

Quantum dissipation and the virial theorem

Aritra Ghosh* and Malay Bandyopadhyay†

*School of Basic Sciences,
Indian Institute of Technology Bhubaneswar,
Argul, Jatni, Khurda, Odisha 752050, India*

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In this short note, we study the celebrated virial theorem for dissipative systems, both classical and quantum. The classical formulation is discussed and an intriguing effect of the random force (noise) is made explicit in the context of the virial theorem. Subsequently, we derive a generalized virial theorem for a dissipative quantum oscillator, i.e. a quantum oscillator coupled with a quantum heat bath. Such a heat bath is modelled as an infinite collection of independent harmonic oscillators with a certain distribution of initial conditions. In this situation, the non-Markovian nature of the quantum noise leads to novel bath-induced terms in the virial theorem. We also consider the case of an electrical circuit with thermal noise and analyze the role of non-Markovian quantum noise in the context of the virial theorem.

I. INTRODUCTION

In 1870, Rudolf Clausius formulated the virial theorem for a mechanical system [1]. For a one-particle system, it says that if the virial $G = m\mathbf{r} \cdot \mathbf{v}$ remains bounded in its time evolution, then

$$\langle K \rangle = -\frac{1}{2} \langle \mathbf{r} \cdot \mathbf{F} \rangle \quad (1)$$

where K is the kinetic energy, \mathbf{r} is the position vector and \mathbf{F} is the external force. Here, angled brackets $\langle \cdot \rangle$ denote ‘time-averaging’. Thus, the virial theorem relates the time-averaged kinetic energy to a suitable time average involving the external force. In particular, if the force is conservative, one has $\mathbf{F} = -\nabla V$ and thus

$$\langle K \rangle = \frac{1}{2} \langle \mathbf{r} \cdot \nabla V \rangle. \quad (2)$$

The result can be appropriately generalized to a system of particles. It has found applications in astrophysics, cosmology, molecular physics, quantum mechanics and statistical mechanics (see for instance [2–6]).

The virial theorem can be straightforwardly extended for quantum mechanical systems [5, 6] where the Heisenberg equations replace the classical Hamilton’s equations of motion. For a quantum mechanical system whose Hamiltonian operator is

$$H = \frac{p^2}{2m} + V(x) \quad (3)$$

where x and p are the position and momentum operators respectively, i.e. $[x, p] = i\hbar$, the quantum mechanical virial theorem gives

$$\left\langle \frac{p^2}{m} \right\rangle = \langle xV'(x) \rangle. \quad (4)$$

This is in exact analogy with eqn (2). Eqn (4) can be easily generalized to multi-particle systems. In particular, for the harmonic oscillator potential, i.e. $V(x) = m\omega_0^2 x^2/2$ one finds that the time-averaged kinetic and potential energies are equal.

Since in real life, one rarely has truly isolated systems, one can now ask how eqn (4) changes if the quantum system interacts with some environment? As we will discuss in the next section, the corresponding classical result remains unchanged even in the presence of an environment. However, in the quantum mechanical case, we shall find that eqn (4) picks up novel environment induced terms which are non-zero in general. An immediate consequence of this is that the time-averaged kinetic and potential energies are no longer equal. The aim of the present work is to obtain a generalized virial theorem for a dissipative quantum system and analyze the environment induced terms in the virial theorem. For that we consider a prototypical system, which consists of a single quantum particle placed in a harmonic potential while it is also interacting with a quantum heat bath. The heat bath is taken to be composed of an infinitely many independent harmonic oscillators [7–9] and the reduced quantum dynamics of the system is described by the quantum Langevin equation [10]. We shall also discuss the result obtained here in the light of the quantum counterpart of energy equipartition theorem studied earlier [11–16].

