Entropy production theorem for a charged particle in an electromagnetic field

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In this work, it is shown that the detailed fluctuation theorem for the total entropy production of a charged particle in a two-dimensional harmonic trap under the action of an electromagnetic field is valid in two physical situations. The proof of the theorem is achieved if the particle is initially distributed with a canonical distribution at equilibrium with the thermal bath. The two examined cases are the following: in the first case, the charged particle in the harmonic trap is subjected to an arbitrary time-dependent electric field; in the second one, the minimum of the harmonic trap is arbitrarily dragged by such an electric field. The theoretical framework is developed within the context of stochastic thermodynamics and the Langevin dynamics for the charged particle.

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I. INTRODUCTION

The fluctuation theorems (FTs) are topics of current interest to the scientific community and continue to be applied to nonequilibrium thermodynamics of small systems in which thermal fluctuations play a very important role [1]. In this context, the study of the FTs for thermodynamic quantities such as work, heat, and entropy production produces essential results for the understanding of nonequilibrium phenomena. It is well known that the second law of thermodynamics states that the entropy of a macroscopic isolated system always increases. The entropy and the entropy production are quantities associated to macroscopic systems and they have a clear physical sense as properties of ensembles. However, when such concepts are applied to small systems and in short-time intervals, it becomes clear that there exists a probability to find situations which do not match the ensemble averages. The FTs offer a way to quantify such deviations, which in fact becomes important for such small systems within short times [2,3]. In general, FTs relate probability distribution functions along forward and backward trajectories for a small system. In the case of the entropy this statement suggests a definition of the entropy along a stochastic trajectory. This and other thermodynamic concepts, such as the first-law-like energy balance involving applied or extracted work, exchanged heat, and changes in internal energy, were consistently defined along a single stochastic trajectory in the context of stochastic thermodynamics by Seifert [4,5]. Stochastic thermodynamics has been developed for mesoscopic systems such as colloidal particles or single (bio)molecules driven out of equilibrium by time-dependent forces but still in contact with a heat bath of well-defined temperature. The main results reported in [4,5] are the following: the total entropy production (TEP), denoted as Δs_{tot} , along a single stochastic trajectory, which involves both the particle entropy and entropy production in the surrounding medium, satisfies the integral fluctuation theorem (IFT). It is expressed as $\langle e^{-\Delta s_{tot}} \rangle = 1$ for any initial condition when the particle is arbitrarily driven by time-dependent external forces over a finite time interval (*the transient case*). It is also shown that in the *nonequilibrium steady state* over a finite time interval, a stronger fluctuation theorem, called the detailed fluctuation theorem (DFT), holds, that is, $P(\Delta s_{tot})/P(-\Delta s_{tot}) = e^{\Delta s_{tot}}$, where $P(\Delta s_{tot})$ is the probability of entropy generating trajectory and $P(-\Delta s_{tot})$ is that of annihilating trajectory.

Last year, Saha et al. [6] used the concepts of stochastic thermodynamics and the definition of the entropy along a single stochastic trajectory to prove that even in the transient case the DFT for a Brownian particle in a harmonic trap also holds for two exactly solvable models, namely, (i) the Brownian particle is in a harmonic trap and it is subjected to an external time-dependent force and (ii) the minimum of the trap potential is arbitrarily dragged with a time-dependent protocol. They also showed that the average entropy production over a finite time interval gives a better bound for the average work performed on the system than that obtained from the Jarzynski equality. Perhaps, it would be pertinent to comment here that in the conclusions of Ref. [6] the following sentence is remarked: "Analysis of the total entropy production in presence of magnetic field is carried out separately. The results will be published elsewhere." However, such an analysis has not yet been reported.

The purpose of the present paper is to prove, also in the transient case, the validity of the DFT for the total entropy production for the case of a Brownian harmonic oscillator in the presence of an electromagnetic field in two physical situations for arbitrary time-dependent electric field driven over a finite time interval: (i) the charged Brownian particle in a two-dimensional harmonic trap is subjected to the action of an arbitrary time-dependent electric field and (ii) the minimum of the harmonic trap is arbitrarily dragged by the electric field. The goal is achieved by means of the explicit solution of the Smoluchowski equation (SE) associated with the Langevin equation for the charged particle under the assumption of an initial canonical distribution at equilibrium with the thermal bath. It will be shown that this solution is essential for the calculation of the particle entropy along a single stochastic trajectory. The calculation of the explicit solution of the SE is not an easy task. Furthermore, it will be

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better calculated by means of a mathematical strategy consisting in two transformations [7,8]: one is given in terms of a stochastic variable $\mathbf{X}(t)$ and the other corresponds to a time-dependent rotation of this variable. In this scheme of solution, the DFT is proved in a very simple and effective way.

The structure of the work is as follows: in Sec. II, the two-dimensional (on the *x*-*y* plane) Langevin equation for the charged harmonic oscillator in the presence of the electromagnetic field is introduced. The process along the *z* axis, which is independent of the planar process, has already been studied in [6], so it is not considered here. The concepts of stochastic thermodynamics and the definition of the trajectory-dependent entropy are given to establish the TEP. The TEP requires the calculation of the charged particle joint probability density giving the initial condition. This calculation is done with an initial canonical distribution. In Sec. III, the DFT is proved for the above two mentioned physical situations. The concluding remarks are given in Sec. IV.

