Dragging of an electrically charged particle in a magnetic field

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We study the statistical properties of the total work associated with the Langevin equation for an electrically charged Brownian particle in a two-dimensional harmonic trap and in the presence of a uniform magnetic field. The calculations are performed under the overdamped approximation. The center of the harmonic trap is dragged in an arbitrary time-dependent way. As a result we have found the relation of the averaged work and the variance in the work distribution in the presence of the magnetic field. In addition, the Jarzynski equality (JE) is considered when the potential associated with the working force contains a time-dependent term, giving a way to calculate the change in the free energy. The particular cases in Jayannavar and Sahoo's work [Phys. Rev. E **75**, 032102 (2007)] and their use of the JE are also discussed.

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The study of nonequilibrium processes in macroscopic systems has been a subject of permanent interest in the literature. The difficulties found when we are interested in nonequilibrium phenomena have been treated following different approaches, going from Brownian dynamics through linear response, Green-Kubo formulas, irreversible thermodynamics, and so on. It is well known that most of these approaches are limited to considering systems in the neighborhood of an equilibrium state. Then, the main question to be answered goes to the search for general properties characterizing the behavior away from equilibrium. In this sense, the Jarzynski equality (JE) [1] as well as all the fluctuation theorems [2–8] play a role in the understanding of the time evolution in systems away from an equilibrium state [9–12]. The Jarzynski equality relates nonequilibrium quantities to free energies; in particular, the properties of the work distribution measured through the average work and its variance give an expression for the free energy. In this paper we calculate in a general way the statistical properties of the work distributions for an electrically charged Brownian particle in the presence of a magnetic field which is in a harmonic trap dragged by an arbitrary time-dependent force. In fact, this problem was considered by Jayannavar and Sahoo [13] for two particular cases: (i) The center of the harmonic trap is dragged with a uniform velocity, whereas in the other model (ii) the charged particle is subjected to an ac force. Our results go further, in the sense that we consider an arbitrary time-dependent motion for the center in the harmonic trap and an additional time-dependent force is added to clarify the origin of the free energy found by Jayannavar and Sahoo. Our proposal will be displayed as follows: the system is the same as in Ref. [13], i.e., we consider a charged particle motion in the x-y plane in the presence of a time-dependent potential $U(\mathbf{x},t)$ with $\mathbf{x}=(x,y)$ the position vector, and under the action of a uniform magnetic field which is allowed to point along the z axis, i.e., $\mathbf{B}=(0,0,B)$. In this case the two-dimensional equation of motion can be written as

$$m\frac{d\mathbf{u}}{dt} = -\gamma\mathbf{u} + \mathcal{W}\mathbf{u} - \mathrm{grad}_{\mathbf{x}}U + \mathbf{A}(t), \tag{1}$$

where $\gamma > 0$ is the friction coefficient, q the charge of the particle, m its mass, and $\mathbf{A}(t)$ the fluctuating force that satisfies the properties of Gaussian white noise with zero mean value $\langle A_i(t)\rangle = 0$ and a correlation function given by

$$\langle A_i(t)A_j(t')\rangle = 2\lambda\,\delta_{ij}\,\delta(t-t'), \tag{2}$$

with $i,j=x,y$. λ is a constant that measures the noise intensity and, according to the fluctuation-dissipation theorem, is related to the friction constant by $\lambda=\gamma k_B T$, and k_B is the Boltzmann constant. $\mathcal{W}$ is a real antisymmetric matrix given by

$$\mathcal{W} = \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix}, \tag{3}$$

where $\omega = qB/c$ is the Larmor frequency which takes into account the coupling coming from the Lorentz force. First, we consider in general a time-dependent harmonic trap and its corresponding associated harmonic force, such that

$$U_C(\mathbf{x},t) = \frac{k}{2}|\mathbf{x}-\mathbf{x}^*|^2, \quad \mathbf{F}(\mathbf{x},\mathbf{x}^*) = -k(\mathbf{x}-\mathbf{x}^*), \tag{4}$$

