Quantum energy partition and dissipative diamagnetism: A novel approach

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In this paper, we demonstrate a remarkable connection between the recently proposed quantum energy equipartition theorem and dissipative diamagnetism exhibited by a charged particle moving in a two dimensional harmonic potential in the presence of a uniform external magnetic field. The system is coupled to a quantum heat bath through coordinate variables with the latter being modelled as a collection of independent quantum oscillators. In the full frequency domain: $\omega \in (-\infty, \infty)$, the equilibrium magnetic moment $M_e$ can be expressed as an integral over the bath spectrum involving the relaxation function $\Phi(\omega)$, and subsequently, it is possible to propose a fruitful connection between the quantum counterpart of energy equipartition theorem and magnetic moment of the oscillator. We discuss an alternate picture, which emerges upon restricting the integration domain to $\omega \in [0, \infty)$. In these limits, the magnetic moment can be written as an integral over a distribution function $P_\omega(\omega)$ which has two wings corresponding to positive and negative segments. At high temperatures, these two contributions identically cancel each other. However, at low temperatures, the cancellation is incomplete resulting in a non-zero diamagnetic moment. A comparative study of the present results with those obtained from the more traditional Gibbs approach is performed and a perfect agreement is obtained.

I. INTRODUCTION

Statistical mechanics provides the microscopic basis for explaining the macroscopic properties of a system described by thermodynamics, as enunciated by Boltzmann and Gibbs. The remarkable underlying idea is that for a system in thermodynamic equilibrium the observed attributes can be computed from the weighted average of the values of the relevant observables at all possible phase points that lie on a constant time slice. The averaging is done with the aid of a weight function – the Boltzmann-Gibbs measure – also known as the density matrix $\rho$.

A contrasting view however is to consider time-dependent equations of motion of observables that contain dissipative terms originating from the coupling to the environment. A particular example is that of the Langevin equations which, with built-in fluctuation-dissipation (FD) theorem, can yield ‘equilibrium’ results in agreement with statistical mechanics. The validity of the FD theorem rests on the assumption of ‘mixing’ which requires that all points in the phase space are explored over an infinitely long time. Appropriately therefore the latter ‘Brownian motion’ model is dubbed as the “Einstein approach to statistical mechanics”. A nice aspect about this method is that in addition to equilibrium quantities, non-equilibrium and approach-to-equilibrium properties can also be calculated [2–9].

In recent years the Einstein approach to statistical mechanics has been further extended to the domain of thermodynamics as well, giving rise to what is called stochastic thermodynamics. The idea is to rewrite the Langevin equations by delineating the subsystem dynamics (including external field-induced terms) from the heat bath-induced dissipative terms to put them in the context of the ‘differential’ heat, energy and work ‘operators’ as in the first law of thermodynamics. Here, operators are written within quotes to emphasize that only when averaged over the noise terms inherent in the Langevin equations can they be ascribed thermodynamic interpretations. The stochastic thermodynamics approach is not only physically motivated but it also allows one to go beyond thermodynamics into the microscopic realm of fluctuating time-dependent observables of the system. The method is also extremely useful in the topically important applications to thermal ratchets, nano Brownian motors, etc., especially in the context of classical biological processes. In the present work, we transit from the domain of classical to quantum phenomena and assess stochastic thermodynamics of quantum Langevin equations as appropriate for dissipative quantum mechanics [10]. We consider an exactly solvable model of a quantum charged particle such as an electron in a two-dimensional parabolic well subjected to a transverse magnetic field and additionally, in (linear) interaction with a bath of quantum harmonic oscillators. This problem of the dissipative cyclotron motion of an electron is of great interest in dissipative Landau diamagnetism [5, 9, 11, 12] and other condensed matter physics issues such as that of the quantum Hall effect [13, 14].

One particular aspect of dissipative quantum systems which has generated a considerable amount of interest in the recent times is the quantum counterpart of the energy equipartition theorem [15–21]. According to this result which has been proven under quite general considerations [19], the mean kinetic energy of a quantum
particular interacting linearly with a heat bath can always be expressed as

$$E_k = \int_0^\infty \mathcal{E}_k(\omega)P_k(\omega)d\omega$$

where $\mathcal{E}_k(\omega) = \frac{d\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right)$ is the mean kinetic energy of a single heat bath oscillator of frequency $\omega$ with $d$ denoting the number of spatial dimensions. Here, $P_k(\omega)$ refers to a suitable probability distribution function, i.e. it is both positive definite and normalized. Its exact functional form depends on the dissipative mechanism under consideration, i.e. on the distribution of bath modes over the entire bath spectrum. Thus, one may physically interpret eqn (1) as if the system’s kinetic energy $E_k$ receives systematic contributions from the kinetic energy of bath oscillators over the entire spectrum with such contributions being modulated by the probability distribution function $P_k(\omega)$. In other words, $E_k(\omega)P_k(\omega)d\omega$ corresponds to the contribution arising from the frequency interval between $\omega$ and $\omega + d\omega$.

In this paper, our primary focus is on the magnetic moment of a two dimensional dissipative charged oscillator placed in a transverse magnetic field. Given the above setup, it is natural to ask whether an interpretation similar to that of eqn (1) can be associated to the magnetic moment. We begin our analysis by reformulating eqn (1) by extending the range of integration from $-\infty$ to $\infty$.

The following result shall be proved,

**Theorem 1** The mean kinetic energy of a two dimensional dissipative charged oscillator of mass $m$, electric charge $e$ and placed in magnetic field $B = B\hat{z}$ can be expressed as,

$$E_k = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \mathcal{E}_k(\omega)\omega^2[\Phi(\omega) + \Phi(-\omega)]$$

(2)

where $\mathcal{E}_k(\omega) = \frac{\hbar\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right)$ is the mean kinetic energy of a two dimensional bath oscillator of frequency $\omega$ and the function $\Phi(\omega)$ is given by,

$$\Phi(\omega) = \frac{\text{Re}[\tilde{\gamma}(\omega)]}{\left(\omega^2 - \omega_0^2 - \omega_0c + \omega\text{Im}[\tilde{\gamma}(\omega)]\right)^2 + (\omega\text{Re}[\tilde{\gamma}(\omega)])^2}$$

(3)

Here, $\tilde{\gamma}(\omega)$ is the Fourier transform of the friction kernel appearing in the quantum Langevin equation, $\omega_0$ is the system’s eigenfrequency and $\omega_c = eB/m$ is the cyclotron frequency.

