Langevin dynamics in crossed magnetic and electric fields: Hall and diamagnetic fluctuations

Dibyendu Roy* and N. Kumar†
Raman Research Institute, Bangalore 560080, India
(Received 28 August 2008; published 14 November 2008)

Based on the classical Langevin equation, we have revisited the problem of orbital motion of a charged particle in two dimensions for a normal magnetic field crossed with or without an in-plane electric bias. We are led to two interesting fluctuation effects: First, we obtain not only a longitudinal "work-fluctuation" relation as expected for a barotropic type system, but also a transverse work-fluctuation relation perpendicular to the electric bias. This "Hall fluctuation" involves the product of the electric and the magnetic fields. Second, for the case of harmonic confinement without bias, the calculated probability density for the orbital magnetic moment gives nonzero even moments, not derivable as field derivatives of the classical free energy.

DOI: 10.1103/PhysRevE.78.052102 PACS number(s): 05.10.Gg, 05.40.−a, 75.20.−g, 75.47.−m

I. INTRODUCTION

Consider the classical motion of a charged particle in a plane under the influence of a normal (out-of-plane) magnetic field crossed in general with a parallel "in-plane" electric field, in the presence of a dissipative coupling to the environment (bath). This two-dimensional (2D) motion has two notable general features—first, the cyclotron circularly orbits about the magnetic field under the Lorentz force that classically does no work, and second, there is the well-known transverse drift identified as the Hall effect which is a dissipative transport (nonequilibrium) phenomenon. The orbital motion holds surprises—the best known of these being the absence of classical orbital diamagnetism in equilibrium, as embodied in the classic theorem due to Bohr and van Leeuwen, and, indeed, regarded by some to be a surprise of theoretical physics [1]. A notable point here is the subtle role played by the spatial confinement (the boundary) that interrupts the otherwise complete circular (diamagnetic) orbits leading to a skipping cuspidal motion at the boundary which is retrograde (paramagnetic) and exactly cancels the bulk diamagnetic contribution [2–4]. Diamagnetism, or rather its absence classically, [5] is, of course, a well-known equilibrium phenomenon. We, however, find interesting fluctuation effects here. Thus, while the orbital diamagnetic moment is zero in the mean, its higher (even) moments do exist under confinement, but cannot be obtained as field derivatives of the classical free energy. The other surprising effect manifests in the nonequilibrium steady state as a transverse work-fluctuation relation in addition to the well-known longitudinal work-fluctuation theoretic results of much current interest [6–9]. In the light of these, we revisit the classical problem of orbital motion of a charged particle in two dimensions in the presence of a normal magnetic field. First, we will consider the work fluctuations in the presence of a parallel (in-plane) electric bias. Keeping in mind the nonequilibrium steady-state situation of interest here, we follow the Einsteinian statistical approach based on the Langevin equation whose solution in the long-time limit gives the nonequilibrium steady-state results for the system driven externally (e.g., biased electrically). The main results are the following: For nonzero electric bias, a "work fluctuation" expression is obtained as, of course, expected for a barotropic-type system. In addition, however, a transverse work fluctuation is also obtained perpendicular to the electric bias—a "Hall fluctuation" theorem. This "Hall fluctuation" involves the product of the electric and the magnetic fields. Inasmuch as classically the magnetic field does not work on a moving charge, this cross effect (Hall fluctuation) seems to be related to the time-reversal symmetry breaking effect of the externally applied magnetic field. This is quite distinct from the time-reversal asymmetry (irreversibility) arising out of dissipation. It is apt to point out at this stage that the physical scheme we have in mind here is experimentally an obvious variation on the well-known Haynes-Shockley [10] setup for studying the drift concomitant with the spread (diffusion) of minority charge carriers photoinjected in an electrically biased semiconducting sample. Indeed, the fact that the minority carriers can disappear through the electron-hole recombination process, provides for a study of finite lifetime effects in our nonequilibrium steady state [3]. This should be an interesting way of probing the effect of confinement, or the boundary, that may not be effective when the carrier lifetime is very short.