where $\mathbf{x}^*$ is the position of the minimum of the harmonic potential with $\dot{\mathbf{x}}^* = \mathbf{u}^*(t)$, and k the force constant of this potential. For $t=0$, the minimum of the potential is at the origin, $\mathbf{x}_0^* = \mathbf{0}$, and it moves with a velocity $\mathbf{u}^*(t)$, which in principle can be an arbitrary function of time. We also consider the overdamped approximation of Eq. (1) where the corresponding dynamical equation becomes

$$\frac{d\mathbf{x}}{dt} = -\Lambda\mathbf{x} + \Lambda\mathbf{x}^* + k^{-1}\Lambda\mathbf{A}(t), \tag{5}$$

where Λ is a 2×2 matrix given by

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$$\Lambda = \begin{pmatrix} \bar{\gamma} & \Omega \\ -\Omega & \bar{\gamma} \end{pmatrix}, \tag{6}$$

such that $\bar{\gamma}=k/\gamma_e$, with $\gamma_e=\gamma[1+(\omega^2/\gamma^2)]$, which corresponds to a redefinition of the friction coefficient, and $\Omega=k\omega/(\gamma^2+\omega^2)$. As established in Ref. [2], the total work W_{tot} done on a system during a time τ is defined (in the two-dimensional case) by

$$W_{\mathrm{tot}} = \int_0^\tau \mathbf{u}^* \cdot \mathbf{F}(\mathbf{x},\mathbf{x}^*)dt, \tag{7}$$

or equivalently [2]

$$W_{\mathrm{tot}} = \Delta U_C + W_{\mathrm{Br}}, \tag{8}$$

where $\Delta U_C=(k/2)[|\Delta\mathbf{x}(\tau)|^2-|\Delta\mathbf{x}(0)|^2]$ with $\Delta\mathbf{x}(t)=\mathbf{x}(t)-\mathbf{x}^*(t)$, and

$$W_{\mathrm{Br}} = \int_0^\tau \mathbf{u} \cdot \mathbf{F}(\mathbf{x},\mathbf{x}^*)dt \tag{9}$$

represents the work done (dissipated work) on the Brownian particle by the harmonic force $\mathbf{F}(\mathbf{x},\mathbf{x}^*)$ given in Eq. (4); $\mathbf{u}$ is the Brownian particle velocity. We now give a proof for one instance of the fluctuation theorem when there is a constant magnetic field. We proceed as follows: we separate the average motion from the stochastic motion [2], where $\langle \mathbf{x}(t)\rangle$ is the deterministic solution of Eq. (5), that is,

$$\frac{d\langle \mathbf{x}\rangle}{dt} = -\Lambda\langle \mathbf{x}\rangle + \Lambda\mathbf{x}^*, \tag{10}$$

with the initial condition $\langle \mathbf{x}_0\rangle=\mathbf{0}$. Then we look at the deviation from this average motion through the change of variable

$$\mathbf{X} = \mathbf{x} - \langle \mathbf{x}\rangle. \tag{11}$$

In this case the expression for the total work in terms of the $\mathbf{X}$ variable, taking into account the expression of the harmonic force (4), reads

$$W_{\mathrm{tot}} = -k\int_0^\tau [\mathbf{u}^*\cdot\mathbf{X} + \mathbf{u}^*\cdot(\langle\mathbf{x}\rangle - \mathbf{x}^*)]dt. \tag{12}$$

Since $\langle \mathbf{X}\rangle=\mathbf{0}$ we have that the average work $\langle W_{\mathrm{tot}}\rangle$ is then

$$\langle W_{\mathrm{tot}}\rangle = -k\int_0^\tau \mathbf{u}^*\cdot[\langle\mathbf{x}\rangle - \mathbf{x}^*]dt. \tag{13}$$