The function $\Phi(\omega)$ has been called the relaxation function in [22]. Now, noting that the integrand is an even function, one straightforwardly recovers eqn (1) by converting the integration limits to $\omega \in [0, \infty)$, and if the following identification is made,

$$P_k(\omega) = \frac{\omega^2}{\pi} [\Phi(\omega) + \Phi(-\omega)],$$

(4)

It follows that $P_k(\omega)$ is a positive definite and normalized in $\omega \in [0, \infty)$. A similar statement as above can be made for the potential energy, i.e.

**Theorem 2** The mean potential energy of a two dimensional dissipative charged oscillator of mass $m$, electric charge $e$ and placed in magnetic field $B = B\hat{z}$ can be expressed as,

$$E_p = \frac{\omega_0^2}{2\pi} \int_{-\infty}^{\infty} d\omega \mathcal{E}_p(\omega)[\Phi(\omega) + \Phi(-\omega)]$$

(5)

where $\mathcal{E}_p(\omega) = \frac{\hbar\omega}{2\pi} \coth\left(\frac{\beta\omega}{2}\right)$ is the mean potential energy of a two dimensional bath oscillator with frequency $\omega$.

With this background, we state the following result,

**Theorem 3** The equilibrium magnetic moment $M_z$ of a dissipative charged oscillator in two dimensions can be expressed as,

$$M_z = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega m(\omega)\omega^2[\Phi(\omega) - \Phi(-\omega)]$$

(6)

where $m(\omega) = -\mu_B \coth\left(\frac{\beta\omega}{2}\right)$ is the thermal Bohr magneton.

Thus, the equilibrium magnetic moment of the charged dissipative oscillator can be expressed as an integral over the bath spectrum.

Another aspect of this work is to demonstrate the equivalence between the Einstein method (based on quantum Langevin equation) and the usual Gibbs approach to quantum thermodynamics. It should be specially emphasized that the approach to equilibrium ($t \to \infty$), i.e. the order of taking limits: $\omega_0 \to 0$ (coming from confining well) and $t \to \infty$ plays a vital role in recovering the results of dissipative Landau diamagnetism [3].

With this preamble, the rest of the paper is organized as follows. In the next section, in order to set up our notation, we briefly describe our model and the quantum Langevin equation describing its dissipative dynamics. Following this, in section-(III), we compute the mean energy of the charged dissipative oscillator from the quantum Langevin equation, thereby proving theorems-(1) and (2) stated above. When the integrals in eqns (2) and (5) are expressed in the range $\omega \in [0, \infty)$, the situation corresponds to the previously studied quantum counterpart of energy equipartition theorem for both kinetic and potential energies of the oscillator [21]. This is highlighted in subsection-(III A). Then, in subsection-(III B), we re-express the basic result of quantum energy partition in a novel manner, whose significance shall be disclosed later. In section-(IV), we prove theorem-(3) and its physical significance in the context of diamagnetism is discussed in some detail. In subsection-(IV A), we
demonstrate the connection of eqn (IV) with the results presented in subsection-(III B). Thereafter, in section-(V), we express the equilibrium magnetic moment of the oscillator in the form of an infinite series and discuss the role of the system parameters on the behaviour of the magnetic moment. The equivalence between Einstein method and Gibbs approach are established. Further, the role of boundary and the significance of approach to equilibrium are demonstrated. We conclude our paper in section-(VI).

II. THE MODEL

In this section, we set up our notation and recall some definitions for future reference. We consider here a two dimensional quantum particle of mass $m$ and charge $e$ confined to a harmonic potential of eigenfrequency $\omega_0$ and acted upon by a transverse magnetic field $B$. Further, it is linearly coupled to a heat bath which comprises of an infinite number of independent two dimensional oscillators. Thus, the total Hamiltonian reads,

$$H = \frac{(p - eA)^2}{2m} + m\omega_0^2 r^2 + \sum_j \left[ \frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 (q_j - \frac{c_j}{m_j\omega_j^2} r) \right]^2$$

where $p$ and $r$ are the momentum and position operators, $p_j$ and $q_j$ are the corresponding variables for the $j$th reservoir particle and $A$ is the vector potential. The usual commutation relations between coordinates and momenta hold. Integrating out the reservoir variables from Hamilton’s equations of motion and assuming that the system and the bath were in a coupled Gibbs canonical state initially, one obtains a quantum Langevin equation (see for example [10] and references therein),

$$m\dot{r}(t) + \int_{-\infty}^{t} \mu(t-t')\dot{r}(t')dt' + m\omega_0^2 r(t) - \frac{e}{c}(\dot{r}(t) \times B) = f(t)$$

where $\mu(t)$ is the dissipation kernel given by,

$$\mu(t) = \sum_{j=1}^{N} m_j\omega_j^2 \cos(\omega_j t) \Theta(t)$$

defined to vanish for $t < 0$ in order to be consistent with the principle of causality and $f(t)$ is an operator valued random noise whose spectral properties are characterized by the following symmetric correlation and the commutator,

$$\langle f_\alpha(t) f_\beta(t') \rangle = \delta_{\alpha\beta} \frac{2m\gamma_0}{\pi} \int_{0}^{\infty} d\omega \hbar\omega \coth \left( \frac{\hbar\omega}{2kB_T} \right) \times \cos[\omega(t-t')]$$

$$\langle [f_\alpha(t), f_\beta(t')] \rangle = \delta_{\alpha\beta} \frac{2m\gamma_0}{i\pi} \int_{0}^{\infty} d\omega \hbar\omega \sin[\omega(t-t')]$$

Here $\alpha$ and $\beta$ are being used to indicate Cartesian indices $x$ and $y$. The angular brackets in eqns (10) and (11) imply thermal averaging over the heat bath. Let us recall that the bath spectral function $J(\omega)$ characterizing the spectral distribution of the bath degrees of freedom is defined as,

$$J(\omega) = \frac{\pi}{2} \sum_{j=1}^{N} \frac{c_j^2}{m_j\omega_j} \delta(\omega - \omega_j)$$