II. LANGEVIN DYNAMICS AND STOCHASTIC THERMODYNAMICS

Let us consider a particle of charge q trapped in a harmonic potential which experiences Brownian motion in a thermal bath at temperature T; also, it is in the presence of an electromagnetic field. The magnetic field is a constant vector given by $\mathbf{B} = (0, 0, B)$ and the electric field is an arbitrary time-dependent vector defined as $\mathbf{E}(t)$. Due the orientation of the magnetic field, the motion can be split into two independent processes: one on the x-y plane, perpendicular to the magnetic field, and the other parallel to this field. We are interested only in the x-y plane on which all the other vectors except the magnetic field lie, so that the two-dimensional harmonic trap reads as $V(\mathbf{x}) = (k/2)|\mathbf{x}|^2$, where $\mathbf{x} = (x, y)$ is the position vector on the plane and k is a constant. The external time-dependent electric force is then $\mathbf{F}_{e}(t) = q\mathbf{E}(t)$. The overdamped approximation of the planar Langevin equation for the charged harmonic oscillator in this case can be written as

$$\frac{d\mathbf{x}}{dt} = -\Lambda \mathbf{x} + k^{-1} \Lambda \mathbf{F}_e(t) + k^{-1} \Lambda \mathbf{g}(t), \qquad (1)$$

where Λ is the matrix

$$\Lambda = \begin{pmatrix} \tilde{\gamma} & \tilde{\Omega} \\ -\tilde{\Omega} & \tilde{\gamma} \end{pmatrix}.$$
 (2)

In terms of the dimensionless parameter $C = qB/c\gamma$, where γ is the friction coefficient, the elements of matrix Λ are defined as $\tilde{\gamma} = k/\gamma(1+C^2)$ and $\tilde{\Omega} = kC/\gamma(1+C^2)$. The vector $\mathbf{g}(t)$ is the fluctuating force with zero mean value $\langle g_i(t) \rangle = 0$ and correlation function $\langle g_i(t)g_j(t') \rangle = 2\lambda \delta_{ij}\delta(t-t')$, with i, j=x, y and λ is the noise intensity which according to the fluctuation-dissipation relation satisfies $\lambda = \gamma T$, where the Boltzmann constant k_B has been absorbed in the temperature *T*.

According to stochastic thermodynamics [4,5,9], the firstlaw-like balance between the applied work *W*, the change in internal energy ΔU , and the dissipated heat Q to the bath can be calculated along a trajectory $\mathbf{x}(t)$ over a finite time interval t. This first-law-like reads as

$$Q = W - \Delta U, \tag{3}$$

where the work can be calculated from the relation [6,10,11]

$$W = \int_0^t \frac{\partial U(\mathbf{x}, t')}{\partial t'} dt'.$$
 (4)

On the other hand, the change in the medium entropy Δs_m over the time interval is $\Delta s_m = Q/T$ and the nonequilibrium Gibbs entropy *S* of the system in the present problem is defined as

$$S(t) = -\int f(\mathbf{x}, t) \ln f(\mathbf{x}, t) d\mathbf{x} = \langle s(t) \rangle.$$
 (5)

This definition suggests the definition of a trajectorydependent entropy for the particle as

$$\mathbf{s}(t) = -\ln f[\mathbf{x}(t), t], \tag{6}$$

where the probability density $f(\mathbf{x}, t)$ is obtained through the solution of the SE and it is evaluated along the stochastic trajectory. For a given trajectory $\mathbf{x}(t)$, the entropy s(t) depends on the given initial data $f(\mathbf{x}_0) \equiv f(\mathbf{x}_0, 0)$, where $f(\mathbf{x}_0)$ is the probability density of the particle at initial time t=0 and thus contains information about the whole ensemble. The change in the system entropy for any trajectory of duration t is then

$$\Delta s = -\ln\left[\frac{f(\mathbf{x},t)}{f(\mathbf{x}_0)}\right].$$
(7)

Now, the change in TEP along a trajectory over a finite time interval t is shown to be [4,5]

$$\Delta s_{tot} = \Delta s_m + \Delta s. \tag{8}$$

Using this definition, Seifert derived the IFT, $\langle e^{-\Delta s_{tot}} \rangle = 1$, where the angular brackets denote average over the statistical ensemble of realizations or over the ensemble of finite time trajectories [4,5]. Also, he showed that in the nonequilibrium steady state over a finite time interval, the DFT holds. The latter is stated as

$$\frac{P(\Delta s_{tot})}{P(-\Delta s_{tot})} = e^{\Delta s_{tot}}.$$
(9)

This theorem has also been proved, even in the transient case, for a Brownian particle in a harmonic trap only if the system is initially prepared in equilibrium [6].

In what follows, it will be shown that this is also the case for a charged Brownian particle in an electromagnetic field. For this purpose it is necessary to calculate the joint probability density (JPD) $f(\mathbf{x},t)$ as required by Eq. (7). Let us first proceed to solve the SE for the transition-probability density (TPD) $P(\mathbf{x},t|\mathbf{x}_0)$ associated with Eq. (1). The SE is given by [8,12]

$$\frac{\partial P}{\partial t} + \mathbf{b}(t) \cdot \nabla_{\mathbf{x}} P = \nabla_{\mathbf{x}} \cdot (\Lambda \mathbf{x} P) + \tilde{\lambda} \nabla_{\mathbf{x}}^2 P, \qquad (10)$$

