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Landau Diamagnetism in a Dissipative and Confined System

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Starting from a quantum Langevin equation of a charged particle in a magnetic field we present a fully dynamical calculation of the orbital diamagnetism, from which the effect of dissipation on Landau diamagnetism can be assessed. The treatment throws light on subtle issues of confined boundaries and the approach to equilibrium of a quantum dissipative system. Additional results are presented for the diamagnetism in a confined parabolic potential. [S0031-9007(97)03710-1]

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The problem of a charged quantum particle in the presence of a magnetic field serves in quantum mechanics as a paradigm of exactly solvable models [1], results of which made possible a major breakthrough in solid state physics when Landau gave the theory of diamagnetism [2]. Today, the physics of Landau levels is of great interest in, e.g., the quantum Hall effect [3] and high temperature superconductivity [4]. The issue that we address in this Letter is what happens to the dynamics of a charged particle in an external magnetic field when it is in contact with a dissipative quantum bath. The analysis of this question puts the problem in the general context of dissipative quantum mechanics, a subject that has seen a recent revival, mainly through the work of Leggett and co -workers $[5-7]$. It turns out that the dynamics of a charged particle in a magnetic field (like a free quantum particle [8] or a quantum oscillator [9]), in the presence of what is called an Ohmic bath, can be tackled exactly.

The Leggett approach is based on the Feynman-Vernon model in which a particle, moving in an arbitrary potential, is assumed to be linearly coupled with a collection of quantum harmonic oscillators [10]. While the starting point is a many body Hamiltonian of a particle interacting with bosonic excitations, Caldeira and Leggett show that the projected dynamics of the particle is dissipative. In particular, when the number of oscillator modes is infinitely large and their spectral density is of the Ohmic character, one has quantum Brownian motion in the sense that in the corresponding classical limit, the underlying Wigner distribution function obeys the well known

Fokker-Planck equation [6]. We may remark in passing that the Ohmic spectral density is indeed the relevant one when the bath is constituted of fermions and the important excitations are those of electrons and holes, near the Fermi surface [11]. For the purpose of investigating quantum transport properties we find it more convenient to use an equivalent formulation given by Ford and co-workers [12,13], and Zwanzig [14], employing the Heisenberg picture. Starting again from the Feynman-Vernon Hamiltonian these authors derive a quantum Langevin equation for the particle at hand. We use the latter as the basis of our further discussion of transport properties. In particular, we focus attention to the important issue of diamagnetism and the role of the boundary of the system inside which the electrons move. The diamagnetism is first calculated as a fully time-dependent quantity. Its asymptotic $(t \rightarrow \infty)$ limit yields the equilibrium answer. For the sake of pedagogical interest we may refer to the celebrated Bohr–Van Leeuwen theorem which states that "diamagnetism does not exist in classical statistical mechanics" [15]. The reason for this is an intriguing one: The contribution of the bulk electrons to the diamagnetic moment cancels exactly the contribution of the boundary electrons in classical theory [2]. Landau, of course, provided a quantum formulation as mentioned earlier, without apparently worrying about what the boundary does [16,17]. We now raise the question: Does Landau diamagnetism survive dissipation?

Another way of framing the same question is: Since dissipation is known to lead to classical-like motion of

a quantum system, should one expect to see the Bohr– Van Leeuwen theorem restored in the limit of infinite damping? We show that a proper analysis of this question requires a careful treatment of the boundary, bringing out subtle roles of thermodynamic limit and approach to equilibrium. The confined boundaries are, of course, of great interest in their own right in view of the present upsurge of activity in mesoscopic structures. In the last part of this Letter, we present results for the diamagnetism when the electrons are constrained to move in a twodimensional parabolic potential in the plane normal to the applied field.

The Feynman-Vernon Hamiltonian for a particle of charge *e* in a magnetic field **B** can be written as

$$
\mathcal{H} = \frac{1}{2m} \left(\mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2
$$

$$
+ \sum_{j} \left[\frac{1}{2m_j} \mathbf{p}_j^2 + \frac{1}{2} m_j \omega_j^2 (\mathbf{q}_j - \mathbf{r})^2 \right], \quad (1)
$$

where **p** and **r** are the momentum and position operators of the particle, \mathbf{p}_i and \mathbf{q}_j are the corresponding variables for the reservoir particles, and **A** is the vector potential. For the Ohmic dissipation model, the distribution of oscillators is such that [8]

$$
J(\omega) = \frac{\pi}{2} \sum_j m_j \omega_j^3 \delta(\omega - \omega_j) = \gamma \omega, \qquad (2)
$$

where γ is the constant friction. Integrating out the reservoir variables from Hamilton's equations of motion one obtains a quantum Langevin equation [13]

$$
m\ddot{\mathbf{r}} + m\gamma \dot{\mathbf{r}} - \frac{e}{c} (\dot{\mathbf{r}} \times \mathbf{B}) = \mathbf{f}(t), \qquad (3)
$$

