Work, heat and fluctuation relations in single-electron transport

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in collaboration with
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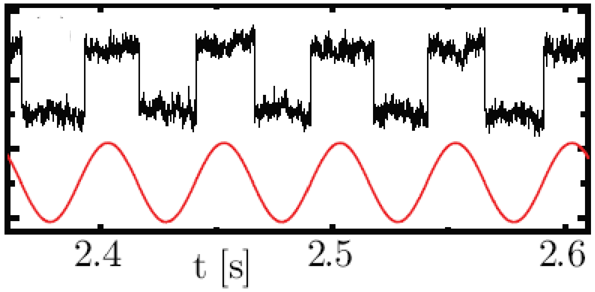
Olli-Pentti Saira, Youngsoo Yoon, Timothe Faivre (experiment)



Low temperature laboratory

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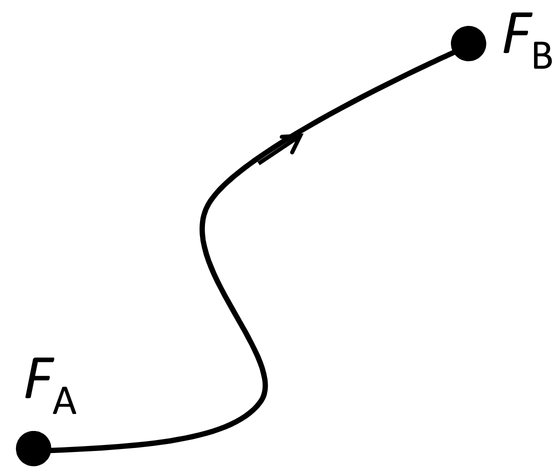
Fluctuation relations

Jarzynski equality, C. Jarzynski, PRL 78, 2690 (1997)

$$\langle e^{-\beta(W-\Delta F)}\rangle = 1$$



This is a powerful expression (equality!):

1. Since $\langle e^{x}\rangle \geq e^{\langle x\rangle}$

we have $\langle W\rangle \geq \Delta F$ **(2nd law)**

2. For Gaussian noise (near-equilibrium fluctuations) one obtains

$$W_{\text{diss}} \equiv \langle W\rangle - \Delta F = \beta(\langle W^2\rangle - \langle W\rangle^2)/2$$

$$\frac{P_\tau(\Delta S)}{P_\tau(-\Delta S)} = e^{\Delta S/k_B}$$

Equilibrium Information from Nonequilibrium Measurements in an Experimental Test of Jarzynski's Equality

Jan Liphardt,[1,4] Sophie Dumont,[2] Steven B. Smith,[3] Ignacio Tinoco Jr.,[1,4] Carlos Bustamante[1,2,3,4]*

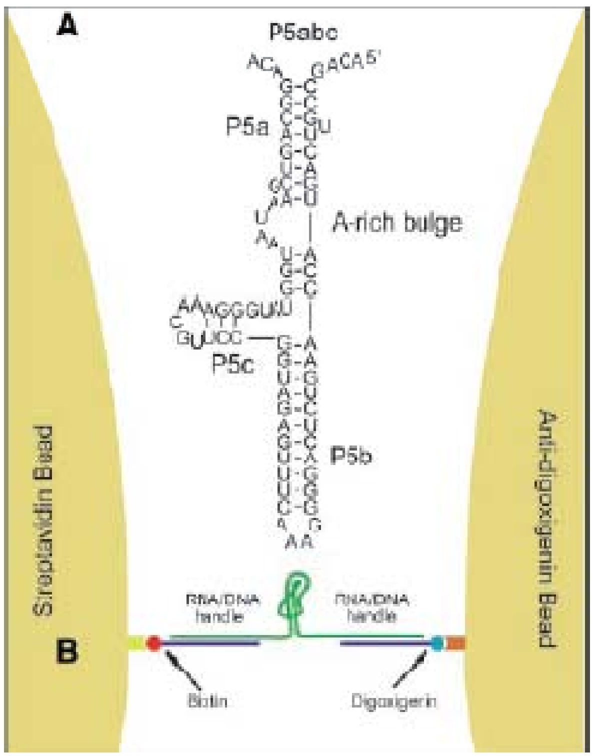


Fig. 1. (A) Sequence and secondary structure of the P5abc RNA. (B) RNA molecules were attached between two beads with RNA-DNA hybrid handles.

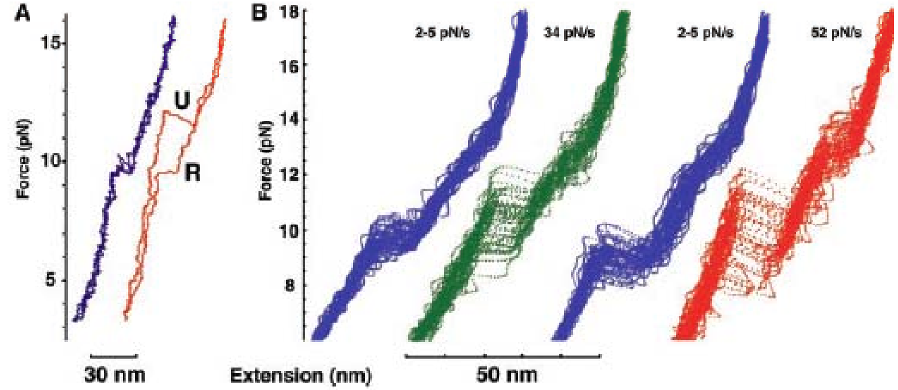
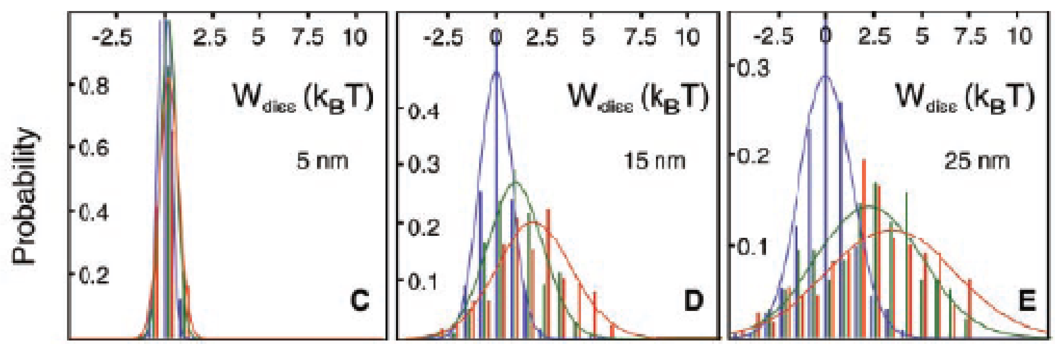


Fig. 2. Force-extension unfolding curves of P5abc at three different switching rates. (A) Typical force-extension unfolding (U) and refolding (R) curves of the P5abc RNA in 10 mM EDTA in reversible (blue, 2 to 5 pN/s) and irreversible (red, 52 pN/s) switching conditions. (B) Two experiments are shown: one in which a molecule was unfolded at rates of 2 to 5 pN/s and 34 pN/s (left pair, blue and green), and another in which the molecule was unfolded at rates of 2 to 5 pN/s and 52 pN/s (right pair, blue and red). Curves (superposition of about 40 curves per experiment) were smoothed by convolution with a Gaussian kernel.



(C to E) Histograms of dissipated work values at $z = 5$, 15, and 25 nm. Dissipated work values for a given switching rate were pooled. Blue, 272; green, 119; red, 153 dissipated work values. Solid lines: Gaussian with mean and standard deviation of data.

Experimental Free Energy Surface Reconstruction from Single-Molecule Force Spectroscopy using Jarzynski's Equality

Nolan C. Harris, Yang Song, and Ching-Hwa Kiang*

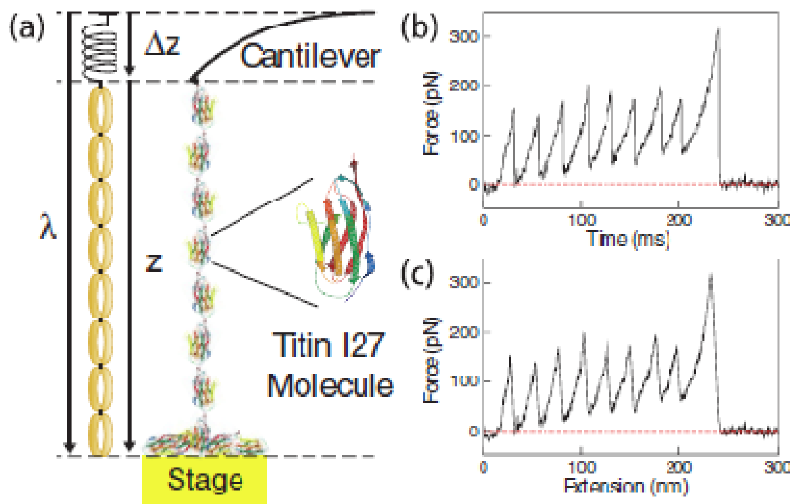
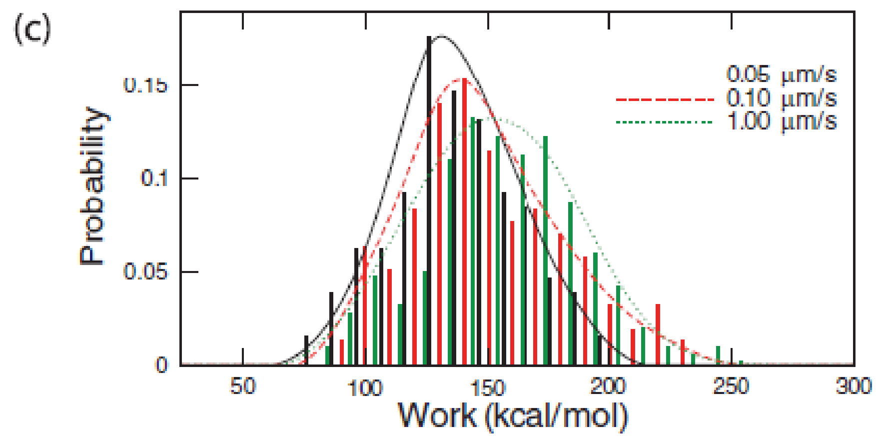
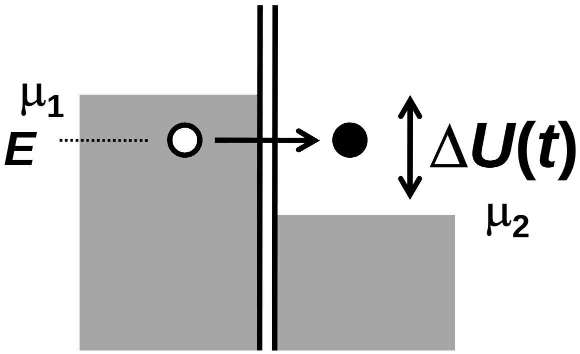


FIG. 1 (color). Single-molecule pulling experiments using AFM. (a) One end of the molecule is attached to the cantilever tip and the other end to a gold substrate, whose position is controlled by a piezoelectric actuator. An analogue of the single-molecule force measurements is illustrated. The cantilever spring obeys Hooke's law, whereas the protein molecular spring follows the wormlike chain model (illustrated using rubber bands).



Statistics of generated heat and work in driven single-electron transitions

Proposal: D. V. Averin and J. P. Pekola, arXiv:1105.0416, EPL **96**, 67004 (2011).

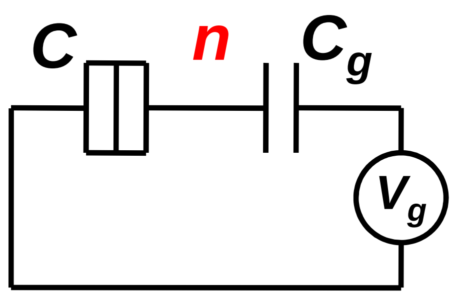


Dissipation generated by tunneling in a biased junction

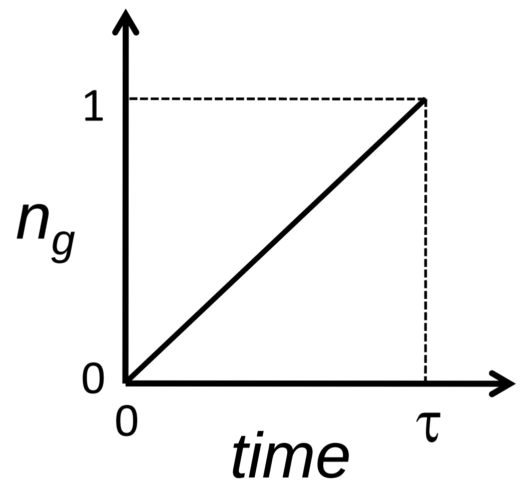
$$= (\mu_1 - E) + (E - \mu_2) = \mu_1 - \mu_2 = \Delta U$$

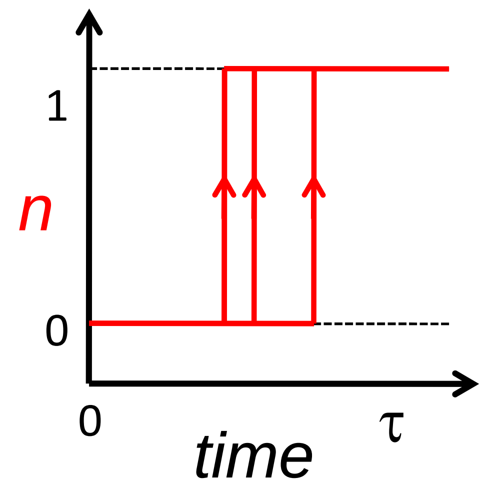
Generated heat $Q = \Delta U$ due to relaxation (typically electron-phonon scattering)

