Statistics of the dissipated energy in driven single-electron transitions

D. V. AVERIN\(^1\)(a) and J. P. PEKOLA\(^2\)

\(^1\) Department of Physics and Astronomy, Stony Brook University, SUNY - Stony Brook, NY 11794-3800, USA
\(^2\) Low Temperature Laboratory, Aalto University - P.O. Box 13500, 00076 Aalto, Finland, EU

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Abstract – We analyze the distribution of heat generated in driven single-electron transitions and discuss the related non-equilibrium work theorems. In the adiabatic limit, the heat distribution is shown to become Gaussian, with the heat noise that, in spite of thermal fluctuations, vanishes together with the average dissipated energy. We show that the transitions satisfy Jarzynski equality for arbitrary drive and calculate the probability of the negative heat values. We also derive a general condition on the heat distribution that connects it to the Jarzynski equality.

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One of the basic statements of statistical mechanics is that any system manipulated adiabatically, at frequencies below its energy relaxation rate, remains in a state close to the instantaneous thermal equilibrium. As a result, the energy is transferred into or out of the system reversibly, with the overall increase of the entropy of the “universe” that can be made arbitrarily small. This statement underlies the notion of reversible computing [1,2] and practical attempts to realize this computation scheme [3]. However, as a statistical statement, it applies in general only to average values, whereas the fluctuations can lead to deviations from it in any given realization of a switching process [4–6]. Such fluctuations are particularly important in small systems making it interesting to understand statistical fluctuations in switching of the nanostructures. The question of the distribution of the generated heat, or of the work done on the system, is addressed in fluctuation theorems [7–9] that have been of interest in the non-equilibrium statistical mechanics [10] and in information theory [11] for several decades, and recently attracted attention also in the mesoscopic transport — see, e.g., [12]. The aim of this work is to calculate the distribution of the generated heat for one of the most basic models of nanoscale information processing: “single-electron tunneling” (SET) [13]. There, the information is encoded in the position of individual electrons in a system of mesoscopic conductors, and is processed through electron tunneling between the neighboring conductors. For the purpose of studying the heat distribution, this model combines several attractive features. It is understood to a high precision, sufficient, e.g., for the development of metrological applications [14,15]. It is also considered as the basis of a practical scheme of reversible computing [16–18], and is sufficiently simple for explicit calculations. We show that, counterintuitively, even for discrete electron transitions, the width of the heat distribution can be smaller than the energy \(k_B T\) of thermal fluctuations, and vanishes for adiabatic switching together with the average generated heat. We also discuss the “Jarzynski equality” (JE) [7], one of the better-known work theorems, as applied to SET switching.

Our discussion is valid for driven single-electron transitions in general. Yet for the sake of clarity, we consider the specific example of a single-electron box (SEB) [19,20], a small conducting island coupled through a tunnel junction with conductance \(G_T\) and capacitance \(C\) to a large external electrode, and biased with respect to it by the gate voltage \(V_g\) applied through the capacitance \(C_G\), see fig. 1. The island can carry extra electric charge \(n e\), where \(n\) is an integer, and its energy is

\[
U(n) = U_0(n) - 2EC_Gn, \quad U_0(n) = EC_Gn^2.
\]

Here \(U_0\) is the box energy as a capacitor with the total capacitance, \(C_G = C + C_g\), i.e., \(E_G \equiv e^2/(2C_G)\), and the second term is the interaction of the charge on the island and the source of the gate voltage, \(n_G \equiv -C_g V_g/e\).

\(^{(a)}\)E-mail: dmitri.averin@stonybrook.edu
In the simplest regime of relatively low temperatures $T$, $\beta \equiv 1/k_BT \gg E_C$, and $V_g$ restricted to the range $0 \leq n_g \leq 1$, the box dynamics can be limited to just two states, one electron on and off the island, $n = 1$ and $n = 0$. Our discussion will be limited to the situation where the states are degenerate in energy. In practice, an SEB can be made by standard nanofabrication techniques, and the charge state $n$ can be detected by an SET electrometer in real time, see, e.g., [21]. The problems of work and heat relations in generic driven two-level systems in different situations have been discussed previously by Ritort [22] and by Subrt and Chvosta [23].