 \sim

where $f(t)$ is the operator form of the "noise." Its spectral properties are characterized by the symmetric correlation and the commutator,

$$
\langle \{ f_{\alpha}(t), f_{\beta}(t') \} \rangle = \delta_{\alpha\beta} \frac{2m\gamma}{\pi} \int_0^{\infty} d\omega \, \hbar \omega
$$

$$
\times \coth\left(\frac{\hbar \omega}{2k_B T} \right) \cos[\omega(t - t')] , \quad (4)
$$

$$
\langle [f_{\alpha}(t), f_{\beta}(t')] \rangle = \delta_{\alpha\beta} \frac{2m\gamma}{i\pi} \int_0^{\infty} d\omega \ \hbar \omega \sin[\omega(t - t')],
$$
\n(5)

 α , β being Cartesian indices *x*, *y*, and *z*. The angular brackets in Eqs. (4) and (5) imply thermal averaging over the heat bath.

For the sake of definiteness we assume the magnetic field to be directed along the *Z* axis and concentrate on the motion in the *xy* plane, the motion along *Z* being merely that of a free, quantum particle, in a dissipative environment. This is most conveniently done in terms of the following variables:

$$
z = x + iy, \qquad F = f_x + if_y,
$$

$$
\overline{\gamma} = \gamma + i\omega_c, \qquad \omega_c = \frac{eB}{mc},
$$
 (6)

where ω_c is called the cyclotron frequency. Thus the motion in the *xy* plane is governed by the equation

$$
\ddot{z} + \overline{\gamma} \dot{z} = \frac{F(t)}{m},\qquad(7)
$$

whose solution reads

$$
z(t) = \frac{1}{\gamma} \dot{z}(t_0) \{1 - \exp[-\overline{\gamma}(t - t_0)]\} + \int_{t_0}^t d\tau \exp(-\overline{\gamma}\tau) \int_{t_0}^{\tau} dt' \exp(\overline{\gamma}t') \frac{F(t')}{m},
$$
\n(8)

where we have set $z(t_0) = 0$, without loss of generality. From Eq. (8) and its time derivative, several correlation functions of interest for magnetotransport behavior, e.g., the velocity-correlation and mean-squared displacement, can be calculated [18].

Our main interest here, however, is in investigating the issue of diamagnetism in a dissipative environment, for which we need to calculate the time-dependent quantity

$$
M_z(t) = \frac{|e|}{2c} \langle (x\dot{y} - y\dot{x}) \rangle = \frac{|e|}{4c} \operatorname{Im} \langle (\dot{z}z^+ + z^+ \dot{z}) \rangle. \tag{9}
$$

The solution given in Eq. (8) allows us, of course, to compute M_z as a function of time. This task can be carried out on the basis of our results for the magnetotransport behavior, presented in [18]. Here, however, we are interested in only an equilibrium property, and therefore, in order to check whether we can recover the (expected) Landau answer in equilibrium, we first consider the limits $t_0 = 0$ and $t = \infty$. We find

$$
M_{z} = -\frac{|e|\hbar}{2\pi cm} \int_{-\infty}^{\infty} \frac{\gamma d\omega}{\gamma^{2} + (\omega - \omega_{c})^{2}} \coth\left(\frac{\hbar \omega}{2k_{B}T}\right).
$$
\n(10)

It is clear then that when the friction $\gamma = 0$, the Lorentzian in ω reduces to $\pi \delta(\omega - \omega_c)$ and therefore

$$
M_z^0 = -\frac{|e|\hbar}{2mc} \coth\left(\frac{\hbar \omega_c}{2k_B T}\right). \tag{11}
$$

Interestingly, this is just a piece of the Landau answer which arises in the equilibrium calculation if one is not careful in computing the role of the "boundary" electrons [2]. As has been lucidly discussed by Peierls [17], it is the boundary electrons which have the so-called "skipping orbits" that lead to "edge currents," which make an essential contribution to diamagnetism.

