Nonequilibrium work distributions for a trapped Brownian particle in a time-dependent magnetic field

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We study the dynamics of a trapped, charged Brownian particle in the presence of a time-dependent magnetic field. We calculate work distributions for different time-dependent protocols numerically. In our problem, thermodynamic work is related to variation of the vector potential with time as opposed to the earlier studies where the work is related to time variation of the potentials, a quantity that depends only on the coordinates of the particle. Using the Jarzynski and the Crooks equalities, we show that the free energy of the particle is independent of the magnetic field, thus complementing the Bohr–van Leeuwen theorem. We also show that our system exhibits a parametric resonance in a certain parameter space.

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Equilibrium statistical mechanics provides us an elegant framework to explain the properties of a broad variety of systems in equilibrium. Close to equilibrium the linear response formalism is very successful in the form of the fluctuation-dissipation theorem and Onsager's reciprocity relations. But no such universal framework exists to study systems driven far away from equilibrium. Needless to say, most processes that occur in nature are far from equilibrium. In recent years there has been considerable interest in the nonequilibrium statistical mechanics of small systems. This has led to the discovery of several rigorous theorems, called fluctuation theorems (FTs) and related equalities [1–11] for systems far away from equilibrium. Some of these theorems have been verified experimentally [12–16] on single nanosystems in physical environments where fluctuations play a dominant role. We will focus on the Jarzynski equality [4] and Crooks equality [5], which deal with systems that are initially in thermal equilibrium and are driven far away from equilibrium irreversibly. The Jarzynski identity relates the free energy change (ΔF) of the system when it is driven out of equilibrium by perturbing its Hamiltonian (H_λ) with an externally controlled time-dependent protocol $\lambda(t)$ to the thermodynamic work (W) done on the system, given by

$$W = \int_0^\tau \dot{\lambda}\frac{\partial H_\lambda}{\partial \lambda}dt, \tag{1}$$

over a phase space trajectory. Here τ is the time through which the system is driven. The Jarzynski identity is

$$\langle e^{-\beta W}\rangle = e^{-\beta \Delta F}. \tag{2}$$

The angular brackets denote the average over all possible realizations of a process that takes the system from the initial equilibrium state to a final state at time τ. The Crooks equality concerns the ratio of the work distributions P_f and P_b. Here the subscripts f and b refer to the externally controlled forward and backward protocols, respectively, by which the the system evolves. This relation is given by

$$\frac{P_f(W)}{P_b(-W)} = e^{\beta W_d}, \tag{3}$$

Here, the dissipative work $W_d = W - W_r$ and W_r is the reversible work, which is same as the free energy difference (ΔF) between the initial and the final states of the system when driven through a reversible, isothermal path. If the system is driven reversibly all along the path, the work distribution is $\delta(W-\Delta F)$, $W_d=0$, and $P_f = P_b$. Thus, the above identities are trivially true for a reversibly driven system. The Jarzynski identity follows from Eq. (3). The Crooks relation follows from a more general Crooks identity which relates the ratio of the work probabilities of the forward reverse paths to the dissipative work expended along the forward trajectory. One can also obtain the free energy difference by using the exact fluctuation theorem. The theorem further gives conditions on external protocols depending on the symmetry of the underlying potential [17].

Here, we will study the applicability of the Jarzynski and Crooks equalities in the case of a velocity-dependent as well as a time-dependent Lorentz force, which is derivable from a generalized potential $U = q[\phi - \mathbf{A}(t)\cdot\mathbf{v}]$. Here, $\mathbf{A}$ is a time-dependent vector potential, ϕ is a scalar potential, q is the charge of the particle, and $\mathbf{v}$ is its velocity. Different time-dependent protocols for magnetic fields are considered. Consequently, we find that the free energy differences obtained using the Jarzynski and Crooks equalities are consistent with the prediction from the Bohr–van Leeuwen theorem [18–20]. This theorem states that in the case of classical systems the free energy is independent of magnetic field and hence there is an absence of diamagnetism in classical thermodyanamical equilibrium systems. We finally also show that our system, in the presence of an ac magnetic field, exhibits parametric resonance in a certain parameter regime.