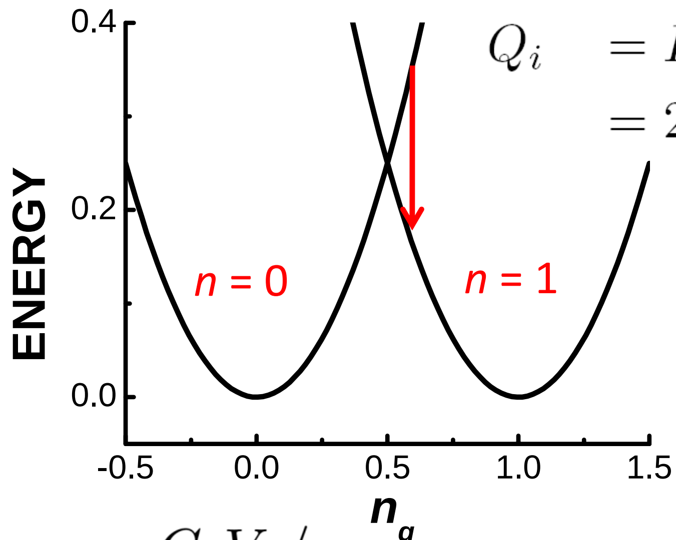
Generated heat in driven single-electron transitions



Single-electron box







$$n_g = -C_g V_g / e$$

$$Q_i = E_0(n_{g,i}) - E_1(n_{g,i}) = E_C(n_{g,i} - 0)^2 - E_C(n_{g,i} - 1)^2$$
$$= 2E_C(n_{g,i} - 1/2) \equiv 2E_C \delta n_{g,i}$$

The total dissipated heat in a ramp:

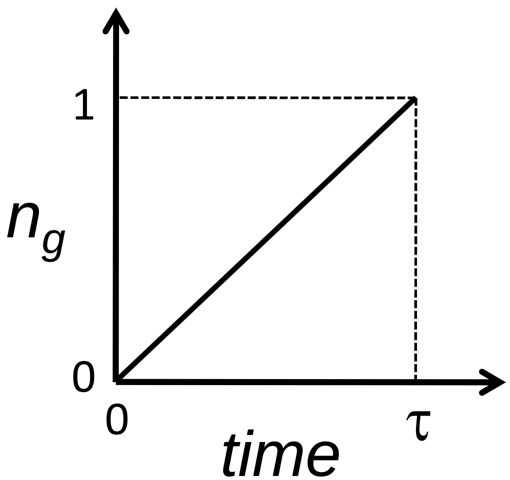
$$Q = 2E_C \sum_i \pm \delta n_{g,i}$$

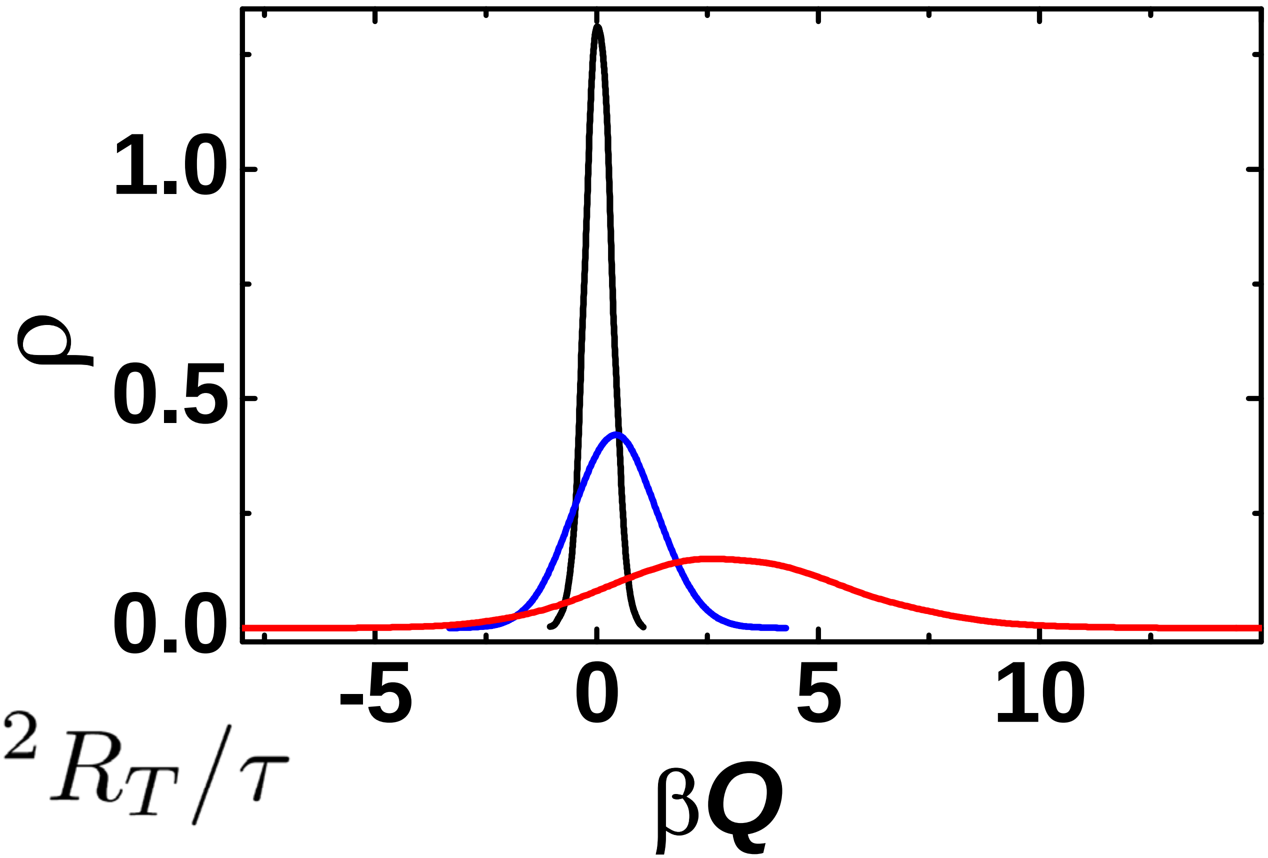
Distribution of heat

Take a normal-metal SEB

$$\Gamma_{\pm} = \pm(G_T/e^2)\Delta U/(1 - e^{\mp\beta\Delta U})$$

with a linear gate ramp





ν = 0.1, 1, 10 (black, blue, red)

$$\nu = 2E_C\beta^2 e^2 R_T/\tau$$

Moments of generated heat

Central moments from the correlation functions of charge, which in turn are obtained from the basic master equation.

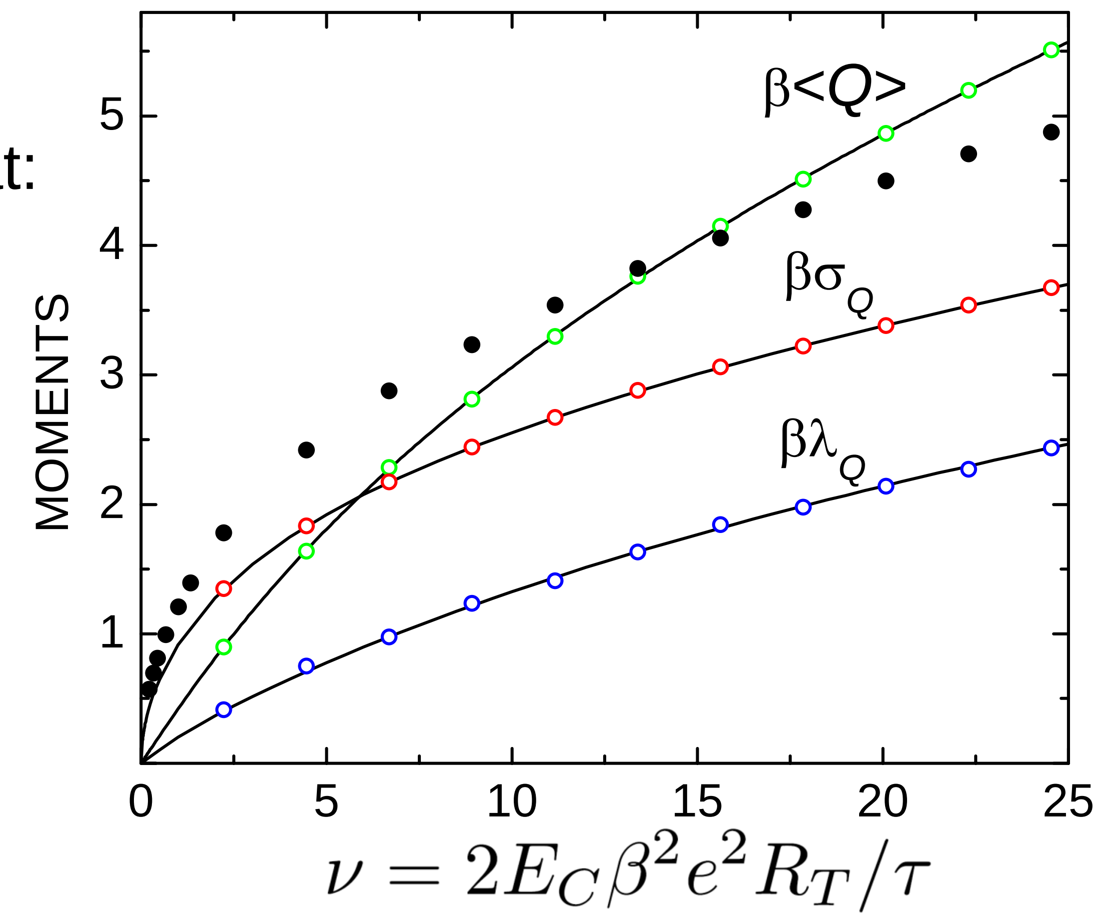
$$\tilde{Q} = Q - \langle Q \rangle$$

Noise of the generated heat:

$$\sigma_Q \equiv \langle \tilde{Q}^2 \rangle^{1/2}$$

The thrird cumulant of the generated heat:

$$\lambda_Q \equiv \langle \tilde{Q}^3 \rangle^{1/3}$$



For slow ramp:

$$\sigma_Q^2 = 2k_B T \langle Q \rangle$$

Fluctuation relations in a single-electron box

$$\langle e^{-\beta(W-\Delta F)}\rangle \stackrel{?}{=} 1$$

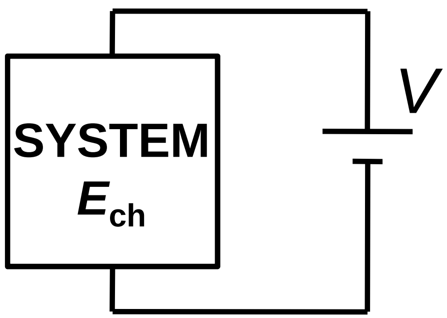
Jarzynski equality

$$\langle e^{-\beta Q}\rangle \stackrel{?}{=} 1$$

H, F and W in the SEB

$$H(n, n_g) = E_{\rm ch} - Q_g V_g$$

This is the energy minimized in a voltage biased circuit $E_{\rm ch} + E_{\rm battery}$



$$= E_{\rm ch} + \left[E_{\rm battery,0} - \int V_g I_g dt\right]$$

$$= E_{\rm ch} - V_g Q_g \; (+E_{\rm battery,0})$$

E_{ch} is the "bare" charging energy of the capacitors $E_{\rm ch} = \sum_i \frac{1}{2} C_i V_i^2$

$$Z(n_g) = e^{-\beta H(0,n_g)} + e^{-\beta H(1,n_g)} \qquad F(n_g) = -\beta^{-1} \ln Z(n_g)$$

Free-energy difference between the end points of the gate voltage trajectory

$$\Delta F = F(n_{g,B}) - F(n_{g,A})$$

Work done (by the gate)

In general: $$W_{\rm th} = \int dt \frac{\partial H}{\partial t} = \int dt \dot{\lambda} \frac{\partial H}{\partial \lambda}$$

For a SEB box:

$$W_{\rm th} = \int V_g dQ_g - Q_g V_g = -\int Q_g dV_g$$

$$W_{\rm th} - \Delta F = E_C (1 - 2 \int_0^1 n dn_g)$$

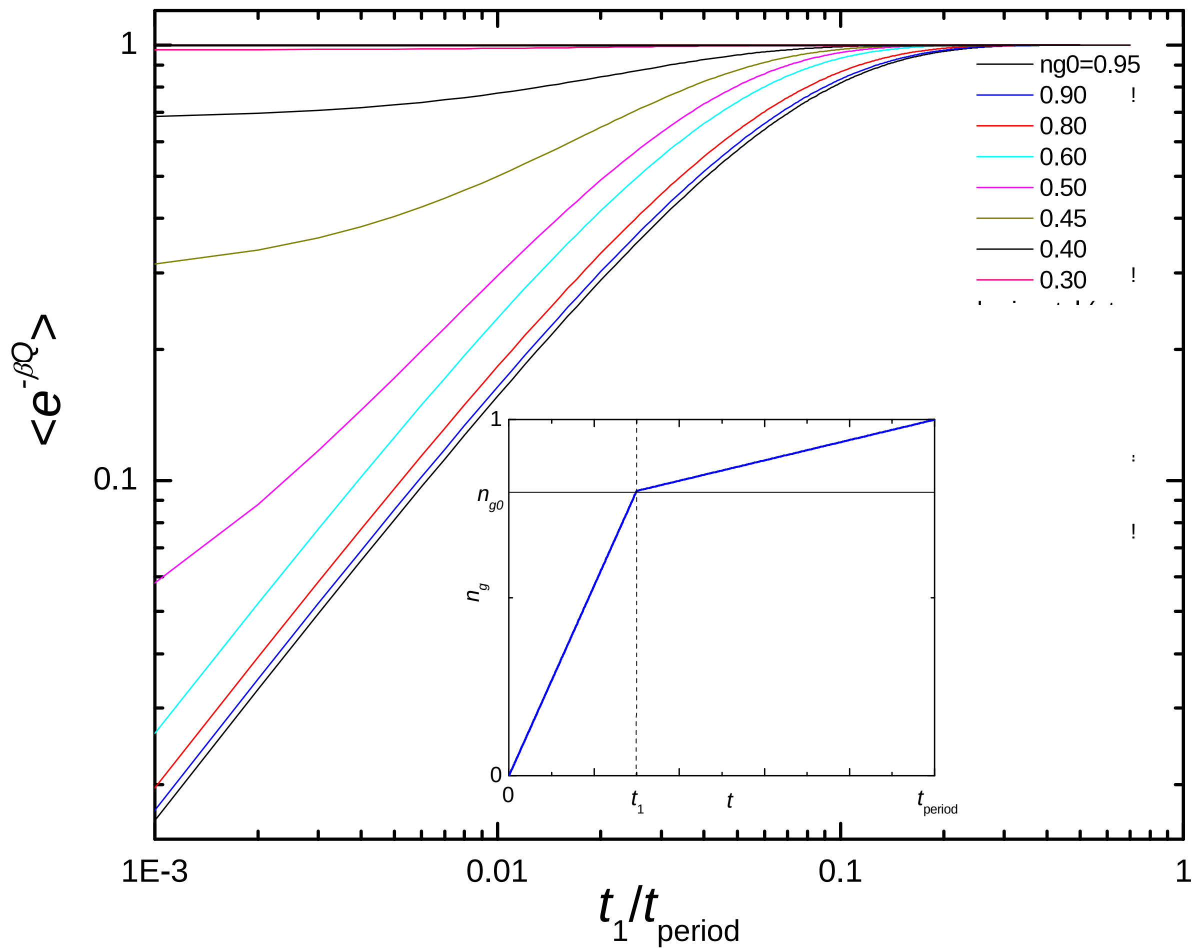
for the gate sweep 0 -> 1

This is to be compared to: $$Q = 2E_C \sum_i \pm \delta n_{g,i}$$

Evaluation of $\langle e^{-\beta Q} \rangle$

$$\langle e^{-\beta Q} \rangle = \sum_{i,f} p_i \, w(f \to i)$$

(By similar arguments as Crooks, 1998)