From eqns (9) and (12), it follows that,

$$\mu(t) = \frac{2}{\pi} \int_{0}^{\infty} \frac{J(\omega)}{\omega} \cos(\omega t) d\omega.$$

A particularly simple example is that of Ohmic dissipation wherein, the bath spectrum function reads $J(\omega) = m\gamma_0\omega$ or equivalently, $\mu(t) = \frac{m\gamma_0}{\omega}(t)$. This corresponds to memoryless friction, i.e. the drag force experienced by the quantum Brownian particle is instantaneous, analogous to that described by the Stokes’ law for its classical counterpart. In what follows, we shall compute the energy and magnetic moment of the system for a rather general dissipation mechanism.

III. ENERGY OF THE OSCILLATOR

In this section, we shall compute the mean energy of the dissipative oscillator from the quantum Langevin equation (eqn (8)). If $(x(t), y(t))$ is a solution of the quantum Langevin equation, then the mean potential energy at any time instant $t$ is defined as,

$$E_p(t) = \frac{m\omega_0^2}{2} \langle x(t)^2 + y(t)^2 \rangle.$$

For our convenience, let us define the variable $Z = x + iy$. Then the solution to eqn (8) can be expressed as (see also [2] [3]),

$$Z(t) = N \int_{0}^{t} d\tau \left[ e^{\omega+(t-\tau)} - e^{\omega-(t-\tau)} \right] f(\tau)$$

where $f(t) = f_x(t) + if_y(t)$ and,
\[
\omega_{\pm} = \frac{1}{2} \sqrt{\text{Re}[\tilde{\mu}(\omega)] + \text{Im}[\tilde{\mu}(\omega)] + i \omega_c} \pm \frac{1}{2} \sqrt{\text{Re}[\tilde{\mu}(\omega)] + \text{Im}[\tilde{\mu}(\omega)] - i \omega_c}^2 - 4\omega_0^2, \quad N = \frac{1}{m(\omega_+ - \omega_-)}. \tag{16}
\]

Thus, one can compute the mean potential energy of the system as,
\[
E_p(t) = \frac{m \omega_0^2}{2} \langle Z(t)Z^\dagger(t) + \text{c.c.} \rangle. \tag{17}
\]

\[
E_p(t) = \frac{m|N|^2 \omega_0^2}{2\pi} \int_{-\infty}^{\infty} d\omega \zeta_{\omega} \coth \left( \frac{\beta \hbar \omega}{2} \right) \left[ \int_0^t dt \left( e^{\omega_+ (t-t') - i\omega t'} - e^{\omega_+ (t-t') + i\omega t'} \right) \times \left( e^{\omega_- (t-t') - i\omega t'} - e^{\omega_- (t-t') + i\omega t'} \right) \right]
\]

which means in the steady state, i.e. \( t \to \infty \), one has the equilibrium mean potential energy given by,
\[
E_p = \frac{m|N|^2 \omega_0^2}{2\pi} \int_{-\infty}^{\infty} d\omega \zeta_{\omega} \left| \frac{1}{\omega - i\omega_-} - \frac{1}{\omega - i\omega_+} \right|^2 \left| + \text{terms with } \omega \to -\omega \right| \tag{19}
\]

Here, \( \tilde{\mu}(\omega) \) represents the Fourier transform of the friction kernel and \( \zeta_{\omega} = \frac{N}{\pi} \coth \left( \frac{\beta \hbar \omega}{2} \right) \) is the potential energy of a two dimensional bath oscillator. Now, we can re-write eqn (19) in following form,
\[
E_p = \frac{\omega_0^2}{2\pi} \int_{-\infty}^{\infty} d\omega \zeta_{\omega} \left[ \Phi(\omega) + \Phi(-\omega) \right] \tag{20}
\]

if we define the function \( \Phi(\omega) \) as,
\[
\Phi(\omega) = m|N|^2 \left| \frac{1}{\omega - i\omega_-} - \frac{1}{\omega - i\omega_+} \right|^2 \frac{\text{Re}[\gamma(\omega)]}{\left( \omega^2 - \omega_0^2 - i\omega \right)^2 + (\omega \text{Re}[\gamma(\omega)])^2}. \tag{21}
\]

Here \( \gamma(\omega) = \frac{\mu(\omega)}{m} \). This proves theorem-1. The function \( \Phi(\omega) \) has dimensions of \( \omega^{-3} \). In figures-(1), we have plotted the \( \omega_0^2 \Phi(\omega/\omega_0) \) and \( \omega_0^2 \Phi(-\omega/\omega_0) \) for two different dissipation mechanisms, namely Ohmic and Drude. It turns out that the mean potential energy of the oscillator receives non-uniform contributions over the bath spectrum. From eqn (21), it is clear that for \( \omega_c \neq 0 \), \( \Phi(\omega) \) is not an even function which can also be observed from the plots. It should be noted that this feature arises exclusively due to the external magnetic field.

We now turn to the kinetic energy which is defined as,
\[
E_k(t) = \frac{m}{2} \langle \dot{x}(t)^2 + \dot{y}(t)^2 \rangle = \frac{m}{4} \langle \dot{Z}(t)\dot{Z}^\dagger(t) + \text{c.c.} \rangle. \tag{22}
\]

With some straightforward manipulations, it follows that,
\[
\dot{Z}(t) = N \int_0^t dt \left( \omega_+ e^{\omega_+ (t-t') - i\omega t'} - \omega_- e^{\omega_- (t-t') - i\omega t'} \right) f(t). \tag{23}
\]