subject to the initial condition $P(\mathbf{x}, 0 | \mathbf{x}_0) = \delta(\mathbf{x} - \mathbf{x}_0)$. Besides it has been defined $\mathbf{b}(t) = k^{-1} \Lambda \mathbf{F}_e(t)$ and $\lambda = \lambda / \gamma^2 (1 + C^2)$, both are magnetic-field dependent. The solution for $f(\mathbf{x}, t)$, assuming the initial condition $f(\mathbf{x}_0) = \delta(\mathbf{x}_0)$, has been given in [8]. Now, the function $f(\mathbf{x}, t)$ will be calculated assuming an initial canonical distribution for $f(\mathbf{x}_0)$. Thus, it is convenient to give briefly the algebraic steps leading to the solution. The strategy of solution relies upon two transformations: the first one is the change of variable $\mathbf{X} = \mathbf{x} - \langle \mathbf{x} \rangle$ and the other is the transformation $\mathbf{X}' = e^{\widetilde{W}t}\mathbf{X}$, such that $\langle \mathbf{x} \rangle$ is the deterministic solution of Eq. (1) and the other coordinates \mathbf{X}' and \mathbf{X} satisfy the following differential equations:

$$\frac{d\langle \mathbf{x} \rangle}{dt} = -\Lambda \langle \mathbf{x} \rangle + \mathbf{b}(t), \qquad (11)$$

$$\frac{d\mathbf{X}}{dt} = -\tilde{\gamma}\mathbf{X} - \tilde{W}\mathbf{X} + \mathbf{G}(t), \qquad (12)$$

$$\frac{d\mathbf{X}'}{dt} = -\tilde{\gamma}\mathbf{X}' + \mathbf{G}'(t), \qquad (13)$$

where $\mathbf{G}(t) = k^{-1}\Lambda \mathbf{g}(t)$, $\mathbf{G}'(t) = \mathcal{R}(t)\mathbf{G}(t)$, and $\Lambda = \tilde{\gamma}\mathbf{I} + \tilde{W}$, with **I** representing the unit matrix and \tilde{W} representing the antisymmetric matrix which satisfies $\mathcal{R}(t) = e^{\tilde{W}t}$. $\mathcal{R}(t)$ is an orthogonal rotation matrix with the property $\mathcal{R}^{-1}(t) = e^{-\tilde{W}t}$, and

$$\widetilde{W} = \begin{pmatrix} 0 & \widetilde{\Omega} \\ -\widetilde{\Omega} & 0 \end{pmatrix}, \quad \mathcal{R}(t) = \begin{pmatrix} \cos \widetilde{\Omega}t & \sin \widetilde{\Omega}t \\ -\sin \widetilde{\Omega}t & \cos \widetilde{\Omega}t \end{pmatrix}. \quad (14)$$

The solution of Eq. (10) is attained by solving the SE associated with Eq. (13) which is very similar to the ordinary Brownian motion. Thus, the solution of this SE is well known [12,13] and it is given by

$$P'(\mathbf{X}',t|\mathbf{X}'_{0}) = \frac{k}{2\pi T(1-e^{-2\tilde{\gamma}t})} \exp\left\{-\frac{k|\mathbf{X}'-e^{-\tilde{\gamma}t}\mathbf{X}'_{0}|^{2}}{2T(1-e^{-2\tilde{\gamma}t})}\right\}.$$
(15)

Coming back to the original variable \mathbf{x} , it can be shown that the solution of SE (10) is then [8]

$$P(\mathbf{x},t|\mathbf{x}_0) = \frac{k}{2\pi T(1-e^{-2\tilde{\gamma}t})} \exp\left(\frac{-k|\mathbf{x}-e^{-\Lambda t}[\bar{\mathbf{b}}(t)+\mathbf{x}_0]|^2}{2T(1-e^{-2\tilde{\gamma}t})}\right),$$
(16)

where $\mathbf{\bar{b}}(t) = \int_0^t e^{\Lambda s} \mathbf{b}(s) ds$. Having obtained the TPD [Eq. (16)], a more general JPD $f(\mathbf{x}, t)$ can be calculated from the integral

$$f(\mathbf{x},t) = \int f(\mathbf{x}_0,0) P(\mathbf{x},t|\mathbf{x}_0) d\mathbf{x}_0.$$
 (17)

In particular, if we assume that $f(\mathbf{x}_0, 0)$ is canonically distributed at equilibrium with the thermal bath at temperature *T*, then

$$f(\mathbf{x}_0) = \frac{k}{2\pi T} \exp\left(-\frac{k|\mathbf{x}_0|^2}{2T}\right).$$
 (18)

By substituting Eq. (18) into Eq. (17), it can be shown after some algebra that

$$f(\mathbf{x},t) = \frac{k}{2\pi T} \exp\left(-\frac{k|\mathbf{x} - \langle \mathbf{x} \rangle|^2}{2T}\right),\tag{19}$$

with $\langle \mathbf{x} \rangle = e^{-\Lambda t} \mathbf{\overline{b}}(t) = k^{-1} e^{-\Lambda t} \int_0^t e^{\Lambda s} \Lambda \mathbf{F}_e(s) ds$, which, by means of a partial integration, can also be written as

$$\langle \mathbf{x} \rangle = k^{-1} \mathbf{F}_e(t) - k^{-1} \mathcal{R}^{-1}(t) \int_0^t e^{-\tilde{\gamma}(t-t')} \mathbf{V}(t') dt', \quad (20)$$

where it has been taken into account that $\langle \mathbf{x}_0 \rangle = 0$, the vector $\mathbf{V}(t) \equiv \mathcal{R}(t)\mathbf{v}_e(t)$, and $\mathbf{v}_e(t) = d\mathbf{F}_e(t)/dt \equiv \dot{\mathbf{F}}_e(t)$. The JPD for the **X** variable can then be easily obtained from Eq. (19) to yield

$$f(\mathbf{X},t) = \frac{k}{2\pi T} \exp\left(-\frac{k|\mathbf{X}|^2}{2T}\right),\tag{21}$$

which is clearly stationary and, therefore, the initial distribution satisfies $f(\mathbf{X}_0) = (k/2\pi T) \exp(-k|\mathbf{X}_0|^2/2T)$. For the purposes required in Sec. III, we write the solution of Eq. (12), which reads

$$\mathbf{X}(t) = e^{-\tilde{\gamma}t} \mathcal{R}^{-1}(t) \mathbf{X}_0 + \mathcal{R}^{-1}(t) \int_0^t e^{-\tilde{\gamma}(t-t')} \mathbf{G}(t') dt'.$$
 (22)

III. DETAILED FLUCTUATION THEOREM

Let us now proceed to prove the DFT for the two physical situations considered in Sec. I of this work.