Electron tunneling in the SEB dissipates energy into the box electrodes, which for the normal-metal box can be modeled as systems of non-interacting electrons. When an electron with energy $\epsilon$ tunnels in or out, it carries heat $\epsilon - \mu$, where $\mu$ is the chemical potential of the electrode. The energy $\epsilon$ is conserved in tunneling, and therefore the total amount of heat deposited in the two electrodes in the electron transfer process, $\pm[(\epsilon - \mu_2) - (\epsilon - \mu_1)]$, is equal to the difference between the chemical potentials of the electrodes, $\pm(\mu_1 - \mu_2)$, at the time $t$ of the transition. In SET systems, the effective position of the chemical potential of the electrodes depends on the charge configuration in the system, and the difference $(\mu_1 - \mu_2)$ for the box electrodes is given by the change of the energy $(1)$, equal to $\Delta U(t) = \pm E_C(2n_g(t) - 1)$ for the transitions between the states $n = 0$ and $n = 1$. The total heat $Q$ generated in one period of the gate voltage is then

$$Q = E_C \sum_{\tau_i} \pm(2n_g(\tau_i) - 1) = E_C \int dt(2n_g(t) - 1)I(t),$$

where the sum is over all back-and-forth $\pm$ transitions at the time instants $\tau_i$ during one ramp, and $I(t) = \sum_{\tau_i} \delta(\tau_i)$ is the associated particle current in the junction. The total change $\Delta U^{(\text{tot})}$ of the energy $(1)$ in one ramp of the gate voltage can be expressed then in the form similar to the first law of thermodynamics,

$$\Delta U^{(\text{tot})} = -Q + W_{\text{th}}, \quad W_{\text{th}} = -2E_C \int ndn_g(t),$$

where the “thermodynamic” work [24,25] is different [26,27] from the usual expression for work $W$ done on the box by the source of the gate voltage, since the energy $(1)$ includes the interaction with the voltage source. The analogous change of energy $U_0$ which does not include the interaction is indeed expressed in terms of the electrostatic work $W$ as

$$\Delta U^{(\text{tot})}_0 = -Q + W, \quad W = 2E_C \int n_g dn(t).$$

Both the heat $Q$ and work $W$ are observables that can in principle be measured experimentally. The heat can be measured directly, or by detecting the position of the gate $n_g(\tau)$ at each transition. Both $Q$ and $W$ fluctuate between different ramps of the gate voltage because of the randomness of electron tunneling. We calculate the distribution of heat $Q$ over an ensemble of ramps assuming the regime when the transition $n = 0 \to n = 1$ happens with certainty. For the charge trajectories $n(t)$ like this,

$$\Delta U^{(\text{tot})}_0 = E_C,$$

and eq. (3) shows that the heat and work are directly related, $W = Q + E_C$. For specific calculations, we consider a normal-metal box, for which the electron tunneling rates are $\Gamma_{\pm} = \pm(G_T/e^2\Delta U/(1 - e^{\mp\beta\Delta U}))$ [13]. The master equation for the occupation probabilities $p_{n\tau}$ of the two charge states, reduces in this case to $\dot{p} = \Gamma_D - \Gamma_{\pm}\delta$ for $p = p_1 - p_0$, where $\Gamma_D = \Gamma_+ - \Gamma_- = G_T\Delta U/e^2$, and $\Gamma_{\pm} = \Gamma_+ + \Gamma_\mp = (G_T\Delta U/e^2)\coth(\beta\Delta U/2)$. It gives the probability $p_{jk}(t_1, t_2)$ for the system to be in the state $k$ at time $t_2$, if it was in the state $j$ at time $t_1$ as

$$p_{jk}(t_1, t_2) = \frac{1}{2} \left[ 1 + \frac{(-1)^{j+1}e^{-\beta\Delta E_{jk}}}{\sum_{\tau} \int d\Gamma_{\pm} d\Gamma_D(r)e^{-\beta\Delta E_{jk}}} d\Gamma_{\pm}(r) \right].$$