The paper is organized as follows. Section-(II) is mostly introductory where we re-derive the classical virial theorem and discuss two simple classical dissipative systems. We emphasize upon the role of environment induced noise in this context. Then, in section-(III), we derive a generalized virial theorem for a dissipative quantum oscillator, i.e. for a quantum oscillator interacting with a heat bath. We compute the bath induced terms in the virial theorem and show that they consistently go to zero as $\hbar \rightarrow 0$. In section-(IV), we consider a linear electric circuit with thermal noise of quantum origin and

*ag34@iitbbs.ac.in

†malay@iitbbs.ac.in

analyze the role of non-Markovian noise in the context of the virial theorem. We end with some discussion in section-(V).

II. VIRIAL THEOREM FOR CLASSICAL DISSIPATIVE SYSTEMS

The virial theorem is typically derived in the following way. Let $H(q^i, p_i)$ describe a Hamiltonian system, with coordinates q^i and momenta p_i . Then, one defines $G := q^i p_i$ (repeated indices summed over), which is called the virial. Now, the dynamics of G is simply

$$\frac{dG}{dt} = \{G, H\} \quad (5)$$

where $\{\cdot, \cdot\}$ is the Poisson bracket. One can then perform time-averaging on both sides, i.e. write

$$\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \frac{dG}{dt} dt = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \{G, H\} dt. \quad (6)$$

If G remains bounded in its time evolution, then one gets the simple result

$$\langle \{G, H\} \rangle = 0 \quad (7)$$

where angled brackets $\langle \cdot \rangle$ denote time-averaging. Eqn (7) has been referred to as a hypervirial theorem, or simply a generalized virial theorem [6] (see also [17–19]). For a typical conservative mechanical system, one has $H(q^i, p_i) = K(p_i) + V(q^i)$ where $K = \sum_i p_i^2 / 2m_i$ and V are the kinetic and potential energies respectively. Thus, eqn (7) gives

$$\langle \{G, K\} \rangle = -\langle \{G, V\} \rangle \quad (8)$$

which using the fact that $G = q^i p_i$ and the Leibniz rule for the Poisson bracket leads to

$$\left\langle \sum_i \frac{p_i^2}{m_i} \right\rangle = \left\langle \sum_i q_i \frac{\partial V(q^i)}{\partial q^i} \right\rangle. \quad (9)$$

This agrees with eqn (1) obtained by Clausius. Although, eqn (7) only describes conservative systems, it has been extended to the case of contact Hamiltonian dynamics, which describe simple dissipative systems in [19]. Let us consider two simple dissipative systems below.

A. Damped oscillator

The damped oscillator is associated with the following equation of motion:

$$m\ddot{x} + \mu\dot{x} + kx = 0 \quad (10)$$

where symbols have their usual meanings. Thus, the force acting on the particle of mass m is $\mathcal{F} = -\mu\dot{x} - kx$.

Since this force is not conservative (for $\mu \neq 0$), we cannot apply eqn (7) straightforwardly to this problem. However, eqn (1) gives

$$\langle m\dot{x}^2 \rangle = \langle kx^2 \rangle + \mu \langle x\dot{x} \rangle \quad (11)$$

or equivalently,

$$\left\langle \frac{p^2}{m} \right\rangle = \langle m\omega_0^2 x^2 \rangle + \gamma \langle xp \rangle \quad (12)$$

where $k = m\omega_0^2$ and $\mu = m\gamma$. Eqn (12) is the same as that obtained via a generalized virial theorem in the contact Hamiltonian framework in [19]. As we shall show in the next subsection, this result [eqn (11)] differs significantly from that for a Brownian particle where the equation of motion contains random force (noise terms).

B. Brownian oscillator

Consider the case of a Brownian particle suspended in a fluid and moving in harmonic potential. Then, the equation of motion is the Langevin equation

$$m\ddot{x} + \mu\dot{x} + m\omega_0^2 x = F(t) \quad (13)$$

where $F(t)$ is a Gaussian random noise, whose power spectrum is white, i.e.