II. FLUCTUATION THEOREM—THE CLASSICAL HALL BAR

Consider a classical 2D system of noninteracting electrons (charge $-e$) under the externally applied crossed electric and magnetic fields, in the presence of a dissipative environment at temperature T (the bath) in the high friction limit. Let the electric field (E) be in the x direction and the magnetic field (B) in the z direction. We can now write the Langevin equations of motion for the electron in the overdamped limit, i.e., ignoring the inertial effects [11] as

$$\gamma\dot{x} = -eE - \frac{eB}{c}\dot{y} + \eta_x(t)$$

and

*dibyendu@rri.res.in
†nkumar@rri.res.in

$$\gamma \dot{y} = \frac{eB}{c}\dot{x} + \eta_y(t),$$

where γ is the friction coefficient due to the underlying bath and $\eta_x(t)$ and $\eta_y(t)$ are the concomitant random (stochastic) forces generated by the bath. The electrical drift mobility is defined as e/γ for electrons. We assume as usual the random forces to be Gaussian white noise with $\langle \eta_{\alpha,\beta}(t)\rangle=0$ and $\langle \eta_\alpha(t)\eta_\beta(t')\rangle=\eta_0^2\delta(t-t')\delta_{\alpha\beta}$. Here $\langle\cdots\rangle$ denotes average over the stochastic ensemble at time t. Solving the above two linearly coupled equations for the velocities $\dot{x}$ and $\dot{y}$, we obtain

$$\dot{x} = \frac{\beta}{1+\beta^2}\left(-\frac{\alpha}{\beta} + \frac{\eta_x(t)}{\beta\gamma} - \frac{\eta_y(t)}{\gamma}\right), \tag{1}$$

$$\dot{y} = \frac{\beta}{1+\beta^2}\left(-\alpha + \frac{\eta_x(t)}{\gamma} + \frac{\eta_y(t)}{\beta\gamma}\right), \tag{2}$$

with $eB/\gamma c=\beta$ and $eE/\gamma=\alpha$. In the overdamped limit, the information of the electron's motion is captured in the probability distribution $P(x,y,t)$ of the x and y positions at time t. We are interested in finding the marginal probability distributions $[P(x,t), P(y,t)]$ of the displacements x and y, respectively, $P(x,t)=\int P(x,y,t)dy$ and $P(y,t)=\int P(x,y,t)dx$. From the van Kampen lemma [12], we can write a continuity equation for the marginal density $\pi(x,t)$ evolving stochastically under Eq. (1) with $P(x,t)=\langle \pi(x,t)\rangle$ as

$$\begin{aligned}\frac{\partial \pi(x,t)}{\partial t} &= -\frac{\partial}{\partial x}[\dot{x}\pi(x,t)]\\ &= \frac{\beta}{1+\beta^2}\left(\frac{\alpha}{\beta}\frac{\partial \pi(x,t)}{\partial x} - \frac{1}{\beta\gamma}\frac{\partial}{\partial x}[\eta_x(t)\pi(x,t)]\right.\\ &\quad \left. + \frac{1}{\gamma}\frac{\partial}{\partial x}[\eta_y(t)\pi(x,t)]\right).\end{aligned} \tag{3}$$

The Fokker-Planck equation for the marginal probability distribution $P(x,t)$ is now obtained by the noise averaging of Eq. (3). We apply Novikov theorem [12] for the Gaussian noise and find

$$\frac{\partial P(x,t)}{\partial t} = \frac{\alpha}{1+\beta^2}\frac{\partial P(x,t)}{\partial x} + \frac{\eta_0^2}{2\gamma^2(1+\beta^2)}\frac{\partial^2 P(x,t)}{\partial x^2}. \tag{4}$$

The last equation describes the diffusion of electrons with drift. Similarly, the Fokker-Planck equation for the marginal probability distribution $P(y,t)$,

$$\frac{\partial P(y,t)}{\partial t} = \frac{\alpha\beta}{1+\beta^2}\frac{\partial P(y,t)}{\partial x} + \frac{\eta_0^2}{2\gamma^2(1+\beta^2)}\frac{\partial^2 P(y,t)}{\partial y^2}. \tag{5}$$

It is easier to solve the differential Eqs. (4) and (5) by the Fourier transform method with initial conditions $P(x,t=0)=\delta(x)$ and $P(y,t=0)=\delta(y)$. It is given as

$$P(x,t) = \sqrt{\frac{\gamma^2(1+\beta^2)}{2\pi\eta_0^2 t}}\exp\left[-\frac{\gamma^2(1+\beta^2)}{2\eta_0^2 t}\left(x + \frac{\alpha}{1+\beta^2}t\right)^2\right].$$

