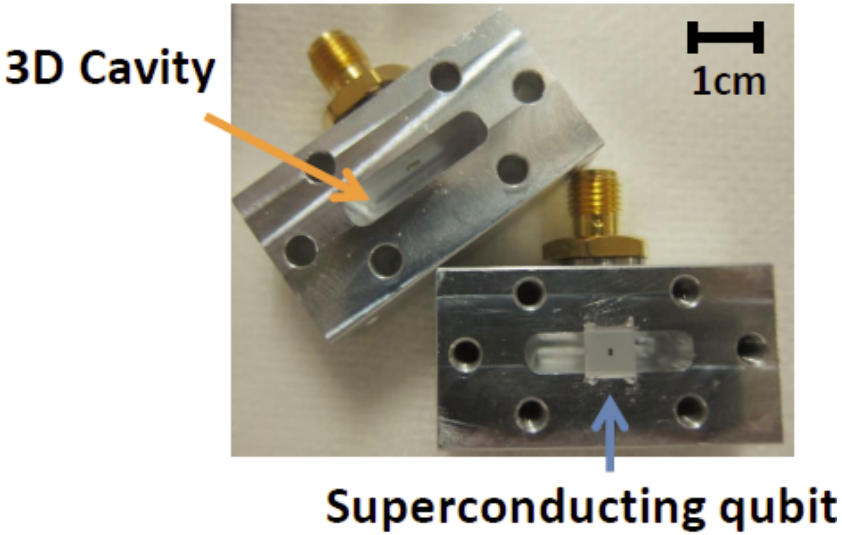
The state of superconducting qubit is measured via 3D cavity.

Free energy difference: $\Delta F = 0$

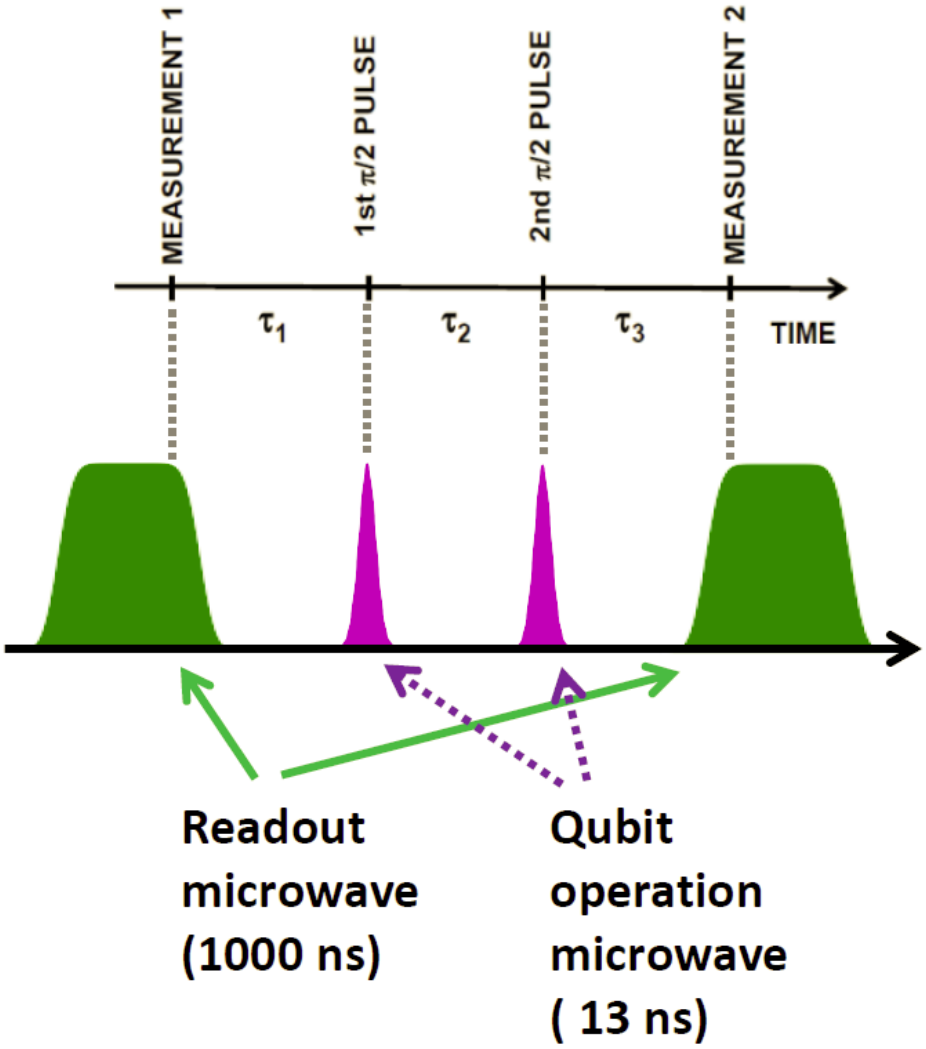
Population of 1st meas.
→Temp. of system
(≈ 100 mK)

Parameters

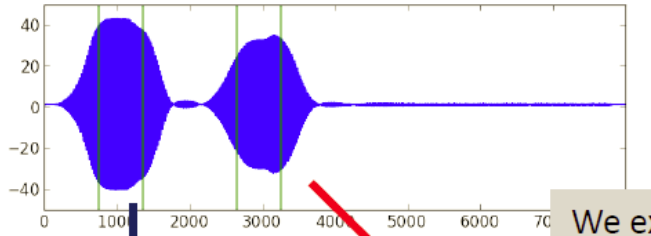
Readout frequency	10.9213 GHz
Qubit frequency	6.7159 GHz
T_1	24.0 μs
T_2^*	4.3 μs
T_2 echo	5.3 μs



Two-point measurement protocol



Readout microwave signal
(Cumulated number : 10000)

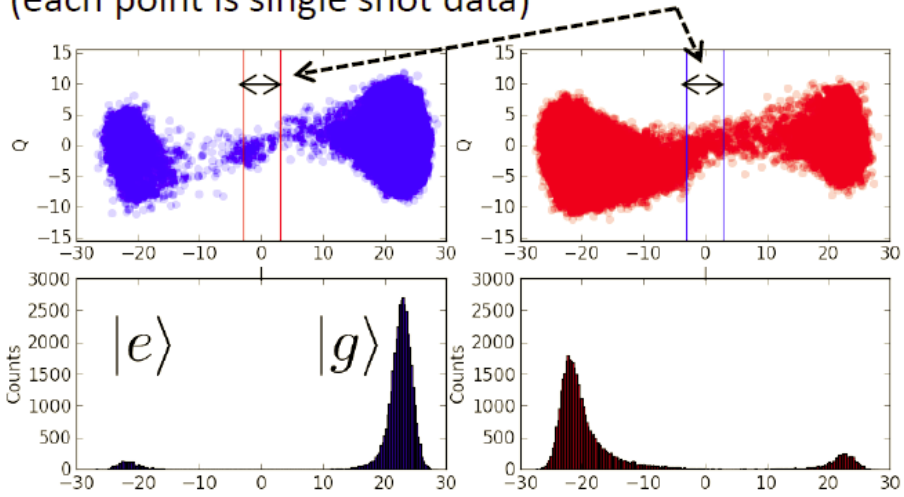


τ_1 = 600 ns
τ_2 = 50 ns
τ_3 = 100 ns

1st RO **2nd RO**

We exclude the data in this region (due to readout error). The counts are small.

Complex amplitude distribution
(each point is single shot data)



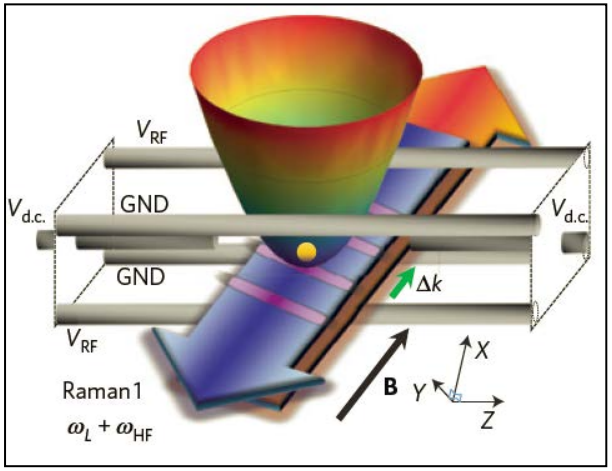
Distinguish $|e\rangle$ and $|g\rangle$

Projection measurement of the qubit

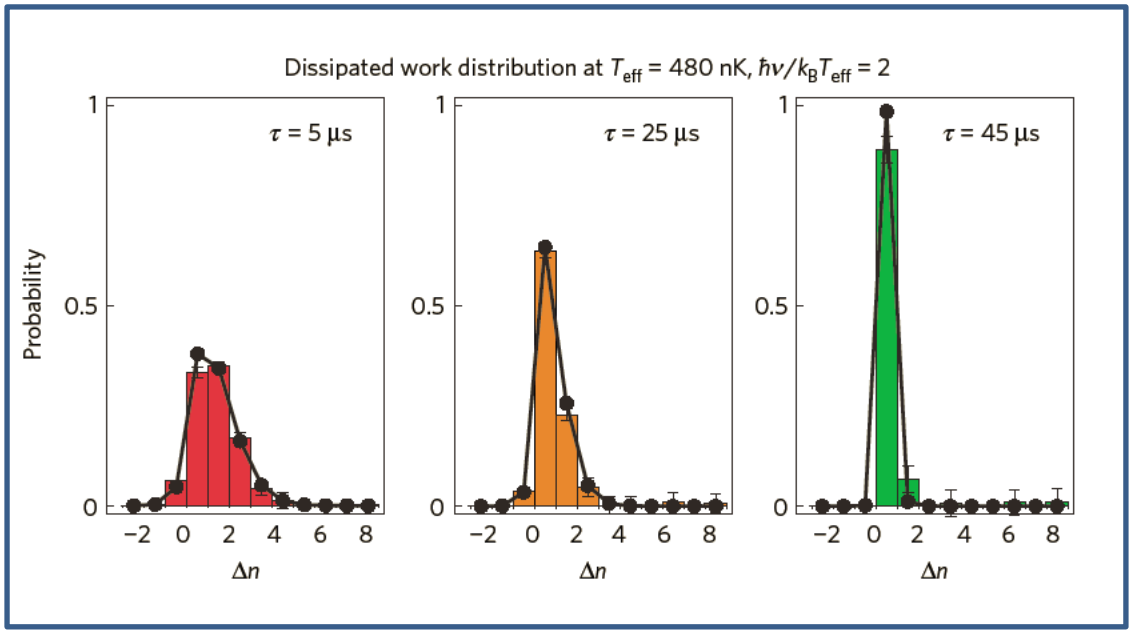
nature physics Vol. 11, 194 (2015) ARTICLES
PUBLISHED ONLINE: 22 DECEMBER 2014 | DOI: 10.1038/NPHYS3197

Experimental test of the quantum Jarzynski equality with a trapped-ion system

Shuoming An[1], Jing-Ning Zhang[1], Mark Um[1], Dingshun Lv[1], Yao Lu[1], Junhua Zhang[1], Zhang-Qi Yin[1], H. T. Quan[2,3]* and Kihwan Kim[1]*



The counter propagating laser beams drive transitions between states in the $^{171}Yb^{+}$ ion



The distribution function of the (dissipated) works is obtained using the two-measurement protocol similar to the one considered here.