$$\langle F(t)F(t') \rangle = \Gamma \delta(t - t') \quad (14)$$

for some $\Gamma > 0$. The Gaussian nature of the noise ensures that all odd moments vanish, i.e. one also has $\langle F(t) \rangle = 0$ and similarly for other odd moments. Since the net external force on the particle is $\mathcal{F} = -\mu\dot{x} - m\omega_0^2 x + F(t)$, from eqn (1), we get the following result:

$$\langle m\dot{x}^2 \rangle = \langle m\omega_0^2 x^2 \rangle + \mu \langle x\dot{x} \rangle - \langle xF(t) \rangle. \quad (15)$$

It is straightforward to show by solving eqn (13) that $\langle xF(t) \rangle = 0$. Now, $\langle x\dot{x} \rangle$ is the position-velocity cross-correlation function. In the steady state, this too vanishes! Therefore, eqn (15) simply gives

$$\left\langle \frac{m\dot{x}^2}{2} \right\rangle = \left\langle \frac{m\omega_0^2 x^2}{2} \right\rangle \quad (16)$$

meaning that the time-averaged kinetic and potential energies are equal. This is in sharp contrast to eqn (11) where $\langle x\dot{x} \rangle \neq 0$. This demonstrates the crucial role of the noise term in the equation of motion which ensures that the position-velocity correlation function identically vanishes in the steady state. Thus, the presence and the nature of noise terms can essentially control the form of the virial theorem.

The presence of a noise term also introduces a thermal interpretation to the averages. For instance, one

can solve eqn (13) and compute $\langle x^2 \rangle$ and $\langle \dot{x}^2 \rangle$ explicitly. They are found to be equal and give [20, 21]

$$\left\langle \frac{m\dot{x}^2}{2} \right\rangle = \left\langle \frac{m\omega_0^2 x^2}{2} \right\rangle = \frac{\Gamma}{4\mu}. \quad (17)$$

Let us now note that the fluid in which the Brownian particle is immersed in has a temperature T and the particles are distributed according to the Maxwell's speed distribution. After repeated collisions, i.e. exchanging energy with the fluid, the Brownian particle shall also reach a steady state, attaining the same temperature T . Thus, it is described by the canonical distribution

$$\rho = \frac{e^{-\beta\left(\frac{m\dot{x}^2}{2} + \frac{m\omega_0^2 x^2}{2}\right)}}{Z} \quad (18)$$

where $\beta = 1/k_B T$ and $Z = (2\pi k_B T / m\omega_0)$ is the partition function normalizing ρ . Thus, the thermally-averaged kinetic energy is

$$K_{\text{th}} = Z^{-1} \int dx d\dot{x} \left(\frac{m\dot{x}^2}{2} \right) e^{-\beta\left(\frac{m\dot{x}^2}{2} + \frac{m\omega_0^2 x^2}{2}\right)} = \frac{k_B T}{2} \quad (19)$$

and similarly $V_{\text{th}} = \frac{k_B T}{2}$. Thus, once again the (thermally-)averaged kinetic and potential energies are equal. In the steady state, the time-averaged values agree with the thermally-averaged values, i.e. $\langle K \rangle = K_{\text{th}}$ and $\langle V \rangle = V_{\text{th}}$. This requires that we pick $\Gamma = 2\mu k_B T$ and then everything fits consistently.

Therefore, the presence of a noise term in the equation of motion can dramatically alter the virial theorem. We emphasize upon two main features of the noise:

1. The presence of noise leads to the kinetic and potential energies being equal in the steady state for the potential $V(x) = \frac{m\omega_0^2 x^2}{2}$. If the noise was absent, then the time-averaged kinetic and potential energies are not equal [eqn (11)].
2. The noise associates a natural thermal character to the averages, i.e. the time-averages are the same as thermal-averages. While eqn (11) has no thermal interpretation, eqn (16) has one and the averages are equal to $\frac{k_B T}{2}$ in accordance with the equipartition theorem.

We are now in a position to discuss a generalized virial theorem for dissipative quantum systems.