To obtain quantitative results for distribution of the generated heat $Q$, we take the time dependence of the gate voltage to be linear, $E_C(2n_g(t) - 1) = \eta t$. Since the transitions, and hence the current $I(t)$, are suppressed away from the resonance, $t \to \pm\infty$, one can separate out the average heat $\langle Q \rangle$, reducing the equation for heat fluctuations $\dot{Q} = Q - \langle Q \rangle$ in this case to $\dot{Q} = \eta \int dt\dot{h}(t)$, where $\dot{h}(t)$ is the random realization of the charge on the SEB relative to its average in the gate ramp, $\dot{h}(t) = I(t) - \langle I(t) \rangle$. This means that the central moments of the heat fluctuations can be calculated through the correlation functions $K^{(m)}$ of the charge,

$$\langle Q^{(m)} \rangle = \eta^m \int dt_1 \ldots dt_m K^{(m)}(t_1, \ldots, t_m).$$
Fig. 2: (Colour on-line) The average and the higher moments of the distribution of the dissipated heat in single-electron transitions as functions of the ramp rate of the gate voltage driving the transitions. For comparison, open dots show the results (including the fourth central moment—dots without a line) of direct Monte Carlo simulations of the transitions. The simulations also give the overall shape of the distribution shown in the inset. Increasing ramp rate, $\nu = 0.1, 1, 10$, leads to broadening of the distribution.

which in turn can be obtained directly from the solution (4) of the master equation,

$$K^{(m)}(t_1, \ldots, t_m) = p_j(t_1)\tilde{n}_j(t_1)p_jk(t_1, t_2)\tilde{n}_k(t_2)\cdots p_j(t_{m-1}, t_m)\tilde{n}_j(t_m).$$

(6)

Here $p_j(t) \equiv p_{0,j}(-\infty, t)$ are the probabilities of the two charge states evolving from the state $n = 0$ at $t \rightarrow -\infty$, and $\tilde{n}_j(t) = j - \langle n(t) \rangle = j - p_j(t)$ is the value of the charge fluctuation $\tilde{n}(t)$ in the state $j = 0, 1$. Summation over all repeated indices is implied in eq. (6).

Equations (4)–(6) allow one, in principle, to find any central moment of the heat distribution. We calculate explicitly the heat noise $\sigma_Q \equiv \langle Q^2 \rangle^{1/2}$ and the third moment $\lambda_Q \equiv \langle Q^3 \rangle^{1/3}$ that coincides with the third cumulant of the distribution. For $m = 2$, one gets

$$K^{(2)}(t_1, t_2) = p_0(t_1)p_1(t_1)\exp(-\int_{t_1}^{t_2} dt' \Gamma_\Sigma^\nu(t')),$$

$$t_1 \leq t_2.$$  

(7)

Since the charge dynamics we are considering is essentially classical, the correlator at $t_1 > t_2$ is determined by the condition $K^{(2)}(t_1, t_2) = K^{(2)}(t_2, t_1)$. The correlator (7) substituted in eq. (5) gives the heat noise $\sigma_Q$.

The first few moments of the generated heat are shown in fig. 2 as functions of the dimensionless ramp rate $\nu \equiv \eta(\nu^*)^2/G_\Sigma$. Despite the thermal fluctuations of energies of tunneling electrons, the heat noise $\sigma_Q$ becomes smaller than $k_B T$ and vanishes together with the average dissipated energy $\langle Q \rangle$ in the limit of adiabatic reversible evolution, $\nu \rightarrow 0$. This means that, similarly to continuous diffusive processes [24], for discrete SET transitions, the dissipation is suppressed in the adiabatic limit not only on average, but for the individual ramps as well. Quantitatively, the instantaneous equilibrium probability $p = \Gamma_D/\Gamma_\Sigma$ obtained from eq. (4), combined with eqs. (5) and (7) gives the heat noise for $\nu \leq 1$:

$$\sigma_Q^2 = c\nu(k_B T)^2 = 2k_B T\langle Q \rangle,$$

(8)

with $c = (8/\pi^2)\sum_{n=0}^{\infty}(2n+1)^{-3} \approx 0.85$. The second equality in (8) [24,25,28] follows from comparison to the average dissipated energy $\langle Q \rangle = \eta \int dt \dot{n}(t)$ obtained using eq. (4) to find the first-order adiabatic correction to $\langle \dot{n}(t) \rangle = p_1(t)$. This equality resembles the standard fluctuation-dissipation theorem relating (in this case, quasi-) equilibrium fluctuations of the dissipated energy and the average linear response to a slow change inducing this dissipation. Numerical evaluation of both quantities for arbitrary $\nu$ (as in fig. 2) shows that this relation holds very accurately up to $\nu \approx 5$.

