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Role of quantum heat bath and confinement in the low-temperature thermodynamics of cyclotron motion

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In this Brief Report we show how the low-temperature thermodynamics of the dissipative motion of an electron in a magnetic field is sensitive to the nature of the spectral density function, $J(\omega)$, of the quantum heat bath. In all cases of couplings considered here the free energy and the entropy of the cyclotron motion of the electron fall off to zero as power law in conformity with the third law of thermodynamics. The power of the power law however depends on the nature of $J(\omega)$. We also separately discuss the influence of confinement.

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The low-temperature thermodynamic behavior of small systems has received attention due to the importance of quantum dissipative environment [1]. In order to critically assess this issue, the dissipative cyclotron motion of a charged quantum oscillator has been extensively studied [2,3]. The main conclusion is that while the free oscillator has an exponential suppression of the low-temperature specific heat, strong coupling with the quantum bath makes the specific heat vanish at zero temperature as a power law in temperature, in conformity with the third law. It is easy to trace the origin of the exponential suppression to the discreteness of the so-called Landau levels of the charged oscillator in the presence of the magnetic field. In contrast, the power law emerges from the disappearance of the energy gap due to a continuous spectrum of the energy, as a result of the presence of the bath. In this Brief Report we explore the issue of what role the nature of the coupling with the bath and the boundary plays in determining the power of the power law for a charged magneto-oscillator.

The magnetic response of a charged quantum particle has an important bearing on the problem of Landau diamagnetism [4–7], quantum Hall effect [4,8], atomic physics [9], and two-dimensional electronic systems [10]. The further effect of quantum dissipation because of the coupling with an infinitely large collection of quantum harmonic oscillators had been investigated in a series of papers by Ford *et al.* from the point of view of a quantum Langevin equation (QLE) [11]. These authors have not only considered the diamagnetic response but have also provided a treatment for the free energy from which all thermodynamic attributes can be evaluated. The problem has indeed turned out to be illustrative for clarifying the essential role of the boundary mimicked by confining the charged particle in a harmonic oscillator potential [7], and unifying the Einstein and Gibbs approaches to statistical mechanics [6].

In this Brief Report, our focus of attention is not dissipative diamagnetism but the low-temperature thermodynamic property of the dissipative cyclotron motion of an electron. Lately Hänggi *et al.* have advanced the intriguing thesis that quantum dissipation has an important bearing on the third law [1]. They confirm this by showing that the low-temperature specific heat of both a free particle and a single Einstein oscillator assumes a power law in temperature because of dissipation, whereas their corresponding free parts, i.e., free from heat bath influence, are characterized by constancy or exponential suppression in temperature, respectively [1]. This work was further expanded in [3] by also bringing the problem of dissipative diamagnetism within the ambit of the third law. One common feature in all the above treatments, be it for a free particle, or an Einstein oscillator or a charged particle in a magnetic field, is the assumed form of the interaction with the environment, which has almost exclusively been taken to be a linear coupling between the coordinate of the system at hand and the coordinate of the bath oscillator. The question we address here is: how does the low-temperature entropy behave if the nature of coupling or more specifically the nature of the spectral density function of the heat bath is altered?

Our starting point is the so-called system plus reservoir Hamiltonian

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p} - \frac{e\vec{A}}{c}\right)^2 + \frac{1}{2}m\omega_0^2\vec{r}^2 + \sum_{j=1}^{N}\left[\frac{1}{2m_j}(\vec{p}_j^2 + m_j^2\omega_j^2\vec{q}_j^2) + g_j(\vec{r},\vec{p},\vec{q}_j,\vec{p}_j)\right] \quad (1)$$

of a charged oscillator of mass m, charge e and frequency ω_0 with $\{\vec{r},\vec{p}\}$ and $\{\vec{q}_j,\vec{p}_j\}$ are the sets of three-dimensional coordinate and momentum operators of the system and bath oscillators, respectively, $\vec{A}$ is the vector potential of the applied magnetic field $\vec{B}(\vec{B}=\vec{\nabla}\times\vec{A})$ and g_j is the coupling that assumes different forms depending on the nature of the interaction [12,14]. For the much studied classical [15] and quantum Brownian motion [16,17]

$$g_j = -c^j\vec{r}\cdot\vec{q}_j + (c^j)^2\frac{\vec{r}^2}{2m_j\omega_j^2}. \quad (2a)$$

On the other hand, for system-momentum and environment-momentum coupling [14,18,19]

$$g_j = -e^j\frac{\vec{p}\cdot\vec{p}_j}{mm_j} + (e^j)^2\frac{\vec{p}^2}{2m_jm^2}. \quad (2b)$$

The latter case is relevant for a Josephson junction under the effect of a blackbody electromagnetic field [20]. The quanti-

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ties c^j and e^j are the respective coupling constants. The second term in each of the above Eqs. (2a) and (2b) is the so-called "counter term" to make the Hamiltonian bounded from below [12]. It is pertinent to mention that the equation of motion ensuing from Eq. (1) and following the steps given in Ref. [11], even for the assumed form of the coupling in Eq. (2b), has the explicit presence of the Lorentz force term, and are therefore, not gauge-specific. However, the issue of gauge invariance of the total Hamiltonian (including heat bath effects) is being investigated in detail and the results will be reported elsewhere [13].