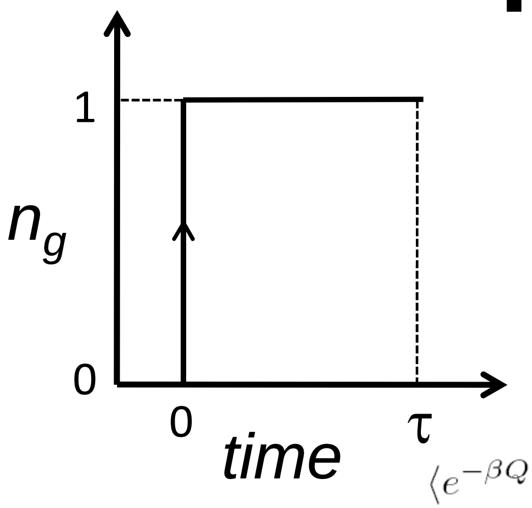
For symmetric trajectories (linear ramp, harmonic drive around the degeneracy,...)

$$\langle e^{-\beta Q} \rangle = 1$$

In general

$$\langle e^{-\beta Q} \rangle \leq 1$$

Example: Abrupt trajectory



Assume long equilibration time before and after the jump:

$$
\begin{aligned}
\langle e^{-\beta Q}\rangle &= p_i(0)p_f(0|n_i=0)e^{-\beta Q_{0\to 0}} + p_i(0)p_f(1|n_i=0)e^{-\beta Q_{0\to 1}} \\
&+ p_i(1)p_f(0|n_i=1)e^{-\beta Q_{1\to 0}} + p_i(1)p_f(1|n_i=1)e^{-\beta Q_{1\to 1}} \\
&= \frac{e^{\beta E_C}}{1+e^{\beta E_C}}\frac{1}{1+e^{\beta E_C}}\cdot 1 + \frac{e^{\beta E_C}}{1+e^{\beta E_C}}\frac{e^{\beta E_C}}{1+e^{\beta E_C}}e^{-\beta E_C} \\
&+ \frac{1}{1+e^{\beta E_C}}\frac{1}{1+e^{\beta E_C}}e^{\beta E_C} + \frac{1}{1+e^{\beta E_C}}\frac{e^{\beta E_C}}{1+e^{\beta E_C}}\cdot 1 = \frac{4e^{\beta E_C}}{(1+e^{\beta E_C})^2} \ll 1
\end{aligned}
$$

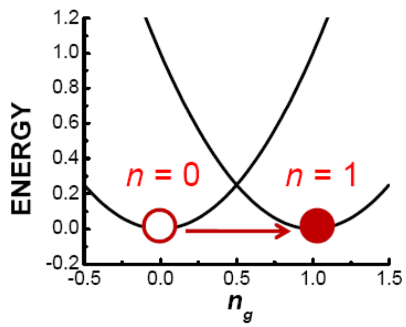
$$
\begin{aligned}
\langle e^{-\beta(W_{\rm th}-\Delta F)}\rangle &= p_i(0)p_f(0|n_i=0)e^{-\beta(W_{\rm th}-\Delta F)_{0\to 0}} + p_i(0)p_f(1|n_i=0)e^{-\beta(W_{\rm th}-\Delta F)_{0\to 1}} \\
&+ p_i(1)p_f(0|n_i=1)e^{-\beta(W_{\rm th}-\Delta F)_{1\to 0}} + p_i(1)p_f(1|n_i=1)e^{-\beta(W_{\rm th}-\Delta F)_{1\to 1}} \\
&= \frac{e^{\beta E_C}}{1+e^{\beta E_C}}\frac{1}{1+e^{\beta E_C}}e^{-\beta E_C} + \frac{e^{\beta E_C}}{1+e^{\beta E_C}}\frac{e^{\beta E_C}}{1+e^{\beta E_C}}e^{-\beta E_C} \\
&+ \frac{1}{1+e^{\beta E_C}}\frac{1}{1+e^{\beta E_C}}e^{\beta E_C} + \frac{1}{1+e^{\beta E_C}}\frac{e^{\beta E_C}}{1+e^{\beta E_C}}e^{\beta E_C} = 1.
\end{aligned}
$$

Single-electron box with an arbitrary n_g: 0 -> 1 gate ramp

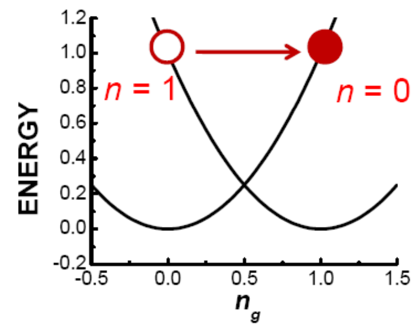
Jarzynski equality:

The generated heat Q is not always equal to $(W_{\text{th}} - \Delta F)$:

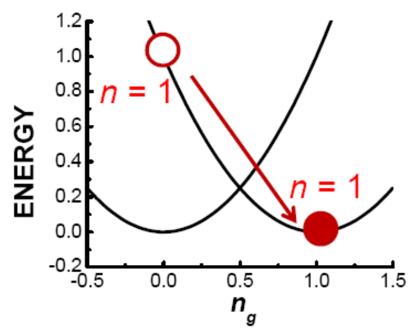
$(W_{\text{th}} - \Delta F)_{0\to 1} = Q$



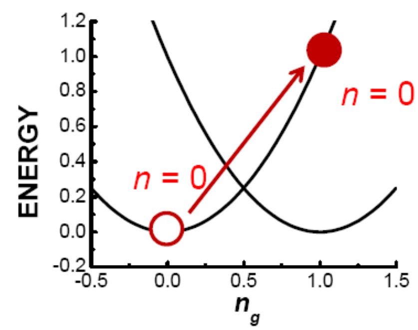
$(W_{\text{th}} - \Delta F)_{1\to 0} = Q$



$(W_{\text{th}} - \Delta F)_{1\to 1} = Q - E_C$



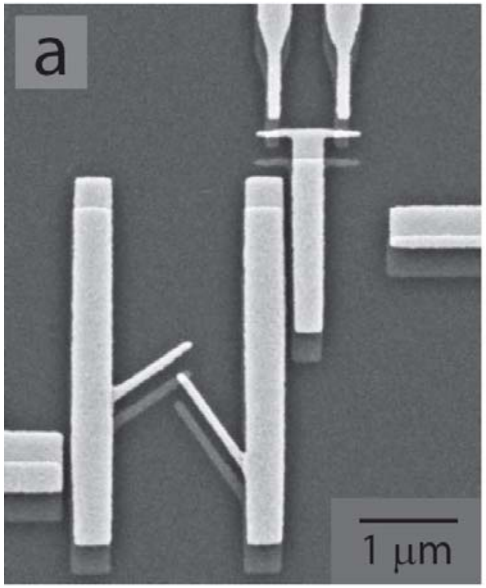
$(W_{\text{th}} - \Delta F)_{0\to 0} = Q + E_C$

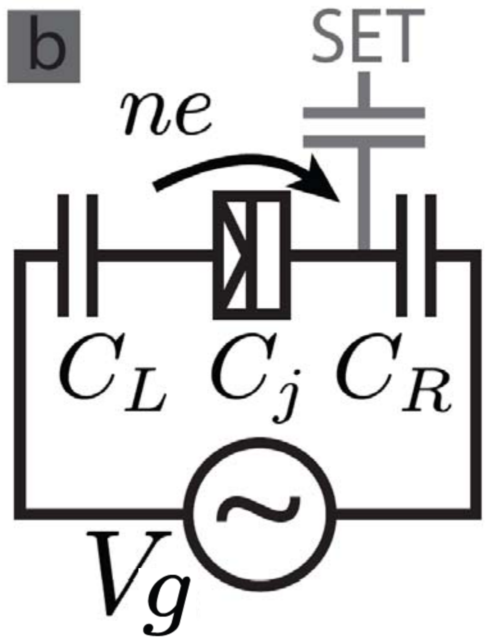


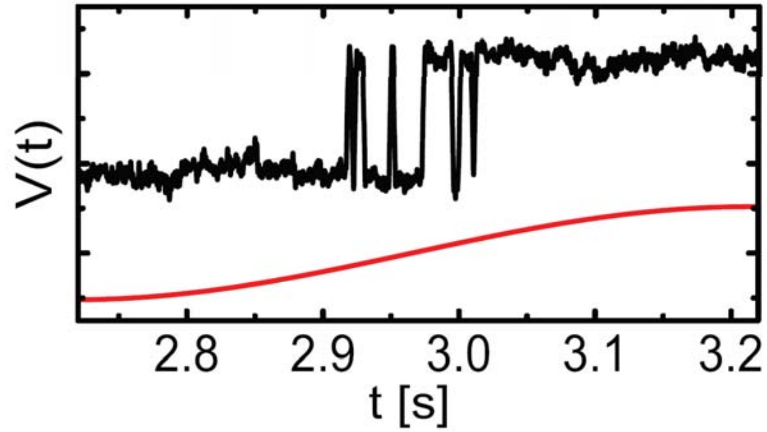
This difference yields for an arbitrary trajectory: $\langle e^{-\beta(W_{\text{th}} - \Delta F)} \rangle = 1$