III. GENERALIZATION TO QUANTUM DISSIPATION

We shall now consider formulating a quantum mechanical virial theorem suited for dissipative systems. A dissipative system is one that interacts with an environment, i.e. the total Hamiltonian is $H = H_S + H_B + H_{SB}$, where

H_S and H_B are the Hamiltonians of the system and the bath respectively, while H_{SB} is that describing the interaction between the system and the bath. Thus, in the Schrodinger picture, the dynamics of the system and the bath collectively is unitary, i.e.

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = (H_S + H_B + H_{SB}) |\psi(t)\rangle. \quad (20)$$

However, one is only interested in the dynamics of the system while it is in contact with the heat bath. To obtain that, one conveniently traces over the degrees of freedom of the bath so that one gets a reduced dynamical description for the system and the time evolution is no longer unitary. One way to trace over the bath degrees of freedom is to consider the path integral formulation of quantum mechanics and subsequently compute the influence functional which takes care of the environmental effects [7]. A distinct approach is to consider the Heisenberg equations for the system and bath variables wherein, one solves those of the bath and substitutes them into the equations of motion describing the system degrees of freedom. This naturally leads to a quantum Langevin equation [10], with a built-in fluctuation dissipation theorem.

In this paper, we consider the latter approach to dissipative quantum systems. Our system is particle of mass m moving on one dimension in the presence of some potential $V(x)$. The bath is modelled as a collection of infinite harmonic oscillators with a distribution of frequencies and initial conditions while the system-bath coupling is taken to be bilinear. Thus, the total Hamiltonian reads

$$H = \frac{p^2}{2m} + V(x) + \sum_{j=1}^N \left[\frac{p_j^2}{2m_j} + \frac{m_j \omega_j^2}{2} (q_j - x)^2 \right] \quad (21)$$

where q_j and p_j are the coordinates and momenta of the bath degrees of freedom, i.e. $[q_j, p_j] = i\hbar \delta_{ij}$. It should be remarked that we have considered an additional potential term $V_r(x) = x^2 \sum_{j=1}^N m_j \omega_j^2$ in order to ensure that the Hamiltonian is translationally invariant or equivalently, the system-bath coupling is homogenous in space. Addition of $V_r(x)$ is often called 'potential renormalization'.

Now, one can use the usual commutation relations between the variables appearing in eqn (21) to derive the Heisenberg equations for the system and bath variables. Subsequently, one can solve the equations of motion for the bath and substitute them into those of the system. The resulting reduced equation of motion describing the 'open' quantum system is

$$m\ddot{x} + \int_{-\infty}^t \mu(t-t') \dot{x}(t') dt' + V'(x) = F(t) \quad (22)$$

where the function $\mu(t)$ is the dissipation kernel whose

expression is

$$\mu(t) = \Theta(t) \sum_{j=1}^N m_j \omega_j^2 \cos(\omega_j t). \quad (23)$$

The presence of the step function $\Theta(t)$ ensures that $\mu(t)$ vanishes for negative arguments, consistent with the principle of causality. Now, assuming that the system and the bath were coupled at the distant past, $F(t)$ is a Gaussian noise whose explicit expression is

$$F(t) = \sum_{j=1}^N m_j \omega_j^2 \left[\left(q_j(0) - x(0) \right) \cos(\omega_j t) + \frac{p_j(0)}{m_j \omega_j} \sin(\omega_j t) \right]. \quad (24)$$

Notice that the noise depends upon the initial conditions of the system as well as the bath oscillators. The initial conditions can be taken to be distributed according to a canonical distribution and this implements the random nature of $F(t)$ leading to a thermal interpretation of the dynamics. This is not a quantum mechanical feature, the same arguments go through for the classical case. Furthermore, it should also be noted that the thermodynamic limit corresponds to $N \rightarrow \infty$ which shall be assumed to be the case even if it is not explicitly mentioned. The spectral properties of the noise are given by the following correlation function and commutator:

$$\begin{aligned} \langle \{F(t), F(t')\} \rangle &= \frac{2}{\pi} \int_0^\infty d\omega \hbar \omega \text{Re}[\tilde{\mu}(\omega)] \coth\left(\frac{\hbar \omega}{2k_B T}\right) \\ &\quad \times \cos[\omega(t - t')] \end{aligned} \quad (25)$$

$$\langle [F(t), F(t')] \rangle = \frac{2}{i\pi} \int_0^\infty d\omega \hbar \omega \text{Re}[\tilde{\mu}(\omega)] \sin[\omega(t - t')] \quad (26)$$

where $\tilde{\mu}(\omega)$ is the Fourier transform of $\mu(t)$ [eqn (37)].