Used together with eq. (16) below, the second equality in (8) also means that the distribution function $\rho(Q)$ of the dissipated energy is Gaussian,

$$\rho(Q) = ((\beta/4\pi\langle Q \rangle)^{1/2} e^{-\beta(Q - \langle Q \rangle)^2/4\langle Q \rangle}.$$  

(9)

This conclusion agrees with the behavior of $\lambda_Q$ shown in fig. 2, which, as described below, satisfies $\lambda_Q \propto \nu \ll \sigma_Q \propto \sqrt{\nu}$ for $\nu \ll 1$. In the adiabatic limit, $Q$ is produced by many back-and-forth transitions and its distribution should indeed become Gaussian by the central limit theorem.

In the opposite limit of the rapid gate voltage ramp, $\nu \gg 1$, the heat distribution can be found in the “single-jump” approximation assuming that in this case, the system has time for only one electron transition from the initial ($n = 0$) to the final ($n = 1$) charge state. Then,

$$\rho(x = \beta Q) = \frac{x/\nu}{1 - e^{-x}} \exp \left\{ -\frac{1}{\nu} \int_{-\infty}^{x} \frac{u}{1 - e^{-u}} \right\}.$$  

(10)

One can check that this distribution reproduces well the large $\nu$ behavior of the moments plotted in fig. 2. The leading part of these asymptotes can be obtained analytically by completely neglecting the $1/\nu$ parts of the distribution, reducing it to $\rho(Q) = (Q/\sigma_Q)^{1/2} e^{-Q^2/2\sigma_Q^2}$, with $\sigma_Q \equiv (\Sigma_{n=0}^{\infty}(2n+1)^{-3} \approx 0.85$. For arbitrary $\nu$, the third cumulant $\lambda_Q$ can be calculated from eqs. (5) and (6). Equation (6) combined with eq. (4) gives after some algebra for $m = 3$:

$$K^{(3)}(t_1, t_2, t_3) = p_0(t_1)p_1(t_1)p_2(t_2)\left[ p_0(t_2) - p_0(t_3) \right] e^{-\int_{t_1}^{t_2} dt' \Gamma_\Sigma^\nu(t')}, \quad t_1 \leq t_2 \leq t_3.$$  

(11)

In all other time intervals, the correlator $K^{(3)}$ is defined, similarly to $K^{(2)}$, by the condition that it is symmetric
adiabatic limit

expression for the probabilities, dissipated energy in the SET transitions considered in finite probability recently by applying rotating electric field to a dimeric dimer\[29\]: One can envision extracting electrical energy basis of implementation of an SET version of “Maxwell’s integrals of eq. (11) as required in eq. (5) can be evaluated with respect to permutations of the time arguments. The integrals of eq. (11) as required in eq. (5) can be evaluated numerically and give $\lambda_Q$ shown in fig. 2. For $\nu \gg 1$, this can be done analytically, with the result agreeing with that of the large-$\nu$ approximation given above. In the adiabatic limit $\nu \ll 1$, one can use the quasiequilibrium expression for the probabilities, $p_{0,1} = (1 + \Gamma_D/\Gamma_{\Sigma})/2$, and get $\lambda_Q = c' v k_B T$, with $c' \simeq 0.22$.