Thus, one can express the kinetic energy at time instant \( t \) in the following form,
\[
E_k(t) = \frac{m|N|^2}{4\pi} \int_{-\infty}^{\infty} d\omega \omega^2 \Phi(\omega) d\omega
\]
\[
\omega^2 \omega_0 \Phi(\omega/\omega_0)
\]
\[
\omega^2 \omega_0 \Phi(-\omega/\omega_0)
\]

or, in the steady state,

\[
E_k = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \omega^2 E_k(\omega) [\Phi(\omega) + \Phi(-\omega)] \tag{25}
\]

where \(E_k(\omega) = \frac{\hbar \omega}{2} \coth(\frac{\beta \hbar \omega}{2})\) is the mean kinetic energy of a two dimensional bath oscillator of frequency \(\omega\). This is identical to eqn (2) and completes the proof of theorem-(1). We should also note that upon combining eqns (20) and (25) and identifying \(E(\omega) = E_k(\omega) + E_p(\omega)\) as the mean energy per degree of freedom of a bath oscillator of frequency \(\omega\), we can express the total energy of the system (kinetic + potential) as an integral over the bath spectrum. In figures-(2), we have plotted the \(\omega^2 \omega_0 \Phi(\omega/\omega_0)\) and \(\omega^2 \omega_0 \Phi(-\omega/\omega_0)\) for Ohmic and Drude baths. As before, it can be observed that the terms involving \(\Phi(\omega)\) and that involving \(\Phi(-\omega)\) contribute in an unequal manner to the mean kinetic energy. As remarked earlier, this is a consequence of the applied magnetic field.

A. Quantum counterpart of energy equipartition

Consider the function \(P_k(\omega)\) defined in eqn (4). Then, since the integrand of eqn (25) is an even function, we may convert the integration limits to \(\omega \in [0, \infty)\) and rewrite eqn (25) as,

\[
E_k = \int_{0}^{\infty} E_k P_k(\omega) d\omega. \tag{26}
\]

This exactly corresponds to the quantum counterpart of energy equipartition theorem explored in the recent years [15–21]. Since Re\(\tilde{\gamma}(\omega)\) > 0, as a consequence of the second law (see, for example [10]), from eqn (21) \(\Phi(\omega)\) is positive definite by inspection. Thus \(P_k(\omega)\) is positive definite, as expected from a probability distribution function. It may further be shown that it is also normalized.

Next, consider defining a function \(P_p(\omega)\) as,

\[
P_p(\omega) = \frac{\hbar \omega^2}{2} \Phi(\omega) + \Phi(-\omega) \tag{27}
\]

such that eqn (20) can be expressed as,

\[
E_p = \int_{0}^{\infty} E_p P_p(\omega) d\omega. \tag{28}
\]

This corresponds to the quantum counterpart of energy equipartition theorem for the potential energy of the oscillator (see for example [16, 17, 21]). By the same arguments as above, the function \(P_p(\omega)\) is positive definite. Its normalization for \(\omega \in [0, \infty)\) can also be proved straightforwardly. Thus, the functions \(P_k(\omega)\) and \(P_p(\omega)\) are genuine probability distribution functions. Both of them are sensitive to various control parameters such as trapping frequency \(\omega_0\), magnetic field \(\omega_c\) and the nature of dissipation mechanism \(\tilde{\gamma}(\omega)\). The role of such factors has been explored earlier [16, 21].

B. Energy partition: Alternate form

We will now extend the result discussed in the previous subsection to the frequency domain \(\omega \in (-\infty, \infty)\). Upon putting \(\omega \to -\omega\) in the second term appearing in eqn (20), i.e. the integral involving \(\Phi(-\omega)\) gives,

\[
E_p = \frac{\hbar \omega^2}{2} \int_{-\infty}^{\infty} d\omega E_p(\omega) \Phi(\omega). \tag{29}
\]
Since \( \text{Re}[\bar{\gamma}(\omega)] > 0 \) as a consequence of the second law \[10\], it turns out that \( \Phi(\omega) \) is positive definite. Furthermore, it follows that (see subsection-\[\text{V B}\]),
\[
\int_{-\infty}^{\infty} \Phi(\omega) d\omega = \frac{\pi}{\omega_0^2} \tag{30}
\]
which means that the function \( \pi^{-1}\omega_0^2\Phi(\omega) \) is normalized in the interval \( \omega \in (-\infty, \infty) \). In conclusion, one may interpret \( P_p(\omega) = \pi^{-1}\omega_0^2\Phi(\omega) \) as a probability distribution function over the interval \( \omega \in (-\infty, \infty) \). This result differs slightly from the form of the quantum counterpart of energy equipartition theorem, discussed in recent literature in which the integration limits in the latter are from \( \omega = 0 \) to \( \omega = \infty \). The connection between the two can however be made straightforwardly if in eqn (20), we convert the integration limits to \( \omega \) to \( \omega = \infty \) and define a probability distribution \( P_p(\omega) \) (different from \( P_p(\omega) \)) via eqn (27). We should keep in mind that the distribution functions \( P_p(\omega) \) and \( P_p(\omega) \) are different functions defined over domains \( (-\infty, \infty) \) and \( \{0, \infty\} \) respectively.

Let us now consider the kinetic energy of the oscillator. The integral appearing in eqn (25) can be re-written as,
\[
E_k = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \omega^2 \mathcal{E}_k(\omega) \Phi(\omega). \tag{31}
\]
The following result can be proven directly (see subsection-\[\text{V B}\]),
\[
\int_{-\infty}^{\infty} \omega^2 \Phi(\omega) d\omega = \pi \tag{32}
\]
which imply that the function \( \mathcal{P}_k(\omega) = \pi^{-1}\omega^2\Phi(\omega) \) acts as a suitable probability distribution function for the kinetic energy in the frequency domain \( \omega \in (-\infty, \infty) \). We should also note that upon combining eqns (20) and (25) and identifying \( \mathcal{E}(\omega) = \mathcal{E}_k(\omega) + \mathcal{E}_p(\omega) \) as the mean energy per degree of freedom of a bath oscillator of frequency \( \omega \), we can express the total energy of the system (kinetic + potential) as an integral over the bath spectrum. As with the case of potential energy, the functions \( P_k(\omega) \) and \( P_p(\omega) \) are distinct. We shall show that the latter has profound implications in the context of dissipative diamagnetism.