Intermediate summary (for the "quantum" part)

- TMP turns out to be an independent tool for studying thermodynamic relations in driven systems.

- The central result is the relationship

$$\Delta \equiv \langle e^{-\beta U} \rangle - 1 = \left[\tau_3 - \tau_1 \langle \cos(\delta\varphi_2) \rangle \right] \Gamma_\Sigma \coth^2 \left(\frac{\beta\hbar\omega_0}{2} \right).$$

✓ If the system is well characterized and the r.h.s. is known , then JE can be checked only by measuring the values of the internal energy.

✓ Contrary, determining the Δ versus times τ_i from experiment (say, via registering of absorber or emitted photons) one can judge on the underlying dephasing mechanism from the relation

$$\langle \cos(\delta\varphi_2) \rangle = \frac{\tau_3}{\tau_1} \left[1 - \left(\frac{\partial \ln \Delta}{\partial \ln \tau_3} \right)^{-1} \right]$$

✓ If both sides are measured independently the protocol can be used as a primary thermometer for the quantum system

How it can be done?

$$\Delta \equiv \langle e^{-\beta U} \rangle - 1 = [\tau_3 - \tau_1 \langle \cos(\delta\varphi_2) \rangle] \, \Gamma_\Sigma \coth^2 \left(\frac{\beta\hbar\omega_0}{2} \right).$$

Measured
(statistics of *U*)

Measured
(Ramsey protocol)

Measured
(spectroscopy)

The only adjustable parameter is β.

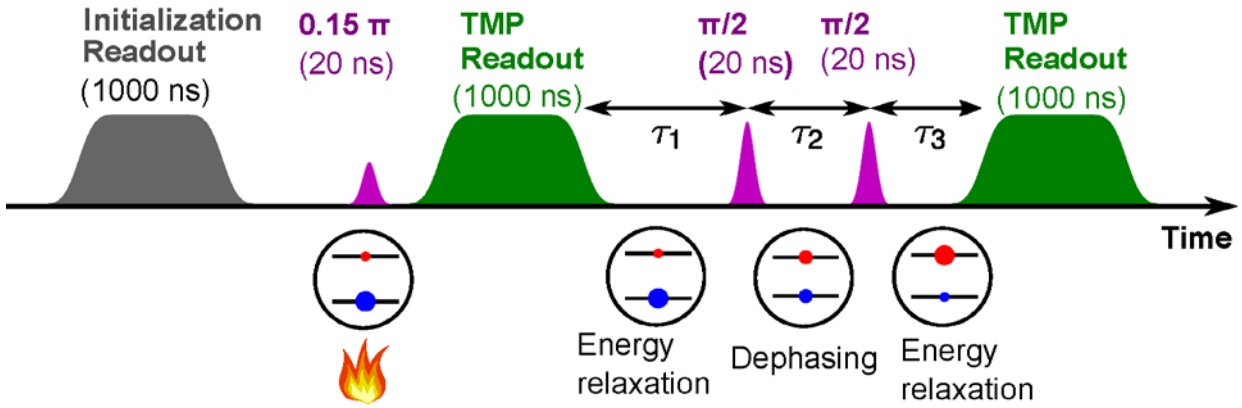
Problem:

In a realistic situation the temperature is unknown because the final temperature may be higher than the initial one due to heating by the measurement and rotating pulses.

↓

one has to check whether the “r.h.s.” temperature is the same as the “l.h.s.” one

To match the temperatures we utilize a protocol shown below



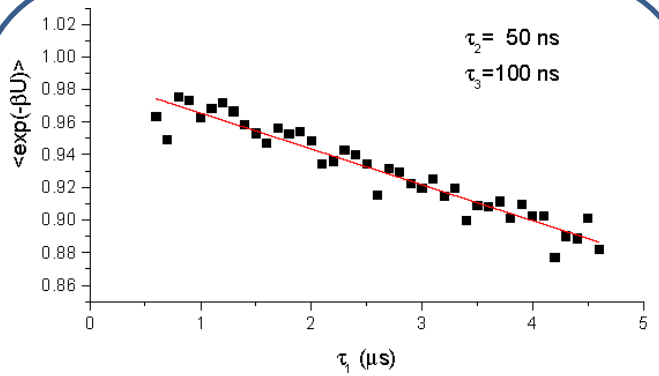
The qubit is first initialized by measurement and pre-selection of the ground state.

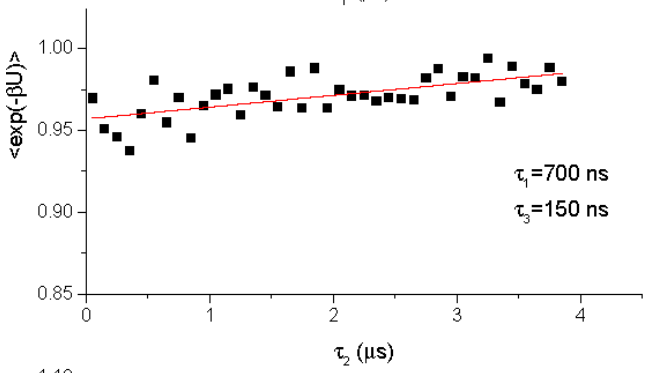
Then the qubit is excited by a pulse with duration providing rotation of the qubit by the angle θ around x-axis. After that a second readout is performed. This readout serves as a beginning of a TMP.

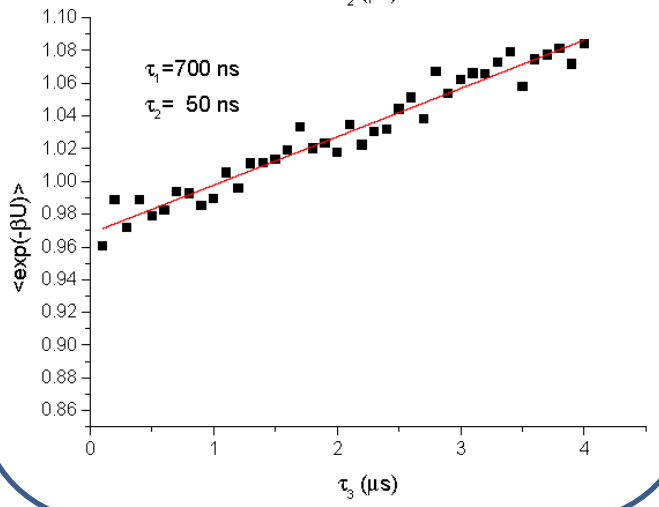
The exponential average $\langle e^{-\beta_i U} \rangle$ is calculated using an effective temperature related to the rotation angle produced by the first (preheating) pulse as

$$\Theta_i \equiv \frac{1}{k_B \beta_i} = \frac{\hbar \omega_0}{2 \ln(\cot \theta/2)}$$

The l.h.s. temperature can be independently evaluated from the statistics of the 1st readout starting TMP.







The pulse duration is chosen to get $\langle e^{-\beta_i U} \rangle \to 1$ at $\tau_i \to 0$.

In this limit the system is effectively closed and there is no difference between the internal energy change *U* and work *W*.

Hence, if the Jarzynski equation is fulfilled for $\beta_i = \beta$ then $\frac{1}{k_B \beta}$ is the qubit temperature. Therefore the qubit works as a primary thermometer.

The best fit for our experimental setup corresponds to $\theta = 0.15\pi$. is equivalent to the initial qubit temperature of 112 mK while statistics of the read-outs provides 117 mK.

This work is in progress – there exist unanswered questions regarding fidelity of the experimental procedure.

Conclusion to the third block

By analysis of the exponential average $\langle e^{-\beta U} \rangle$ for a controlled transmon qubit we have confirmed the energy fluctuation relation for this quantum system.

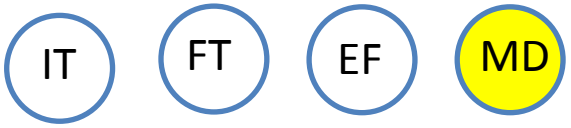
$$\Delta \equiv \langle e^{-\beta U} \rangle - 1 = [\tau_3 - \tau_1 \langle \cos(\delta\varphi_2) \rangle] \, \Gamma_\Sigma \coth^2 \left(\frac{\beta \hbar \omega_0}{2} \right).$$

This could be achieved by the known two-measurement protocol by a proper excitation of the qubit using a resonant pulse. The duration of this pulse and its intensity were chosen to preheat a qubit to a temperature equal to that of the final state.

Thus the measurement provides a fast thermometer of the environment.

Fitting of the τ_2-dependence of $\langle e^{-\beta U} \rangle$ evidences exponential relaxation $\propto e^{-t/\tau_\varphi}$ with $\tau_\varphi = 21\ \mu$s. This value is close to one obtained from qubit dynamics.

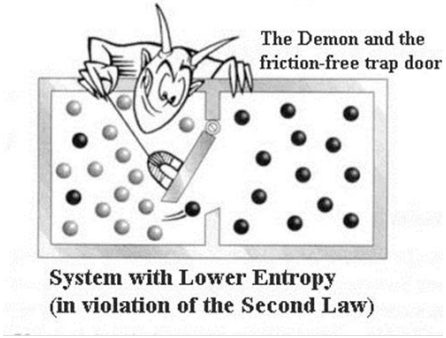
Block # 4



4. Maxwell's demon devices
   - Second law of thermodynamics and Maxwell's demon (MD)
   - The Szilard engine: Realization with a single electron
   - Optimal protocol for a given extracted power
   - Role of measurement errors

More detailed plan

J. C. Maxwell (1831-1879)



Maxwell's demon (1867-)

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

Second law of thermodynamics

The second law in Clausius's version states: "It is impossible to devise an engine which, working in a cycle, shall produce no effect other than the transfer of heat from a colder to a hotter body."

Entropy formulation: "In any cyclic process the total entropy of the physical systems involved in the process will either increase or remain the same."