Also, from the solution of Eq. (10) we can show that

$$\langle \mathbf{x}\rangle = \mathbf{x}^*(t) - e^{-\Lambda t}\int_0^t e^{\Lambda t'}\mathbf{u}^*(t')dt'. \tag{14}$$

Now, the matrix Λ can also be written as $\Lambda=\bar{\gamma}I+\bar{\mathcal{W}}$, where $\bar{\mathcal{W}}$ is a real antisymmetric matrix and $e^{\Lambda t}=e^{\bar{\gamma}t}\mathcal{R}(t)$, with $\mathcal{R}(t)=e^{\bar{\mathcal{W}}t}$ an orthogonal rotation matrix such that $\mathcal{R}^T(t)=\mathcal{R}^{-1}(t)$, i.e., the transpose is its inverse and therefore $\mathcal{R}^{-1}(t)=e^{-\bar{\mathcal{W}}t}$. In this case

$$\bar{\mathcal{W}} = \begin{pmatrix} 0 & \Omega \\ -\Omega & 0 \end{pmatrix}, \quad \mathcal{R}(t) = \begin{pmatrix} \cos\Omega t & \sin\Omega t \\ -\sin\Omega t & \cos\Omega t \end{pmatrix}. \tag{15}$$

Under these conditions we substitute Eq. (14) into Eq. (13) to get

$$\langle W_{\mathrm{tot}}\rangle = k\int_0^\tau dt'\,\mathbf{u}^*\cdot\mathcal{R}^{-1}(t')\int_0^{t'} e^{-\bar{\gamma}(t'-t'')}\mathbf{U}^*(t'')dt'', \tag{16}$$

where we have defined $\mathbf{U}^*(t)=\mathcal{R}(t)\mathbf{u}^*(t)$. If we take into account that the scalar product of two vectors $\mathbf{a}$ and $\mathbf{b}$ can also be written as $\mathbf{a}\cdot\mathbf{b}=\mathbf{a}^T\mathbf{b}$, the average value of the work can be written as

$$\langle W_{\mathrm{tot}}\rangle = k\int_0^\tau dt'\int_0^{t'} e^{-\bar{\gamma}(t'-t'')}\mathbf{U}^*(t')\cdot\mathbf{U}^*(t'')dt''. \tag{17}$$

On the other hand, the variance of the work is $V=\langle W_{\mathrm{tot}}^2\rangle-\langle W_{\mathrm{tot}}\rangle^2$, so that from Eq. (12) it can be written as

$$V = k^2\int_0^\tau\int_0^\tau \langle \mathbf{X}(t_1)\cdot\mathbf{u}^*(t_1)\mathbf{X}(t_2)\cdot\mathbf{u}^*(t_2)\rangle dt_1dt_2. \tag{18}$$

To evaluate this expression, we need the explicit solution of the variable $\mathbf{X}$, which according to Eqs. (5) and (11) satisfies the Langevin equation

$$\frac{d\mathbf{X}}{dt} = -\Lambda\mathbf{X} + k^{-1}\Lambda\mathbf{A}(t). \tag{19}$$

The required solution can be written as

$$\mathbf{X}(t) = e^{-\bar{\gamma}t}\mathcal{R}^{-1}(t)\mathbf{X}_0 + k^{-1}\mathcal{R}^{-1}(t)\mathbf{C}(t), \tag{20}$$

where the vector

$$\mathbf{C}(t) = \int_0^t e^{-\bar{\gamma}(t-t')}\Lambda\bar{\mathbf{A}}(t')dt', \tag{21}$$

and $\bar{\mathbf{A}}(t)=\mathcal{R}(t)\mathbf{A}(t)$. If we use again the property of the scalar product between two arbitrary vectors, as was established above, we can show that

$$\mathbf{X}(t)\cdot\mathbf{u}^*(t) = e^{-\bar{\gamma}t}\mathbf{U}^*(t)\cdot\mathbf{X}_0 + k^{-1}\mathbf{U}^*(t)\cdot\mathbf{C}(t). \tag{22}$$