IV. MAGNETIC MOMENT OF THE OSCILLATOR

The magnetic moment of the oscillator can be computed from the following correlation function \[34\],
\[
M_z = \frac{|c|}{2c} \langle \sigma(t) \dot{y}(t) - y(t) \dot{x}(t) \rangle \tag{33}
\]
\[
= \frac{|c|}{4c} \text{Im} \langle \dot{Z}(t) Z(t)^\dagger + Z(t)^\dagger \dot{Z}(t) \rangle. \tag{34}
\]

FIG. 3. Plot of \( F(\omega/\omega_0) = \omega_0 m(\omega/\omega_0)P_M(\omega/\omega_0) \) as a function of \( \omega/\omega_0 \) in units of \( \mu_B \) for an Ohmic bath with \( \gamma_0/\omega_0 = 0.3 \) and \( \omega/\omega_0 = 0.1 \). Here \( \alpha = \hbar \omega_0/k_B T \).

where \( Z(t) \) and \( \dot{Z}(t) \) are given by eqns (15) and (23). With a few straightforward manipulations, it follows that in the steady state,
\[
M_z = -\frac{e\hbar}{4\pi mc} \int_{-\infty}^{\infty} d\omega \omega^2 \coth \left( \frac{\beta \hbar \omega}{2} \right) \left[ \Phi(\omega) - \Phi(-\omega) \right]. \tag{35}
\]
Therefore, upon identifying \( \mathcal{M}(\omega) = -\frac{e\hbar}{2mc} \coth \left( \frac{\beta \hbar \omega}{2} \right) \), eqn (35) corresponds to eqn (9) thereby proving theorem-\[9\]. One can cast eqn (35) in a form analogous to the quantum counterpart of energy equipartition theorem, i.e.
\[
M_z = \int_{0}^{\infty} m(\omega) P_M(\omega) d\omega \tag{36}
\]
where,
\[
P_M(\omega) = \frac{\omega^2}{\pi} \left[ \Phi(\omega) - \Phi(-\omega) \right]. \tag{37}
\]
Note that unlike the functions \( P_k(\omega) \) and \( P_p(\omega) \) (defined in eqns (4) and (27) respectively), \( P_M(\omega) \) is not positive definite and as such cannot be interpreted as a probability distribution function. In figure-(3), we plot a dimensionless form of the integrand \( F(\omega/\omega_0) = \omega_0 m(\omega/\omega_0)P_M(\omega/\omega_0) \) as a function of \( \omega/\omega_0 \) in units of \( \mu_B \) for the Ohmic bath. The plot signifies the spectral distribution of the magnetic moment such that the total area under these plots gives the equilibrium magnetic moment of the dissipative oscillator. One should note that in general, the areas enclosed on the positive and negative sides of the \( y \)–axis are unequal leading to a total non-zero magnetic moment. The parameter \( \alpha \) is defined as \( \alpha = \hbar \omega_0/k_B T \) whose numerical value signifies departure from classical statistical mechanics.

Our results show the existence of an interesting picture, which can be considered as complementary to the existing ones. We show that the equilibrium state of the dissipative magnetic system is characterized by a wide magnetic moment distribution. The areas enclosed by the positive and negative wings are in
This is manifestly negative due to the fact that the bath oscillator in frequency range $\omega$ quantity equipartition theorem and eqn (39). In eqn (31), the difference between the quantum counterpart of energy and eqn (39) offers a new perspective to dissipative diamagnetism, that the diamagnetic moment at equilibrium can be expressed as a sum taken over an appropriate probability distribution function and indicates towards the connection between the quantum counterpart of energy equipartition theorem and dissipative diamagnetism.

It is imperative to check whether eqn (39) gives $M_z = 0$ for zero external field, i.e. $\omega_c = 0$. Let us first note that from eqns (9) and (12), for any dissipation function $\mu(t)$, the real and imaginary parts of its Fourier transform are respectively even and odd functions in $\omega$. Then, putting $\omega_c = 0$ makes $\Phi(\omega)$ (hence, $P_k(\omega)$) an even function making eqn (39) vanish because $m(\omega)$ is odd. On the other hand, eqn (31) is non-zero (as expected) since $\mathcal{E}_k(\omega)$ is an even function.

Another interesting limit is the classical limit, i.e. $\hbar \rightarrow 0$. In this limit, one has,

$$\frac{\beta \hbar \omega}{2} \coth \left( \frac{\beta \hbar \omega}{2} \right) \rightarrow 1. \quad (40)$$

Therefore, eqn (38) gives,

$$M_z = -\frac{e}{\beta mc\pi} \int_{-\infty}^{\infty} d\omega \Phi(\omega). \quad (41)$$

This integral can be evaluated for specific choices of parameters. It may be checked that the final answer is vanishingly small, consistent with the Bohr-van Leeuwen theorem.

### V. EQUIVALENCE OF EINSTEIN AND GIBBS APPROACH

In this section we are going to demonstrate the equivalence of two distinct approaches to the statistical mechanics of dissipative quantum systems, viz., the ensemble approach of Gibbs and the quantum Brownian motion approach due to Einstein utilizing the paradigmatic model of dissipative diamagnetism. For this purpose we try to connect this magnetization expression in eqn (37) to some of the well known results in the field of dissipative diamagnetism. For definiteness, in this section we shall consider Ohmic dissipation, where $\gamma(\omega) = \gamma_0$.