In an earlier related work [20,21], charged particle dynamics in the overdamped limit is studied in the presence of a harmonic trap and static magnetic field. The work distribution was obtained analytically for different protocols. It is shown that the work distribution depends explicitly on the magnetic field but not the free energy difference (ΔF).

The model Hamiltonian for our isolated system is

$$H=\frac{1}{2m}\left[\left(p_x+\frac{qB(t)y}{2}\right)^2+\left(p_y-\frac{qB(t)x}{2}\right)^2\right]+\frac{1}{2}k(x^2+y^2), \tag{4}$$

where k is the stiffness constant of harmonic confinement. The magnetic field $B(t)$ is applied in the z direction. The x and y components of the vector potential, A_x A_y are given by $-qB(t)y/2$ and $qB(t)x/2$, respectively. We have chosen a symmetric gauge here. The above Hamiltonian remains invariant under time-reversal symmetry. In this case, however, in addition to changing $t\rightarrow -t$ we must reverse the sign of the magnetic fields. This implies that the externally controlled protocol B under time reversal becomes $-B$ [5,22–24]. The particle-environment interaction is modeled via a Langevin equation including inertia [25], namely,

$$m\ddot{x}=\frac{q}{2}[y\dot{B}(t)+2\dot{y}B(t)]-kx-\Gamma\dot{x}+\eta_x(t), \tag{5}$$

$$m\ddot{y}=-\frac{q}{2}[x\dot{B}(t)+2\dot{x}B(t)]-ky-\Gamma\dot{y}+\eta_y(t), \tag{6}$$

where Γ is the friction coefficient and η_x and η_y are the Gaussian white noise along the x and y directions, respectively. This thermal noise has the following properties:

$$\langle\eta_i\rangle=0, \quad \langle\eta_i(t)\eta_j(t')\rangle=\delta_{ij}2\Gamma k_BT\delta(t-t'), \tag{7}$$

so that the system approaches a unique equilibrium state in the absence of time-dependent potentials. Denoting the protocol $\lambda(t)=(q/2)B(t)$, the thermodynamic work done by an external magnetic field on the system up to time τ is

$$W=-\frac{q}{2}\int_0^\tau(x\dot{y}-y\dot{x})\dot{B}(t)dt. \tag{8}$$

We want to emphasize that this thermodynamic work is related to the time variation of the vector potential and can be identified as the time variation of the magnetic potential $-\boldsymbol{\mu}\cdot\mathbf{B}$, $W=-\int_0^\tau\boldsymbol{\mu}\cdot(d\mathbf{B}/dt)dt$, where the induced magnetic moment is $(q/2)(x\dot{y}-y\dot{x})=(q/2)(\mathbf{r}\times\mathbf{v})$. To obtain the value of the work and its distribution, we have solved Eqs. (5) and (6) numerically using the Verlet algorithm [26]. We first evolve the system upto a large time greater than the typical relaxation time so that the system is in equilibrium, and then apply a time-dependent protocol for the magnetic field. We have calculated values of the work numerically for 10^5 different realizations to get better statistics. The values of work obtained for different realizations can be viewed as random samples from the probability distribution $P(W)$. We have fixed the friction coefficient, mass, charge, and k_BT to be unity. All the physical parameters are taken in dimensionless units.

First we have taken the magnetic field to vary linearly in time, i.e., $\mathbf{B}=B_0(t/\tau)\hat{z}$. Work distributions for both forward and backward protocols are obtained. In Fig. 1 we have plotted the distributions $P_f(W)$ and $P_b(-W)$, for forward and backward protocols, respectively, which are depicted in the insets of Fig. 1.