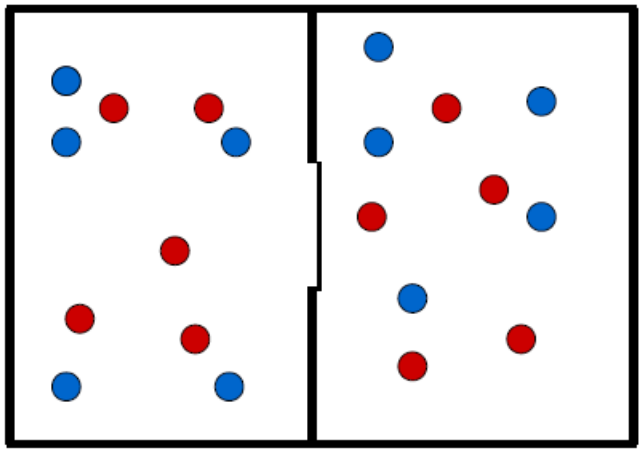
Maxwell devised his demon in a thought experiment to demonstrate that the second law is only a statistical principle that holds *almost* all the time, and not an absolute law set in stone.

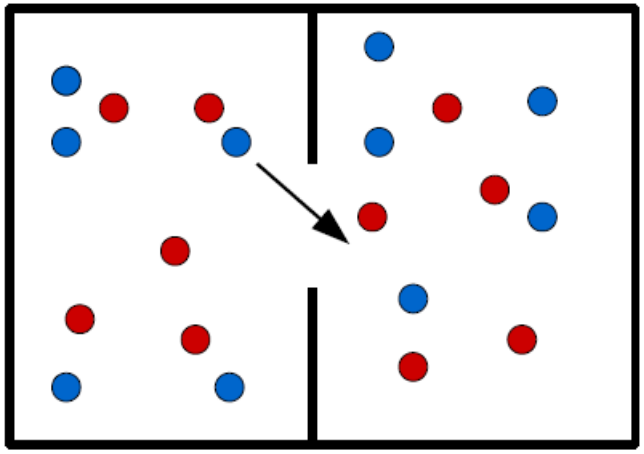
Entropy is, in thermodynamics, a state variable S whose change is defined as $\delta S = \delta Q/T$ for a reversible process at temperature T, where δQ is the heat absorbed. Thus, what the demon attempts to do is to decrease the entropy of the whole system for the cyclic process.

Maxwell's thought experiment

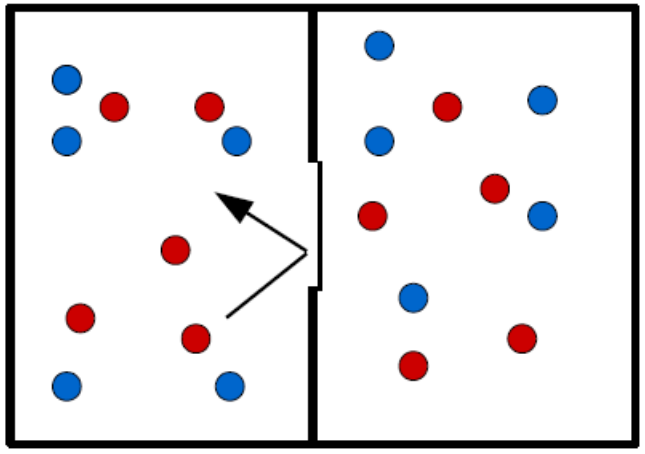
We have a container with gas. The container is divided in two parts by a wall with a small door that can be opened and closed.

In a gas the molecules move with different velocities, the average is given by the temperature. Let us make it simple and imagine that there are some which are fast (●) and some which are slow (●).

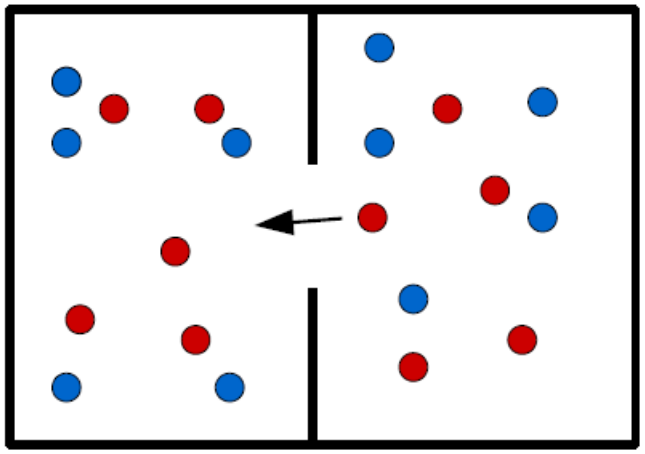


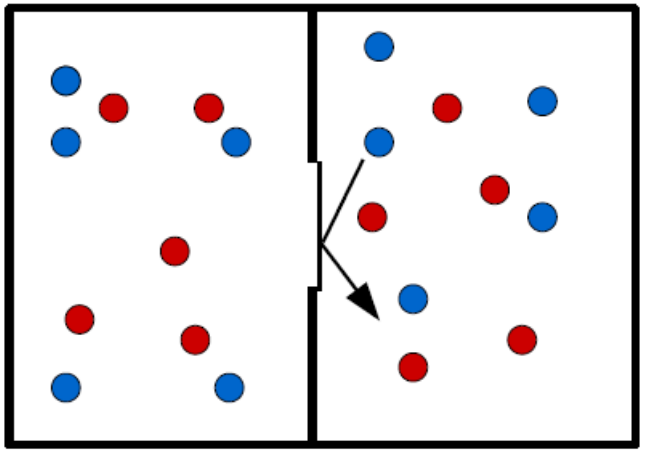


If a slow molecule comes to the door from the left we open it and let it pass through



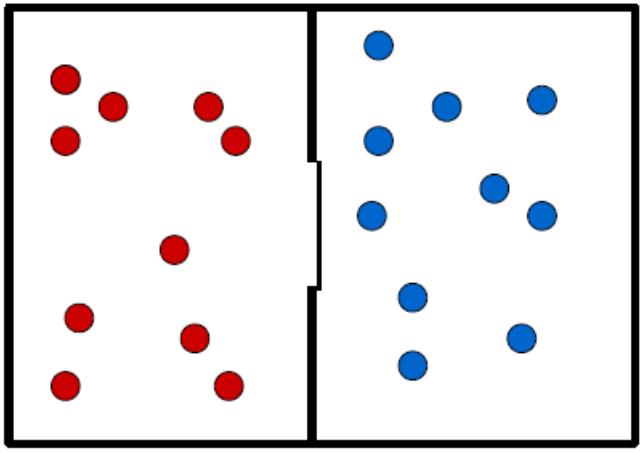
If a fast molecule comes from the left we keep the door closed





From the right we let fast molecules pass and stop the slow.

In this way we sort the molecules so that the fast are on the left and the slow on the right.

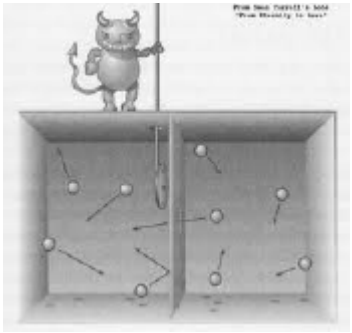


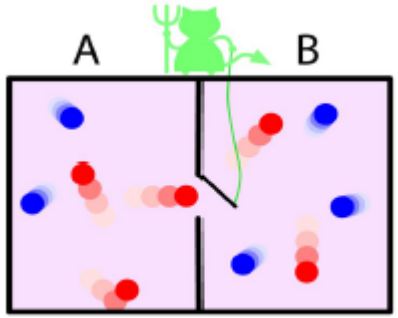
We created a temperature difference without any work done .
(The door must be without friction, we could worry about this, but it turns out not to be a problem).

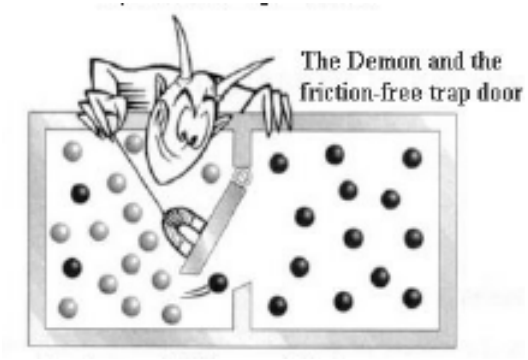
We have done impossible!!

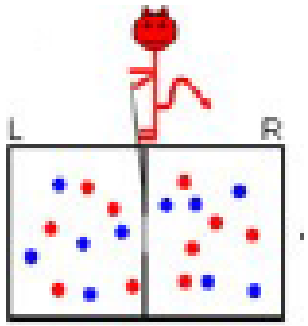
Of course it is difficult to follow the motion of molecules.

Maxwell imagined the help of a very small and fast assistant, which was later called his demon. The demon can see the molecules and open or close the door.





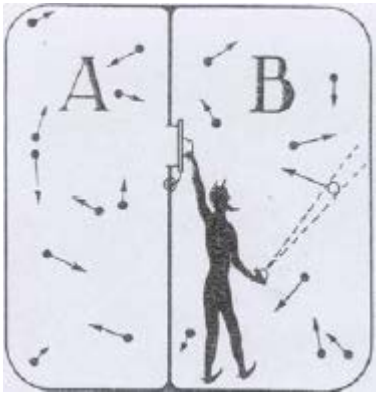




Demon:

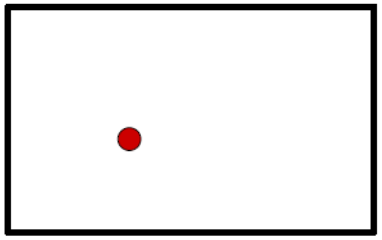
a supernatural being of Greek mythology intermediate between gods and men.

Merriam-Webster dictionary

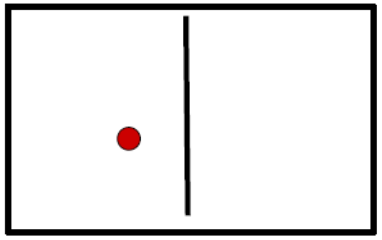


But can we build it? Without some mysterious demon but using the laws of physics?