A. Particle in a harmonic trap subjected to a time-dependent electric field

For this physical situation one has the effective potential $U(\mathbf{x},t) = (k/2)|\mathbf{x}|^2 - \mathbf{x} \cdot \mathbf{F}_e(t)$. In this case the thermodynamic work is

$$W = \int_0^t \frac{\partial U(\mathbf{x}, t')}{\partial t'} dt' = -\int_0^t \mathbf{x}(t') \cdot \mathbf{v}_e(t') dt', \qquad (23)$$

and the internal energy change reads

$$\Delta U = \frac{k}{2} |\mathbf{x}|^2 - \mathbf{x} \cdot \mathbf{F}_e(t) - \frac{k}{2} |\mathbf{x}_0|^2, \qquad (24)$$

where $\mathbf{F}_{e}(0)=0$ is assumed for simplicity. On the other hand, $\Delta \bar{s}_{tot}$ is calculated from Eqs. (3), (18), (19), and (24), and it is (see Appendix C)

$$\Delta \overline{s}_{tot} = \frac{W - \Delta U}{T} - \ln \left[\frac{f(\mathbf{x}, t)}{f(\mathbf{x}_0)} \right]$$
$$= \frac{1}{T} \left[W + \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \mathbf{x} \cdot \mathbf{F}_e - k\mathbf{x} \cdot \langle \mathbf{x} \rangle \right].$$
(25)

Equations (23) and (25) show that the work and the change in entropy are linear functions of $\mathbf{x}(t)$ and since \mathbf{x} is also a linear function of the Gaussian random variable $\mathbf{g}(t)$ [as can be easily seen from the solution of Eq. (1)], $\Delta \overline{s}_{tot}$ is also a Gaussian random variable whose probability density satisfies the Gaussian distribution function,

$$P(\Delta \overline{s}_{tot}) = \frac{1}{\sqrt{2\pi\overline{\sigma}_s^2}} \exp\left(-\frac{(\Delta \overline{s}_{tot} - \langle \Delta \overline{s}_{tot} \rangle)^2}{2\overline{\sigma}_s^2}\right).$$
 (26)

Here $\bar{\sigma}_s^2 \equiv \langle \Delta \bar{s}_{tot}^2 \rangle - \langle \Delta \bar{s}_{tot} \rangle^2$ is the entropy variance and $\langle \Delta \bar{s}_{tot} \rangle$ is the entropy mean value. This last quantity satisfies

$$\langle \Delta \overline{s}_{tot} \rangle = \frac{1}{T} \bigg[\langle W \rangle - \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \langle \mathbf{x} \rangle \cdot \mathbf{F}_e \bigg], \qquad (27)$$

and $\langle W \rangle$ is the work mean value given by

$$\langle W \rangle = -\int_0^t \langle \mathbf{x}(t') \rangle \cdot \mathbf{v}_e(t') dt', \qquad (28)$$

where the mean value $\langle \mathbf{x} \rangle$ is given by solution (20). It can be checked from Eq. (25), after a long but straightforward algebra, that the entropy variance can be written as

$$\overline{\sigma}_{s}^{2} = \frac{1}{T^{2}} \{ \sigma_{w}^{2} + [\langle W \mathbf{x} \rangle - \langle W \rangle \langle \mathbf{x} \rangle] \cdot [2\mathbf{F}_{e} - 2k \langle \mathbf{x} \rangle] + \mathbf{F}_{e} \cdot \mathbf{\Xi} \cdot \mathbf{F}_{e} - 2k \langle \mathbf{x} \rangle \cdot \mathbf{\Xi} \cdot \mathbf{F}_{e} + k^{2} \langle \mathbf{x} \rangle \cdot \mathbf{\Xi} \cdot \langle \mathbf{x} \rangle \},$$
(29)

where $\sigma_w^2 \equiv \langle W^2 \rangle - \langle W \rangle^2$ is the variance of the work and $\Xi \equiv [\langle \mathbf{x} \mathbf{x} \rangle - \langle \mathbf{x} \rangle \langle \mathbf{x} \rangle]$ is a tensor. It is shown in Appendix A that the work mean value takes the form

$$\langle W \rangle = \frac{1}{k} \int_0^t dt' \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt'' - \frac{|\mathbf{F}_e(t)|^2}{2k},$$
(30)

and the variance of the work the expression

$$\sigma_w^2 = \frac{2T}{k} \int_0^t dt' \int_0^{t'} e^{-\widetilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt''.$$
(31)

Upon comparison of Eqs. (30) and (31), one sees that

$$\sigma_w^2 = 2T[\langle W \rangle + (|\mathbf{F}_e|^2/2k)]. \tag{32}$$

This result is similar to that calculated in Ref. [6] in the absence of magnetic field. Therefore, result (32) represents a generalization when an electromagnetic field is present. In this latter result, the effect of the electromagnetic field appears in the expression of the work mean value given by Eq. (28), through $\mathbf{V}(t) = \mathcal{R}(t) \dot{\mathbf{F}}_{e}(t)$, which is explicitly written as

$$\mathbf{V}(t) = q \begin{pmatrix} \cos \tilde{\Omega}t & \sin \tilde{\Omega}t \\ -\sin \tilde{\Omega}t & \cos \tilde{\Omega}t \end{pmatrix} \dot{\mathbf{E}}_e(t).$$
(33)

As it can be seen, this expression accounts for a timedependent rotation of the electric field rate of change due the magnetic field.