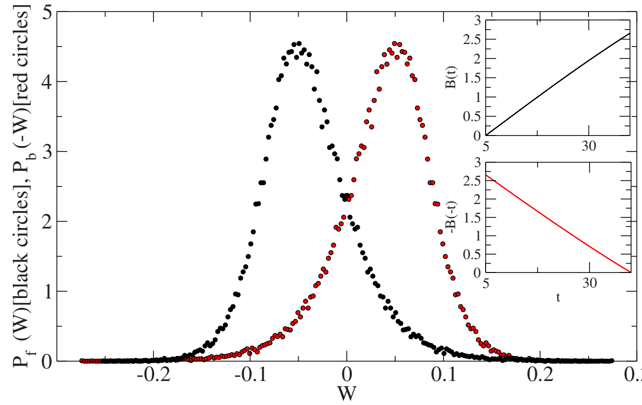

FIG. 1. (Color online) Forward $P_f(W)$ and backward $P_b(-W)$ work probability distributions for a ramped magnetic field.

Using the Jarzynski equality [Eq. (2)] we computed the free energy difference ΔF. We obtained $\langle e^{-\beta W}\rangle$ to be unity (1.0 ± 0.04) implying that $\Delta F=0$. It may be noted that $\Delta F=F(B)-F(0)$, where B is the value of the field at the end of the protocol. In the begining of the protocol, the value of B is zero. For different values of the final magnetic field we obtained $\Delta F=0$ within our numerical accuracy. This implies that the free energy itself (and not the free energy difference) is independent of the magnetic field, thereby satisfying the Bohr–van Leeuwen theorem as stated earlier. We can also employ Crooks equality [Eq. (3)] to determine the free energy difference. It follows from Crooks equality that the P_f and P_b distributions cross at value $W=\Delta F$. This value, where the two distributions cross each other (that is, $W=0$), can be readily inferred from Fig. 1. This again suggests that $\Delta F=0$, which is consistent with the result obtained using Jarzynski equality.

To strengthen our assertion (that is, that the free energy is independent of magnetic field) further, in Figs. 2 and 3 we have plotted $P_f(W)$ and $P_b(-W)$ for two different protocols as shown in the insets of the corresponding figures. For Fig. 3 we have considered a sinusoidally varying magnetic field

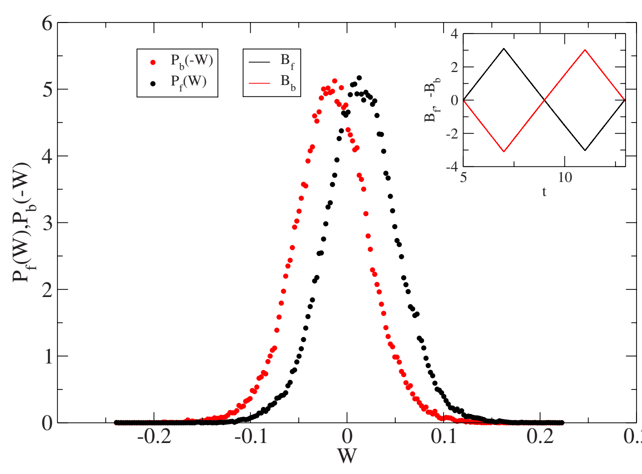

FIG. 2. (Color online) $P_f(W)$ and $P_b(-W)$ for symmetric ramp for $B(t)$.

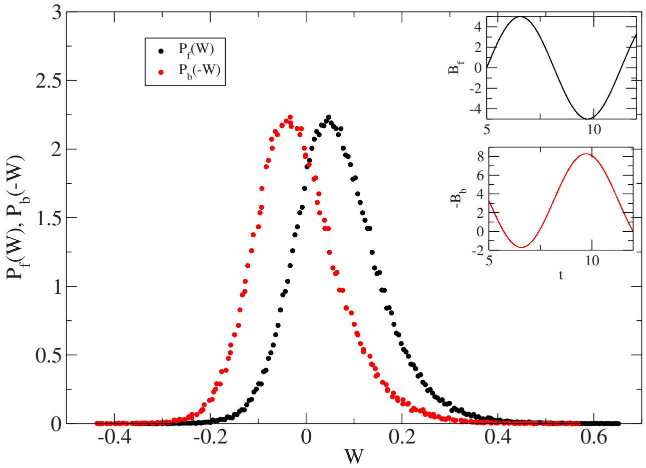

FIG. 3. (Color online) $P_f(W)$ and $P_b(-W)$ for oscillatory magnetic field.