In terms of the components we have

$$\begin{aligned}\langle \mathbf{X}(t_1)\cdot\mathbf{u}^*(t_1)\mathbf{X}(t_2)\cdot\mathbf{u}^*(t_2)\rangle &= e^{-\bar{\gamma}(t_1+t_2)}U_i^*(t_1)U_j^*(t_2)\langle X_{0i}X_{0j}\rangle \\ &\quad + k^{-2}U_i^*(t_1)U_j^*(t_2)\langle C_i(t_1)C_j(t_2)\rangle.\end{aligned} \tag{23}$$

The initial distribution for $\mathbf{X}_0$ is assumed to be the canonical equilibrium distribution [2,13], that is, $P_{\mathrm{eq}}(\mathbf{X}_0)=(k\beta/2)\exp(-k\beta|\mathbf{X}_0|^2/2)$ where $\beta=1/k_BT$ with k_B Boltzmann's constant and T the temperature, and therefore $\langle X_{0i}X_{0j}\rangle=(k\beta)^{-1}\delta_{ij}$. For the vector $\mathbf{C}(t)$, the correlation function becomes

$$\langle C_i(t_1)C_j(t_2)\rangle = \int_0^{t_1}\int_0^{t_2} e^{-\bar{\gamma}(t_1+t_2-t_1'-t_2')}\Lambda_{il}\Lambda_{jm} \times \langle \bar{A}_l(t_1')\bar{A}_m(t_2')\rangle dt_1' dt_2'. \tag{24}$$

Using the definitions given in the text, we can show that

$$\langle C_i(t_1)C_j(t_2)\rangle = \frac{k}{\beta}(e^{-\bar{\gamma}|t_1-t_2|} - e^{-\bar{\gamma}(t_1+t_2)})\delta_{ij}. \tag{25}$$

So the variance now reduces to

$$V = \frac{k}{\beta}\int_0^{\tau}\int_0^{\tau} dt_1 dt_2 e^{-\bar{\gamma}|t_1-t_2|} U_i^*(t_1)U_i^*(t_2). \tag{26}$$

Finally, for times $t_1 < t_2$ or $t_2 < t_1$ we have

$$V = 2\frac{k}{\beta}\int_0^{\tau} dt' \int_0^{t'} e^{-\bar{\gamma}(t'-t'')}\mathbf{U}^*(t')\cdot\mathbf{U}^*(t'')dt'', \tag{27}$$

and therefore we conclude that

$$\langle W_{\text{tot}}^2\rangle - \langle W_{\text{tot}}\rangle^2 = \frac{2}{\beta}\langle W_{\text{tot}}\rangle. \tag{28}$$

This result is the same as that obtained by van Zon and Cohen [2] for an arbitrary time-dependent dragged velocity $\mathbf{u}^*$ in the absence of the magnetic field. Thus, it is a generalization to their results when a magnetic field is present. The same result (28) was obtained by Jayannavar and Sahoo [13] when the harmonic potential minimum is dragged with constant velocity, that is, $\mathbf{u}^*=(u,u)$, with u a constant. Equation (28) leads to the transient work-fluctuation theorem [2,7,11], that is,

$$\frac{P(W)}{P(-W)} = \exp(\beta W). \tag{29}$$

The last equation shows that the transient work fluctuation theorem also holds in the presence of a magnetic field.