Therefore, in order to obtain the correct result for *Mz* we must consider anew the dissipative dynamics of the charge in a finite volume. As the latter is difficult to implement mathematically, we employ a trick due originally to Darwin [19]. Darwin was interested in calculating M_z^0 from the equilibrium trace formula and, in order to obtain the correct Landau expression, had to first put in a contrived constraining parabolic potential $\frac{1}{2}k(x^2 + y^2)$ in the Hamiltonian, complete the calculation of the trace, and then switch k to zero. We adopt the same approach here, in which case, the equation of motion (7) is modified to

$$
\ddot{z} + \overline{\gamma} \dot{z} + (k/m)z = F(t)/m. \tag{12}
$$

The solution to Eq. (12) [with $z(0) = 0$] now reads

$$
z(t) = \frac{\dot{z}(0)}{w_+ - w_-} \left[\exp(w_+ t) - \exp(w_- t) \right] + \frac{1}{w_+ - w_-} \int_0^t d\tau \left[\exp w_+ (t - \tau) \right. - \exp w_- (t - \tau) \left[\frac{F(\tau)}{m} \right],
$$
(13)

where

$$
w_{\pm} = -\frac{1}{2}\overline{\gamma} \pm \frac{1}{2}\sqrt{(\overline{\gamma})^2 - \omega_0^2}, \qquad \omega_0^2 = \frac{4k}{m}.
$$
\n(14)

substituting the result in Eq. (9) and letting $t \to \infty$, we finally obtain

$$
M_z = \frac{|e|\gamma}{2\pi mc} \frac{1}{|w_+ - w_-|^2} \operatorname{Im} \int_{-\infty}^{\infty} d\omega \,\hbar\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right) \left(\frac{1}{\omega + i w_+^*} - \frac{1}{\omega + i w_-^*}\right) \left(\frac{w_+}{\omega - i w_+} - \frac{w_-}{\omega - i w_-}\right). \tag{15}
$$

Before taking the Darwin limit (i.e., $k \to 0$ or $\omega_0 \to 0$) in Eq. (15) it is important to compute the integral over ω . This we do by closing the contour in the upper-half plane and noting that the cotangent function has poles at $h\omega/2k_BT = in\pi$, *n* integer. The result is

$$
M_{z} = -\frac{|e|\hbar\zeta}{mc} \operatorname{Im} \left\{ \sum_{n=1}^{\infty} \frac{n^{2}\pi^{2}}{(n\pi + \nu_{+}^{*})(n\pi - \nu_{+})(n\pi + \nu_{-}^{*})(n\pi - \nu_{-})} + \frac{1}{(\nu_{+}^{*} - \nu_{-}^{*})} \right. \\ \times \left. \left[\frac{(\nu_{+}^{*})^{2} \cot(\nu_{+}^{*})}{(\nu_{+} + \nu_{+}^{*})(\nu_{+}^{*} + \nu_{-})} - \frac{(\nu_{-}^{*})^{2} \cot(\nu_{-}^{*})}{(\nu_{-} + \nu_{-}^{*})(\nu_{-}^{*} + \nu_{+})} \right] \right\}, \tag{16}
$$

where

$$
\zeta = \frac{\hbar \gamma}{2k_B T}, \qquad \nu_{\pm} = \frac{\hbar \omega_{\pm}}{2k_B T}.
$$
 (17)

Equation (16) is our final result for the orbital (diamagnetic) magnetization of a charged particle in a quantum dissipative environment, and moving in a confining parabolic potential. If the latter is switched off (i.e., $\omega_0 \rightarrow 0$)

$$
\nu_{+} \approx \frac{\nu_0^2}{4} \frac{(\zeta - i\nu_c)}{\zeta^2 + \nu_c^2}, \qquad \nu_{-} \approx -(\zeta + i\nu_c),
$$

$$
\nu_c = \frac{\hbar \omega_c}{2k_B T}, \qquad \nu_0 = \frac{\hbar \omega_0}{2k_B T}.
$$
 (18)

The result for the magnetization then becomes

$$
M_{z} = \frac{|e|\hbar}{2mc} \left\{ \sum_{n=1}^{\infty} \frac{4n\pi\zeta\nu_{c}}{(\nu_{c}^{2} + \zeta^{2} - n^{2}\pi^{2})^{2} + 4n^{2}\pi^{2}\nu_{c}^{2}} + \frac{\nu_{c}}{\zeta^{2} + \nu_{c}^{2}} - \frac{1}{2} \frac{\sinh(2\nu_{c})}{\sinh^{2}(\nu_{c}) + \sin^{2}(\zeta)} \right\},
$$
(19)

which in the limit of zero damping $(\zeta = 0)$ yields the Landau answer

$$
M_z^0 = \frac{|e|\hbar}{2mc} \left[\frac{1}{\nu_c} - \coth(\nu_c) \right].
$$
 (20)

Equation (19) is our central result which generalizes the Landau expression to be applicable in a situation in which the system has scattering processes that can lead to decoherence of Landau orbits. In a sense it is the analog of the Drude formula for electrical conductivity [20].