It is often convenient to define a bath spectral function $J(\omega)$ describing the spectral distribution of the bath degrees of freedom as

$$J(\omega) = \frac{\pi}{2} \sum_{j=1}^N m_j \omega_j^3 \delta(\omega - \omega_j). \quad (27)$$

Combining eqns (23) and (27), one gets

$$\mu(t) = \frac{2}{\pi} \int_0^\infty \frac{J(\omega)}{\omega} \cos(\omega t) d\omega. \quad (28)$$

We have now set-up our notation and have introduced all the preliminaries in order to derive a generalized virial theorem for the dissipative quantum system. For definiteness, we consider Ohmic dissipation for which $J(\omega) = m\gamma\omega$ or $\mu(t) \sim \delta(t)$.

Now let us derive a generalized virial theorem for the dissipative quantum system described above. Since we are interesting in the system (S), we define a symmetrized virial operator for the system as $G = \frac{xp+px}{2}$ which means

$$\frac{d\langle G \rangle}{dt} = \frac{\langle [G, H] \rangle}{i\hbar} = \frac{\langle [xp, H] + [px, H] \rangle}{2i\hbar}. \quad (29)$$

Note that the Hamiltonian H appearing in the equations above is the total Hamiltonian [eqn (21)] which also contains H_B and H_{SB} . Let us analyze the quantity $\langle [xp, H] + [px, H] \rangle$. Some straightforward manipulations using eqn (21) gives

$$\langle [xp, H] + [px, H] \rangle = \left\langle \frac{p^2}{m} \right\rangle - \langle xV'(x) \rangle + \sum_{j=1}^N m_j \omega_j^2 \langle q_j(t)x(t) \rangle - \frac{1}{2} \sum_{j=1}^N m_j \omega_j^2 \int_{-\infty}^t dt' \langle x(t)\dot{x}(t') + \dot{x}(t')x(t) \rangle \cos[\omega_j(t - t')]. \quad (30)$$

Let us define

$$I_1 = \frac{1}{2} \sum_{j=1}^N m_j \omega_j^2 \langle q_j(t)x(t) + x(t)q_j(t) \rangle = \frac{1}{2} \langle x(t)F(t) + F(t)x(t) \rangle, \quad (31)$$

$$I_2 = \frac{1}{2} \sum_{j=1}^N m_j \omega_j^2 \int_{-\infty}^t dt' \langle x(t)v(t') + v(t')x(t) \rangle \cos[\omega_j(t - t')] = \int_{-\infty}^t dt' \mu(t - t') C_{xv}(t - t') \quad (32)$$

where we have used eqns (24) and (28), and have defined the position-velocity correlation function $C_{xv}(t - t') = \frac{1}{2} \langle x(t)v(t') + v(t')x(t) \rangle$ for velocity operator

$$v(t) = \dot{x}(t).$$

If one now takes the steady state limit, one would have

$d\langle G \rangle/dt = 0$ meaning that the left-hand side of the equation above vanishes. This will give eqn (4) together with novel bath induced terms which can be determined by evaluating the steady state expressions for I_1 and I_2 . One may interpret here, $c_j = m_j \omega_j^2$ as coupling constants which couple the system and the environment. Setting $c_j = 0$, one straightforwardly recovers eqn (4) as anticipated. In the steady state, for $V(x) = \frac{m\omega_0^2 x^2}{2}$, one has $\langle K \rangle - \langle V \rangle = \frac{I_2 - I_1}{2}$ and therefore, the kinetic and potential energies are unequal in general [13, 14, 16]. It is the competition between I_1 and I_2 which will decide whether the mean kinetic energy exceeds the mean potential energy or vice versa. We now separately analyze each of these.