The marginal probability density $P(x,t)$ is a Gaussian distribution with mean $\langle x\rangle=-\alpha t/(1+\beta^2)$ and variance $(\langle x^2\rangle - \langle x\rangle^2)=\eta_0^2 t/\gamma^2(1+\beta^2)$. Here $v_{xd}=-\alpha/(1+\beta^2)$ is the drift velocity along the x direction. It can also be derived from Eq. (1) by taking the ensemble average on both sides. The above solution, of course, reduces to ordinary diffusion in the limit $E=0$ and $B=0$ with the identification $\eta_0^2=2D\gamma^2$, where D is the diffusion constant. We can now readily derive the usual barotropic-type work fluctuation relation in the direction of electric field,

$$\frac{P(x,t)}{P(-x,t)} = \exp\left(-\frac{2e\gamma E}{\eta_0^2}x\right) = \exp\left(-\frac{eEx}{K_BT}\right) \tag{6}$$

with the Einstein relation, $D\gamma=k_BT$. The interpretation of the above relation is straightforward. Though the system is always far from thermodynamic equilibrium (as the electron continuously dissipates energy in the environment), it reaches a mechanical equilibrium asymptotically under the combined effect (forcing) of the electromagnetic fields and the viscous drag acting in opposition. After the system attains the steady state, if the electron is at a position x_1, say, at $t=0$, then $P(x,t)$ is the conditional probability of finding the particle at position x_2 at later time t with the displacement $x=x_2-x_1$. Now, we reverse the positions keeping time direction as before and start at $t=0$ from the position x_2, then $P(-x,t)$ is the conditional probability of finding the particle at position x_1 at time t. The main feature of the relation (6) is that the right-hand side is time independent. The relation (6) can also be derived from the equilibrium probability distribution (depicting microscopic reversibility) [13]. Using now the normalization condition of the probability distribution, we obtain another useful relation from Eq. (6),

$$\begin{aligned}\left\langle \exp\left(\frac{eEx}{K_BT}\right)\right\rangle &= \int_{-\infty}^{\infty}\exp\left(\frac{eEx}{K_BT}\right)P(x,t)dx\\ &= \int_{-\infty}^{\infty}P(-x,t)dx = 1.\end{aligned} \tag{7}$$

The last two relations [Eqs. (6) and (7)] are similar to the generalized fluctuation-dissipation theorems which were derived in a very different context in Ref. [14].

Next, we investigate the rather interesting transverse fluctuations. Again, using the Fourier transform method, we solve Eq. (5) for the marginal probability distribution $[P(y,t)]$ of y giving

$$P(y,t) = \sqrt{\frac{\gamma^2(1+\beta^2)}{2\pi\eta_0^2 t}}\exp\left[-\frac{\gamma^2(1+\beta^2)}{2\eta_0^2 t}\left(y + \frac{\alpha\beta}{1+\beta^2}t\right)^2\right],$$

where the drift velocity along the y direction is $v_{yd}=-\alpha\beta/(1+\beta^2)$. The ratio of the probability densities for the transverse fluctuations is given by

$$\frac{P(y,t)}{P(-y,t)} = \exp\left(-\frac{e^2EBy}{c\gamma K_BT}\right) = \exp\left(-\frac{eEy}{K_BT}\beta\right), \tag{8}$$

where the interpretation of $P(y,t)$ and $P(-y,t)$ are similar to that for the x direction. We call the last relation the "Hall fluctuation" theorem—it involves the product of the crossed electric and magnetic fields. The magnetic field, of course, does not work on a charge moving in the xy plane. This cross