On the other hand, the tensor Ξ can be calculated most efficiently in terms of the X variable, showing that $\Xi = \langle \mathbf{x}\mathbf{x} \rangle - \langle \mathbf{x} \rangle \langle \mathbf{x} \rangle = \langle \mathbf{X}\mathbf{X} \rangle$. This correlation function is calculated with the help of Eq. (21), giving as a result $\Xi = \langle \mathbf{X}\mathbf{X} \rangle$ $= \langle \mathbf{X}_0 \mathbf{X}_0 \rangle = (T/k)\mathbf{I}$. In a similar way, it can be shown that $\langle W\mathbf{x} \rangle - \langle W \rangle \langle \mathbf{x} \rangle = \langle W\mathbf{X} \rangle$, where

$$\langle W\mathbf{X} \rangle = -\left\langle \left(\int_{0}^{t} \mathbf{v}_{e}(t') \cdot \mathbf{x}(t') dt' \right) \mathbf{X}(t) \right\rangle dt'.$$
 (34)

Again, according to Appendix A, Eq. (34) reduces to

$$\langle W\mathbf{X} \rangle = \frac{T}{k} [k \langle \mathbf{x}(t) \rangle - \mathbf{F}_e(t)].$$
(35)

Upon the substitution of the term Ξ [Eqs. (32) and (35)] into Eq. (29), the total entropy variance becomes

$$\bar{\sigma}_s^2 = \frac{2}{T} \left[\langle W \rangle - \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \langle \mathbf{x} \rangle \cdot \mathbf{F}_e \right] = 2 \langle \Delta \bar{s}_{tot} \rangle.$$
(36)

This result implies the validity of the DFT, in the transient case, for the total entropy production in an electromagnetic field when the initial state of the system is canonically distributed at equilibrium with the thermal bath, thus

$$\frac{P(\Delta \overline{s}_{tot})}{P(-\Delta \overline{s}_{tot})} = e^{\Delta \overline{s}_{tot}}.$$
(37)

B. Dragging of the harmonic trap

Let us now consider the physical situation for which the minimum of the harmonic trap is arbitrarily dragged by the time-dependent electric field. In this case the effective potential reads $U(\mathbf{x},t)=(k/2)|\mathbf{x}-[\mathbf{F}_e(t)/k]|^2$, and the thermodynamic work will be

$$\hat{W} = \int_0^t \frac{\partial U(\mathbf{x}, t')}{\partial t'} dt' = -\int_0^t \mathbf{x}(t') \cdot \mathbf{v}_e(t') dt' + \frac{|\mathbf{F}_e|^2}{2k}.$$
(38)

The change in the internal energy during a time t is now

$$\Delta \hat{U} = \frac{k}{2} \left| \mathbf{x} - \frac{\mathbf{F}_e(t)}{k} \right|^2 - \frac{k}{2} |\mathbf{x}_0|^2.$$
(39)

To calculate the change in the total entropy production defined in this case as $\Delta \hat{s}_{tot}$, a similar procedure to that employed in Sec. III A will be used (see Appendix C). For the present case

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$$\Delta \hat{s}_{tot} = \frac{1}{T} \left[\hat{W} + \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \mathbf{x} \cdot \mathbf{F}_e - k\mathbf{x} \cdot \langle \mathbf{x} \rangle - \frac{1}{2k} |\mathbf{F}_e|^2 \right].$$
(40)

Again \hat{W} and $\Delta \hat{s}_{tot}$ are linear functions of the Gaussian variable **x**, thus $P(\Delta \hat{s}_{tot})$ satisfies the same Gaussian distribution, the one given in Eq. (26). The mean value for the total entropy production becomes

$$\langle \Delta \hat{s}_{tot} \rangle = \frac{1}{T} \Biggl[\langle \hat{W} \rangle - \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \langle \mathbf{x} \rangle \cdot \mathbf{F}_e - \frac{1}{2k} |\mathbf{F}_e|^2 \Biggr], \quad (41)$$

and the work mean value is now

$$\langle \hat{W} \rangle = -\int_{0}^{t} \langle \mathbf{x}(t') \rangle \cdot \mathbf{v}_{e}(t') dt' + \frac{|\mathbf{F}_{e}|^{2}}{2k}.$$
 (42)

The total entropy variance defined as $\hat{\sigma}_s^2 \equiv \langle \Delta \hat{s}_{tot}^2 \rangle - \langle \Delta \hat{s}_{tot} \rangle^2$ becomes

$$\hat{\sigma}_{s}^{2} = \frac{1}{T^{2}} \{ \hat{\sigma}_{w}^{2} + [\langle \hat{W} \mathbf{x} \rangle - \langle \hat{W} \rangle \langle \mathbf{x} \rangle] \cdot [2\mathbf{F}_{e} - 2k \langle \mathbf{x} \rangle] + \mathbf{F}_{e} \cdot \mathbf{\Xi} \cdot \mathbf{F}_{e} - 2k \langle \mathbf{x} \rangle \cdot \mathbf{\Xi} \cdot \mathbf{F}_{e} + k^{2} \langle \mathbf{x} \rangle \cdot \mathbf{\Xi} \cdot \langle \mathbf{x} \rangle \},$$
(43)

where $\hat{\sigma}_w^2 \equiv \langle \hat{W}^2 \rangle - \langle \hat{W} \rangle^2$ is the variance of the work. Checking the calculation in Appendix B, the work mean value takes the form