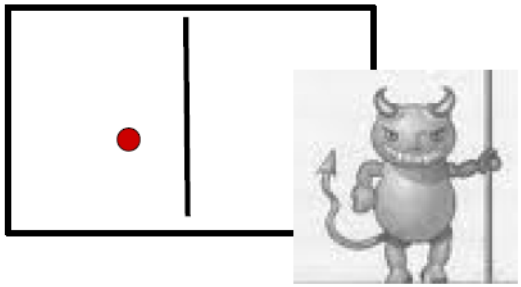
Another scenario: The Szilard engine (single particle gas)



A container with only one molecule

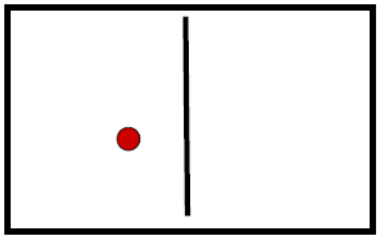


Insert a partition in the middle

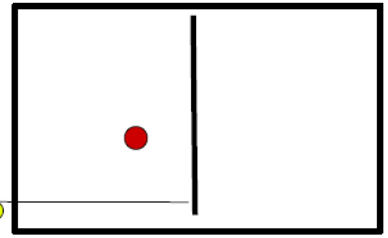


Measure on which side the molecule is (this is the work of the demon)

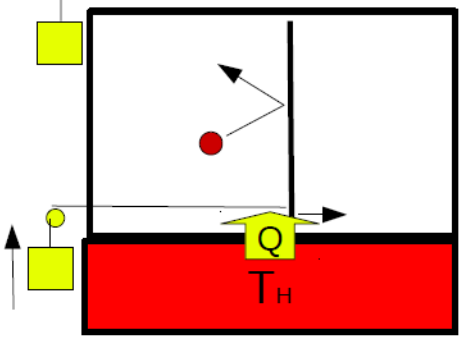
The demon is the only source of knowledge



The demon knows on which side the molecule is

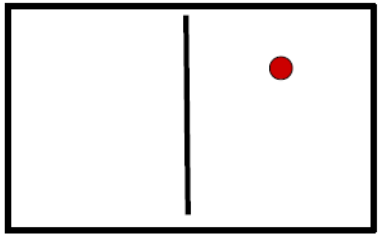


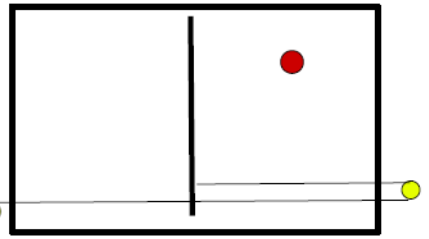
It attaches the weight depending on which side the molecule is on

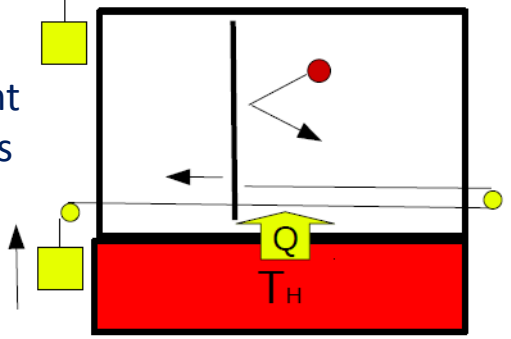


The gas expands and lifts the weight (the expanding gas will cool if we do not attach it to a reservoir).

It measures and tells us the result







Amount of work: $W = kT \ln 2$

The net result:

- Our engine came back to the same state.
- Energy was transferred from the heat bath to the gas
- The weight was lifted

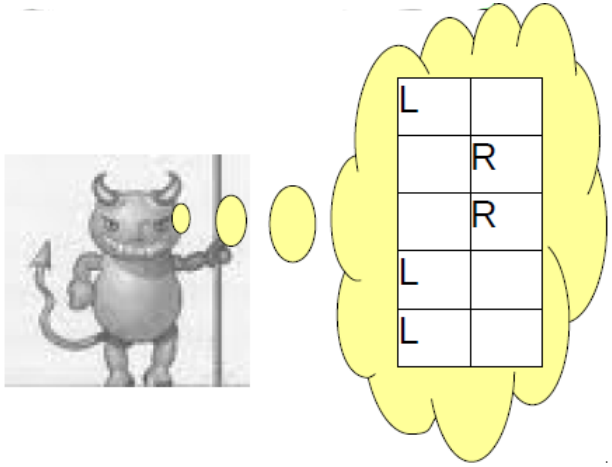
The second law of thermodynamics:
No cycle process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work.

Have we violated this law?

But, what happens to the demon?

The demon is not back to the original state, it still knows which side the molecule was on. It has gained information.

For some time it may work, but if we run for a long time, it will run out of memory!

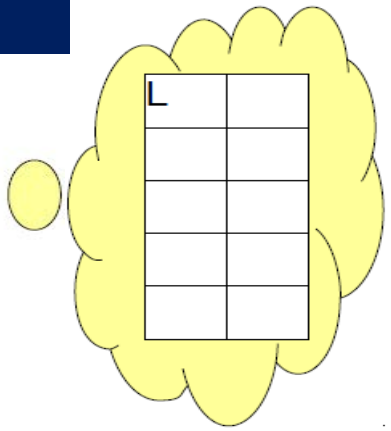


Shannon information: Definition

Claude Shannon (1916-2001)

If the memory has different states *i* and the probability of each is p_i the information is:

$$S = -k \sum_i p_i \ln p_i$$

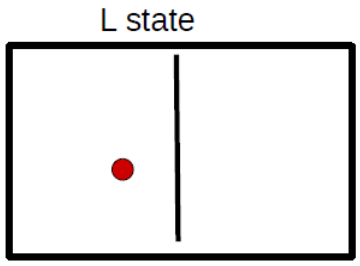


If both sides (L and R) are equally probable, $p_L = p_R = 1/2,\ S = k \ln 2\,.$

The increase in the information is exactly equal to the decrease of entropy in the gas!

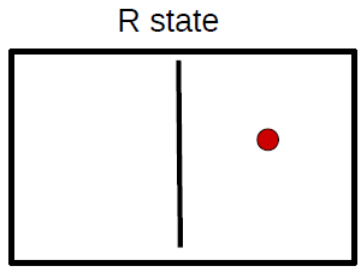
Rolf Landauer (1927-1999)

Landauer's principle: Forgetting is not for free

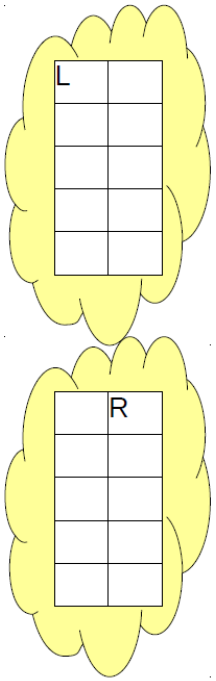


Consider memory:

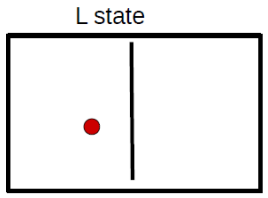
Molecule on left means demon remembers left



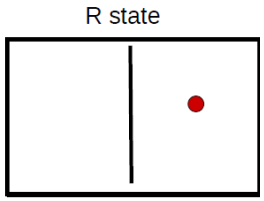
Molecule on right means demon remembers right

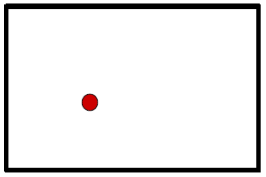


Forgetting means resetting the memory to a fixed state (let us say L):

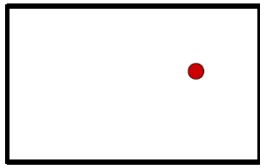


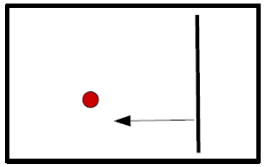
To reset:



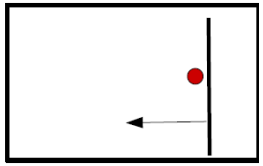


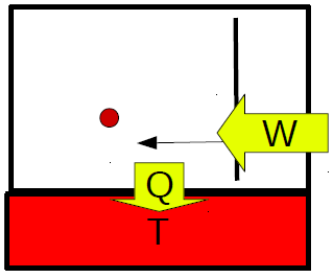
(1) Remove the partition





(2) Insert it on the right and (3) push it to the middle





But now we are compressing the gas. This requires work, and heat has to be given to the bath for the gas not to heat up.

How much work is needed? $W = kT \ln 2$

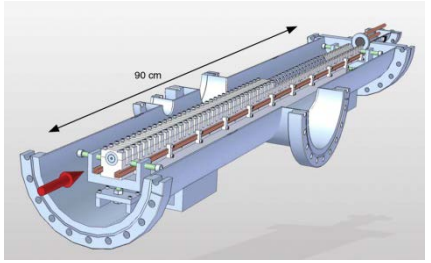
This is exactly the same amount of work as the Szilard engine produced in one cycle.

Our engine produces no work at all after resetting the memory!

MD: Various implementations

Cold atoms in traps

G. Price, et al., Phys. Rev. Lett. 100, 093004 (2008).
J. Thorn, et al., Phys. Rev. Lett. 100, 240407 (2008).
M. Raizen, Science 324, 1403,1406 (2009).

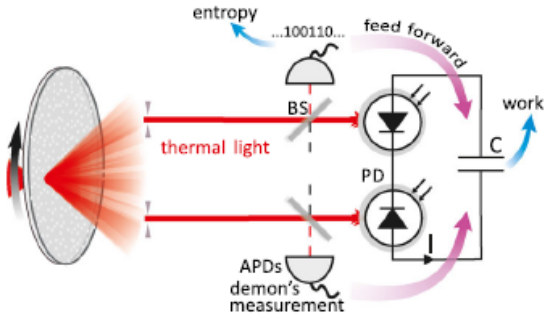


Colloidal particles, Molecules

S. Toyabe, et al., Nat. Phys. 6, 988 (2010).
A. Berut, et al., Nature 483, 187 (2012).
V. Serreli, et al., Nature 445, 523 (2007)

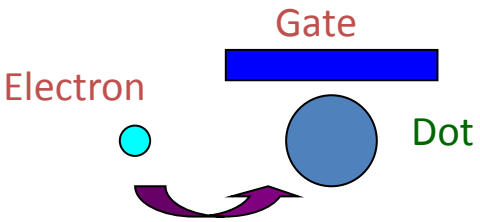
Photons

M. Vidrighin, et al., Phys. Rev. Lett. 116, 050401 (2016).



Electrons

Electronic implementations – Single-electron boxes

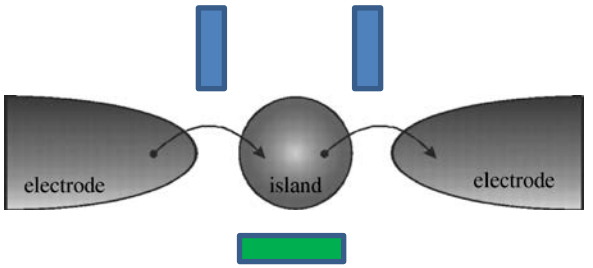


Repulsion at the dot

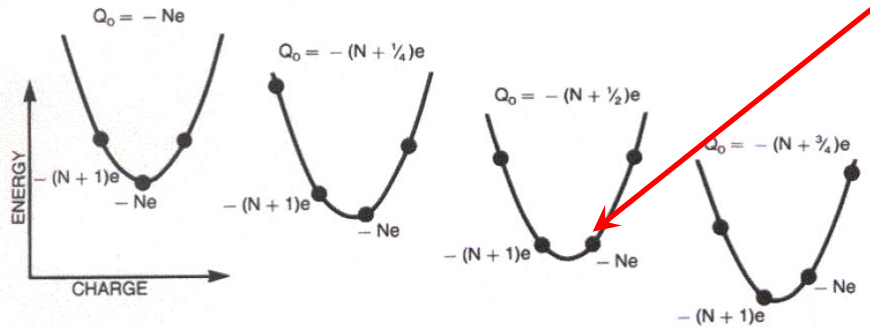
Cost: $E = QV_g + \frac{Q^2}{2C}$

Attraction to the gate

Generic SET:
Gates allow tuning the tunneling rates
Γ_i and the potential E_{dot}.