As mentioned earlier our main focus is the thermodynamics of the charged oscillator in a magnetic field for which there exists the fascinating formula derived in Ref. [11] that expresses the free energy entirely in terms of the free energy of an isolated harmonic oscillator, $f(\omega,T)$ and the familiar response function (generalized susceptibility), $\alpha_\mu(\omega)$ [21]

$$F_\mu(T,B) = \frac{1}{\pi}\int_0^\infty d\omega f(\omega,T)\,\mathrm{Im}\left\{\frac{d}{d\omega}\ln\frac{\alpha_\mu^3(\omega)}{1-\left(\frac{eB\omega}{c}\right)^2\alpha_\mu^2(\omega)}\right\}, \tag{3}$$

where $\mu=1,2$ stands for the two different coupling schemes, and the free energy of a single oscillator with frequency ω is given by

$$f(\omega,T) = k_B T\,\ln\left[1-\exp\left(-\frac{\hbar\omega}{k_B T}\right)\right], \tag{4}$$

with the zero-point energy contribution ignored as the latter makes no difference to the heat capacity and

$$\alpha_\mu(\omega) = \frac{1}{m(\omega_0^2-\omega^2)-i\omega\tilde{\gamma}_\mu(\omega)}. \tag{5}$$

For a brief derivation of Eq. (3) one can consult Refs. [18,20]. The remarkable aspect of the formula (3) is that the entire influence of the quantum heat bath enters through the frequency-dependent "memory friction" $\tilde{\gamma}_\mu(\omega)$. The cubic power in $\alpha_\mu(\omega)$ occurs in Eq. (3) because of the three-dimensional nature of the isotropic oscillator. The other interesting feature is that the effect of the magnetic field is solely contained in the term multiplying e^2. The expression (3) for the free energy can be meaningfully split into a sum of a magnetic field independent term and a field dependent term

$$F_\mu(T,B) = \frac{1}{\pi}\int_0^\infty d\omega f(\omega,T)[I_0^\mu(\omega)+I_B^\mu(\omega)], \tag{6}$$

where

$$I_0^\mu(\omega) = 3\,\mathrm{Im}\frac{d}{d\omega}\ln\,\alpha_\mu(\omega), \tag{7}$$

and

$$I_B^\mu(\omega) = \mathrm{Im}\left\{\frac{d}{d\omega}\ln\left[\frac{1}{1-(eB\omega/c)^2\alpha_\mu^2(\omega)}\right]\right\}. \tag{8}$$

From the free energy and its derivatives with respect to temperature we can of course compute other thermodynamic functions like the entropy and the specific heat.

We now turn our attention to the heat bath induced friction $\tilde{\gamma}_\mu(\omega)$, which is the Fourier transform of the time-domain function that can be written as:

$$\gamma_\mu(t) = \Theta(t)\frac{2}{m\pi}\int_0^\infty d\omega\frac{J_\mu(\omega)}{\omega}\cos(\omega t), \tag{9}$$

$J_\mu(\omega)$ being the spectral density which varies in accordance with the nature of coupling with the bath. Thus,

$$J_1(\omega) = J_{c-c}(\omega) = \pi\sum_{j=1}^N\frac{(c^j)^2}{2m_j\omega_j}\delta(\omega-\omega_j), \tag{10a}$$

and

$$J_2(\omega) = J_{p-p}(\omega) = \pi\sum_{j=1}^N\frac{(e^j)^2}{2m_j}\omega_j^3\delta(\omega-\omega_j). \tag{10b}$$