#### A. Magnetic moment

One can manipulate eqn (37) as follows,
\[ M_z = -\frac{e}{\pi mc\beta} \int_{-\infty}^{\infty} d\omega \left[ \left( \frac{\beta \hbar \omega}{2} \right) \coth \left( \frac{\beta \hbar \omega}{2} \right) \omega [\Phi(\omega) - \Phi(-\omega)] \right] \]
\[ = -\frac{e}{\pi mc\beta} \int_{-\infty}^{\infty} d\omega \left[ \left( \frac{\beta \hbar \omega}{2} \right) \coth \left( \frac{\beta \hbar \omega}{2} \right) \text{Im} \left[ \chi(\omega) - \chi(-\omega) \right] \right] \]
\[ = -\frac{e}{\pi mc\beta} \text{Im} \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\omega \left[ \frac{\omega}{\omega + i\nu_n} + \frac{\omega}{\omega - i\nu_n} \right] \left[ \chi(\omega) - \chi(-\omega) \right] \]
\[ (42) \]

Here we have employed the summation formula: \( x \coth(x) = 1 + 2 \sum_{n=1}^{\infty} (x^2) / [(x^2) + (n\pi)^2] \), where \( x \) is in general complex, and we use the fact that the term unity in the above formula multiplies to \( \text{Im} \left[ \chi(\omega) - \chi(-\omega) \right] \) in the above eqn (42) and thus integrates out to zero and here \( \chi(\omega) = \frac{1}{(\omega^2 - \omega_0^2 + i\nu_n \omega_c - \gamma_0 \nu_n)} \). Note that the term \( 1/(\omega + i\nu_n) \) has a pole at \( \omega = -i\nu_n \) in the lower half of the complex plane and thus contributes to the first term (also lying in the lower half-plane) within the third bracket parentheses of the third line of Eq. (42). Similarly, the pole at \( \omega = +i\nu_n \) in the upper half-plane contributes to the second term (lying in the upper half-plane) within the third bracket parentheses of the third line of Eq. (42). Hence, after performing the contour integration we obtain

\[ M_z = -2 \frac{ie}{mc\beta} \text{Im} \sum_{n=1}^{\infty} \left[ -\nu_n \right] \left[ \frac{\omega_n^2 - \omega_0^2 - i\nu_n \omega_c - \gamma_0 \nu_n}{\nu_n^2} \right] \]
\[ = -2 \frac{e}{mc\beta} \sum_{n=1}^{\infty} \frac{\nu_n^2 \omega_c}{\nu_n^2 + \omega_0^2 + \gamma_0 \nu_n^2 + (\nu_n \omega_c)^2} \]
\[ (43) \]

where, \( \nu_n = \frac{2\pi n}{\beta} \) with \( n = 0, 1, 2, \cdots \). Our final expression [eqn (43)] matches with eqn (55) of [1], as the cut-off \( \omega_D \) goes to infinity. Again, if we consider \( \gamma_0 = 0 \) in eqn (42), we obtain

\[ M_z = -\frac{2B}{\beta} \left( \frac{e}{mc} \right)^2 \sum_{n=1}^{\infty} \frac{\nu_n^2}{(\nu_n^2 + \omega_0^2)^2 + (\nu_n \omega_c)^2} \]
\[ (44) \]

which exactly matches with eqn (35) of Ref. [1] and the latter one is an independent quantum thermodynamic calculation from standard partition function based on the Gibbs method. Further, if we switch off the harmonic trap by putting \( \omega_0 \to 0 \) in eqn (42), we can recover famous Landau diamagnetism result,

\[ M_z = -\frac{2}{B\beta} \sum_{n=1}^{\infty} \frac{\omega_n^2}{(\nu_n^2 + \omega_0^2)} \]
\[ = \frac{e\hbar}{2mc \beta} \left[ \frac{2}{\beta \hbar \omega_c} - \coth \left( \frac{\beta \hbar \omega_c}{2} \right) \right]. \]
\[ (45) \]

It should be specially pointed out that the limits \( t \to \infty \) and \( \omega_0 \to 0 \) do not commute. For obtaining the above result, we have used \( t \to \infty \) in eqn (45), followed by \( \omega_0 \to 0 \) in eqn (44). Reversing the order of these limits gives a different answer, which is only a part of Landau’s result obtained above.

**B. Kinetic and potential energies**

Let us try to represent potential energy and kinetic energy in terms of infinite series of Matsubara frequencies \( \nu_n \). In the process, we shall prove the normalization of \( P_k(\omega) \) and \( P_\nu(\omega) \) defined in subsection IIIB.1. First note that from eqn (29), the average potential energy is given by,

\[ E_p = \frac{\omega_0^2}{2\pi} \int_{-\infty}^{\infty} d\omega \hbar \omega \coth \left( \frac{\beta \hbar \omega}{2} \right) \Phi(\omega) \]
\[ = \frac{\omega_0^2}{\pi \beta} \int_{-\infty}^{\infty} d\omega \left[ 1 + 2 \sum_{n=1}^{\infty} \frac{\omega^2}{\nu_n^2 + \omega^2} \right] \Phi(\omega) \]
\[ (46) \]

The first term \( (n = 0) \) above can be understood to be the classical part, whereas the subsequent terms \( (n = 1, 2, 3, \cdots) \) are quantum corrections. Let us consider the \( n = 0 \) term i.e. the term outside the summation in the second line of Eq. (46). We can rewrite it as,

\[ (E_p)_{n=0} = -\frac{\omega_0^2}{\pi \beta} \int_{-\infty}^{\infty} d\omega \frac{1}{\omega} \text{Im} \left[ \omega^2 - \omega_0^2 - \omega \omega_c + i\gamma_0 \omega \right]^{-1} \]
\[ = \frac{1}{\beta} \]
\[ (47) \]

where picking up the contribution of the pole at \( \omega = 0 \) provides us the final result. One other way of justifying this contribution (i.e. \( \frac{1}{\beta} \)) is that as the temperature goes to infinity (in the classical limit) coth(\( \beta \hbar \omega/2 \)) goes to \( \frac{2}{\hbar \omega} \) and hence, eqn (46) reduces to the \( n = 0 \) term in eqn (46). On the other hand, classical equipartition theorem demands that the this should be equal to \( \frac{1}{2} \). Therefore, we must have the relation,

\[ \int_{-\infty}^{\infty} d\omega \frac{\omega_0^2}{\pi} \Phi(\omega) = 1 \]
\[ (48) \]

which confirms normalization [eqn (30)] of the probability distribution function, \( P_\nu(\omega) = \frac{\omega_0^2}{\pi} \Phi(\omega) \) corresponding to
the potential energy of the dissipative charged magneto-osculator. Now, from eqn (46) we can rewrite

$$E_p = \frac{1}{\beta} + \frac{\omega^2}{\pi \beta} \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\omega \Phi(\omega) \frac{\omega}{\omega^2 + \nu_n^2}$$

$$= \frac{1}{\beta} + \frac{\omega^2}{\pi \beta} \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\omega \frac{\omega}{\omega^2 + \nu_n^2} \text{Re} \left[ i \omega \gamma_0 \right]$$

$$= \frac{1}{\beta} + \frac{\omega^2}{\pi \beta} \sum_{n=1}^{\infty} \text{Re} \left[ \nu_n^2 + \omega_0^2 + \nu_n \omega_c + \gamma_0 \nu_n \right]$$

where, in the last step, we have closed the contour in the upper-half plane and picked up the contribution from the pole at $\omega = i\nu_n$. Finally, we can obtain

$$E_p = \frac{1}{\beta} + \frac{\omega^2}{\beta} \sum_{n=1}^{\infty} \left( \nu_n^2 + \omega_0^2 + \gamma_0 \nu_n + \frac{\gamma_0 \nu_n}{\nu_n} \right)$$

which expresses the mean potential energy of the oscillator as an infinite series.