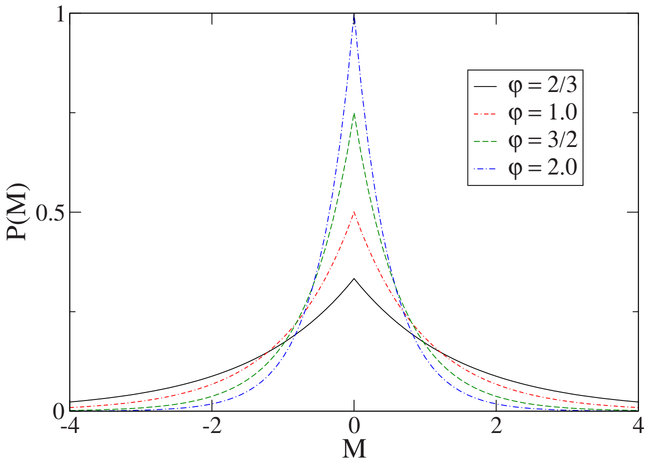

FIG. 1. (Color online) Plot of the probability density $P(M)$ of Eq. (10) vs magnetic moment M for different values of ϕ. Here M is scaled by the Bohr magneton (μ_B).

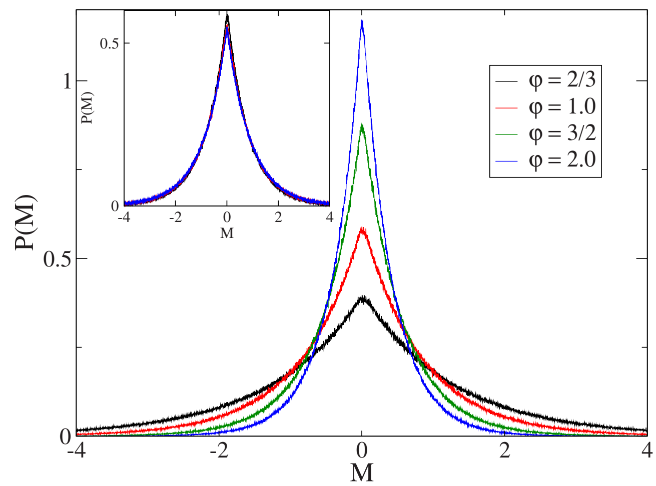

FIG. 2. (Color online) Plot of the probability density $P(M)$ vs magnetic moment M obtained in simulation for the same values of ϕ as in Fig. 1. Peak of the curves decreases with decreasing ϕ. We have used $\gamma=1$, $m=1$ and again M is scaled by μ_B. Inset $P(M)$ for $\phi=1.0$; and for different values of γ and B showing no effect.

"Hall fluctuation" effect can be related ultimately to the time-reversal symmetry breaking effect of the applied magnetic field, which is different from the time irreversibility introduced through the dissipation (γ). We can interpret it variously as arriving from the transverse Hall voltage (the Lorentz force), or effectively as a magnetoresistance in the Hall geometry which occurs due to the enhancement of the path length of an electron's motion caused by the magnetic field. Finally, we give a generalized fluctuation-dissipation theoremlike expression in the presence of the magnetic field,

$$\left\langle \exp\left(\frac{eEy}{K_B T}\beta\right)\right\rangle = 1 .$$

III. DIAMAGNETIC FLUCTUATIONS

Next, we turn to the diamagnetic fluctuations. We derive and briefly discuss the classical equilibrium fluctuations of the orbital diamagnetic moment (which is known to vanish identically in the mean). More specifically, we find the equilibrium probability density for the orbital magnetic moment of a charged particle in two dimensions for a normal magnetic field and a harmonic confinement. The probability density, when properly scaled, turns out to be universal and peaked about a zero mean value. Here, however, we must retain the inertial effect (nonzero electron mass).

Consider the orbital motion of the electron in the xy plane for the normal external uniform magnetic field B along z directions and a harmonic confinement in the xy plane of strength k_0. The Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(p_x - \frac{eBy}{2c}\right)^2 + \frac{1}{2m}\left(p_y + \frac{eBx}{2c}\right)^2 + \frac{1}{2}k_0(x^2+y^2),$$

where we have used the symmetric Landau gauge ($\mathbf{A}=\mathbf{B}\times\mathbf{r}/2$) for the vector potential $\mathbf{A}$. The orbital diamagnetic moment can be expressed as

$$M(t) = \frac{-e}{2c}(x\dot{y} - y\dot{x}) = \frac{-e}{2mc}\left[x\left(p_y + \frac{eBx}{2c}\right) - y\left(p_x - \frac{eBy}{2c}\right)\right]. \tag{9}$$