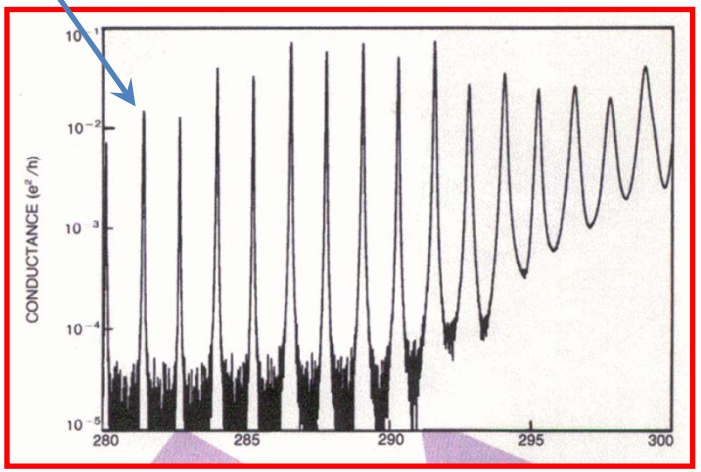


$Q = -Ne$



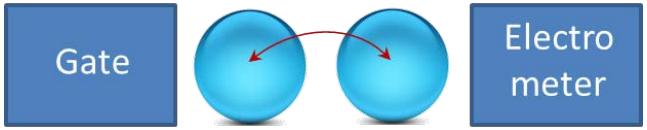
At $V_g = -\left(N + \frac{1}{2}\right)\frac{e}{C}$

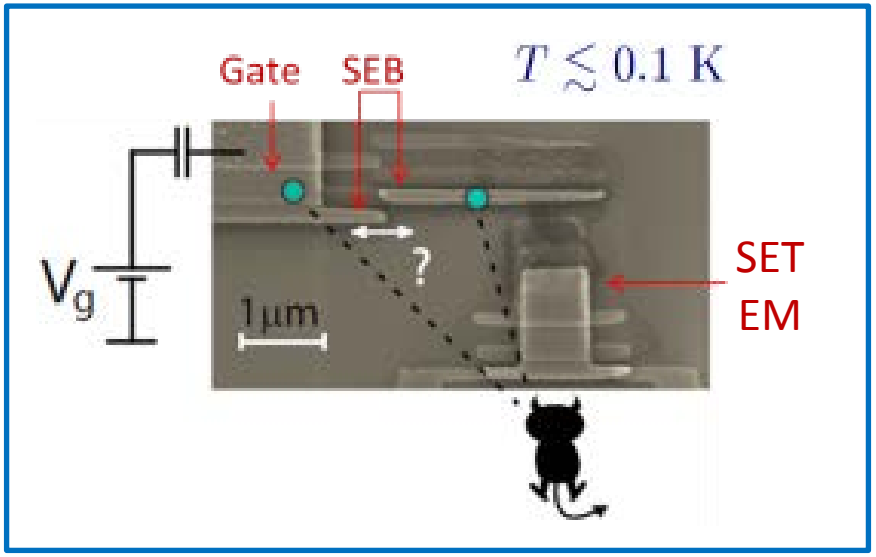
the energy cost vanishes !



Single-electron transistor (SET)

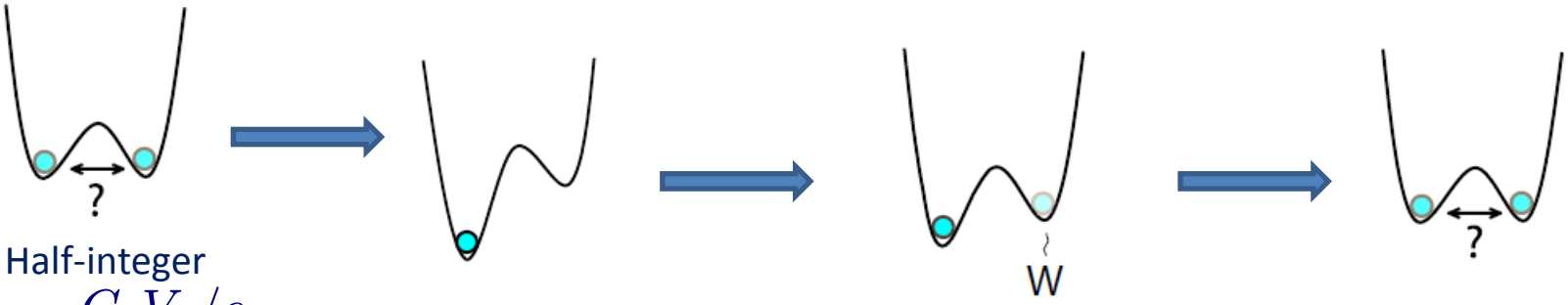
The Szilard engine: Realization with a single electron





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



Half-integer

$n_g = C_g V_g / e$

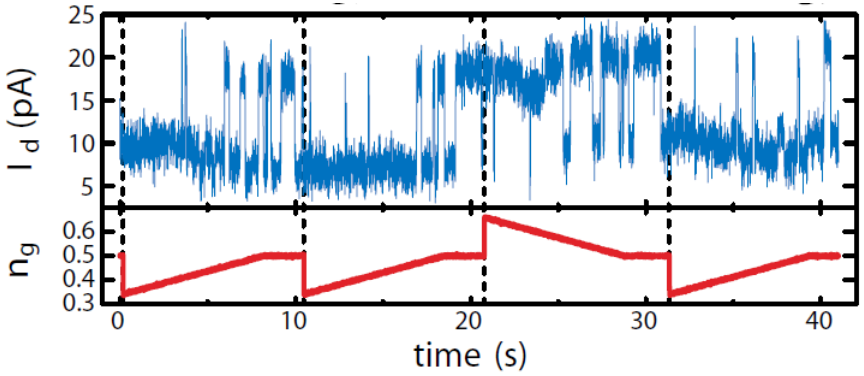
1. SET electrometer measures where the excess particle is

2. Then, n_g is changed rapidly to capture electron on the corresponding island.

3. Finally, n_g is moved slowly back, extracting energy from the heat bath in the process, and completing the cycle.

Experimental realization of a Szilard engine with a single electron

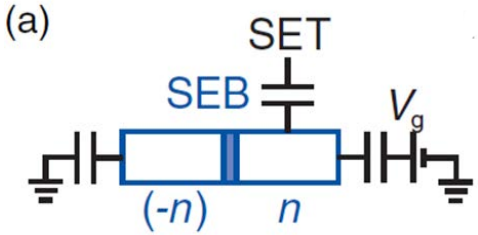
Jonne V. Koski[a,1], Ville F. Maisi[a,b,c], Jukka P. Pekola[a], and Dmitri V. Averin[d]

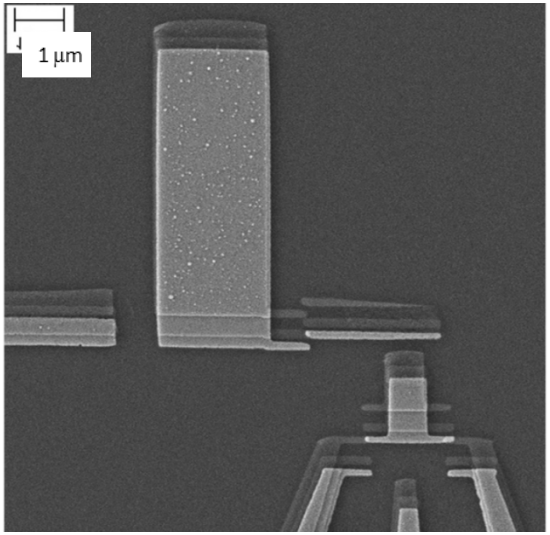


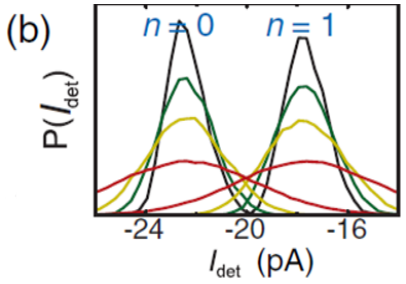
PRL 113, 030601 (2014) PHYSICAL REVIEW LETTERS week ending 18 JULY 2014

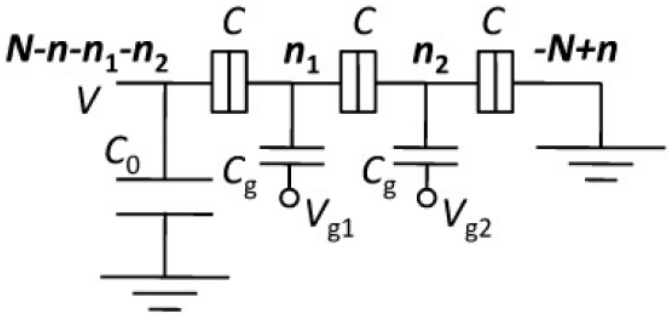
Experimental Observation of the Role of Mutual Information in the Nonequilibrium Dynamics of a Maxwell Demon

J. V. Koski,[1] V. F. Maisi,[1,2,*] T. Sagawa,[3] and J. P. Pekola[1]









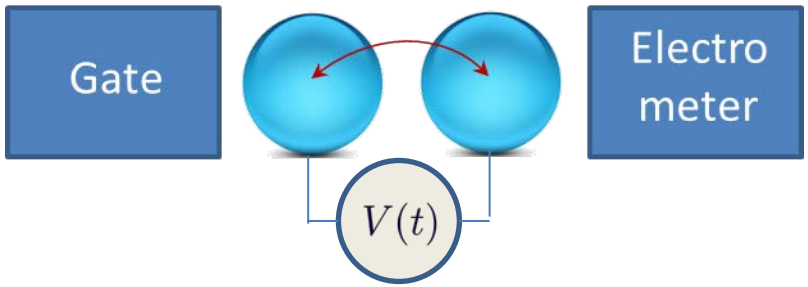
PHYSICAL REVIEW B 84, 245448 (2011)

Maxwell's demon based on a single-electron pump

Dmitri V. Averin,[1] Mikko Möttönen,[2,3] and Jukka P. Pekola[2]

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.