As mentioned earlier, the expression given in Eq. (16) for a confining parabolic potential is interesting in itself as it can be realized in mesoscopic quantum structures [21]. We therefore consider the limiting case of Eq. (16) for zero damping, which leads to

$$
M_{z} = \frac{|e|\hbar}{4mc} \frac{1}{\sqrt{\nu_{0}^{2} + \nu_{c}^{2}}} \left\{ \left(\sqrt{\nu_{0}^{2} + \nu_{c}^{2}} - \nu_{c} \right) \coth\left[\frac{1}{2} \left(\sqrt{\nu_{0}^{2} + \nu_{c}^{2}} - \nu_{c} \right) \right] - \left(\sqrt{\nu_{0}^{2} + \nu_{c}^{2}} + \nu_{c} \right) \coth\left[\frac{1}{2} \left(\sqrt{\nu_{0}^{2} + \nu_{c}^{2}} + \nu_{c} \right) \right] \right\}.
$$
\n(21)

The analysis presented above helps sharpen our notion of the approach to equilibrium. The quantum Langevin equation builds in at the outset, through fluctuationdissipation relations [cf. Eqs. (4) and (5)], the fact that time-dependent quantities approach their equilibrium values, in the asymptotic limit $t \to \infty$. However, we find that the answer is not unique in the sense that the limits $k \to 0$ and $t \rightarrow \infty$ are not interchangeable. The correct Landau expression for diamagnetism results if we first take $t \rightarrow \infty$, i.e., allow the particle to come to thermal equilibrium in the presence of a confining potential, and then switch *k* off to zero. The same situation is encountered in the corresponding classical problem [22]. This aspect has to do with the special role of boundary electrons in producing diamagnetism—although they are fewer in number, they make a giant contribution to the diamagnetic moment [2].

We plot in Figs. 1(a) and 1(b) M_z (divided by $|e|\hbar/2mc$, the Bohr magneton) versus ζ for different values of ν_c , in accordance with Eq. (19). It is seen that *Mz* monotonically approaches zero for a large enough value of the damping ζ , although this approach is slower the larger v_c is. This observation underscores the point made earlier concerning the competition between coherence and dissipation. A large value of v_c gives strong quantum effects which, however, ultimately give way to seemingly classical-like effects when dissipation ζ is strong. Thus the Bohr–Van Leeuwen theorem is restored for large damping. The other point to note, which has also been made earlier, is that for $\zeta = 0$, Eq. (19) reduces to the Landau answer given by Eq. (20).The latter, for large values of the cyclotron frequency v_c , yields a saturation value of the magnetization which equals one (negative) Bohr magneton. This is evident from Fig. 1(b), for $v_c = 20.00$, when only the lowest Landau level is preferentially occupied.

In conclusion, we have presented an exact treatment of the Feynman-Vernon model of a charged particle moving in a magnetic field, in the quantum dissipative regime, have derived interalia the diamagnetic moment for motion in a confined parabolic potential, which is of interest in mesoscopic systems, and have examined the issue of Landau diamagnetism. Normally, diamagnetism is difficult to measure as it is masked by a stronger paramagnetic effect. However, with present technology it is possible to grow two-dimensional electron films. Hence, by applying a magnetic field both perpendicular (yielding diamagnetic as well as paramagnetic contributions) and parallel (with only paramagnetic effect) to the film, it should be possible to experimentally separate out the diamagnetic contribution. By measuring the latter with a controlled amount of scattering impurities it should be possible to verify the results on Landau diamagnetism. The results presented here are particularly relevant for nondegenerate semiconductor structures in which the effect of Fermi statistics can be ignored.

FIG. 1. (a) Plot of $(2mc/|e|\hbar)M_z$ versus the damping parameter ζ for two different values of the dimensionless cyclotron frequency v_c . Upper curve: $v_c = 0.5$; lower curve: $v_c = 1.0$. (b) Same as in (a). Upper curve: $v_c = 10.0$; lower curve: $\nu_c = 20.0$. Note that the approach to zero, for large values of ζ , is now much slower than that depicted in (a).

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