Turning now to the calculation of the average kinetic energy, we have from eqn (25),

$$E_k = \frac{1}{\beta} + \frac{1}{\pi \beta} \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} d\omega \frac{\omega^2}{(\omega + i\nu_n)(\omega - i\nu_n)} \left( \text{Re} \left[ i \omega \gamma_0 \right] \frac{1}{\omega^2 - \omega_0^2 - \omega_c + i\gamma_0 \omega} \right)$$

Finally, picking up the contribution of the pole in the lower half-plane at $\omega = -i\nu_n$ one may obtain

$$E_k = \frac{1}{\beta} + \frac{2}{\beta} \sum_{n=1}^{\infty} \left( \gamma_0 \nu_n \left( \nu_n^2 + \omega_0^2 + \gamma_0 \nu_n \right) + (\nu_n \omega_c)^2 \right)$$

$$\left( \nu_n^2 + \omega_0^2 + \gamma_0 \nu_n \right)^2 + (\omega_c \nu_n)^2$$

Combining eqns (56) and (58), we can obtain the internal energy of the system as,

$$E = \frac{2}{\beta} \left[ 1 + \sum_{n=1}^{\infty} \frac{N(\nu_n)}{D(\nu_n)} \right]$$

where, the numerator $N(\nu_n)$ and the denominator $D(\nu_n)$ are given as follows,

$$N(\nu_n) = \nu_n^2 + \omega_0^2 + \gamma_0 \nu_n \left( 2\nu_n^2 + \gamma_0 \nu_n \right) + (\omega_c \nu_n)^2$$

$$D(\nu_n) = \left[ (\nu_n^2 + \omega_0^2 + \gamma_0 \nu_n)^2 + (\omega_c \nu_n)^2 \right].$$

At this present outset we can compare our results of internal energy (eqns (57) and (58)) obtained from stochastic thermodynamics approach or Einstein approach with that of standard Gibbs thermodynamics method. From eqn (42) of [5] we can write,

$$- \ln Z = 2(\ln \omega_0 + \ln \beta) + \sum_{n=1}^{\infty} \ln X_n,$$
It then follows that eqn (61) matches exactly with eqn (57) establishing the equivalence between the Einstein approach and the Gibbs approach. One can also obtain the \( \gamma_0 = 0 \) limit from eqn (57), which reads,

\[
E_{\gamma_0=0} = \frac{2}{\beta} \left[ 1 + \sum_{n=1}^{\infty} \frac{2(\nu_n^2 + \omega_0^2)\omega_{0n}^2 + (\nu_n\omega_n)^2}{(\nu_n^2 + \omega_0^2)^2 + (\nu_n\omega_n)^2} \right],
\]

which matches with eqn (41) of [6] obtained from an independent calculation of \( E \) from the partition function method.

Similarly, one may obtain the magnetic moment of the oscillator from the partition function \( Z \) using the standard relation,

\[
M_z = \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} = -\frac{1}{\beta} \sum_{n=1}^{\infty} \frac{\partial X_n}{\partial B}
\]

\[
= -\frac{2}{\beta B} \sum_{n=1}^{\infty} \frac{(\omega_{0n}\nu_n)^2}{(\nu_n^2 + \omega_0^2 + \gamma_0\nu_n\omega_n)^2 + (\omega_n\nu_n)^2}.
\]

This is in conformity with eqn (42) of stochastic thermodynamics. The standard thermodynamic expression for \( \gamma_0 = 0 \) also follows from an independent calculation of the partition function as in eqn (35) of [5].

VI. CONCLUSIONS

Considering a paradigmatic model of dissipative diamagnetism, we shed light on certain aspects of diamagnetism in open quantum systems. Starting from the quantum Langevin equation for a dissipative charged particle in a magnetic field, we formulate the energy equipartition theorem of the model system in terms of the relaxation function \( \Phi(\omega) \) and universal power spectrum of quantum noise: \( u(\omega) = \frac{\hbar c}{2} \coth \left( \frac{\hbar c}{2k_B T} \right) \) in the full frequency domain \( \omega \in (-\infty, \infty) \). The mean kinetic and potential energies of the dissipative system can be expressed in accordance with the quantum equipartition theorem, as integral involving \( \Phi(\omega) + \Phi(-\omega) \) and \( u(\omega) \). The latter also corresponds to the mean kinetic/potential energy of a two dimensional bath oscillator. Unlike the previous studies [15, 21], where results were expressed over the frequency domain \( \omega \in [0, \infty) \), our present results are extended for the full domain of frequency. This will help towards a better understanding of the measurable quantities, as they follow the usual Fourier analysis by incorporating negative phasor portion too.

Following this, we consider the main focus of the present study and derive dissipative magnetic moment of our model system as an integral involving \( [\Phi(\omega) - \Phi(-\omega)] \) and the thermal Bohr magneton: \(-\mu_B \coth \left( \frac{\hbar c}{2k_B T} \right) \).

We offer two distinct viewpoints on this result. First, by putting \( \omega \rightarrow -\omega \) in the integral involving \( \Phi(-\omega) \), we find that the magnetic moment can be expressed as \( M_z = \langle m(\omega) \rangle \) where \( m(\omega) \) is the thermal Bohr magneton, and \( \langle \cdot \rangle \) implies can average over the probability distribution function \( P_\omega(\omega) \) which appears in the quantum counterpart of energy equipartition theorem for the kinetic energy. Thus, the quantum counterpart of energy equipartition and magnetic moment of the dissipative oscillator are intimately connected.