On the other hand, we can, in general, establish an alternative form of the total work done on the system if we take into account the definition given in Eq. (8). Let $U(\mathbf{x},t)$ be any potential such that $-\nabla_{\mathbf{x}}U=\mathbf{F}(\mathbf{x},\mathbf{x}^*)$. Since $dU/dt = \nabla_{\mathbf{x}}U\cdot\mathbf{u}+\partial U/\partial t = -\mathbf{F}(\mathbf{x},\mathbf{x}^*)\cdot\mathbf{u}+\partial U/\partial t$, we obtain for W_{Br} [see Eq. (9)] the following:

$$W_{\text{Br}} = -\Delta U + \int_0^{\tau}\frac{\partial U}{\partial t}dt = -\Delta U + W_J, \tag{30}$$

where $\Delta U = U(x(\tau),y(\tau),\tau) - U(x(0),y(0),0)$ and

$$W_J \equiv \int_0^{\tau}\frac{\partial U}{\partial t}dt \tag{31}$$

is the work considered by Jayannavar and Sahoo [13] for two particular cases. In fact, as shown by Jayannavar and Sahoo [13], Eq. (31) gives the work considered by Jarzynski [1] for which the Jarzynski equality holds; this will be commented on further below. Using Eqs. (8) and (30) we conclude that the total work is given by

$$W_{\text{tot}} = \Delta U_C - \Delta U + W_J. \tag{32}$$

In particular, taking $U=U_C$, we have that $W_{\text{tot}}=W_J$. We now study another type of harmonic potential model which corresponds to a generalization of the second case considered by Jayannavar and Sahoo [13]. The calculations given below generalize the case studied by them when the charged particle is subjected to an ac force. In this case the harmonic trap potential would be

$$\begin{aligned} U(\mathbf{x},t) &= \frac{k}{2}|\mathbf{x}|^2 - k\mathbf{x}\cdot\mathbf{x}^*(t) \\ &= \frac{k}{2}|\mathbf{x}-\mathbf{x}^*|^2 - \frac{k}{2}|\mathbf{x}^*|^2 \\ &= U_C(\mathbf{x},t) + U_1(\mathbf{x},t), \end{aligned} \tag{33}$$

where $U_1(\mathbf{x},t) = -(k/2)|\mathbf{x}^*|^2$ and its corresponding harmonic force is clearly given by $\mathbf{F}(\mathbf{x},\mathbf{x}^*) = -k(\mathbf{x}-\mathbf{x}^*)$. Jayannavar and Sahoo's second model is obtained by taking $\mathbf{x}=(x,y)$ and $\mathbf{x}^*(t)=((A/k)\sin\omega t,0)$ in Eq. (33). We now consider the evaluation of W_J given by Eq. (31). For the potential given by Eq. (33) the work W_J will be given in this case by

$$W_J = -k\int_0^{\tau}\mathbf{x}\cdot\mathbf{u}^* dt = -k\int_0^{\tau}(\mathbf{u}^*\cdot\mathbf{X} + \mathbf{u}^*\cdot\langle\mathbf{x}\rangle)dt, \tag{34}$$

and therefore the average work now reads as follows:

$$\langle W_J\rangle = -k\int_0^{\tau}\mathbf{u}^*\cdot\langle\mathbf{x}\rangle dt. \tag{35}$$

The substitution of the solution given by Eq. (14) into Eq. (35) allows us to write the average work as

$$\langle W_J\rangle = k\int_0^{\tau}dt'\int_0^{t'} e^{-\bar{\gamma}(t'-t'')}\mathbf{U}^*(t')\cdot\mathbf{U}^*(t'')dt'' - \frac{k}{2}\Delta|\mathbf{x}^*|^2, \tag{36}$$

where $\Delta|\mathbf{x}^*|^2 = |\mathbf{x}^*(\tau)|^2 - |\mathbf{x}^*(0)|^2$. Now the variance according to Eq. (34) is exactly the same as that given in Eq. (27). So that, by multiplying Eq. (36) by the factor $2/\beta$, we show that the variance can be written as

$$\langle W_J^2\rangle - \langle W_J\rangle^2 = \frac{2}{\beta}(\langle W_J\rangle - \Delta U_1), \tag{37}$$