One of the interesting features of the statistics of the dissipated energy in the SET transitions considered in this work is the existence of the $Q < 0$ region, i.e., a finite probability $P$ of an SET transition taking place with extraction of energy from thermal fluctuations rather than with energy dissipation. This probability could be the basis of implementation of an SET version of “Maxwell’s demon” \[29\]: One can envision extracting electrical energy from thermal fluctuations in multi-junction SET circuits, with the help of a measurement/feedback loop, similar to the “information-to-energy conversion” demonstrated recently by applying rotating electric field to a dimeric particle \[6\]. The magnitude of this probability can be calculated for slow and rapid gate voltage ramps from eqs. (9) and (10):

$$P = \begin{cases} \frac{(1 - \text{erf}((c/\nu)^{1/2})/2)}{\pi^2/(6\nu)}, & \nu \ll 1, \\ \nu \gg 1. \end{cases}$$

(12)

In the adiabatic regime, the probability can be large, $P \rightarrow 1/2$, at the cost of the typical value $Q_c$ of the extracted energy being small on the scale of thermal energy, $Q_c \sim \sqrt{T} k_B T$. In the opposite limit, $\nu \gg 1$, $P$ is small, but $Q_c \sim k_B T$. For arbitrary $\nu$, $P$ can be calculated by direct Monte Carlo simulation of the transitions, see fig. 3, which shows good agreement with the asymptotic behavior (12) in the two limits.

The SET transitions represent a very convenient system for testing the work theorems \[7–10,30\] of non-equilibrium statistical mechanics. To derive them, we do not assume, unlike in the discussion above, any specific energy dependence of the transition rates $\Gamma_{\pm}$ besides the detailed balance, $\Gamma_+(\tau_i) = e^{\beta \Delta U(\tau_i)}\Gamma_-(\tau_i)$, and in principle, allow the transitions to transfer more than one electron across the barrier. The following discussion is thus applicable, with small adjustments, also to normal metal/superconductor (NIS) junctions, which in the box geometry, in addition to SET transitions, demonstrate individual Andreev processes \[21\] transferring pairs of electrons. We also allow the gate voltage to have arbitrary time dependence, and the evolution of the SEB to start and end not in a definite charge state. Instead of transition probabilities (4), it is convenient now to represent the Markovian evolution of the SEB in terms of all possible multi-transition paths between initial $-T/2$ and final $+T/2$ times, so that the average of any function $f(Q)$ of heat is

$$\langle f(Q) \rangle = \sum_{j=0}^{\infty} \sum_{n=0}^{1} p_n \langle f(Q) \rangle_{n,j}. \quad \text{(13)}$$

Here, as before, we restrict the dynamics to the two charge states, $p_n$ is the initial probability of the state $n$, and the averages $\langle f(Q) \rangle_{n,j}$ for trajectories starting at $n$ and making $j$ back-and-forth transitions are

$$\langle f(Q) \rangle_{n,j} = \int_{-T/2}^{T/2} \cdots \int_{-T/2}^{T/2} \int_{-T/2}^{T/2} \cdots \int_{-T/2}^{T/2} \prod_{i=1}^{j} \rho_n(\tau_1, \tau_2, \ldots, \tau_j) f(Q(\tau_1, \ldots, \tau_j)). \quad \text{(14)}$$

The probability density $p_n$ can be expressed in terms of the probability $\eta_{\pm}(\tau_i, \tau_{i+1}) = e^{-\beta \int_{\tau_i}^{\tau_{i+1}} \int_{\tau_i}^{\tau_{i+1}} \cdots d\tau'}$ that the system does not make a $\pm$ transition in the time interval from $\tau_i$ to $\tau_{i+1}$. For odd values of $j$,

$$p_n(\tau_1, \tau_2, \ldots, \tau_j) = \hat{\rho}_{\pm}(T/2, \tau_j) \rho_{\pm}(\tau_1, \tau_2) \cdots \rho_{\pm}(\tau_{j-1}, \tau_j) \cdots \hat{\rho}_{\pm}(\tau_1, T/2), \quad \rho_{\pm}(\tau_i, T/2) = \eta_{\pm}(\tau_i, \tau_{i+1}) \Gamma_{\pm}(\tau_{i+1}),$$

where the two sets of indices refer to the two states $n$, with the upper indices corresponding to $n = 0$, lower $+$ to $n = 1$. For even $j$, the expression is constructed similarly:

$$p_n(\tau_1, \tau_2, \ldots, \tau_j) = \hat{\rho}_{\pm}(T/2, \tau_1) \rho_{\pm}(\tau_1, \tau_2) \cdots \hat{\rho}_{\pm}(\tau_j, T/2) \eta_{\pm}(\tau_j, T/2).$$