Experiment in a single-electron box

O.-P. Saira, Y. Yoon et al., in preparation

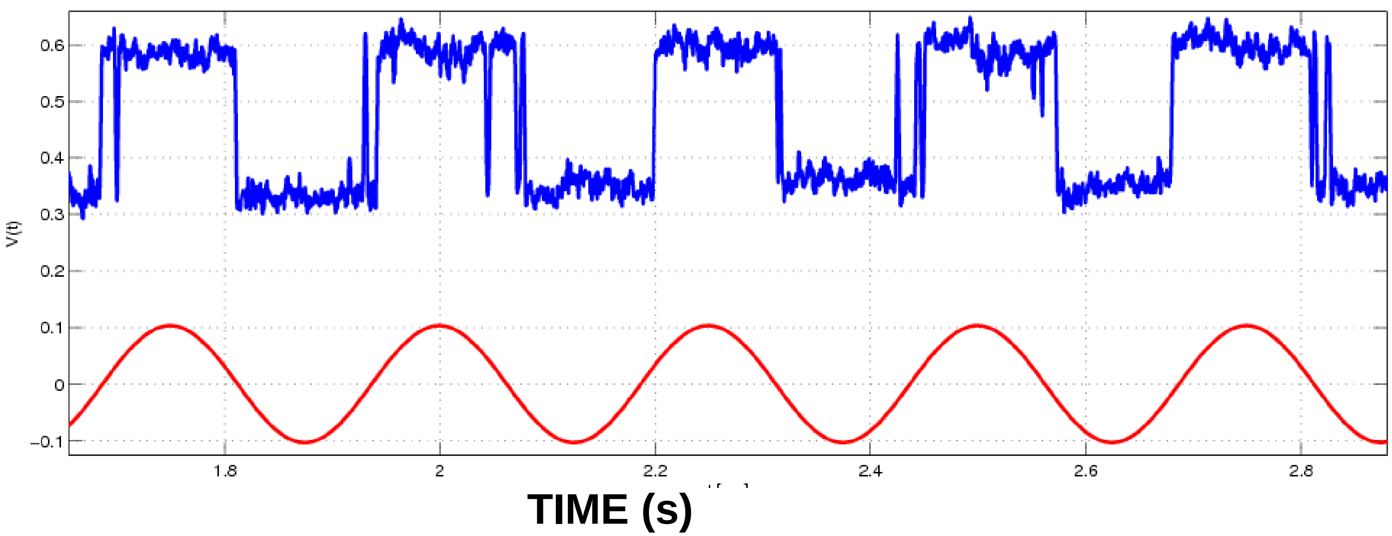




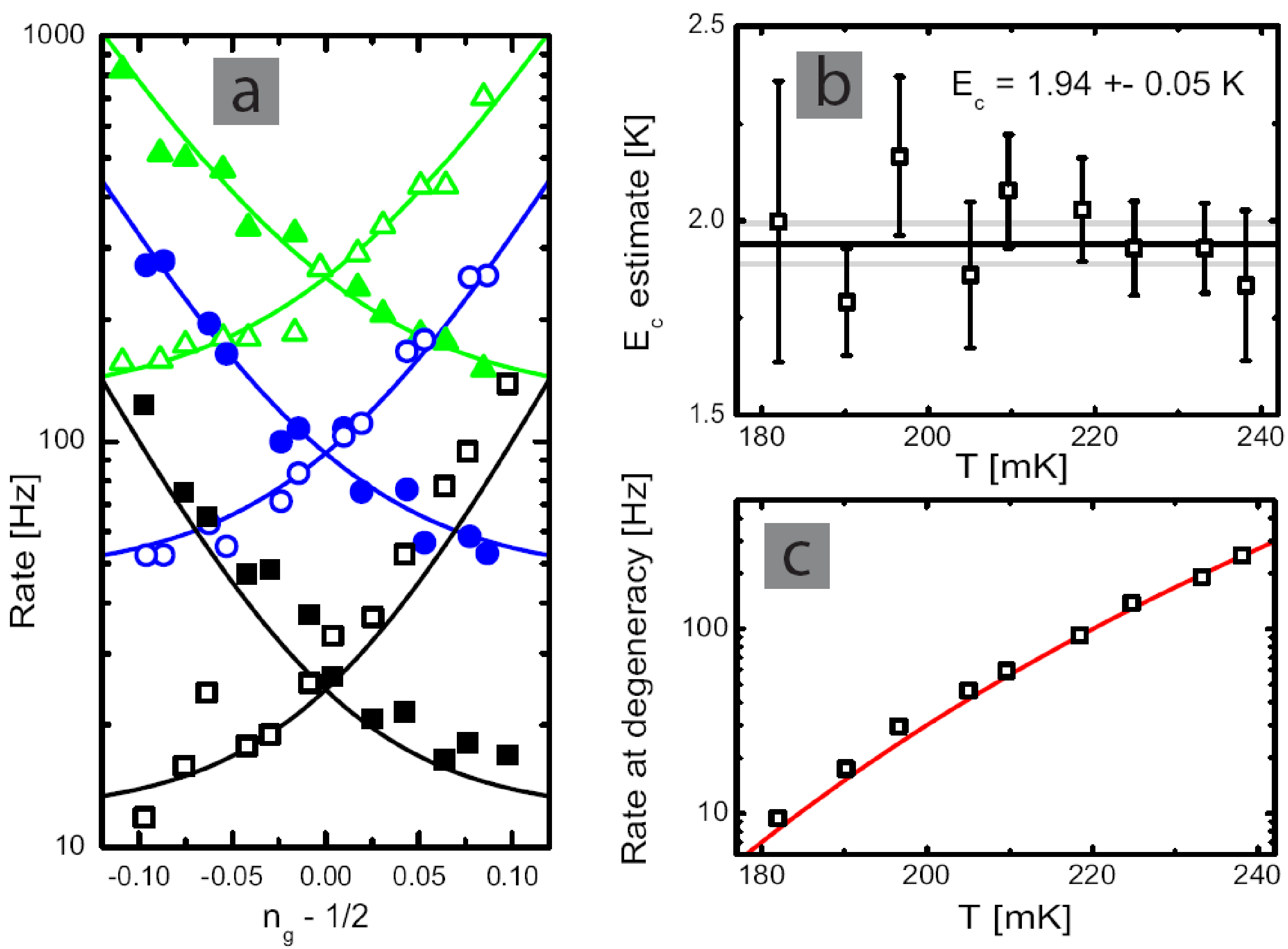


Detector current

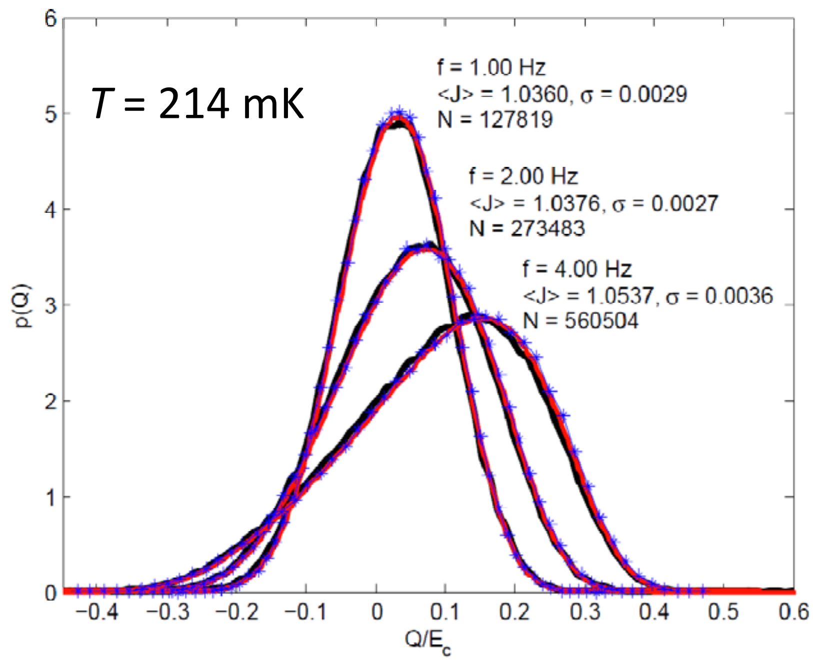
Gate drive

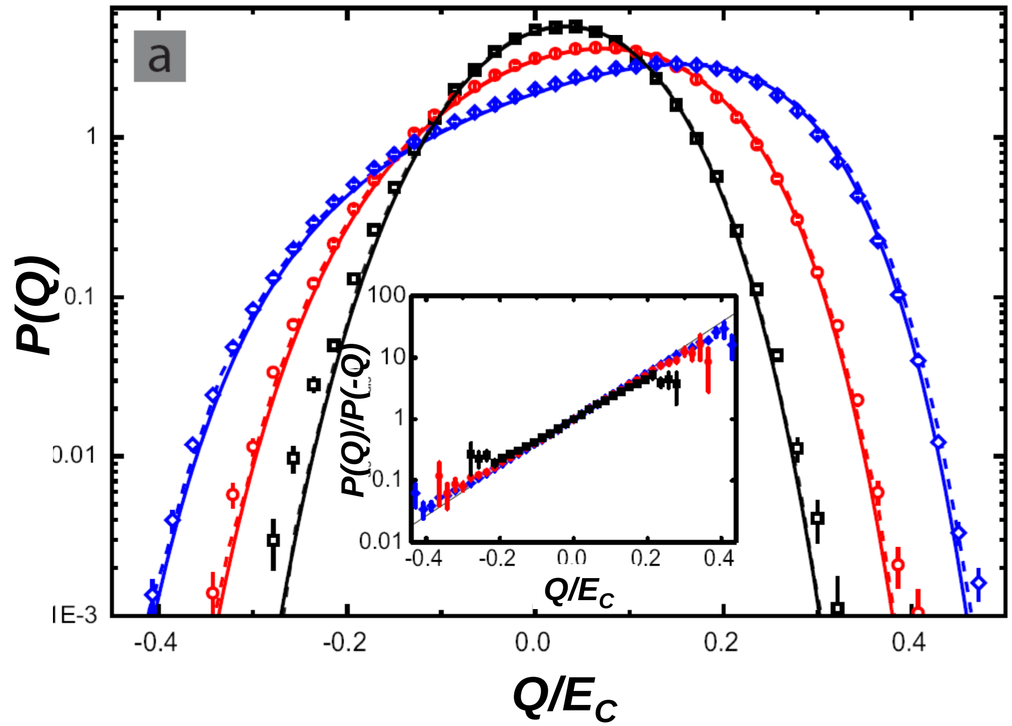


Calibrations



Experimental distributions

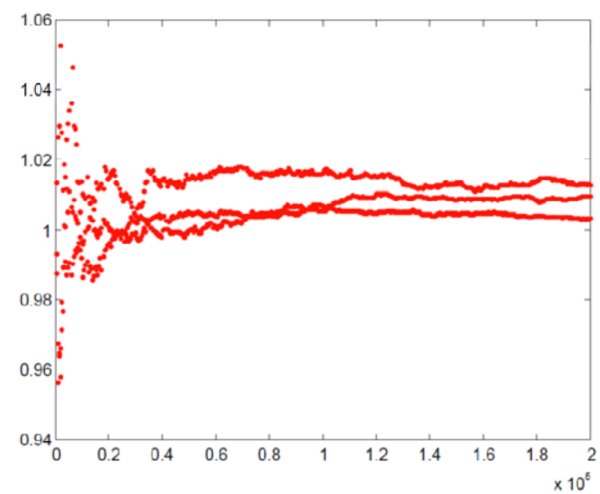




Measured distributions of *Q* at three different ramp frequencies

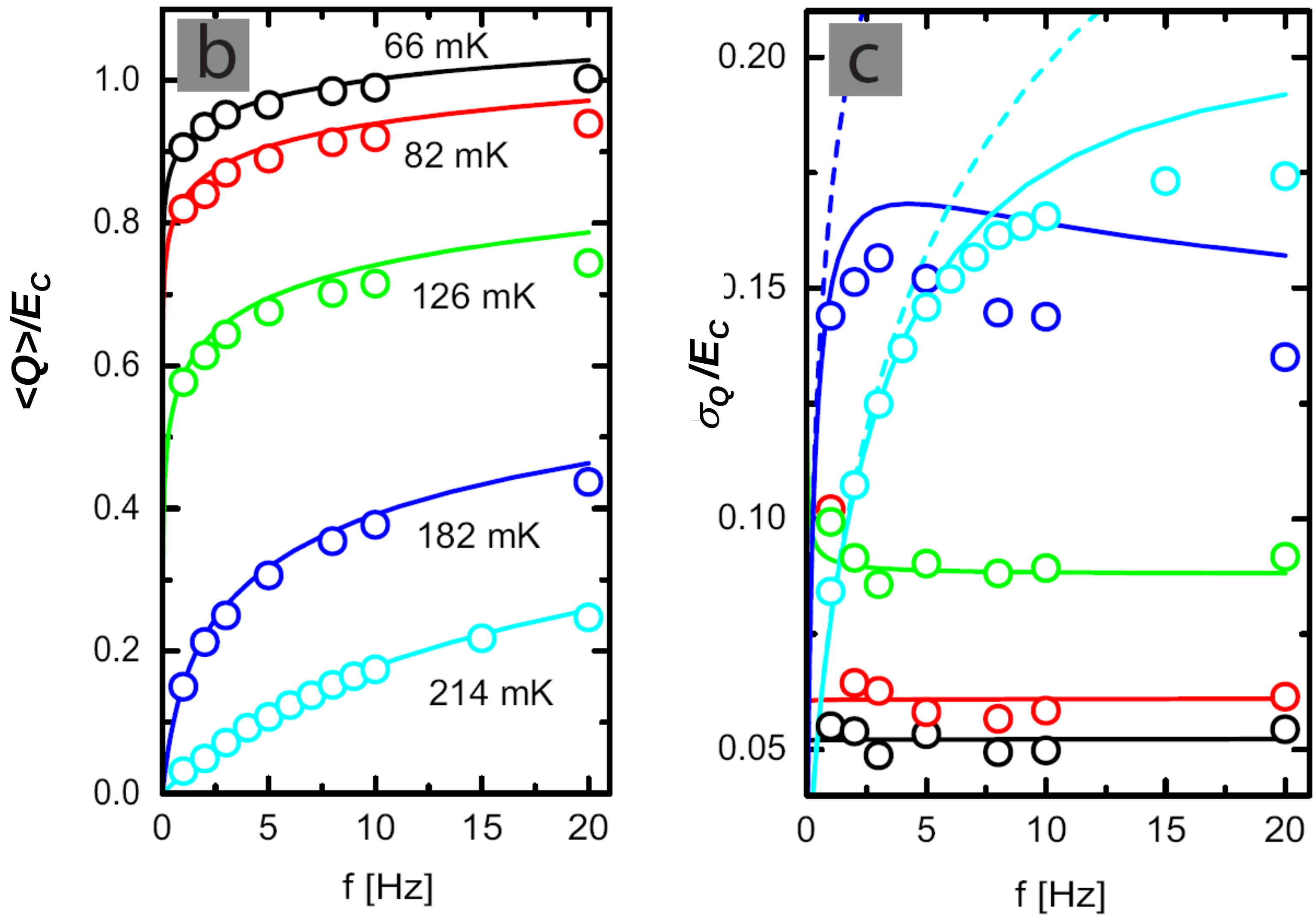
Taking the finite bandwidth of the detector into account yields

$$\langle e^{-\beta(W-\Delta F)}\rangle = 1 \pm 0.03$$

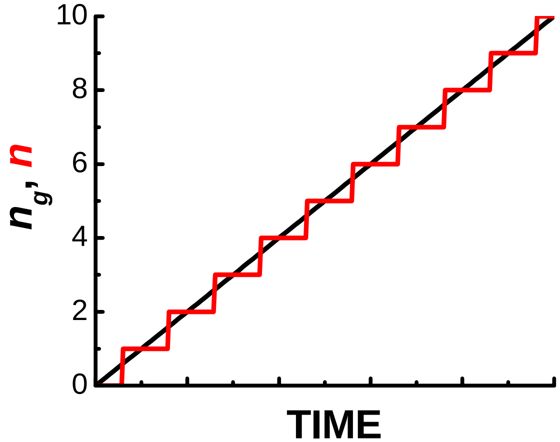


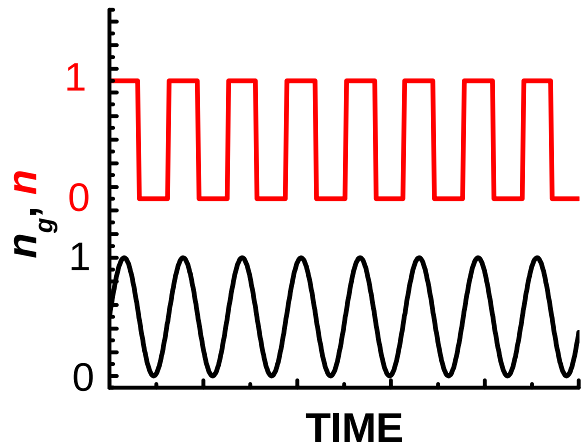
Measurements of the heat distributions at various frequencies and temperatures

symbols: experiment; full lines: theory; dashed lines: $\sigma_Q^2 = 2k_B T\langle Q\rangle$