In the second viewpoint, restricting to the frequency range \( \omega \in [0, \infty) \), the magnetic moment can be expressed as an integral over a distribution function \( P_M(\omega) \) which has a positive as well as a negative wing. Contributions from the two segments exactly cancel each other at high temperatures. This implies that we can correctly recover the Bohr-van Leeuwen results at high temperatures. As one lowers the temperature, it turns out that the cancellation is incomplete, leading to a net magnetic moment. This can be naively related with the Peierls’ concept of bulk current and surface current contributions in the diamagnetic moment.

Finally, we investigate the equivalence of usual Gibbs thermodynamics method and the stochastic thermodynamics (Einstein approach) technique and find that they agree pretty well. Our model system is rather well studied and close to the realistic three dimensional dissipative diamagnetism [11, 12]. Our results on the orbital dissipative diamagnetic moment can be tested via cold atom experiments with hybrid traps for ions and neutral atoms, i.e. by considering a single ion dipped in a BEC [24]. Further one can generate a uniform magnetic field using magnetic coils in the form of Helmholtz configuration. The dissipative environment can be built up via a 3D optical molasses [25] in combination with a magnetic or an optical trap. One can change the temperature by varying the depth of the trap and measure the orbital diamagnetic magnetic moment at low temperatures as well as at high temperatures.

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[1] M. E. Fisher, “Proceedings of Gibbs Symposium”, edited by D. G. Caldi and G. D. Mostow (Yale University Press, New haven, CT, 1989).
[2] S. Dattagupta and J. Singh, “Stochastic motion of a charged particle in a magnetic field: II Quantum Brownian treatment”, Pramana 47 (3), 211-224 (1996).
[3] S. Dattagupta and J. Singh, “Landau diamagnetism in a dissipative and confined system”, Phys. Rev. Lett. 79, 961 (1997).
[4] P. Hanggi, G.-L. Ingold and P. Talkner, “Finite quantum dissipation: the challenge of obtaining specific heat”, New J. Phys. 10, 115008 (2008).
[5] J. Kumar, P. A. Sreeram and S. Dattagupta, “Low-temperature thermodynamics in the context of dissipative diamagnetism”, Phys. Rev. E 79, 021130 (2009).
[6] S. Dattagupta, J. Kumar, S. Sinha and P. A. Sreeram, “Dissipative quantum systems and the heat capacity”, Phys. Rev. E 81, 031136 (2010).
[7] P. Hanggi and G.-L. Ingold, “Quantum Brownian motion and the third law of thermodynamics”, Acta Physica Polonica B 37, 15371550 (2006).
[8] M. Bandyopadhyay, “Quantum thermodynamics of a charged magneto-oscillator coupled to a heat bath”, J. Stat. Mech. P05002 (2009).
[9] M. Bandyopadhyay, Dissipative cyclotron motion of a charged quantum-oscillator and third law, J. Stat. Phys., 140 (3), 603-618 (2010).
[10] G. W. Ford, J.T. Lewis, R.O. O’Connell, “Quantum Langevin equation”, Phys. Rev. A 37, 11 (1988).
[11] M. Bandyopadhyay and S. Dattagupta, “Landau-Drude Diamagnetism: Fluctuation, Dissipation and Decoherence”, J. Phys.: Condens. Matter 18 10029 (2006).
[12] M. Bandyopadhyay and S. Dattagupta, “Dissipative Diamagnetism—A Case Study for Equilibrium and Nonequilibrium Statistical Mechanics”, J. Stat. Phys. 123, 1273 (2006).
[13] R. B. Laughlin, “Quantized Hall conductivity in two dimensions”, Phys. Rev. B 23, 5632 (1981).
[14] K. V. Klitzing, G. Dorda and M. Pepper, “New Method for High-Accuracy Determination of the Fine-Structure Constant Based on Quantized Hall Resistance”, Phys. Rev. Lett. 45, 494 (1980).
[15] P. Bialas and J. Luzcka, “Kinetic energy of a free quantum Brownian particle”, Entropy 20, 123 (2018).
[16] J. Spiechowicz, P. Bialas, and J. Luzcka, “Quantum partition of energy for a free Brownian particle: Impact of dissipation”, Phys. Rev. A 98, 052107 (2018).
[17] P. Bialas, J. Spiechowicz, J. Luzcka, “Partition of energy for a dissipative quantum oscillator”, Sci. Rep. 8, 16080 (2018).
[18] P. Bialas, J. Spiechowicz, J. Luzcka, “Quantum analogue of energy equipartition theorem”, J. Phys. A: Math. Theor. 52, 15 (2019).
[19] J. Luzcka, “Quantum Counterpart of Classical Equipartition of Energy”, J. Stat. Phys. 179, 839-845 (2020).
[20] J. Spiechowicz and J. Luzcka, “Energy of a free Brownian particle coupled to thermal vacuum”, Sci. Rep. 11, 4088 (2021).
[21] J. Kaur, A. Ghosh and M. Bandyopadhyay, “Quantum counterpart of energy equipartition theorem for a dissipative charged magneto-oscillator: Effect of dissipation, memory, and magnetic field”, Phys. Rev. E 104, 064112 (2021).
[22] G. W. Ford and R. F. O’Connell, “Calculation of Correlation Functions in the Weak Coupling Approximation”, Ann. Phys. 276, 144 (1999).
[23] R. Peierls, “Surprises in Theoretical Physics”, (Princeton University Press, Princeton, NJ, 1979), Sec. 4.3.
[24] C. Zipkes, S. Palzer, C. Sias and M. Köhl, “A trapped single ion inside a Bose–Einstein condensate”, Nature 464, 388–391 (2010).
[25] T. W. Hodapp, C. Gerz, C. Furtlechner, C. I. Westbrook, W. D. Phillips and J. Dalibard, “Three-dimensional spatial diffusion in optical molasses”, Appl. Phys. B 60, 135–143 (1995).