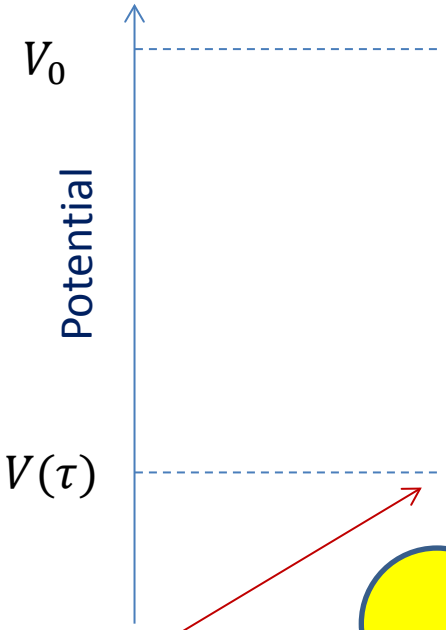
2. Perform a measurement, and if the extra electron is found on one island, quickly raise the potential of the other island to some value $V_0 \equiv V(0^+)$.

3. Reduce the potential of the raised island according to some protocol $V(t)$ until time $t = \tau$, and start over from step 2.

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



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

What is the role of measurement errors?

Perform measurement

If the electron tunnels “uphill” during slow decrease of the potential, then the energy is extracted from the thermal bath.

After finding of an electron at a given dot we quickly raise the potential of the “idle” dot up to V_0, and shift potential of the occupied dot to 0.

In this way we continue the cycle.

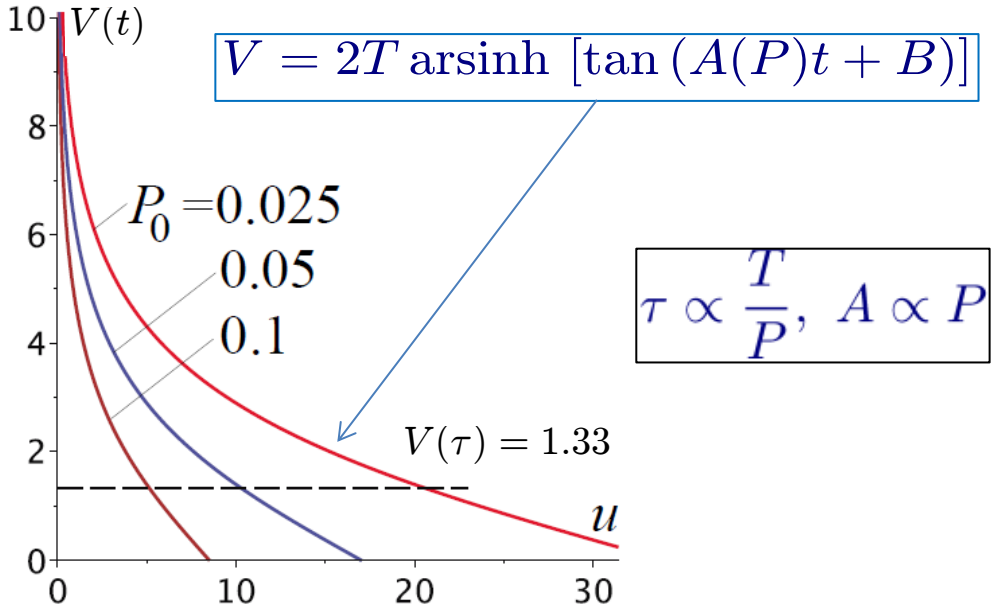
Q: Which *V(t)* and τ correspond to minimum entropy production?

A: $\tau \to \infty$ and any *V(t)* with $V(0) \to \infty$.

This is true only for vanishing power of heat extraction!

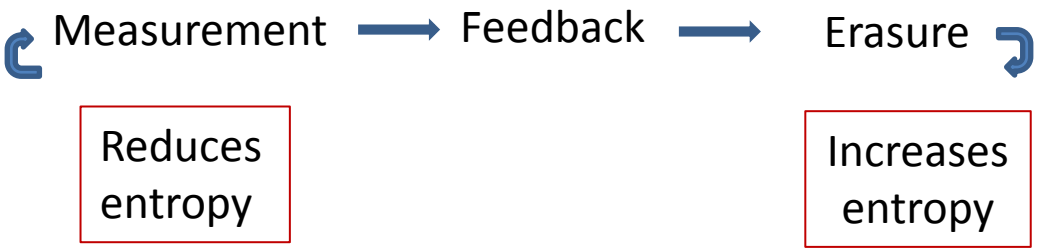
Q: What is the optimal regime for a finite power of heat extraction from the environment?

How the strategy should change in the presence of measurement errors?



Result for error-free case: J. Bergli, Y. M. Galperin and N. B. Kopnin, Phys. Rev. E 88, 062139 (2013)

Role of measurement errors



Can, if no errors, be done fully reversible.

Measurement error:

reduces the information → reduces the entropy decrease

Erasure still gives increase in entropy, the total process becomes irreversible

Another consequence: 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.

Thermodynamics and role of mutual information

If there is a chance that the measurement result is wrong → 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)]:

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

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 sub-spaces corresponding to the logical states $\mathcal{P}_i$.

Both the device and the memory are Szilard engines → 4 logical states

Simple model (continued)

Phase space $\mathcal{P}$, subspaces $\mathcal{P}_i$ corresponding to the logical information stored.

x - point in the phase space.

Probability distribution of the logical states: $P_L(i) = \sum_{x \in \mathcal{P}_i} P(x), \quad i = 0 \vee 1$

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

$$S_{\text{in}} = \sum_i P_L(i) S(\mathcal{P}_i|i) \longrightarrow \boxed{S = H + S_{\text{in}}}$$

Simplified version of the derivation by Sagawa & Ueda

Illustration for ideal gas in 3d box

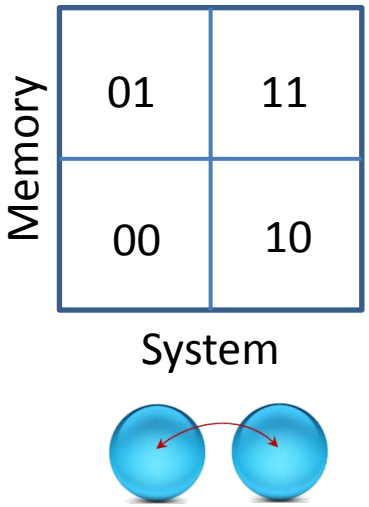
Free energy: $$F(T,V,N) = -NT\ln\left[\frac{Ve}{N}\left(\frac{mT}{2\pi\hbar^2}\right)^{3/2}\right]$$

Entropy: $$S = -\left(\frac{\partial F}{\partial T}\right)_{V,N} = N\left[\frac{3}{2} + \ln\left(\frac{V}{NV_q}\right)\right]$$

$$V_q(T) \equiv \frac{4}{e\sqrt{2}}\left(\frac{\pi\hbar^2}{mT}\right)^{3/2}$$

Single particle, $V \gg NV_q$: $$S = \frac{3}{2} + \ln\left(\frac{V}{V_q}\right).$$

Double-dot system



4 boxes → 4 logical states ($i = 00, 01, 10, 11$), 2 particles

Internal entropy for a logical state i:

$$S_{\text{in}}(i) = S_0 + \ln\left(\frac{x_S x_M}{L^2}\right), \quad S_0 \equiv 3 + 2\ln\left(\frac{V}{V_q}\right) \gg 1.$$

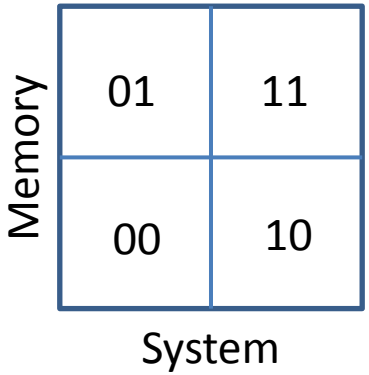
Probability of logical state

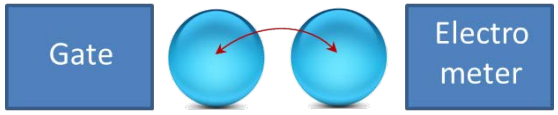
In the following we omit large constant S_0.

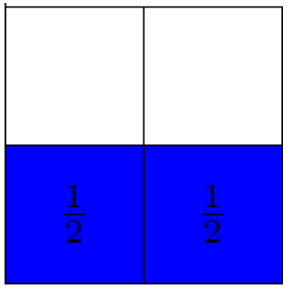
Entropy production and measurement errors: Szilard machine

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.





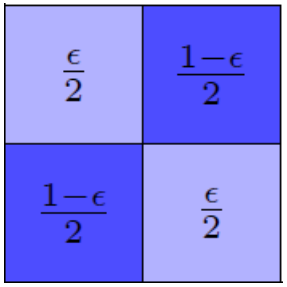


The initial state is such that the system has an equal probability of the particle being on the left or right, and the measurement not yet performed, so that the memory is reset to the left half

$$H = -2 \cdot \frac{1}{2} \ln \frac{1}{2} = \ln 2$$

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

$$S = -\ln 2$$



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

$$H = -2 \cdot \frac{\epsilon}{2} \ln \frac{\epsilon}{2} - 2 \cdot \frac{1-\epsilon}{2} \ln \frac{1-\epsilon}{2} = \ln 2 + S_\epsilon$$

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

$$S = -\ln 2 + S_\epsilon$$

$$S_\epsilon = -\epsilon \ln \epsilon - (1-\epsilon) \ln (1-\epsilon)$$

Details for the initial configuration
(calculation for the last configuration is similar)

For the initial configuration we have two states with probabilities ½ each:

$$H = -\sum_i P_L(i) \ln P_L(i) = -2 \times \frac{1}{2} \ln \frac{1}{2} = \ln 2$$

Putting $x_S = x_M = \frac{L}{2}$ and omitting S_0 we get for the conditional entropy

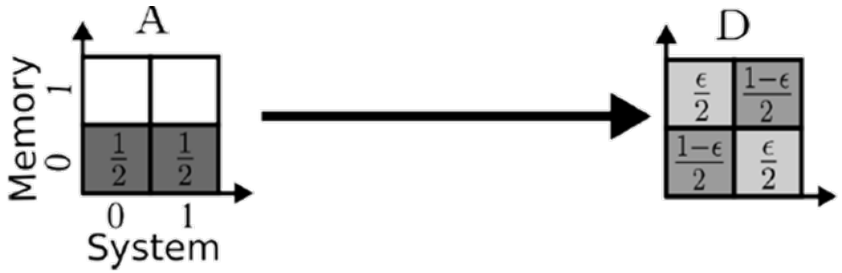
$$S(\mathcal{P}_{00}|00) = S(\mathcal{P}_{10}|10) = \ln \frac{1}{4}$$

$$\rightarrow \qquad S_{\text{in}} = \sum P_L(i) S(\mathcal{P}_i|i) = 2 \times \frac{1}{2} \ln \frac{1}{4} = -2 \ln 2$$