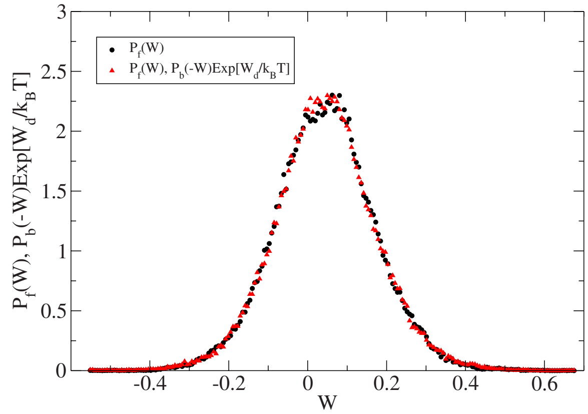

FIG. 4. (Color online) $P_f(W)$ and $P_b(-W)e^{\beta W_d}$ plotted together.

$B=B_1 \sin \omega t$ in the z direction. From the crossing point of P_f and P_b, we observe that $\Delta F=0$, consistent with the earlier result.

In Fig. 4 we have plotted $P_f(W)$ and $P_b(-W)e^{\beta W_d}$, corresponding to the protocol shown in Fig. 3. The two graphs are identical (within numerical error), thus verifying Crooks equality. It may be noted that the reverse protocol also implies reversing the magnetic field [27]. In all our figures the distribution of work is asymmetric and depends on the magnetic field protocol explicitly, as opposed to ΔF. Moreover, all the distributions show a significant tail in the negative work region. This is necessary so as to satisfy the Jarzynski equality.

We now discuss very briefly the occurrence of parametric resonance [28] in our system in the presence of a sinusoidally oscillating magnetic field $B(t)=B_1 \sin \omega t$. In the parameter range $q_1B_1/4\sqrt{2L_1}-\Gamma_1>0$ where $L_1=1+2(k_1-\Gamma_1^2)/q_1^2B_1^2$ (see the Appendix), our system exhibits instability. Here $k_1=k/m$, $\Gamma_1=\Gamma/2m$, and $q_1=q/2m$. The external parametric magnetic field injects energy into the system, and this pumping is expected to be strongest near twice the system frequency ($\sqrt{L_1}$). The trajectory of the Brownian particle grows exponentially in time, also exhibiting oscillatory motion at twice the frequency of external magnetic field. This is shown in Fig. 5, where the coordinates of the particle and the protocol are plotted as a function of time. The parameters are $B_1=60$ and $\omega=1$. For these graphs, the noise strength k_BT is taken as 1. In the presence of this instability (large variation in coordinate values), it becomes difficult to calculate work distributions as it requires a large number of realizations and better accuracy. Further work in analyzing the nature of the parametric resonance and associated work distributions is in progress.

In conclusion, by considering the dynamics of a trapped charged Brownian particle in a time-dependent magnetic field we have verified the Jarzynski and Crooks equalities. As a by-product our result complements Bohr–van Leeuwen theorem. Work done on the system by the external field arises due to the time variation of the vector potential. This is in contrast to earlier studied models where the input energy to the system comes from time variation of the coordinate-dependent potentials. Finally, we have discussed very briefly