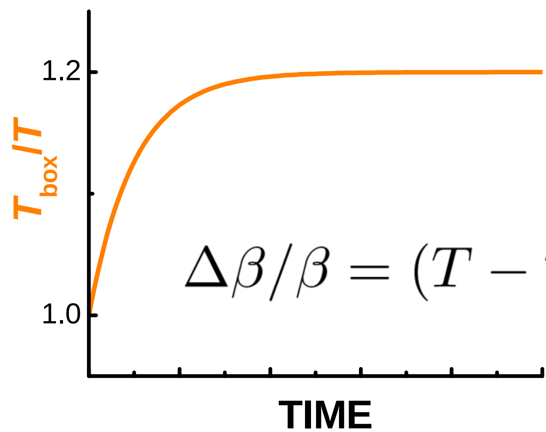


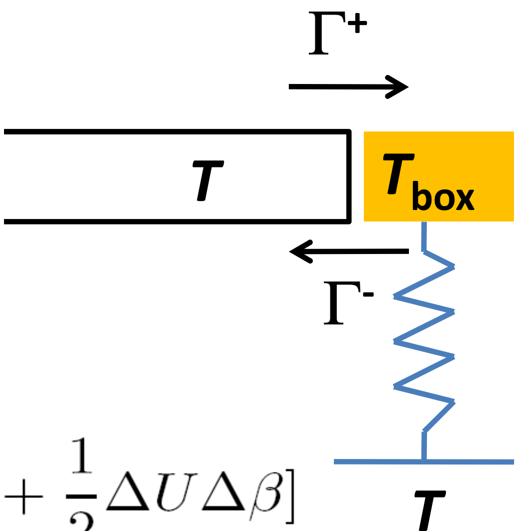
Single-electron box with an overheated island (predictions)





Linear or harmonic drive across many transitions





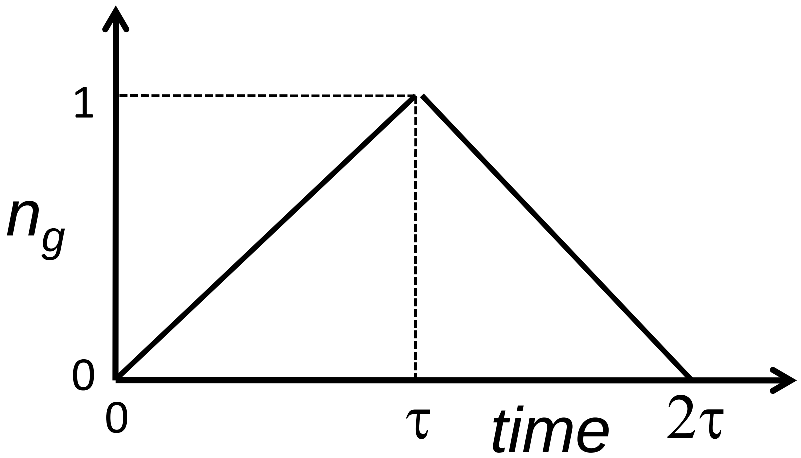
$$\Delta\beta/\beta = (T - T_{\mathrm{box}})/T$$

$$\frac{\Gamma^+}{\Gamma^-} \simeq e^{\beta\Delta U}[1 + \frac{1}{2}\Delta U \Delta\beta]$$

$$\Gamma^+/\Gamma^- \neq e^{\beta\Delta U}$$

$$\langle e^{-\beta(W_{\mathrm{th}} - \Delta F)}\rangle \simeq 1 - \frac{1}{2}\langle Q\rangle\Delta\beta$$

Back-and-forth ramp with heating



Assume one transition in each leg

$$\langle e^{-\beta(W-\Delta F)}\rangle = \int_{-\infty}^{\infty} dE \int_0^{2\tau} d\tau_2 \int_0^{\tau_2} d\tau_1 e^{-\beta[\Delta U(\tau_1)-\Delta U(\tau_2)]} e^{-\int_0^{\tau_1}\Gamma_+(\Delta U(\tau'),T_0)d\tau'} \gamma_+(E,\tau_1) e^{-\int_{\tau_1}^{\tau}\Gamma_-(\Delta U(\tau'),T(E))d\tau'}$$
$$e^{-\int_{\tau}^{\tau_2}\Gamma_-(\Delta U(\tau'),T(E))d\tau'}\Gamma_-(\Delta U(\tau_2),T(E)) e^{-\int_{\tau_2}^{2\tau}\Gamma_+(\Delta U(\tau'),T(E))d\tau'}.$$

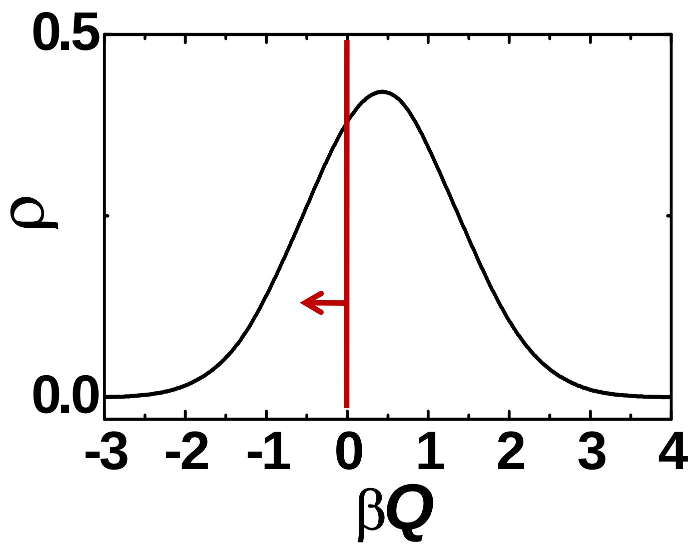
$$\gamma_+(E,\tau_1) = \frac{1}{e^2 R_T} f(E-\Delta U(\tau_1))[1-f(E)] \qquad \frac{T(E)-T_0}{T_0} = \frac{E}{E_C}(\frac{\Delta T}{T})_0$$

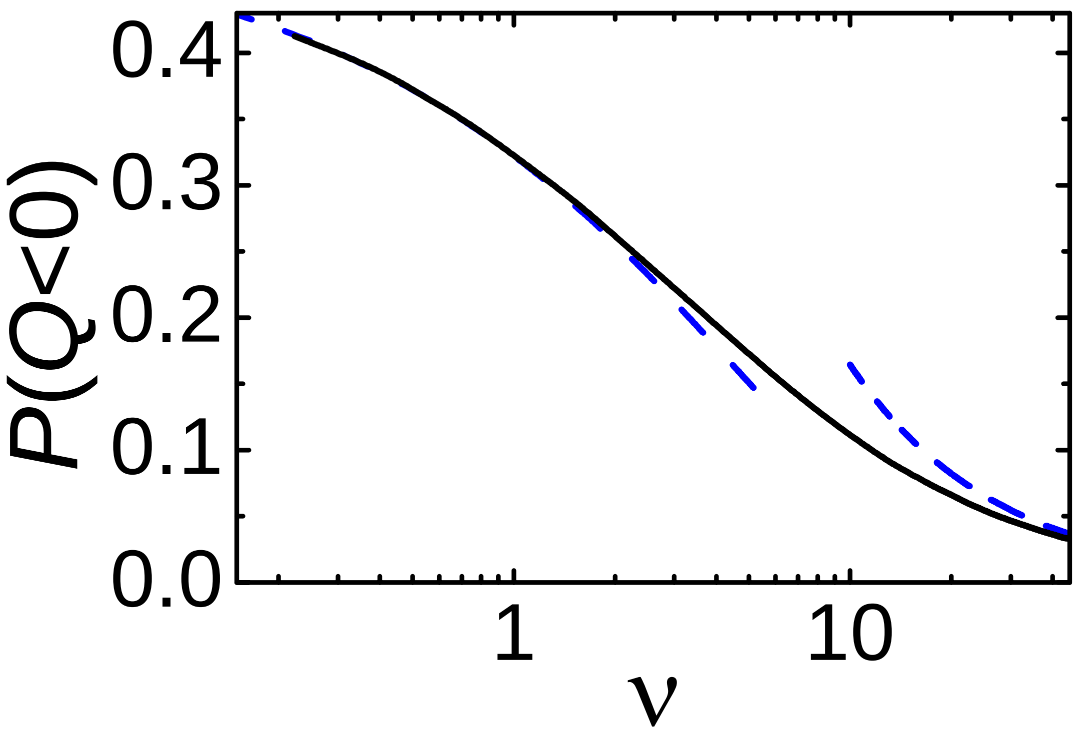
$$\langle e^{-\beta(W-\Delta F)}\rangle \simeq 1 - \frac{\beta\langle\Delta U\rangle^2}{4E_C}(\frac{\Delta T}{T})_0$$