Consequently, the total entropy is

$$S = H + S_{\text{in}} = -\ln 2$$

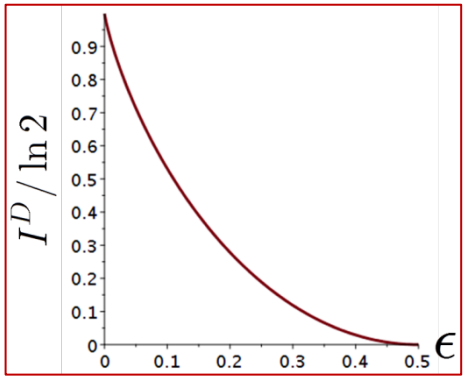
Irreversible transition:



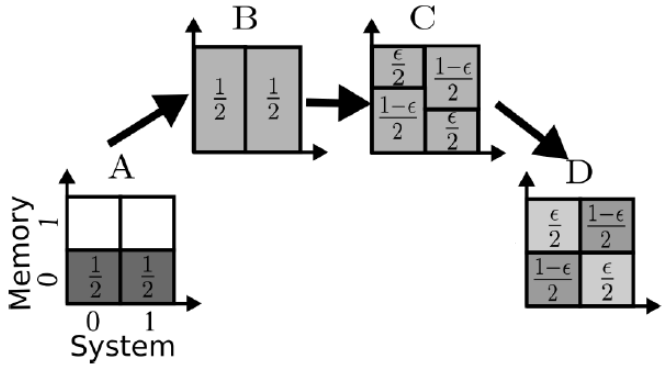
Irreversible entropy increase: $S_\epsilon = -\epsilon \ln \epsilon - (1-\epsilon)\ln(1-\epsilon)$

Logical information: $H^D_{\text{System}} = H^D_{\text{Memory}} = \ln 2$

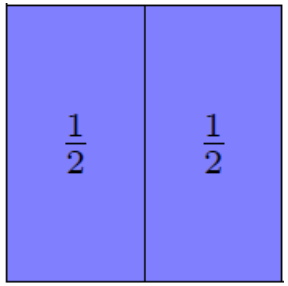
Mutual information: $I^D = H^D_{\text{System}} + H^D_{\text{Memory}} - H^D]$
$= \ln 2 - S_\epsilon$



Reversible transition:

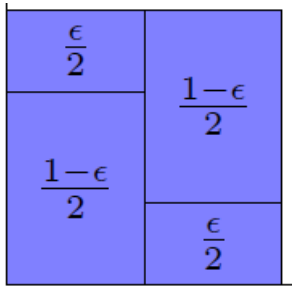


If the correlation is not perfect, $I < H \rightarrow W_{\text{measure}} < 0$, we should be able to reach this state while extracting work if we can do it reversibly.



1. Expand isothermally the memory:

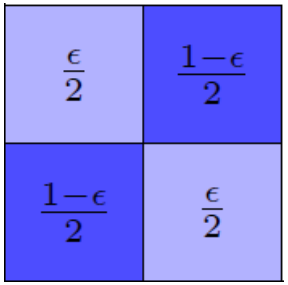
$$\Delta S = \ln 2$$
$$\frac{W}{T} = \frac{Q}{T} = \Delta S = \ln 2$$



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. ε is just a parameter describing at which point we insert the divider.

$$\Delta S = 0$$
$$\frac{W}{T} = 0$$



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.

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

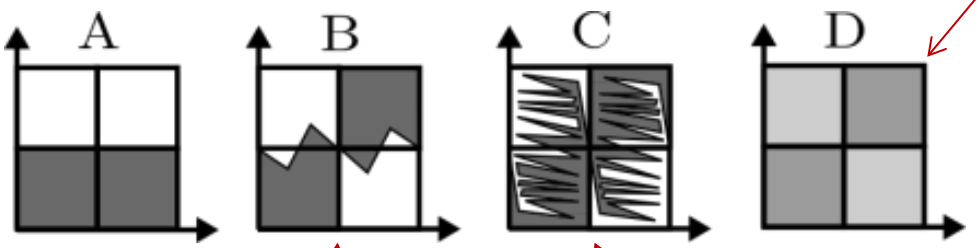
Energy balance: $W_{\text{measure}} = -TS_\epsilon < 0,\ W_{\text{erase}} = T \ln 2$

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

The equality is saturated, but by a reversible process.

What happens when an irreversible measurement with errors takes place?

Initial state



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:

$$\Delta S_{\rm tot} = \underbrace{S_\epsilon}_{\text{measurment}} + \underbrace{\Delta S - Q/T}_{\text{operation}}$$

$$S_{\rm in} = 0 \;\rightarrow\; \Delta S = \Delta H$$

We minimize the entropy production rate

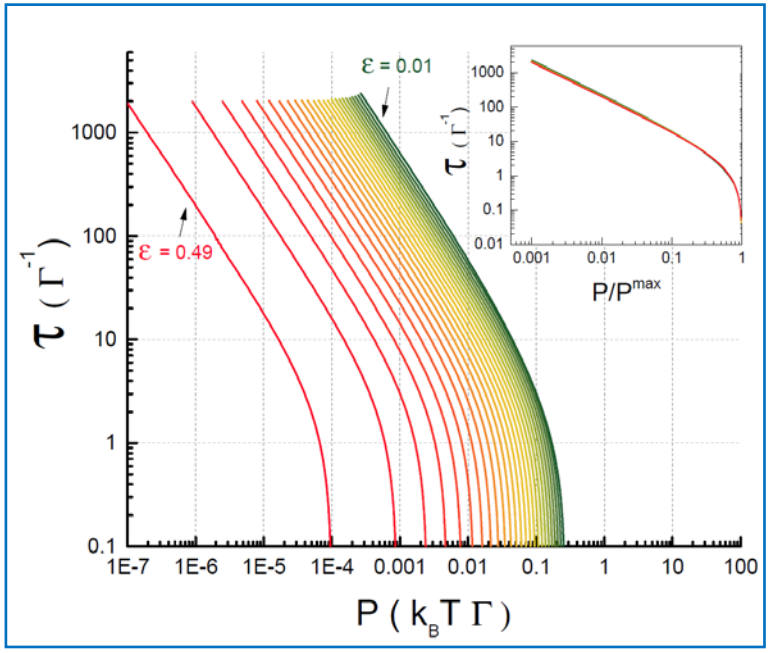
$$\dot{S}_{\rm tot} = \frac{\Delta S_{\rm tot}}{\tau} = \frac{S_\varepsilon}{\tau} + \frac{\Delta H}{\tau} - P$$

power $P = Q/T\tau$

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:

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



Main: 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, $P^{\max}(\epsilon)$, as τ approaches 0.

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

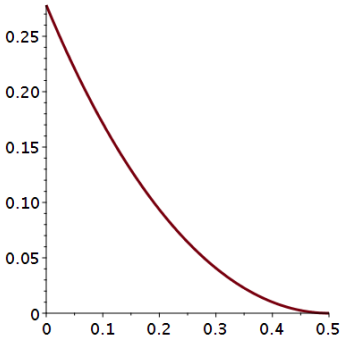
As P approaches its maximum value the period approaches 0 linearly:

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

To a very good approximation,

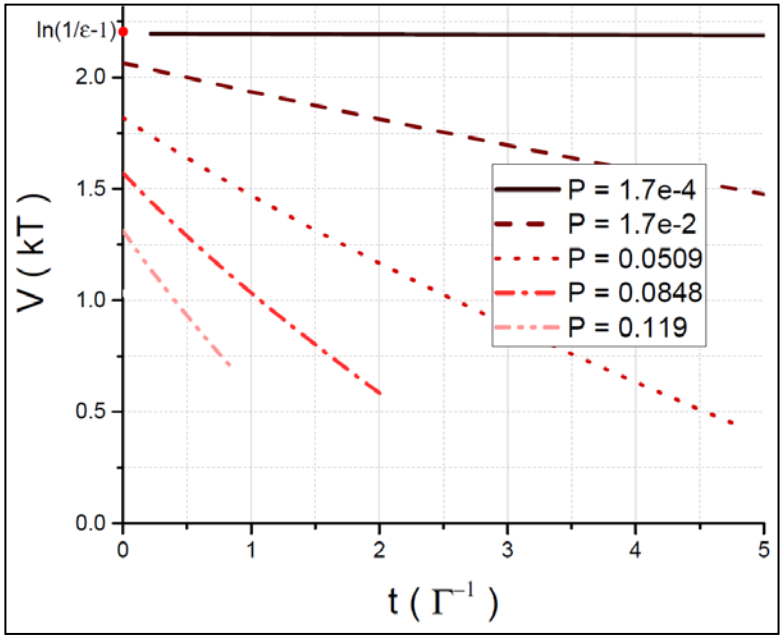
$$P^{\max}(\epsilon) = \frac{\epsilon - 1/2}{\phi} \sinh\left[\phi(\epsilon - 1/2)\right],$$

where $\phi = 1.618$ is the golden ratio.

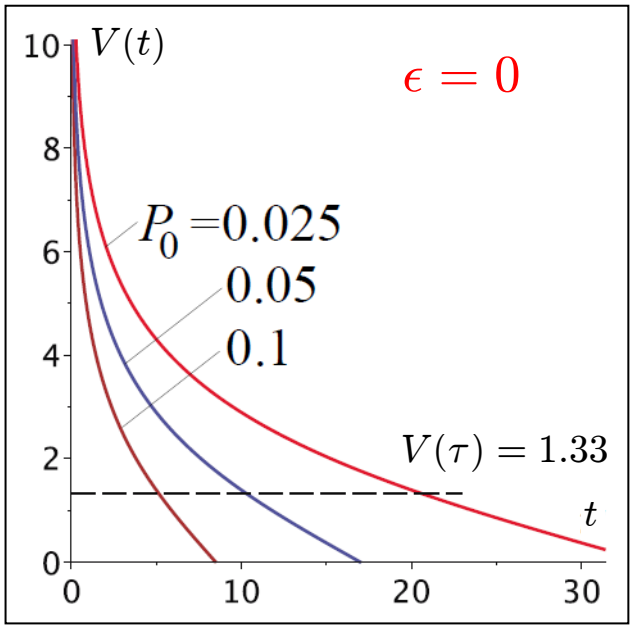


When the power P goes towards zero, the optimal period τ diverges to infinity. In other words, when we approach reversibility by performing the process in an infinite amount of time the power we can extract is zero.