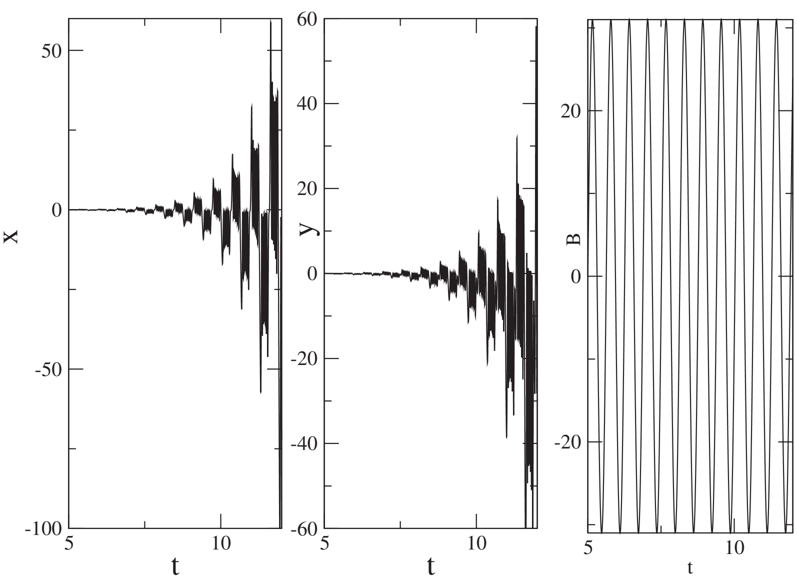

FIG. 5. x and y coordinates of the particle and $B(t)$ plotted as functions of time.

the occurrence of parametric resonance in our system. Our results are amenable to experimental verification.

APPENDIX

In the presence of an oscillatory magnetic field $B(t) = B_1 \sin \omega t$, the mean values of coordinates $\langle x \rangle$ and $\langle y \rangle$ of the particle (averaged over thermal noise) obey the following equation for $z = \langle x \rangle + i\langle y \rangle$:

$$m\ddot{z} + (\Gamma + iqB_1 \sin \omega t)\dot{z} + \left(k + i\frac{qB_1\omega}{2} \cos \omega t\right)z = 0. \tag{A1}$$

With $k = mk_1$, $\Gamma = m\Gamma'$, and $q = mq'$ the above equation becomes

$$\ddot{z} + (\Gamma' + iq'B_1 \sin \omega t)\dot{z} + \left(k_1 + i\frac{q'B_1\omega}{2} \cos \omega t\right)z = 0. \tag{A2}$$

Now, using the following transformation:

$$z(t) = \xi(t)\exp\left(-\frac{1}{2}\int^t (\Gamma' + iq'B_1 \sin \omega t)dt\right), \tag{A3}$$

Eq. (A2) becomes

$$\ddot{\xi} + \left(k_1 - \frac{1}{4}(\Gamma' + iq'B_1 \sin \omega t)^2\right)\xi = 0. \tag{A4}$$

Redefining Γ' and q' as $\Gamma_1 = \Gamma'/2$ and $q_1 = q'/2$, we get

$$\ddot{\xi} + [k_1 - (\Gamma_1 + iq_1B_1 \sin \omega t)^2]\xi = 0. \tag{A5}$$

Again, after transforming t as $t = \sqrt{2}t_1/q_1B_1 - \pi/2\omega$ and ω as $\omega = \omega_1 q_1 B_1/\sqrt{2}$, we get

$$\frac{d^2\xi}{dt_1^2} + (L_1 + \cos 2\omega_1 t_1 + i\epsilon \cos \omega_1 t_1)\xi = 0, \tag{A6}$$

where $L_1 = 1 + 2(k_1 - \Gamma_1^2)/q_1^2 B_1^2$ and $\epsilon = 4\Gamma_1/q_1B_1$. For large B_1, ϵ is small and hence $i\epsilon \cos \omega_1 t_1$ can be treated as a perturbative term as long as ω_1 is far from $2\sqrt{L_1}$. The condition $L_1 > 1$ should be maintained. Thus ξ can be expanded as $\xi = \xi_0 + \epsilon\xi_1 + \cdots$. Using this in Eq. (A6), we get (keeping only the ϵ^0 order term),

$$\frac{d^2\xi_0}{dt_1^2} + (L_1 + \cos 2\omega_1 t_1)\xi_0 = 0. \tag{A7}$$

This exhibits parametric resonance [24] when $\omega_1 \approx \sqrt{L_1}$. Near resonating frequency, ξ_0 varies as $\xi_0 \sim e^{st_1}$, where $s \approx 1/4\sqrt{L_1}$. Hence, z will grow exponentially, if $st_1 - \Gamma_1 t > 0$, i.e., $(q_1B_1/4\sqrt{2L_1})(t + \pi/2\omega) - \Gamma_1 t > 0$.The condition given above can be maintained if $q_1B_1/4\sqrt{2L_1} - \Gamma_1 \geq 0$. For small amplitude of the magnetic field, the trajectories of the particles are stable.

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