The detailed balance for tunneling rates implies immediately that the expression of the average of $f(Q) = e^{-\beta \Delta Q} = \Pi_{f=1}^{F=1} e^{\beta \Delta U(\tau_i)}$, taken according to eqs. (13) and (14), coincides with the transition probability $w$ between the charge states in the time-reversed evolution \[31\] with the same voltage ramp, i.e.,

$$e^{-\beta \Delta Q} = \sum_{i,f} p_i w(f \rightarrow i). \quad \text{(15)}$$

Here $i, f = n(T/2)$ are the initial and final charge states of the system. This equation gives a version of the work equalities discussed previously \[7–10\], in a form convenient for
for the SET transitions. In particular, if the gate voltage ramp satisfies the condition \(n_g(-t) + n_g(t) = 1\), as, e.g., does the linear ramp discussed above, the tunneling rate has the symmetry \(\Gamma_i(-t) = \Gamma_i(t)\). In this case, \(w(f \rightarrow i) = w(i \rightarrow f)\), and eq. (15) gives

\[
\langle e^{-\beta Q} \rangle = 1.
\]  

(16)

This relation was used above to derive the Gaussian form (9) of the heat distribution for adiabatic switching. If the ramp is not antisymmetric relative to the degeneracy point at \(t = 0\), the right-hand side of eq. (15) can be different from 1.

Equation (15) is also reduced to eq. (16) in the situation when the time dependence of the gate voltage is such that both the direct and time-reversed evolution trajectories of the SET start and end in definite charge states. In this case, transition probabilities \(w(i \rightarrow f)\) and \(w(f \rightarrow i)\) in eq. (15) are both equal to 1 for the same pair of states \(i, f\), and the corresponding \(p_i\) is also 1, so that the right-hand side of eq. (15) reduces to 1. Also, for definite initial/final charge states, the change \(\Delta U_0\) of electrostatic energy (1) of the box will be the same for all realizations of the evolution trajectory. Equation (3) shows then that \(W = Q + \Delta U_0\) and the distribution of heat \(Q\) gives also the distribution of electrostatic work \(W\) done by the gate voltage on the box. In particular, eq. (16) can be written in this case as

\[
\langle e^{-\beta (W - \Delta U_0)} \rangle = 1.
\]  

(17)

Definite initial/final charge states imply that the entropy in the charge degree of freedom of the box vanishes and its internal energy \(U_0\) coincides with the free energy \(F\), so that \(\Delta U_0\) in eq. (17) can be replaced in principle with \(\Delta F\). It is important to stress that eq. (17) is valid only for this certain type of the evolution trajectories which connect the same definite initial and final charge states for direct and time-reversed evolution.

For a general equilibrium initial state and a general time dependence of the gate voltage, one can find the average \(\langle e^{-\beta W_{th}} \rangle\) over the distribution of the thermodynamic work that is defined by eq. (2) (in contrast to the regular work \(W\) in eq. (3)). The equilibrium probabilities \(p_f\) are related to the equilibrium probabilities \(p_f\) for the gate voltage at the end of the ramp through the difference \(\Delta F\) of the free energy for the final and the initial values of the gate voltage: \(p_f = p_f e^{\beta(\Delta F_i - \Delta F)}\), where \(E_i, f\) are the energies of the corresponding charge states. Expressing \(E_f - E_i\) with the help of eq. (3), one gets the Jarzynski equality for the distribution of the thermodynamic work

\[
\langle e^{-\beta (W_{th} - \Delta F)} \rangle = 1
\]  

(18)

valid for an arbitrary gate voltage ramp. In practice, validity of this equation will still be limited by overheating effects which were not considered in this analysis.

In summary, we obtained the distribution of heat generated in driven single-electron transitions and its central moments, and analyzed the most common work theorems and their applicability to these transitions.

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