In the limit of low power we find that $\tau = \left(\ln 2 - S_\epsilon\right)/P \to Q_s(\epsilon) = \ln 2 - S_\epsilon = I.$



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

Entropy production

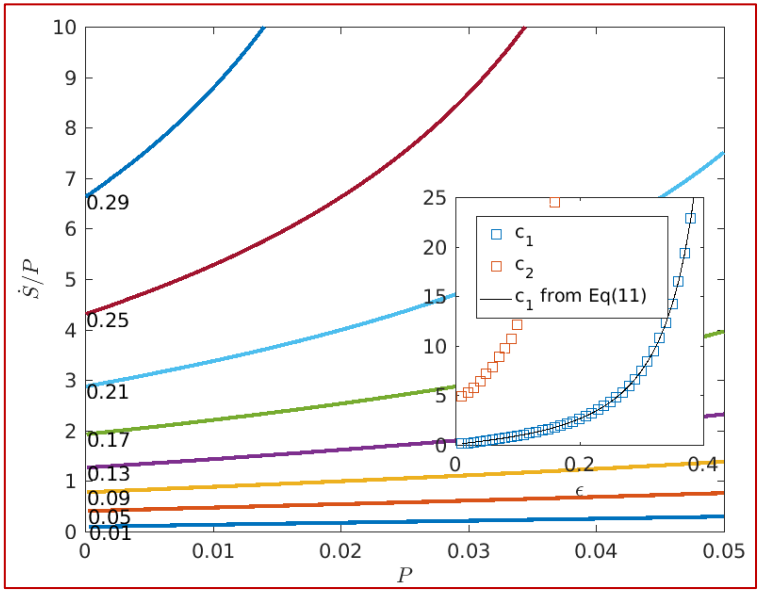
As $P \to P^{\max}$, the entropy production diverges as $\dot{S}_{\rm tot} \propto (P^{\max} - P)^{-1}$.

As $P \to 0$, $\Delta S_{\rm tot} = c_0 + c_1 P$

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

If there are errors, the measurement entropy S_ε exists even for a reversible operation.

As a result $c_0 = S_\varepsilon \to \dot{S}_{\rm tot} = (S_\varepsilon/I)P + c_1^* P^2$



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.

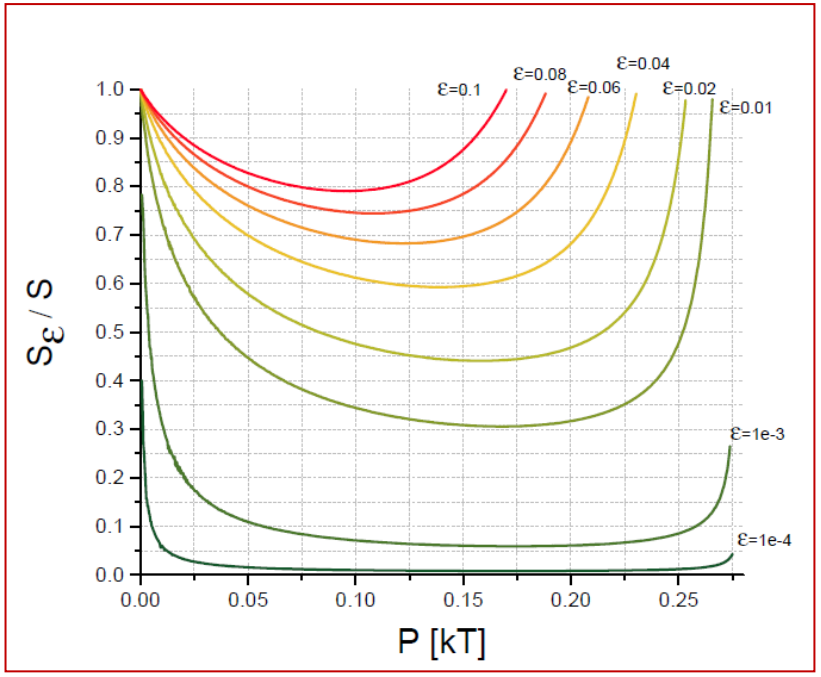
$$c_1 = S_\epsilon(\ln 2 - S_\epsilon)^{-1}.$$

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

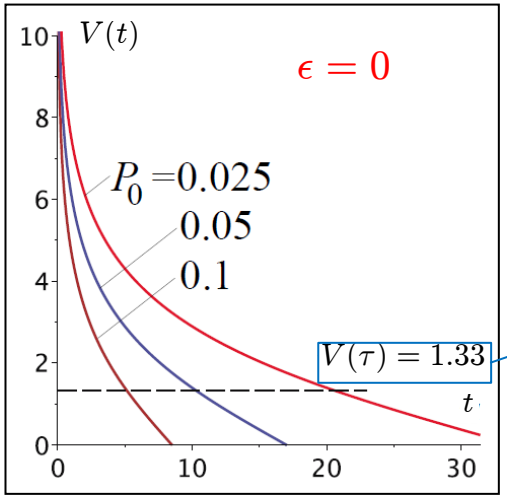
For $P \to 0$, we approach reversible operation ($\Delta S = 0$) and all of the total entropy production is due to the measurement error.

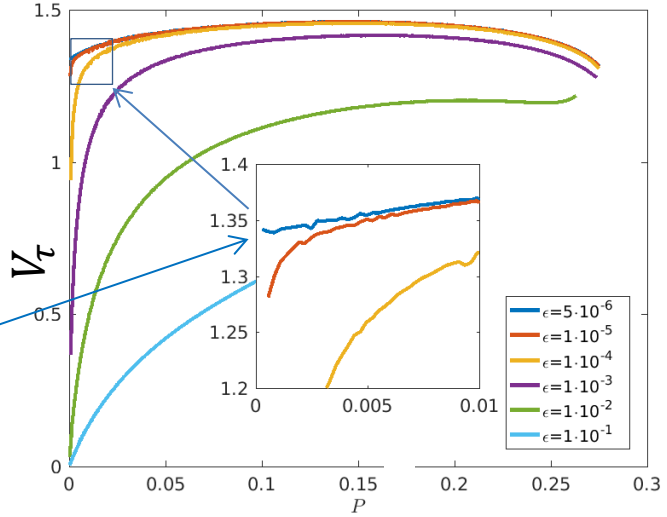
When $P \to P^{\max}$ the measurement entropy dominates again since the there is no time for heat transfer from the environment when $\tau \to 0$.

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.



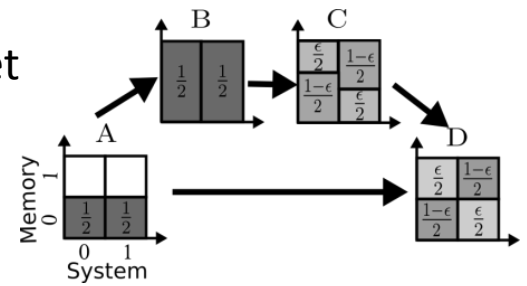
Non-analytical behavior versus ε



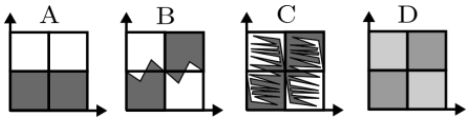


Summary of the results

- 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 from a course graining of either 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.

Sketch of calculations

Master equation:

$$\begin{aligned}\dot{p}_1 &= -\Gamma_{12}p_1 + \Gamma_{21}p_2 = -\Gamma p_1 + \Gamma_{21}, \\ \dot{p}_2 &= \Gamma_{12}p_1 - \Gamma_{21}p_2 = -\Gamma p_2 + \Gamma_{12}\end{aligned} \qquad \Gamma \equiv \Gamma_{12} + \Gamma_{21}$$

Energies of the states: $E_1(t) \equiv 0, \; E_2(t) \equiv V(t)$

Simple model:

$\Gamma = \text{constant}(t)$

Extracted work per cycle: $W_{\text{ex}} = -\sum_{i=1}^{2} \int_0^\tau dt\, p_i \dot{E}_i,$

Change of internal energy: $\Delta U = \sum_{i=1}^{2} [p_i(\tau)E_i(\tau) - p_i(0)E_i(0)]$

Heat transfer: $Q = \Delta U + W_{\text{ex}} = \sum_{i=1}^{2} \int_0^\tau dt\, \dot{p}_i E_i(t)$

Information entropy: $H = -\sum_{i=1}^{2} p_i \ln p_i$

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: $\dot{p} = -p + \frac{1}{e^V + 1}$ Time is measured in $1/\Gamma$; *V* -> in units of *T*

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: $\frac{\Delta S_{\rm tot}}{\tau} = \frac{\Delta H}{\tau} + \frac{S_\epsilon}{\tau} - P$ ← $-\epsilon \ln \epsilon - (1-\epsilon)\ln(1-\epsilon)$

It is sufficient to minimize only

$$I = \frac{\Delta H}{\tau} + \lambda P = \frac{1}{\tau} \int_0^\tau dt\ L(p, \dot{p}, \lambda)$$

Lagrangian: $L(p, \dot{p}, \lambda) = \left[-\ln\left(\frac{p}{1-p}\right) + \lambda \ln\left(\frac{1}{\dot{p}+p} - 1\right)\right] \dot{p}$

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

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, $p(\tau)$: From $(\partial L/\partial \dot{p})_{t=\tau} = 0$, 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: $\dfrac{\partial \Delta S_{\rm tot}/\tau}{\partial \tau} = 0$, or

$$\frac{\partial \Delta S_{\rm tot}}{\partial \tau} = \lambda\frac{\partial P}{\partial \tau} - \frac{1}{\tau^2}(\Delta H + S_\epsilon) + \frac{1}{\tau}\frac{\partial S_\tau}{\partial \tau} = 0$$

$$F_2(\lambda,\tau,p) \equiv \left[\ln\left(\frac{1-p_\tau}{p_\tau}\right) + \lambda\dot{p}_\tau\ln\left(\frac{1}{p_\tau+\dot{p}_\tau}-1\right)\right] - \lambda P - \frac{1}{\tau}\left[\Delta H + S_\epsilon\right] = 0$$

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, ϵ

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

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

Conclusions

We have discussed several aspects of energy and heat exchange in small systems focusing on the situations when the processes leading from one state of the system to another one are non-equilibrium.

We have considered pedagogical examples of a classical ideal gas and of stochastic Brownian motion of a classical particle. For these cases, the Jarzynski fluctuation relation for work distribution and its implication were discussed.

We have also discussed the fluctuation relation for energies U of a simple quantum system (qubit). We have shown that the average $\langle e^{\beta U} \rangle$ is related to the coherence rate of the qubit.

Based on this relation we have discussed a possibility of using the qubit as a primary thermometer.

Finally, we have considered a Maxwell demon device and found at optimal protocol of its operation for a given output power.

THANK YOU FOR YOUR ATTENTION !