Maxwell's demon

Negative heat

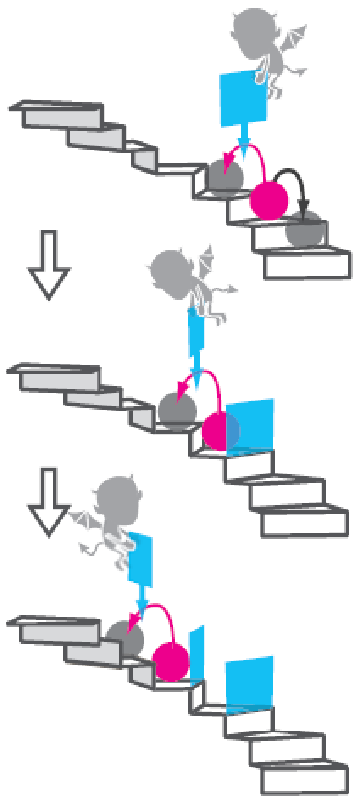
Possible to extract heat from the bath



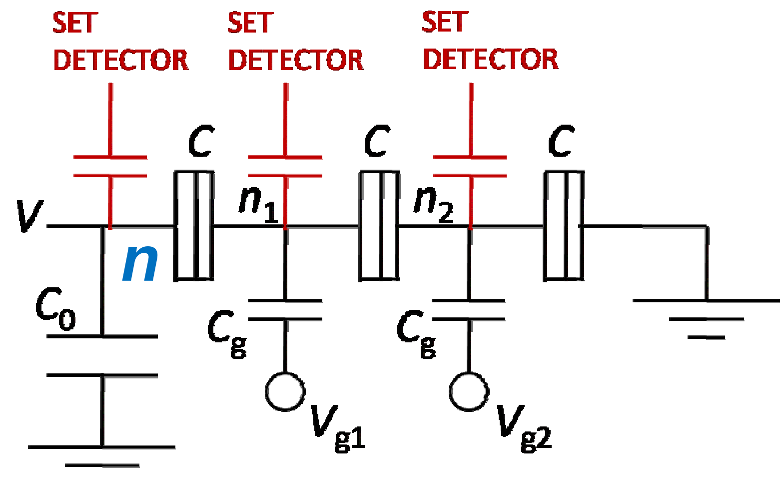


Provides means to make Maxwell's demon using SETs

Maxwell’s demon in an SET trap

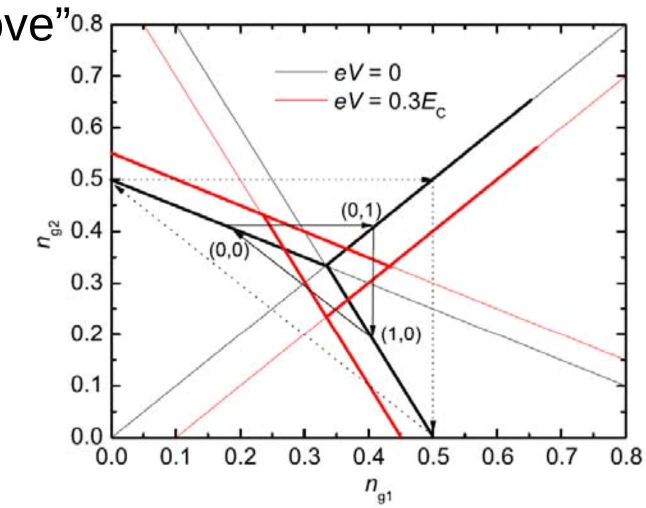


S. Toyabe et al., Nature Physics 2010

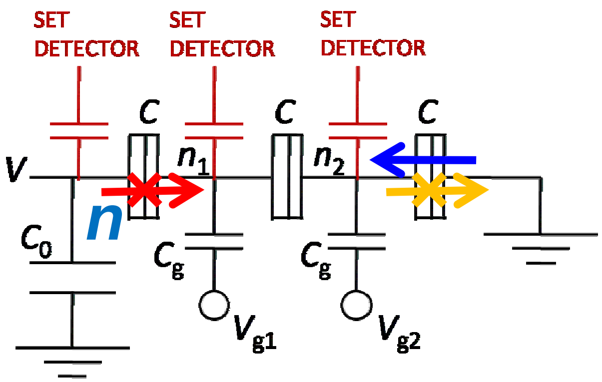


D. Averin, M. Mottonen, J. Pekola, arXiv:1108.5435
see also: G. Schaller et al., PRB (2011)

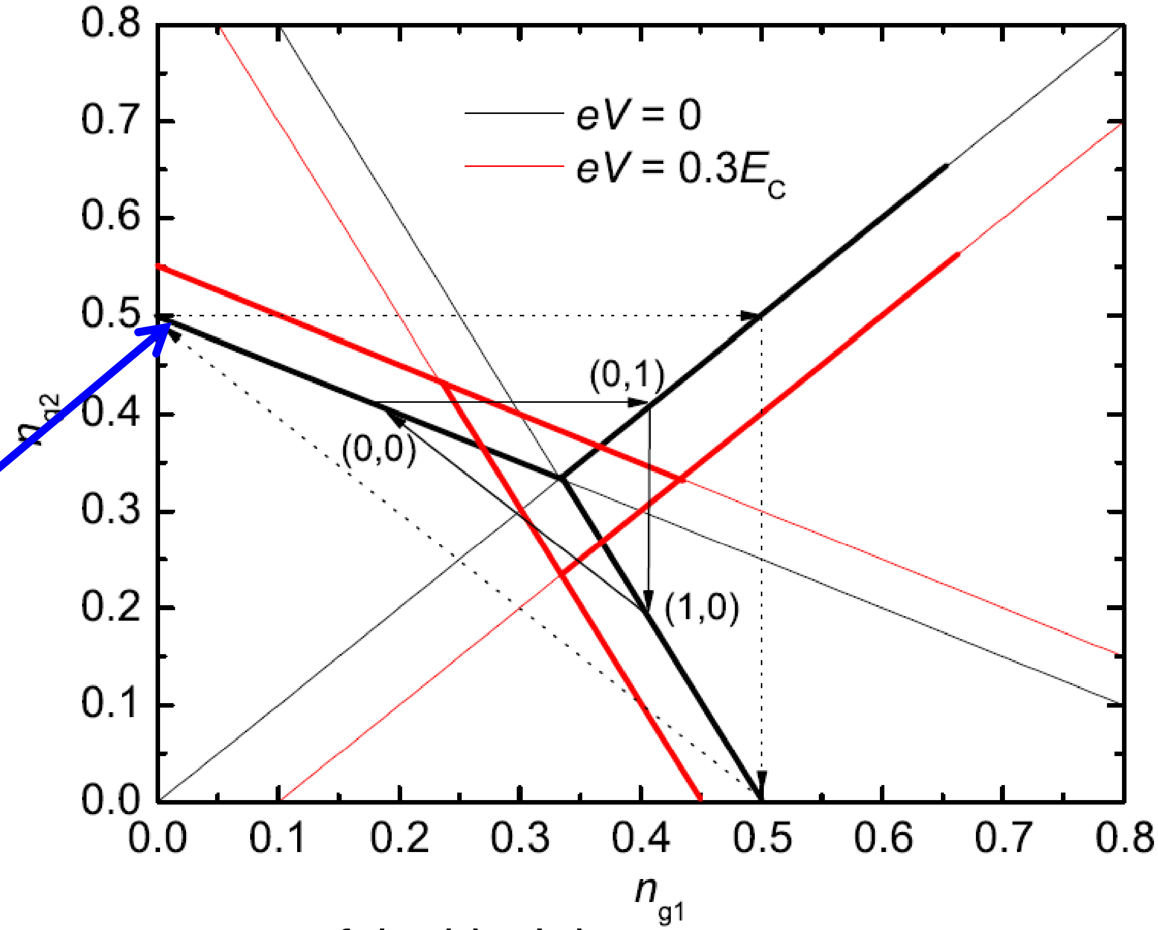
”watch and move”



Demon strategy



Adiabatic ”informationless” pumping: $W = eV$ per cycle
Ideal demon: $W = 0$



Energy costs for the transitions:

$$\Delta U_{1,+} = E_C/2 - eV/3$$
$$\Delta U_{3,-} = eV/3$$

Rate of return (0,1)->(0,0) determined by the energy ”cost” $-eV/3$. If $\Gamma(-eV/3) \ll \tau^{-1}$, the demon is ”successful”. Here τ^{-1} is the bandwidth of the detector. This is easy to satisfy using NIS junctions.

Power of the ideal demon:

$$P = (eV/3)\Gamma(eV/3)$$

Temperature fluctuations

Fluctuation dissipation theorems (FDT)

Classical noise in equilibrium

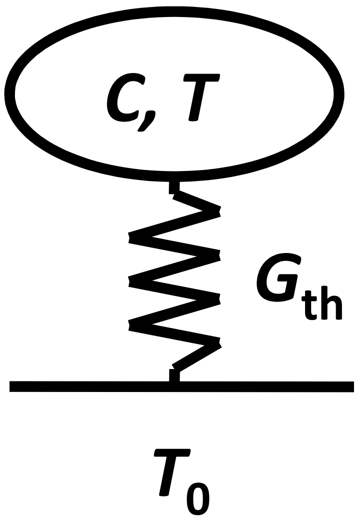
Charge current:

$$I = GV \qquad S_I = 4k_B T G$$

Energy current:

$$\dot{Q} = G_{\mathrm{th}} \Delta T \qquad S_{\dot{Q}} = 2k_B T^2 G_{\mathrm{th}}$$

Classical temperature fluctuations



Assume that T_0 is equal to the average of T (equilibrium fluctuations)

$$S_{\dot{Q}} = 2k_B T^2 G_{\mathrm{th}}$$

(fluctuation-dissipation theorem)

$$\dot{Q} = C\dot{T} + G_{\mathrm{th}}(T - T_0)$$

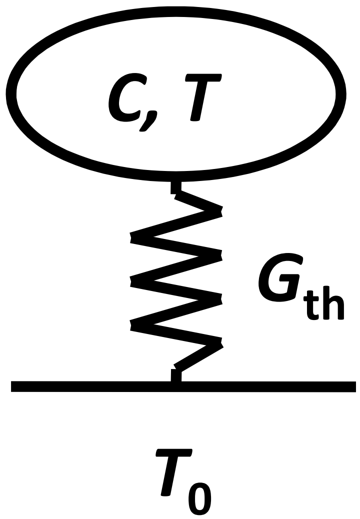
(balance equation)

$$S_{\dot{Q}} = \omega^2 C^2 S_T + G_{\mathrm{th}}^2 S_T$$

(Fourier transform into noise spectra)

$$S_T = \frac{S_{\dot{Q}}}{\omega^2 C^2 + G_{\mathrm{th}}^2}$$

Classical temperature fluctuations

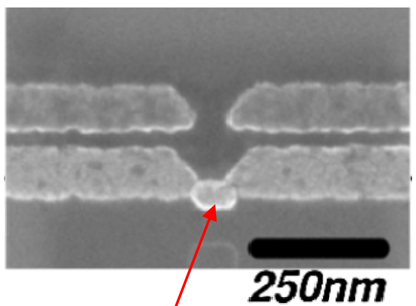


$$S_T(\omega) = \frac{2k_B T^2}{G_{\rm th}} \frac{1}{1+\omega^2 C^2/G_{\rm th}^2}$$

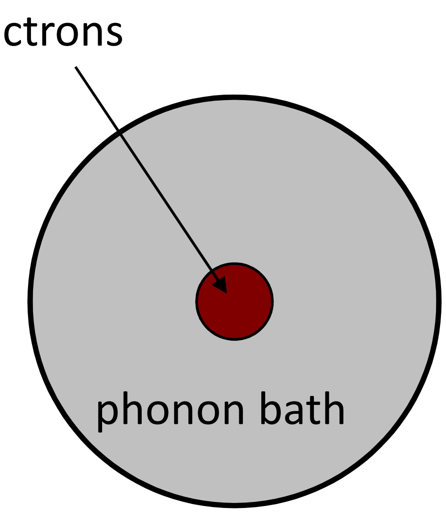
$$\omega_c = G_{\rm th}/C$$

$$\langle \delta T^2 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} S_T(\omega) = k_B T^2/C$$

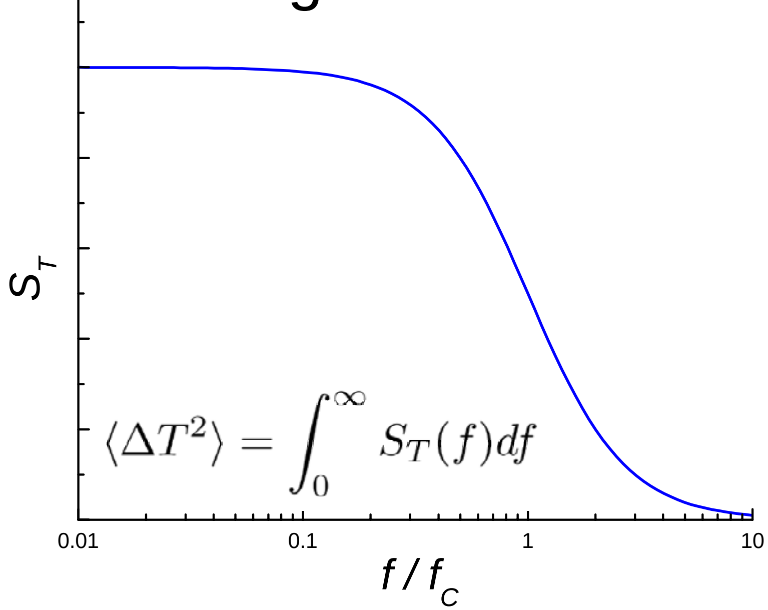
Example system: electrons in the phonon bath



$$\langle \Delta T^2 \rangle \propto T/\mathcal{V}$$

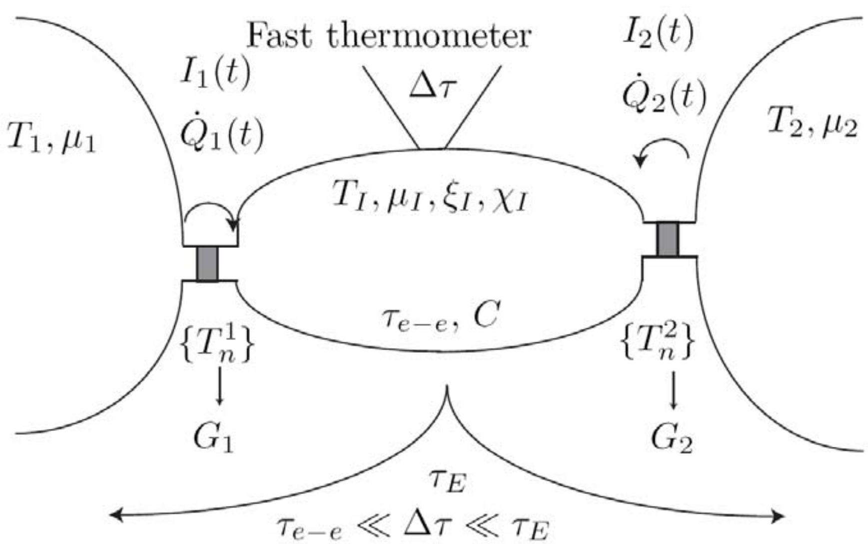


In this grain at T = 100 mK, $\langle \Delta T^2 \rangle$ = (10 mK)^2.

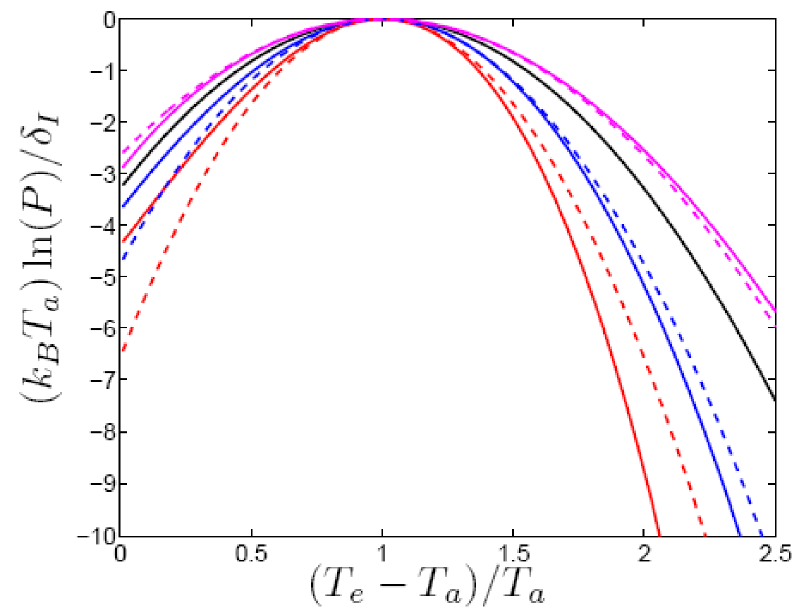


Cut-off frequency f_c determined by electron-phonon relaxation rate, it varies in the range 10 kHz – 10 MHz: suitable for a measurement.

Non-equilibrium temperature fluctuations



Set-up

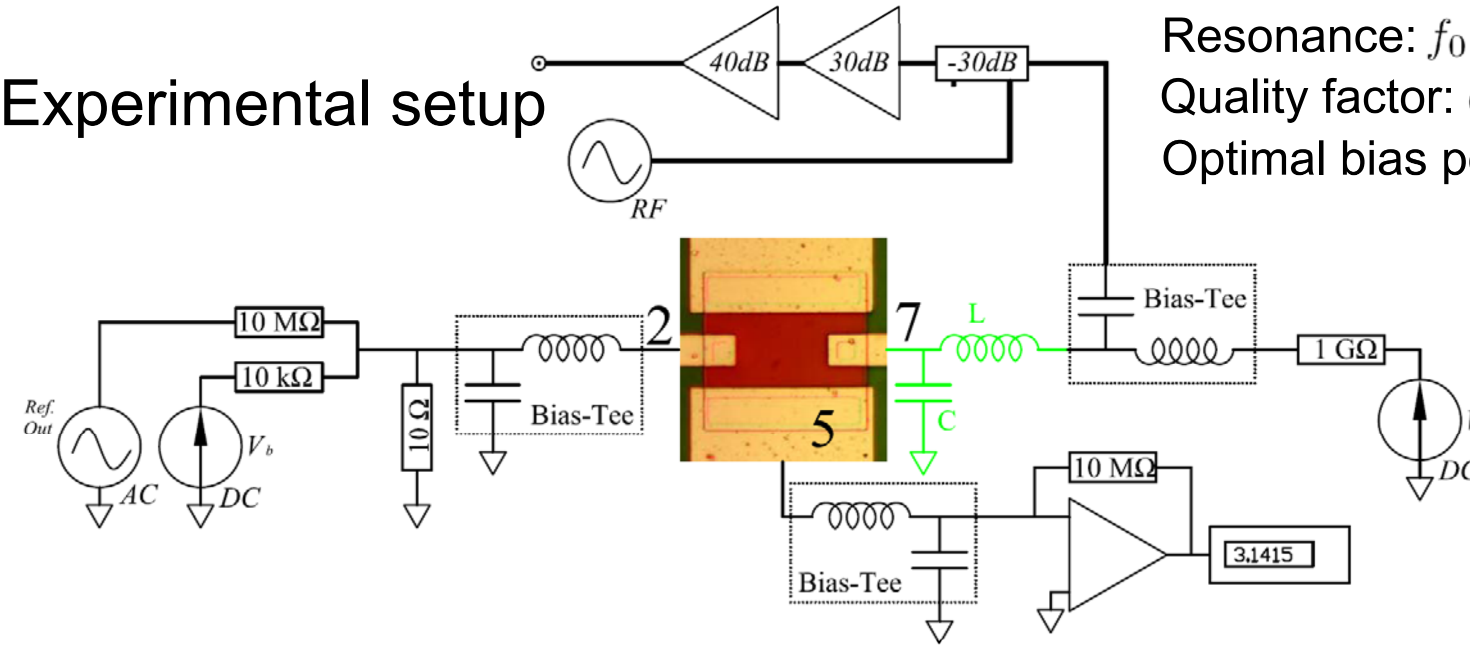


Result, non-gaussian distributions under *T* and *V* bias

Heikkilä and Nazarov, PRL **102**, 130605 (2009)
Laakso, Heikkilä and Nazarov, PRL **104**, 196805 (2010)