We are interested in the asymptotic ($t\to\infty$) distribution of $M(t)$. Now, we can evaluate the probability density $P(M)$ of classical M in the limit $t\to\infty$ (i.e., in equilibrium) through the usual method of finding the equilibrium distribution at finite temperature T,

$$P(M) = \frac{1}{Z}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx\, dy\, dp_x\, dp_y\, e^{-\mathcal{H}/k_B T} \times \delta\left\{M + \frac{e}{2mc}\left[x\left(p_y + \frac{eBx}{2c}\right) - y\left(p_x - \frac{eBy}{2c}\right)\right]\right\}.$$

Here Z is a normalization constant to be determined through $\int_{-\infty}^{\infty}P(M)dM=1$ (in fact Z is the equilibrium partition function for this model). After some simple algebra we obtain the probability density

$$P(M) = \frac{1}{2\mu_B}\left(\frac{\hbar\omega_0}{k_B T}\right)\exp\left(-\frac{\hbar\omega_0}{k_B T}\frac{|M|}{\mu_B}\right), \tag{10}$$

where $\mu_B=e\hbar/2mc$ is the Bohr magneton and $\omega_0=\sqrt{k_0/m}$. As expected $\langle M\rangle=0$, i.e., orbital diamagnetism is identically zero in a confined system. But, we do find finite thermal fluctuations of the orbital diamagnetic moment in confinement. In Fig. 1, we plot $P(M)$ for different values of the dimensionless parameter $\phi=\hbar\omega_0/k_B T$. It is interesting to note that the classical partition function (Z), and hence the free energy ($-k_B T\ln Z$) are independent of the magnetic field B giving vanishing orbital diamagnetism in the mean. But the moments of the orbital magnetic fluctuation of even order are all nonzero. Clearly, then, these orbital magnetic moments cannot be derived through the usual field derivatives of the classical free energy as would be the case for "permanent magnetic moments" intrinsic to the particles. The classical equilibrium simulation of the above model with the Langevin heat bath can be shown to be consistent with the above thermal fluctuations of the magnetic moments. We simulate the coupled set of Langevin equations

$$m\ddot{x} = -\gamma\dot{x} - \frac{eB}{c}\dot{y} - k_0 x + \eta_x(t)$$

and

$$m\ddot{y} = -\gamma\dot{y} + \frac{eB}{c}\dot{x} - k_0 y + \eta_y(t),$$

where again γ and η are, respectively, the friction and the noise, related through $\langle \eta_\alpha(t)\eta_\beta(t')\rangle = 2\gamma k_B T\delta(t-t')\delta_{\alpha\beta}$. Here we use the velocity-Verlet algorithm for the time evolution of the above equations and find steady-state equilibrium distribution of the magnetic moment given by Eq. (9). We plot the distribution $P(M)$ in Fig. 2 for the same parameter values of ϕ as in Fig. 1. Also, we confirm through our simulation that the $P(M)$ is independent of γ and B (see inset of Fig. 2).

IV. CONCLUDING REMARKS

In this paper we have rederived a barotropic-type work-fluctuation relation along with a transverse fluctuation relation for the case of the classical motion of a charged particle in static homogeneous crossed magnetic and electric fields in the presence of dissipation. This is interesting inasmuch as classically the magnetic field does not work on a moving charge particle. Recently, there have been some studies of fluctuation theorems [15] in time-varying electromagnetic fields. But, our approach and the context are quite different from these. As our treatment is based on the classical Langevin equations involving stochastic fluctuating forces and the concomitant dissipation that neglect quantum statistics and the band-structure effects [16], it is expected to be appropriate for a material system which is electronically nondegenerate, i.e., has a low carrier density at a relatively high temperature, and has a low carrier mobility. Clearly, a polar semiconductor with strong electron-phonon interaction is indicated. The inertial mass occurring in our Langevin equations is, of course, to be replaced by the effective mass relevant to the bottom (top) of the conduction (valence) band for the electron (hole) as the band is expected to be close to being parabolic there. We have also derived the probability density for the classical diamagnetic moment giving nonzero orbital magnetic moments of even order. The latter cannot be obtained as field derivatives of the equilibrium free energy which is classically field independent.

ACKNOWLEDGMENT

One of the authors (D.R.) thanks A. Dhar and R. Marathe for fruitful discussions.

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