The idea is to model the spectral density, $J_\mu(\omega)$, and through that, the memory friction $\tilde{\gamma}_\mu(\omega)$. In this Brief Report, we are interested in the low-temperature thermodynamics in the context of the charged magneto-oscillator for which we only need to consider the low frequency contribution. Because, the function $f(\omega,T)$ vanishes exponentially for $\omega > k_B T/\hbar$ and frequencies $\omega \le k_B T/\hbar$ give contribution in Eq. (9). For the coordinate-coordinate (c-c) coupling, we shall consider the case in which spectral density has a power law form at low frequencies. Choosing cutoff at Ω_c, we can describe the reservoir as

$$J_1(\omega) = m\gamma_s\left(\frac{\omega}{\tilde{\omega}}\right)^s\Theta(\Omega_c-\omega), \tag{11}$$

where, Θ is the Heviside step function. Specifying this kind of spectral density function for the heat bath one can easily write down the memory friction function for the c-c coupling at low frequencies [12]

$$\tilde{\gamma}_1(\omega) = \begin{cases} \dfrac{\gamma_s}{\sin(\pi s/2)}\left(\dfrac{\omega}{\tilde{\omega}}\right)^{s-1}, & \text{for } 0<s<2 \\ C_1\left(\dfrac{\omega}{\tilde{\omega}}\right)\left[1-C_2\left(\dfrac{\omega}{\Omega_c}\right)^{s-2}\right], & \text{for } 2<s<4 \\ C_1\left(\dfrac{\omega}{\tilde{\omega}}\right), & \text{for } s\ge 4 \end{cases} \tag{12}$$

with $C_1=\frac{2\gamma_s}{\pi(s-2)}(\frac{\Omega_c}{\tilde{\omega}})^{s-2}$ and $C_2=\frac{\pi(s-2)/2}{\sin[\pi(s-2)/2]}$. Here, $\tilde{\omega}$ is a reference frequency to make the dimension of the coupling constant γ_s that of frequency for all s. In accordance with the references [12,17], $s>1$ is the super-Ohmic case, $s=1$ the Ohmic case and $0\le s<1$ the sub-Ohmic case. These three cases are also relevant for a real physical system. To describe quantum tunneling in a metallic environment one can use the Ohmic spectrum [12]. The super-Ohmic spectrum corresponds to the phonon bath in $d>1$ spatial dimensions and it refers to $s=d$ or $s=d+2$ cases depending on the underlying symmetry of the strain field [12]. The sub-Ohmic spectrum is useful in describing the type of noise in some solid state devices or 1/f noise in Josephson junction [22].

For the momentum-momentum coupling, as it turns out, $\tilde{\gamma}_2(\omega)$ can be expressed as a modified Lorentzian form centered at a frequency Ω [14,23]

$$\tilde{\gamma}_2(\omega) = \frac{2m\gamma\Gamma^2\omega^4}{\Gamma^2\omega^2 + (\Omega^2 - \omega^2)^2}. \tag{13}$$

Note that at low frequencies [$\omega^2 \ll \Omega^2$, but $\Gamma \sim O(\Omega)$] the friction coefficient $\gamma_2(\omega)$, has a quadratic dependence on the frequency. At low frequencies, one can show from Eq. (12) that the spectral density function for this case $J_2(\omega) \sim \omega^3$ which is nothing but a non-Ohmic kind of spectral density function. Thus, one can say that momentum-momentum coupling necessarily leads to a non-Ohmic spectral density at low frequencies which is our observable regime in the present paper. Using Eqs. (5), (15), and (16), the quantities $I_0^\mu(\omega)$ and $I_B^\mu(\omega)$ can be easily calculated, and from these, the free energy can be computed, at least at low frequencies [cf. Eqs. (9), (10a), (10b), and (11)]. But, suffice it to note that as far as the low-temperature thermodynamics is concerned it is only the low frequency behavior of $I_0^\mu(\omega)$ and $I_B^\mu(\omega)$ that matter, in the light of the comment made in preceding paragraph. In assessing these limiting properties it is important however to keep track of two distinct cases $\omega_0 \neq 0$ and $\omega_0 = 0$ [24].

Case of $\omega_0 \neq 0$. For $\omega_0 \neq 0$, one can easily show that $\lim_{\omega\to 0} \alpha_\mu(\omega) = \frac{1}{m\omega_0^2}$. Because the term proportional to B^2 in $I_B^\mu(\omega)$ has a prefactor ω^2 that vanishes identically, $\lim_{\omega\to 0} I_B^\mu(\omega)=0$. Thus, the magnetic field dependence completely disappears from the low-temperature thermodynamic properties, irrespective of s and μ, i.e., the nature of heat bath. Here, we must mention that this case is similar to a two-dimensional harmonic oscillator for which the change in spectral density function causes a difference in the power law of thermodynamic properties at low T [17]. Since B dependent term disappears we need to focus only on the magnetic field independent term which, from Eq. (10), yields

$$\lim_{\omega\to 0} I_0^\mu(\omega) = \frac{3}{m\omega_0^2}\lim_{\omega\to 0}[\omega\gamma_\mu'(\omega) + \gamma_\mu(\omega)]. \tag{14}$$

We are now ready to estimate the temperature dependences of the low-temperature free energy.