Preliminary measurements

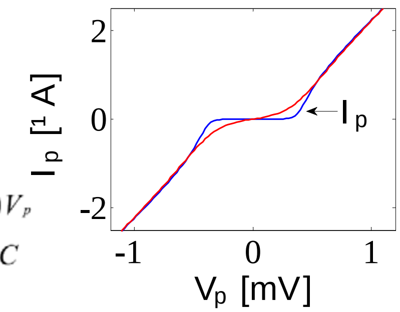
Experimental setup



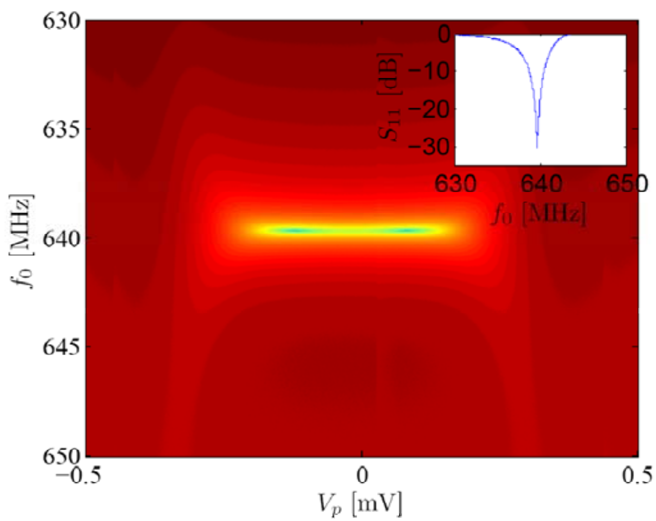
Resonance: $f_0 = 639\,\mathrm{MHz}$

Quality factor: $Q = 280$

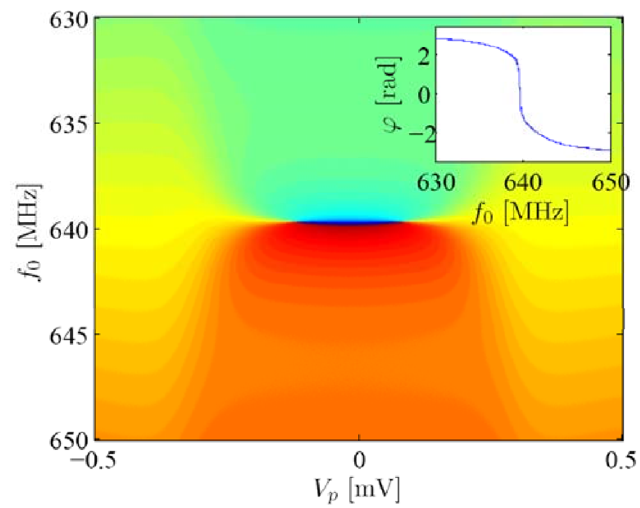
Optimal bias point: $I_p = 0$



Magnitude response:



Phase response:



Summary

Work and heat in driven single-electron transitions analyzed

Fluctuation relations tested analytically, numerically and experimentally

Experiments on an overheated SEB, Maxwell's demon and temperature fluctuations to be done/in progress

Quantum fluctuation relations for superconducting systems?

Landau-Lifshitz, Statistical Physics, Part 2

We can also write out formulae (88.16)–(88.18) in Fourier components with respect to frequency, and we shall do this in a form which generalizes them to the case of quantum fluctuations. According to the general rules of the fluctuation–dissipation theorem, such a generalization is obtained by including an extra factor $(\hbar\omega/2T)\coth(\hbar\omega/2T)$ (which is unity in the classical limit $\hbar\omega \ll T$). In the presence of dispersion of the viscosity and thermal conductivity, the quantities η, ζ and $\varkappa$ are complex functions of the frequency; in the formulae for the fluctuations, they are replaced by the real parts of those functions:

$$(s_{ik}^{(1)} g_l^{(2)})_\omega = 0, \tag{88.19}$$

$$(g_i^{(1)} g_k^{(2)})_\omega = \delta_{ik}\delta(\mathbf{r}_1-\mathbf{r}_2)\hbar\omega T \coth(\hbar\omega/2T)\,\mathrm{re}\,\varkappa(\omega), \tag{88.20}$$

$$(s_{ik}^{(1)} s_{lm}^{(2)})_\omega = \hbar\omega\delta(\mathbf{r}_1-\mathbf{r}_2)\coth(\hbar\omega/2T)\times$$
$$\times[(\delta_{il}\delta_{km}+\delta_{im}\delta_{kl}-\tfrac{2}{3}\delta_{ik}\delta_{lm})\,\mathrm{re}\,\eta(\omega)+\delta_{ik}\delta_{lm}\,\mathrm{re}\,\zeta(\omega)]. \tag{88.21}$$

LL predictions

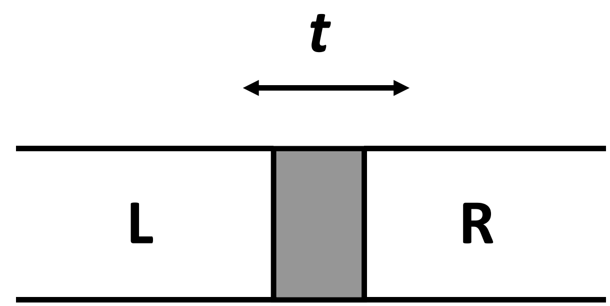
$$S_I(\omega) = 2\hbar\omega \coth(\frac{\hbar\omega}{2k_B T})G$$

Classical: $S_I = 4k_B T G$

$$S_{\dot{Q}}(\omega) = \hbar\omega T \coth(\frac{\hbar\omega}{2k_B T})G_{\rm th}$$

Classical: $S_{\dot{Q}} = 2k_B T^2 G_{\rm th}$

A tunnel junction as a heat conductor



Heat conductance at finite frequencies:

$$\Re\mathrm{e}G_{\mathrm{th}}(\omega) = \frac{\pi^2 G k^2 T}{3e^2}$$

at all frequencies, Wiedemann-Franz law, $G = 1/R_T$

$$S_{\dot{Q}}(\omega) = \hbar\omega T \coth(\hbar\omega/2kT)\Re\mathrm{e}G_{\mathrm{th}}(\omega) + \frac{G}{12e^2}(\hbar\omega)^3 \coth(\hbar\omega/2kT)$$

According to LL:

$$S_{\dot{Q}}(\omega) \to 0,\ T \to 0$$

According to the scattering calculation, or by tunnel hamiltonian based calculation:

$$S_{\dot{Q}}(\omega) \to \frac{G}{12e^2}(\hbar\omega)^3,\ T \to 0$$

D. Averin and J. Pekola, PRL 104, 220601 (2010), D. Sergi, PRB 83, 033401 (2011), Zhan, Denisov and Hänggi, arXivv:1107.3434.

The energy distribution of electrons in a small metal conductor

The distribution is determined by energy relaxation:

Equilibrium –**Thermometer measures the temperature of the bath**

Quasi-equilibrium –**Thermometer measures the temperature of the electron system which can be different from that of the bath**

Non-equilibrium –**There is no temperature to be measured by the electron thermometer**

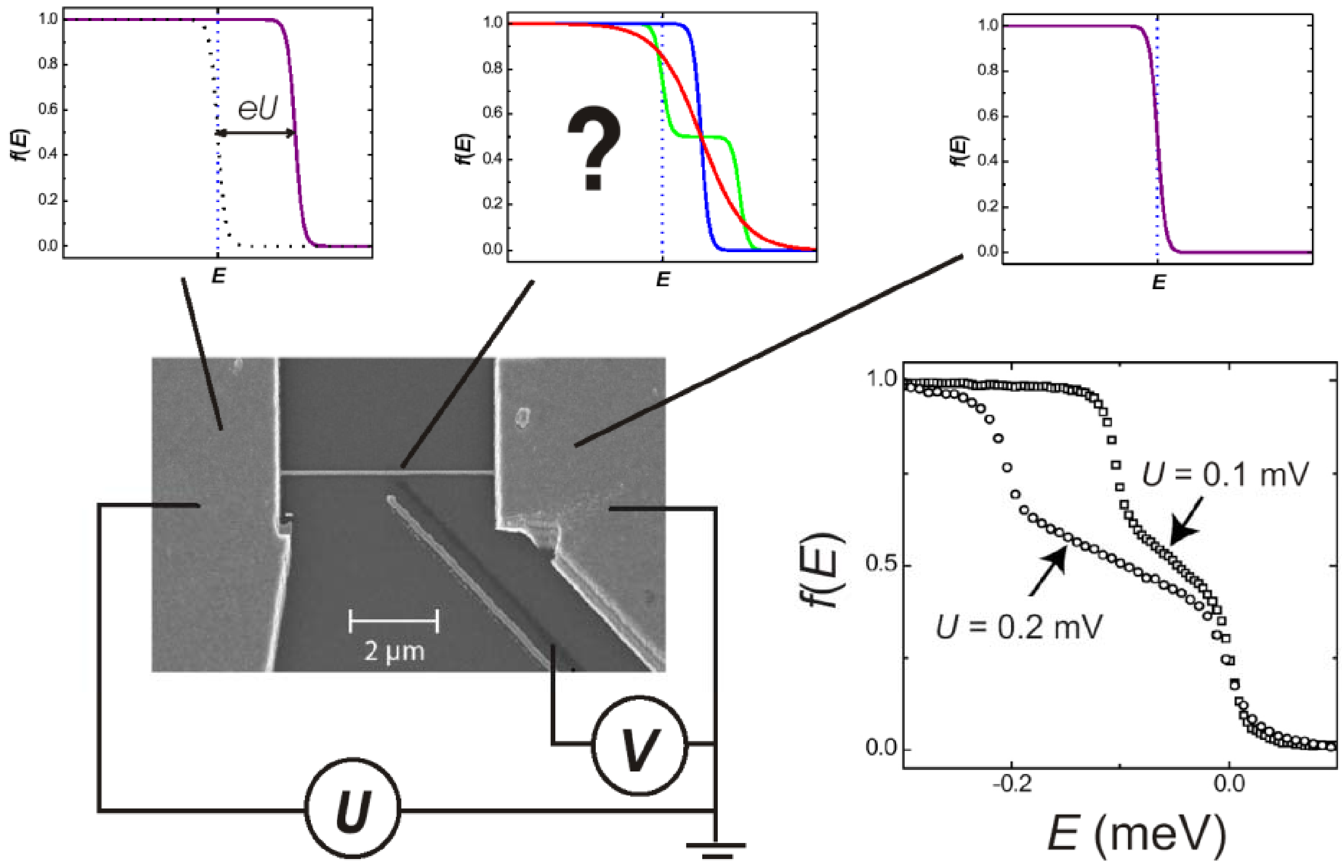
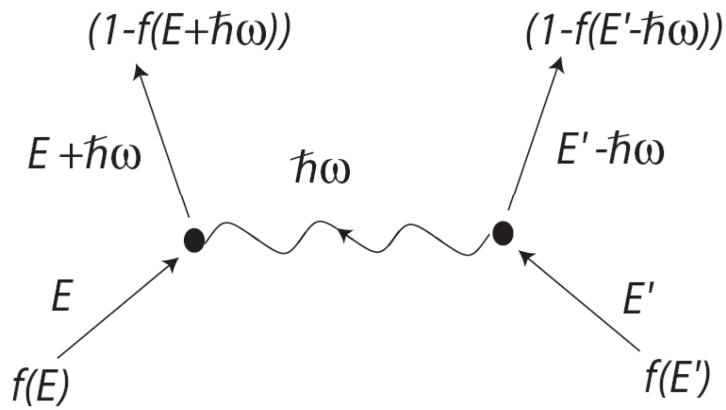
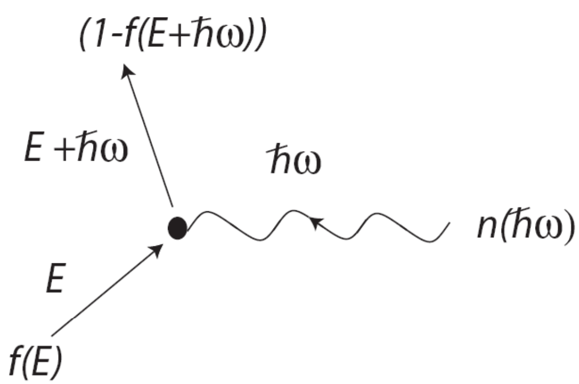


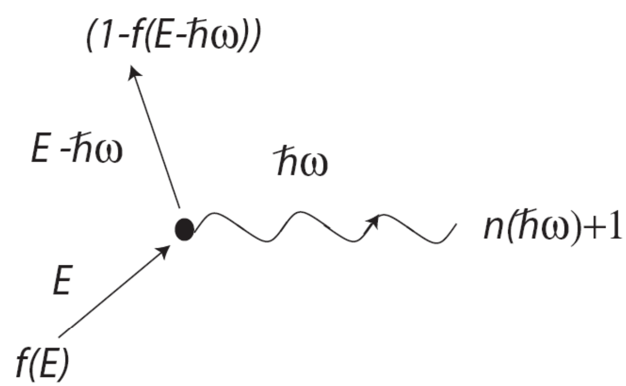
Illustration: diffusive normal metal wire
H. Pothier et al.
PRL 1997