$$\langle \hat{W} \rangle = \frac{1}{k} \int_0^t dt' \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt'', \qquad (44)$$

and its variance becomes

$$\hat{\sigma}_{w}^{2} = \frac{2T}{k} \int_{0}^{t} dt' \int_{0}^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt'', \qquad (45)$$

and therefore $\hat{\sigma}_{w}^{2}=2T\langle \hat{W}\rangle$. It is also clear that $\langle \hat{W}\mathbf{x}\rangle - \langle \hat{W}\rangle \langle \mathbf{x}\rangle = \langle \hat{W}\mathbf{X}\rangle$, where now

$$\langle \hat{W} \mathbf{X} \rangle = \left\langle \left(-\int_0^t \mathbf{v}_e(t') \cdot \mathbf{x}(t') dt' + \frac{|\mathbf{F}_e|^2}{2k} \right) \mathbf{X}(t) \right\rangle.$$
(46)

As shown in Appendix B, this expression reduces to

$$\langle \hat{W} \mathbf{X} \rangle = \frac{T}{k} [k \langle \mathbf{x}(t) \rangle - \mathbf{F}_e(t)].$$
(47)

Upon substitution of the term Ξ , the variance $\hat{\sigma}_{w}^{2}$, and Eq. (47) into Eq. (48), it can be concluded that

$$\hat{\sigma}_{s}^{2} = \frac{2}{T} \left[\langle \hat{W} \rangle - \frac{k}{2} |\langle \mathbf{x} \rangle|^{2} + \langle \mathbf{x} \rangle \cdot \mathbf{F}_{e} - \frac{1}{2k} |\mathbf{F}_{e}|^{2} \right] = 2 \langle \Delta \hat{s}_{tot} \rangle,$$
(48)

and therefore the DFT for the total entropy production as required by Eq. (37) holds. As can be checked from Eq. (37), it is now clear for both models $(s=\overline{s} \text{ and } s=\hat{s})$ that $\langle e^{-\Delta s_{tot}} \rangle = \int e^{-\Delta s_{tot}} P(\Delta s_{tot}) d(\Delta s_{tot}) = \int P(-\Delta s_{tot}) d(\Delta s_{tot}) = 1$ because $P(-\Delta s_{tot})$ is normalized, and therefore the IFT holds.

IV. CONCLUDING REMARKS

The thermodynamic concepts applied to the study of the Brownian motion have been used to prove the validity of the transient DFT for an electrically charged Brownian particle in a two-dimensional harmonic trap under the action of an electromagnetic field. The proof of the theorem has been given for two general physical situations when the system is initially distributed with a canonical distribution at equilibrium with the thermal bath. In both cases, the relation σ_s^2 $=2\langle\Delta s_{tot}\rangle$ is shown to be valid. As shown in Eqs. (27) and (41), the mean value of the total entropy production depends on the influence of the electromagnetic field through the work mean value, the mean value $\langle \mathbf{x} \rangle$, and $\mathbf{F}_{e}(t)$. It must be noted that all the results reported here have been achieved, thanks to an effective mathematical tool capable to solve SE (10) and calculate the mean value and the variance of the total entropy production in a very simple way. Under these conditions, the stochastic thermodynamics concepts have consistently been applied at this level.

On the other hand, in a similar way shown in [6], if the initial distribution is different from the canonical one. DFT in the transient case does not hold. For instance, consider a charged particle in a magnetic field embedded in a thermal bath at temperature T and in a harmonic trap $V(\mathbf{x})$ $=(k/2)|\mathbf{x}|^2$, which is initially prepared in a nonequilibrium state in the absence of any time-dependent perturbation or protocol ($\mathbf{F}_{e}=0$, W=0). For this case, an athermal initial distribution can be proposed as $f(\mathbf{x}_0) = (k/2\pi\sigma_0^2)\exp(k/2\pi\sigma_0^2)$ $[-k|\mathbf{x}_0|^2/2\sigma_0^2]$, with $\sigma_0^2 \neq T$. The probability density defined by Eq. (17) is now $f(\mathbf{x},t) = [k/2\pi\sigma^2(t)]\exp[-k|\mathbf{x}|^2/2\sigma^2(t)]$, where $\sigma^2(t) = T + (\sigma_0^2 - T)e^{-2\tilde{\gamma}t}$. It can be shown that the total entropy production is a quadratic function of \mathbf{x} and \mathbf{x}_0 , which is given by $\Delta s_{tot} = (\alpha/2) |\mathbf{x}_0|^2 + (\beta/2) |\mathbf{x}|^2 + \varepsilon$, where $\alpha = k [(\sigma_0^2 + \varepsilon) |\mathbf{x}_0|^2 + \varepsilon]$ $-T)/T\sigma_0^2$, $\beta = k\{[T - \sigma^2(t)]/T\sigma^2(t)\}$, and $\varepsilon = -\ln[\sigma_0^2/\sigma^2(t)];$ hence, the probability density $P(\Delta s_{tot})$ is not Gaussian. Following the algebraic steps in Ref. [6], it is also shown that the DFT does not hold. In this respect, it is very important to take into account the very recent contribution of Shargel [14] in which some comments in Ref. [6] have been addressed, namely, as proved by Saha et al., the transient fluctuation theorem (TFT), given by Eq. (37) for a Brownian particle in a harmonic potential and driven by an arbitrary timedependent force, is only valid if the particle is initially in thermal equilibrium. However, this is a surprising result because according to Shargel, Eq. (37) fails to distinguish between both the forward and backward path measures and the forward and backward entropy productions, each of which is distinct due to the time-dependent driving. Certainly, in the paper of Saha et al. and also as shown in this work, the TFT holds in a very particular case that strongly depends on the form on which the initial distribution has been constructed. The latter is constructed on the basis of a harmonic potential [see Eq. (18)]. For any other potential or initial distribution the TFT breaks down. This is indeed the case for an athermal initial distribution as commented in the beginning of this paragraph. On the other hand, as shown in Ref. [15], both the Jarzynski relation and DFT for the applied work have been verified for an overdamped colloidal particle in a timedependent nonharmonic potential in the context of the firstlaw-like balance. It is shown that the distribution of the work is non-Gaussian, though the DFT holds for this quantity, contrary to what happens with the total entropy production as shown in [6] and in the present work.