(A1) $\mu=1$ and $0 \leq s < 2$; sub-Ohmic $(0<s<1)$, Ohmic $(s=1)$ and a part of super-Ohmic range $(1<s<2)$ fall into one category, for which

$$\lim_{\omega\to 0} I_0^{(1)}(\omega) = \frac{3s\gamma_s}{\sin(s\pi/2)\omega_0^2}\left(\frac{\omega}{\tilde{\omega}}\right)^{s-1}. \tag{15}$$

From Eq. (9) one obtains,

$$\lim_{T\to 0} F_1(T) = -\frac{3s\hbar\gamma_s}{\sin(s\pi/2)}\left(\frac{\tilde{\omega}}{\omega_0}\right)^2\left(\frac{k_BT}{\hbar\tilde{\omega}}\right)^{s+1}\Gamma(s)\zeta(s+1), \tag{16}$$

where we use the following integral (which is relevant throughout the paper):

$$\int_0^\infty dy y^\nu \ln(1-e^{-y}) = -\Gamma(\nu+1)\zeta(\nu+2), \tag{17}$$

Γ and ζ being the gamma and zeta functions, respectively. Consequently the entropy vanishes as T^s.

(A2) $\mu=1$ and $s>2$; two super-Ohmic regime with $2<s<4$ and $s \geq 4$ fall into this category, for which we have

$$\lim_{\omega\to 0} I_0^{(1)}(\omega) = \frac{12\gamma_s\Omega_c^{s-2}}{\pi(s-2)\omega_0^2}\left(\frac{\omega}{\tilde{\omega}}\right) \tag{18}$$

Thus, the free energy becomes

$$\lim_{T\to 0} F_{(1)}(T) = -\frac{12\hbar\gamma_s\Omega_c^{s-2}}{\pi^2(s-2)}\left(\frac{\tilde{\omega}}{\omega_0}\right)^2\left(\frac{k_BT}{\hbar\tilde{\omega}}\right)^3\Gamma(2)\zeta(3). \tag{19}$$

Correspondingly, the entropy goes to zero as T^2.

(A3) For $\mu=2$;

$$\lim_{\omega\to 0} I_0^2(\omega) = \frac{30}{\omega_0^2}\frac{\gamma}{\Omega^4}\omega^4. \tag{20}$$

As a result the free energy becomes

$$\lim_{T\to 0} F_2(T) = -\frac{30\hbar\gamma}{\pi}\left(\frac{\Omega}{\omega_0}\right)^2\left(\frac{k_BT}{\hbar\Omega}\right)^6\Gamma(5)\zeta(6). \tag{21}$$

The entropy now vanishes as T^5.

Case of $\omega_0=0$. The situation at hand is that of a free charged particle in a constant magnetic field interacting with a quantum dissipative heat bath. Interestingly, in this case, the opposite to what happened under case 1 for $\omega_0 \neq 0$ occurs, in that $I_B^\mu(\omega)$ does not vanish for most of the cases, and thus the field dependent as well as field independent free energy survive. Following the analysis of case A, we now find, for (B1). $\mu=1$; sub-Ohmic $(0 \leq s < 1)$

$$\lim_{\omega\to 0} I_0^1(\omega) = \frac{3\sin(\pi/2s)(2-s)}{\gamma_s}\left(\frac{\omega}{\tilde{\omega}}\right)^{1-s}, \tag{22}$$

$$\lim_{\omega\to 0} I_B^1(\omega) = 0. \tag{23}$$

Thus, the free energy becomes

$$\lim_{T\to 0} F_1(T) = -\frac{3C_3(2-s)\hbar\tilde{\omega}\sin(s\pi/2)}{\gamma_s/\tilde{\omega}}\left(\frac{k_BT}{\hbar\tilde{\omega}}\right)^{3-s}, \tag{24}$$

with $C_3=\Gamma(2-s)\zeta(3-s)$. Hence, the entropy vanishes as T^{2-s}.