Electron-electron and electron-phonon relaxation



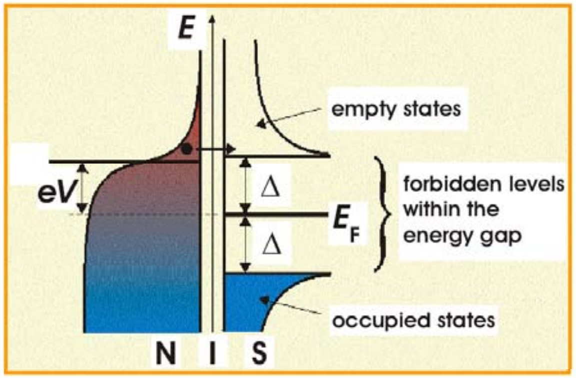
e-e relaxation drives the system towards *quasi-equilibrium*



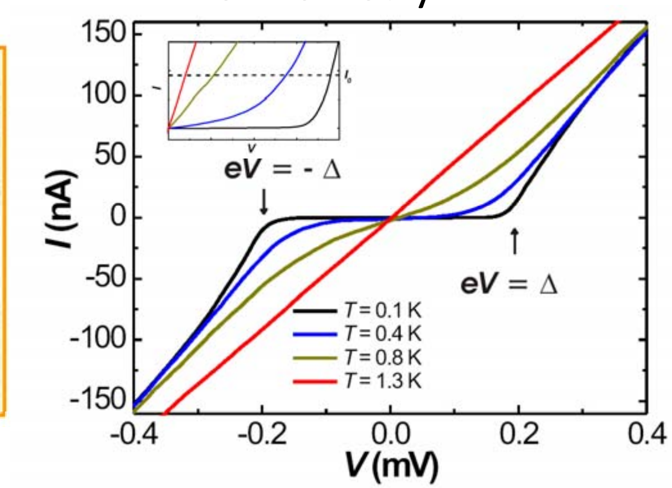


e-p relaxation drives the system towards *equilibrium*
Heat generation

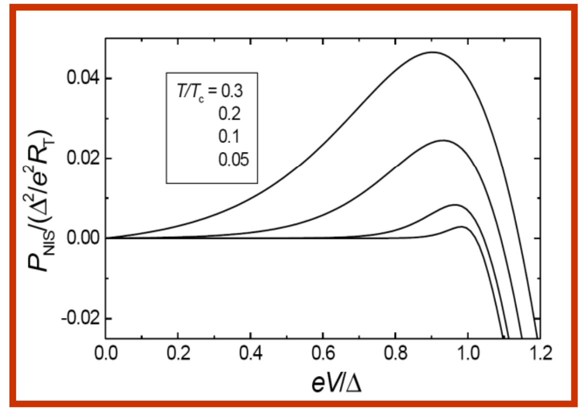
NIS junction as a refrigerator



Thermometry:



Cooling power of a NIS junction:



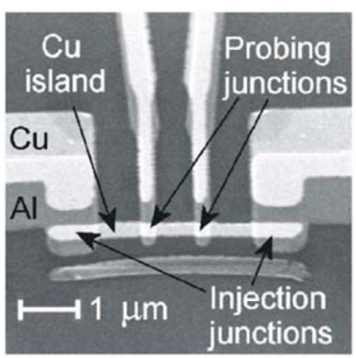
$$P(V) = \frac{1}{eR_T}\int (E-eV)N_S(E)[f_N(E-eV)-f_S(E)]dE$$

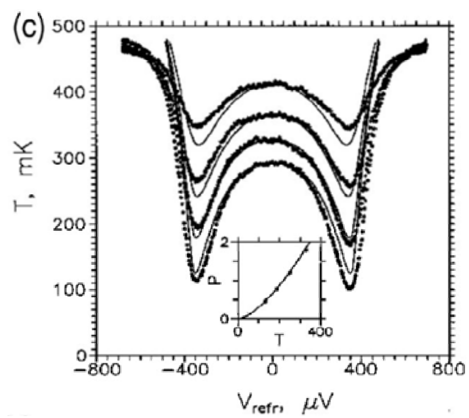
Optimum cooling power is reached at $V \cong \Delta/e$:

$$P_{\mathrm{NIS,max}} \simeq 0.59\frac{\Delta^2}{e^2R_T}\left(\frac{k_BT_N}{\Delta}\right)^{3/2}$$

Efficiency of a NIS junction refrigerator:

$$\eta \simeq k_BT/\Delta$$





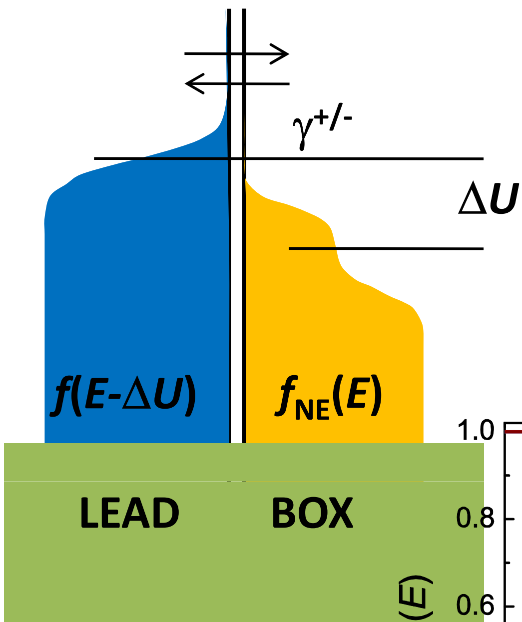
M. Leivo et al., APL 1996

Full non-equilibrium (harmonic drive)

$$N(0)\mathcal{V}\dot{f}_{\rm NE}(E) = [p_0\gamma^+(E,\Delta U) - p_1\gamma^-(E,\Delta U)] - \gamma N(0)\mathcal{V}[f_{\rm NE}(E) - f(E)]$$

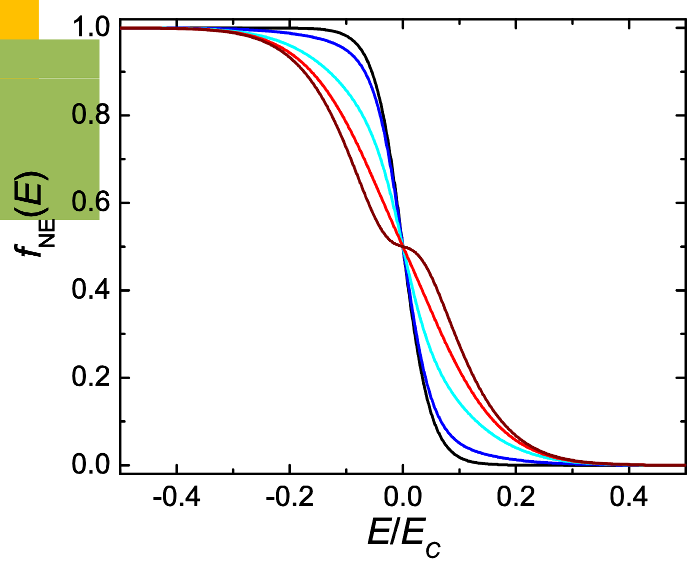
Population of n extra electrons in the box, p_n

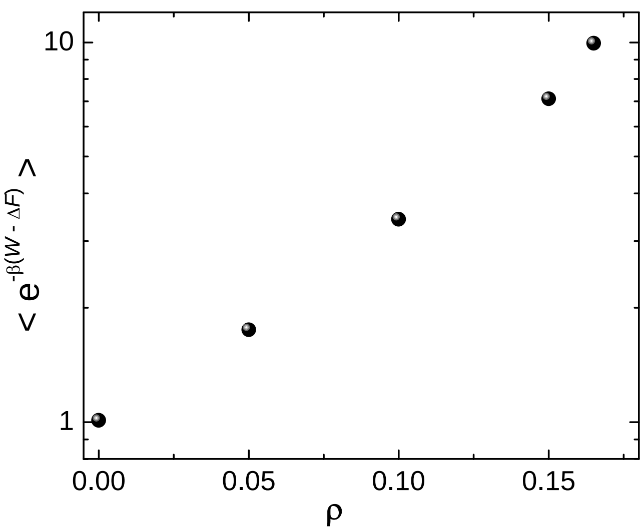
Relaxation rate towards equilibrium



$$\gamma^{\pm}(E,\Delta U) \equiv (e^2R_T)^{-1}f(E\mp\Delta U)[1-f_{\rm NE}(E)]$$

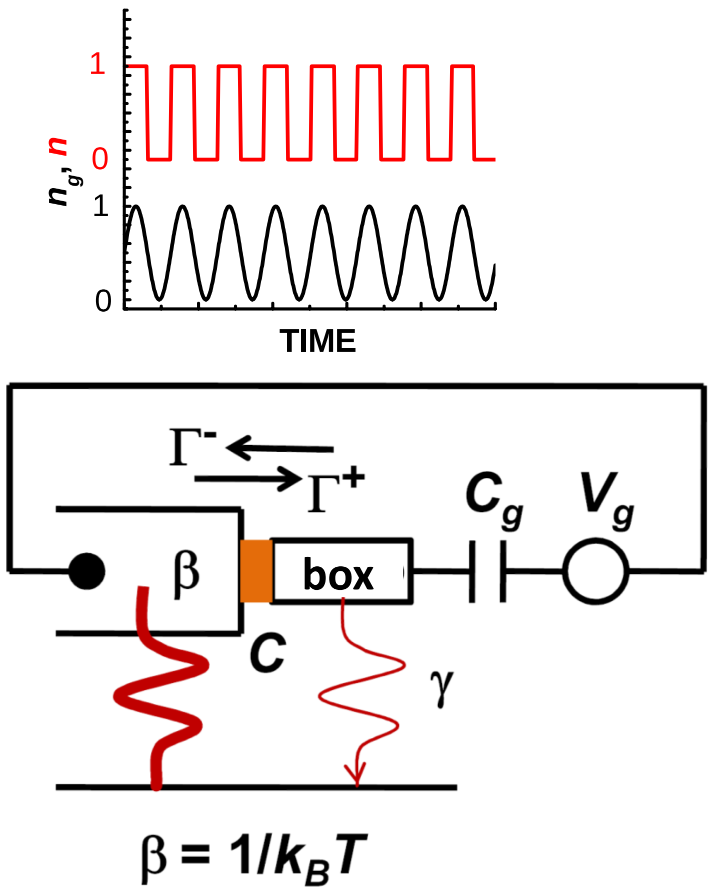
$N(0)\mathcal{V}$ = DOS X Volume of the box

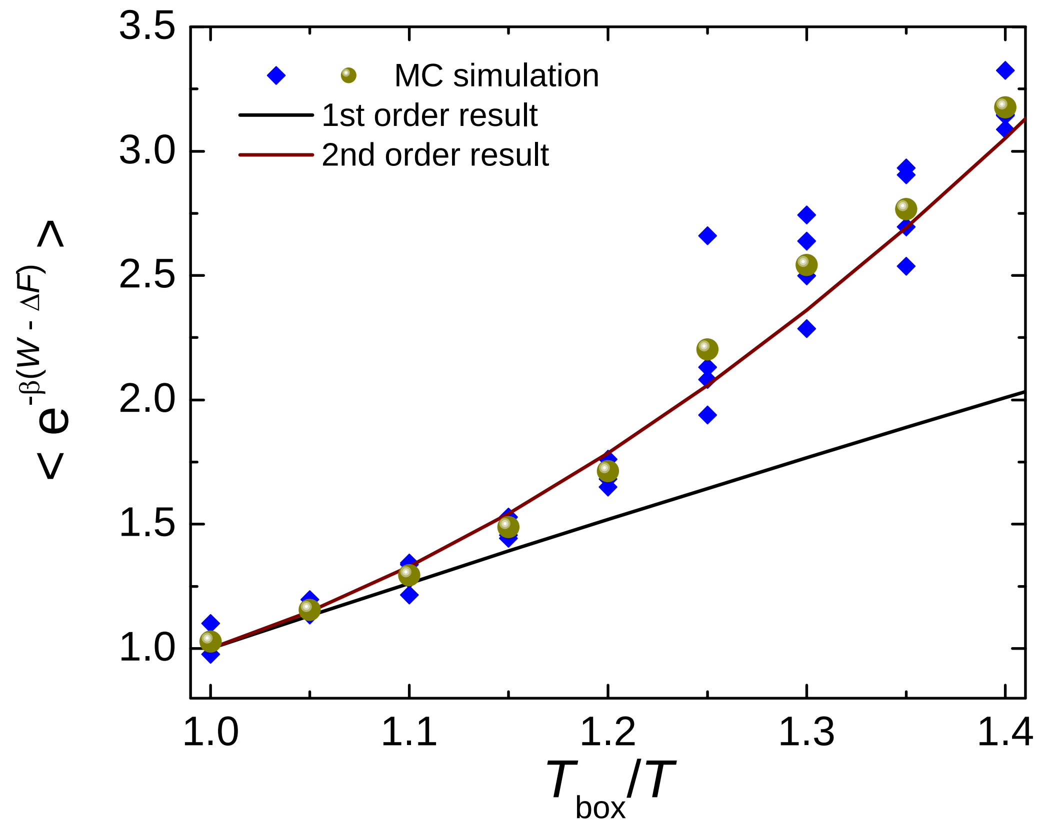




$$\rho \equiv \gamma_T/(\gamma_T + \gamma) \;\text{with}\; \gamma_T = [N(0)\mathcal{V}e^2R_T]^{-1}$$

Numerical simulations and analytic approximation for an overheated island





$$\langle e^{-\beta(W-\Delta F)}\rangle \simeq 1 - \frac{1}{2}\langle Q\rangle\Delta\beta + \frac{1}{6}\langle Q^2\rangle\Delta\beta^2$$