In the validity context of the DFT for the total entropy production, it is also shown in [6] that Eqs. (45) and (46) give a bound for the average work performed on the system over a finite time interval τ , which seems to be better than that obtained from the Jarzynski equality [11]. This statement is explicitly shown in Fig. 3 of Ref. [6] for a particular protocol. It is also clear that the same statement must be valid for the problem studied here due to the validity of the DFT [16–25].

Lastly, the theoretical demonstration of the transient DFT in the absence of an electromagnetic field [6], as well as in its presence, may motivate the carrying out of new experiments similar to those reported in Refs. [2,3].

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APPENDIX A: EXPLICIT CALCULATIONS FOR $\langle W \rangle$, σ_w^2 , AND $\langle WX \rangle$

To calculate the work mean value given by Eq. (30), the change of variable $\mathbf{X} = \mathbf{x} - \langle \mathbf{x} \rangle$ is used. In this case Eq. (28) does not change because $\langle \mathbf{X} \rangle = 0$. So, upon the substitution of Eq. (20) into Eq. (28), one has

$$\begin{split} \langle W \rangle &= -\frac{1}{k} \int_0^t \mathbf{F}_e(t') \cdot \dot{\mathbf{F}}_e(t') dt' \\ &+ \frac{1}{k} \int_0^t dt' \mathbf{v}_e \cdot \mathcal{R}^{-1}(t') \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t'') dt''. \end{split}$$
(A1)

The second term of this equation can be further rewritten in such a way that

$$\langle W \rangle = \frac{1}{k} \int_0^t dt' \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt'' - \frac{|\mathbf{F}_e(t)|^2}{2k}.$$
(A2)

On the other hand, for the variance σ_w^2 as given by Eq. (31) is written as

$$\sigma_w^2 = \int_0^t \int_0^t \mathbf{v}_e(t_1) \cdot \langle \mathbf{X}(t_1)\mathbf{X}(t_2) \rangle \cdot \mathbf{v}_e(t_2) dt_1 dt_2$$
$$= 2 \int_0^t dt' \int_0^{t'} \mathbf{v}_e(t') \cdot \langle \mathbf{X}(t')\mathbf{X}(t'') \rangle \cdot \mathbf{v}_e(t'') dt'', \quad (A3)$$

where the symmetry of the correlation function $\langle \mathbf{X}(t_1)\mathbf{X}(t_2)\rangle$ has been used. To evaluate the integral in Eq. (A3), the stationary property of the process $\mathbf{X}(t)$ is used. Therefore, its correlation function also satisfies that $\langle \mathbf{X}(t'-t'')\mathbf{X}_0 \rangle$. It can be seen from the initial probability density $f(\mathbf{X}_0)$ given in Sec.

II that $\langle \mathbf{X}_0 \mathbf{X}_0 \rangle = (T/k)\mathbf{I}$, where **I** is the unit matrix. By assuming that $\langle \mathbf{g}(t)\mathbf{X}_0 \rangle = 0$, then from Eq. (22) it has

$$\langle \mathbf{X}(t)\mathbf{X}_{0}\rangle = \frac{T}{k}e^{-\tilde{\gamma}t}\mathcal{R}^{-1}(t)\mathbf{I},$$
 (A4)

which implies

$$\langle \mathbf{X}(t'-t'')\mathbf{X}_0 \rangle = \frac{T}{k} e^{-\tilde{\gamma}(t'-t'')} \mathcal{R}^{-1}(t') \mathcal{R}(t'') \mathbf{I}.$$
 (A5)

Upon the substitution of Eq. (A5) into Eq. (A3), the variance of the work is then

$$\sigma_w^2 = \frac{2T}{k} \int_0^t dt' \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt''.$$
(A6)

The correlation function $\langle W\mathbf{x} \rangle - \langle W \rangle \langle \mathbf{x} \rangle = \langle W\mathbf{X} \rangle$ will be calculated by making use of Eq. (23). In this case

$$\langle W\mathbf{X} \rangle = -\left\langle \left(\int_{0}^{t} \mathbf{v}_{e}(t') \cdot \mathbf{x}(t') dt' \right) \mathbf{X}(t) \right\rangle$$
$$= -\int_{0}^{t} \mathbf{v}_{e}(t') \cdot \langle \mathbf{X}(t) \mathbf{X}(t') \rangle dt'.$$
(A7)

According to Eq. (A5), this correlation function now reads

$$\langle W\mathbf{X} \rangle = -\frac{T}{k} \int_{0}^{t} e^{-\tilde{\gamma}(t-t')} \mathcal{R}^{-1}(t) \mathcal{R}(t') \mathbf{I} \cdot \mathbf{v}_{e}(t')$$
$$= -\frac{T}{k} \mathcal{R}^{-1}(t) \int_{0}^{t} e^{-\tilde{\gamma}(t-t')} \mathbf{V}(t') dt'.$$
(A8)