(B2) $\mu=1$; Ohmic $(s=1)$ Following Ref. [2] one can write:

$$\lim_{\omega\to 0} I_0^1(\omega) = \frac{3}{\gamma_1}, \tag{25}$$

$$\lim_{\omega\to 0} I_B^1(\omega) = \frac{2}{\gamma_1} - \frac{2\gamma_1}{\gamma_1^2 + \omega_c^2}, \tag{26}$$

where cycltron frequency $\omega_c = eB/mc$ through which magnetic field enters into the thermodynamic functions. Thus, the free energy becomes

$$\lim_{T\to 0} F_1(T,B) = -\left[\frac{\pi\gamma_1}{3\hbar(\gamma_1^2+\omega_c^2)} + \frac{\pi}{\hbar\gamma_1}\right](k_B T)^2. \quad (27)$$

So, the entropy vanishes linearly with temperature, but the prefactor has an explicit dependence on the magnetic field and the second term is inversely proportional to γ_1.

(B3a) $\mu=1$, super-Ohmic with $1<s<2$,

$$\lim_{\omega\to 0} I_0^1(\omega) = \frac{3\,\sin(s\pi/2)(2-s)}{\gamma_s}\left(\frac{\omega}{\tilde{\omega}}\right)^{1-s}, \quad (28)$$

$$\lim_{\omega\to 0} I_B^1(\omega) = \frac{2}{3}\lim_{\omega\to 0} I_0^1(\omega) - \frac{2\gamma_s(2-s)}{\sin(s\pi/2)\omega_c^2}\left(\frac{\omega}{\tilde{\omega}}\right)^{s-1}, \quad (29)$$

Thus, the free energy becomes

$$\lim_{T\to 0} F_1(T) = -\frac{C_3(2-s)\hbar\tilde{\omega}\,\sin(s\pi/2)}{\gamma_s/\tilde{\omega}}\left(\frac{k_B T}{\hbar\tilde{\omega}}\right)^{3-s}. \quad (30)$$

(B3b) $\mu=1$, super-Ohmic with $2<s<4$,

$$\lim_{\omega\to 0} I_0^1(\omega) = \frac{3C_1C_2\Omega_c(2-s)}{(1+C_1^2)\tilde{\omega}}\left(\frac{\omega}{\Omega_c}\right)^{s-3}, \quad (31)$$

$$\lim_{\omega\to 0} I_B^1(\omega) = \frac{2C_1C_2\Omega_c(2-s)}{(1+C_1^2)\tilde{\omega}}\left(\frac{\omega}{\Omega_c}\right)^{s-3}. \quad (32)$$

Hence,

$$\lim_{T\to 0} F_1(T) = -\frac{C_1C_2C_4(s-2)\Omega_c^3\hbar}{\pi(1+A^2)\tilde{\omega}}\left(\frac{k_B T}{\hbar\Omega_c}\right)^{s-1}, \quad (33)$$

with $C_4=\Gamma(s-2)\zeta(s-1)$.

(B3c) $\mu=1$, super-Ohmic with $s\geq 4$; for which one can show that $\lim_{T\to 0} F_1(T,B)=0$.

(B4) Finally, for $\mu=2$,

$$\lim_{\omega\to 0} I_B^2(\omega) = -\frac{16\gamma}{\Omega^4\omega_c}\omega^3 - \frac{12\gamma}{\Omega^4}\omega^2, \quad (34)$$

$$\lim_{\omega\to 0} I_0^2(\omega) = -\frac{6\gamma}{\Omega^4}\omega^2. \quad (35)$$

Now, the free energy becomes

$$\lim_{T\to 0} F_2(T) \simeq \frac{6\gamma}{\hbar^3\Omega^4}(k_B T)^4\Gamma(2)\zeta(3). \quad (36)$$

Thus, the entropy maintains the following power law: $\lim_{T\to 0} S(T)=\frac{24\gamma}{\hbar^3\Omega^4}(k_B T)^3\Gamma(2)\zeta(3)$. Again, the prefactor as well as the temperature dependence are very much different from that of a confined particle [Eq. (24)].

In conclusion, we find that different spectral density functions of the heat bath, i.e., various kinds of density of states of the heat bath and the confinement of the particle lead to distinct low-temperature thermodynamic properties. The $\omega_0\neq 0$ and $\omega_0=0$ cases for coordinate-coordinate coupling ($\mu=1$) yield identical temperature dependence for the Ohmic heat bath, but the prefactors depend differently on the friction coefficients and the magnetic field. On the other hand, for other values of s with $\mu=1$ and for the velocity-velocity coupling ($\mu=2$), the temperature dependence as well as the prefactors in terms of their dependencies on the friction coefficients and the magnetic field are quite different for the free particle ($\omega_0=0$) and the confined particle ($\omega\neq 0$). The distinct temperature dependence through power law can be attributed to different density of states factors appropriate to various spectral density function of the heat bath as well as on the confinement of the particle. Although the isolated cyclotron motion gives an exponentially vanishing heat capacity [2,3], but all the cases discussed in this Report naturally yield a satisfactory third law behavior [25].

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