where $\Delta U_1 = -(k/2)\Delta|\mathbf{x}^*|^2$. The direct comparison between Eqs. (37) and (28) shows that the fluctuation theorem Eq. (29) does not hold when we use W_J. In fact, notice that for the potential given by Eq. (33) we have $\Delta U = \Delta U_C + \Delta U_1$ and so $W_J = W_{\text{tot}} + \Delta U_1$, where Eq. (32) was used. Using the last relation in Eq. (37), we conclude that

$$\langle W_{\text{tot}}^2\rangle - \langle W_{\text{tot}}\rangle^2 = \frac{2}{\beta}\langle W_{\text{tot}}\rangle, \tag{38}$$

which means that the fluctuation theorem holds for the total work, as expected. As mentioned before, the work W_J, given by Eq. (31), calculated by Jayannavar and Sahoo [13] corresponds to the one used by Jarzynski to establish the so-called Jarzynski equality, which reads as

$$\langle e^{-\beta W_J} \rangle = e^{-\beta \Delta F}, \tag{39}$$

where the average can be calculated with the help of the full work probability distribution, which in this case is a Gaussian distribution given by [2,13]

$$P(W_J) = \frac{1}{\sqrt{4\pi \langle W_J \rangle / \beta}} e^{-\beta(W_J - \langle W_J \rangle)^2 / 4 \langle W_J \rangle}. \tag{40}$$

For the case of the potential U_C that leads to Eq. (28) we show that

$$\langle e^{-\beta W_J} \rangle = e^{-\beta \Delta F} = 1, \tag{41}$$

which implies $\Delta F = 0$, indicating that the equilibrium free energy of a particle in a harmonic potential is independent of the magnetic field, consistent with the Bohr–van Leeuwen theorem on the absence of orbital diamagnetism in a classical systems of charged particles in thermodynamic equilibrium [14]. Notice that in this case $W_{\mathrm{tot}} = W_J$. The result (41) is the same conclusion arrived at by Jayannavar and Sahoo [13] for the harmonic potential given by Eq. (4), but with a constant value of the velocity $\mathbf{u}^*$. On the other hand, the potential given by Eq. (33) that leads to the condition given by Eq. (37), the JE given by Eq. (39) implies that the free energy difference is then $\Delta F = -(k/2)\Delta |\mathbf{x}^*|^2 = \Delta U_1$, which is magnetic field independent, again confirming the Bohr–van Leeuwen theorem. For Jayannavar and Sahoo's second model we get the same result for ΔF as a particular case, that is, $\Delta F = -(A^2/2k)\sin^2(\omega\tau)$. Our conclusions in this work are then that, no matter what the minimum's velocity of the harmonic potential is, the variance of the total work distribution is twice the average value of the total work when a constant magnetic field is present. This result holds for the models given by Eqs. (4) and (33). When Jarzynski's work is considered, the variance depends on the type of the time-dependent harmonic potential. For the potential given by Eq. (4) the same result stated above holds for Jarzynski's work since $W_{\mathrm{tot}} = W_J$, and for the potential given by Eq. (33) the variance of W_J is given by Eq. (37). This equation clarifies the origin of the free energy identified by Jayannavar and Sahoo [13] since the average $\langle \exp(-\beta W) \rangle \neq 1$, meaning that there is a free energy $\Delta F \neq 0$ when W_J is used instead of the total work. In addition, for W_J the results obtained by Jayannavar and Sahoo show that the corresponding averages change depending on the potential used; for the model given by Eq. (4) the change in the Helmholtz free energy, ΔF, is zero while for the potential given by Eq. (33) $\Delta F = \Delta U_1$. Last, we notice that our result concerning the fluctuation properties of the work is general in the sense that it is valid for any time-dependent motion of the minimum's potential in the harmonic trap. The particular results given by Jayannavar and Sahoo are the same as those obtained by our method. Finally, we would like to point out that the results obtained should not be taken as arguments for favoring one or other definition of work; the two definitions (Jarzynski's work and the total work) complement each other.

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