Upon comparison of Eq. (A8) with Eq. (20), then

$$\langle W\mathbf{X} \rangle = \frac{T}{k} [k \langle \mathbf{x}(t) \rangle - \mathbf{F}_e(t)]. \tag{A9}$$

APPENDIX B: EXPLICIT CALCULATIONS FOR $\langle \hat{W} \rangle$, $\hat{\sigma}_{w}^{2}$, AND $\langle \hat{W} X \rangle$

The mean value of work given by Eq. (38), after substitution of Eq. (20), reads

$$\begin{split} \langle \hat{W} \rangle &= -\frac{1}{k} \int_{0}^{t} \mathbf{F}_{e}(t') \cdot \dot{\mathbf{F}}_{e}(t') dt' \\ &+ \frac{1}{k} \int_{0}^{t} dt' \mathbf{v}_{e} \cdot \mathcal{R}^{-1}(t') \int_{0}^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t'') dt'' + \frac{|\mathbf{F}_{e}|^{2}}{2k}. \end{split}$$

$$\end{split} \tag{B1}$$

Upon elimination of the first and third terms, it reduces to

$$\langle \hat{W} \rangle = \frac{1}{k} \int_0^t dt' \int_0^{t'} e^{-\hat{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt''.$$
(B2)

It is shown that the variance for the stochastic work [Eq. (38)] can also be written as

$$\hat{\sigma}_{w}^{2} = \int_{0}^{t} \int_{0}^{t} \mathbf{v}_{e}(t_{1}) \cdot \langle \mathbf{X}(t_{1})\mathbf{X}(t_{2}) \rangle \cdot \mathbf{v}_{e}(t_{2})dt_{1}dt_{2}$$
$$= 2\int_{0}^{t} dt' \int_{0}^{t'} \mathbf{v}_{e}(t') \cdot \langle \mathbf{X}(t')\mathbf{X}(t'') \rangle \cdot \mathbf{v}_{e}(t'')dt''. \quad (B3)$$

This expression is the same as that given by Eq. (A3), and therefore it reduces to the same expression given by Eq. (A6), that is,

$$\hat{\sigma}_w^2 = \frac{2T}{k} \int_0^t dt' \int_0^{t'} e^{-\tilde{\gamma}(t'-t'')} \mathbf{V}(t') \cdot \mathbf{V}(t'') dt''.$$
(B4)

Under these conditions it is shown that $\hat{\sigma}_{w}^{2}=2T\langle \hat{W}\rangle$.

This correlation function can be written with the help of Eq. (38) to give

$$\langle \hat{W} \mathbf{X} \rangle = \left\langle \left(-\int_{0}^{t} \mathbf{v}_{e}(t') \cdot \mathbf{x}(t') dt' + \frac{|\mathbf{F}_{e}|^{2}}{2k} \right) \mathbf{X}(t) \right\rangle$$
$$= -\int_{0}^{t} \mathbf{v}_{e}(t') \cdot \langle \mathbf{X}(t) \mathbf{X}(t') \rangle dt', \qquad (B5)$$

which is the same as Eq. (A7), so that

$$\langle \hat{W} \mathbf{X} \rangle = -\frac{T}{k} \mathcal{R}^{-1}(t) \int_{0}^{t} e^{-\tilde{\gamma}(t-t')} \mathbf{V}(t') dt' = \frac{T}{k} [k \langle \mathbf{x}(t) \rangle - \mathbf{F}_{e}(t)].$$
(B6)

APPENDIX C: EXPLICIT CALCULATION OF Δs_{tot} AND $\Delta \hat{s}_{tot}$

To obtain the total entropy production $\Delta \bar{s}_{tot}$ given by Eq. (25), we see from Eqs. (18), (19), and (24) that

$$\begin{split} \Delta \overline{s}_{tot} &= \frac{W - \Delta U}{T} - \ln \left[\frac{f(\mathbf{x}, t)}{f(\mathbf{x}_0)} \right] \\ &= \frac{1}{T} \left[W - \frac{k}{2} |\mathbf{x}|^2 + \mathbf{x} \cdot \mathbf{F}_e + \frac{k}{2} |\mathbf{x}_0|^2 \right] \\ &+ \frac{k}{2T} [|\mathbf{x} - \langle \mathbf{x} \rangle|^2 - |\mathbf{x}_0|^2] \\ &= \frac{1}{T} \left[W + \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \mathbf{x} \cdot \mathbf{F}_e - k\mathbf{x} \cdot \langle \mathbf{x} \rangle \right]. \end{split}$$
(C1)

In a similar way, the total entropy production $\Delta \hat{s}_{tot}$, given by Eq. (40), is obtained from Eqs. (18), (19), and (39), yielding

$$\begin{split} \Delta \hat{s}_{tot} &= \frac{\hat{W} - \Delta \hat{U}}{T} - \ln \left[\frac{f(\mathbf{x}, t)}{f(\mathbf{x}_0)} \right] \\ &= \frac{1}{T} \left[\hat{W} - \frac{k}{2} |\mathbf{x} - k^{-1} \mathbf{F}_e|^2 + \frac{k}{2} |\mathbf{x}_0|^2 \right] \\ &+ \frac{k}{2T} [|\mathbf{x} - \langle \mathbf{x} \rangle|^2 - |\mathbf{x}_0|^2] \\ &= \frac{1}{T} \left[\hat{W} + \frac{k}{2} |\langle \mathbf{x} \rangle|^2 + \mathbf{x} \cdot \mathbf{F}_e - k\mathbf{x} \cdot \langle \mathbf{x} \rangle - \frac{1}{2k} |\mathbf{F}_e|^2 \right]. \end{split}$$
(C2)

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