A. Analysis of I_1

Let us begin by evaluating I_1 defined in eqn (31). Physically, this term corresponds to the time-averaged work done on the dissipative system by the quantum noise. Remarkably, it vanishes for the classical case [22] but as we will show, it is non-trivial for a dissipative quantum system. I_1 is the symmetrized position-noise correlation function, i.e.

$$I_1 = C_{xF} := \frac{\langle x(t)F(t) + F(t)x(t) \rangle}{2} \quad (33)$$

and we are required to compute the above correlation function for equal times, i.e. the position and noise operators are defined at the same time instant t . For the moment however, let us consider a more general unequal time correlation function, where $\tau = t - t'$ is the time separation, i.e. we consider $C_{xF}(t - t') := \frac{\langle x(t)F(t') + F(t')x(t) \rangle}{2}$ and later we will set $t = t'$ or $\tau = 0$. Now, we may write

$$C_{xF}(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{C}_{xF}(\omega) e^{-i\omega\tau} \quad (34)$$

which means if we can find $\tilde{C}_{xF}(\omega)$, we can find $C_{xF}(\tau)$ at $\tau = 0$ easily. Let us begin by considering the quantum Langevin equation [eqn (22)] with $V(x) = \frac{m\omega_0^2 x^2}{2}$. A Fourier transform allows us to solve it and we may write $\tilde{x}(\omega) = \alpha(\omega)\tilde{F}(\omega)$ where

$$\tilde{x}(\omega) = \int_{-\infty}^{\infty} x(t)e^{i\omega t} dt, \quad \tilde{F}(\omega) = \int_{-\infty}^{\infty} F(t)e^{i\omega t} dt \quad (35)$$

and

$$\alpha(\omega) = \frac{1}{m(\omega_0^2 - \omega^2) - i\omega\tilde{\mu}(\omega)} \quad (36)$$

is the susceptibility. In the above expression

$$\tilde{\mu}(\omega) = \int_0^{\infty} \mu(t)e^{i\omega t} dt \quad (37)$$

is the Fourier transformed dissipation kernel. For Ohmic dissipation, one has $\tilde{\mu}(\omega) = m\gamma$, where $\gamma > 0$ is the system-bath coupling strength. Since, $\tilde{x}(\omega) = \alpha(\omega)\tilde{F}(\omega)$, one can write

$$\tilde{C}_{xF}(\omega) = \alpha(\omega)\tilde{C}_{FF}(\omega) \quad (38)$$

where, $\tilde{C}_{FF}(\omega) = \int_{-\infty}^{\infty} C_{FF}(\tau)e^{i\omega\tau}$ is the Fourier transformed noise autocorrelation function. But from eqn (26), $\tilde{C}_{FF}(\omega)$ is just

$$\tilde{C}_{FF}(\omega) = \text{Re}[\tilde{\mu}(\omega)]\hbar\omega \coth\left(\frac{\hbar\omega}{2k_B T}\right) \quad (39)$$

meaning that from eqns (33) and (34)

$$I_1 = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \omega \text{Re}[\tilde{\mu}(\omega)]\alpha(\omega) \coth\left(\frac{\hbar\omega}{2k_B T}\right) \quad (40)$$

where we have set $\tau = 0$ in eqn (34). For Ohmic dissipation, one simply has

$$\begin{aligned} I_1 &= \frac{\hbar\gamma}{2\pi} \int_{-\infty}^{\infty} \frac{\omega d\omega}{(\omega_0^2 - \omega^2) - i\omega\gamma} \coth\left(\frac{\hbar\omega}{2k_B T}\right) \\ &= \frac{\gamma}{\beta\pi} \int_{-\infty}^{\infty} \frac{d\omega}{(\omega_0^2 - \omega^2) - i\omega\gamma} \left(\frac{\hbar\omega}{2k_B T}\right) \coth\left(\frac{\hbar\omega}{2k_B T}\right) \\ &= \frac{\gamma}{\beta\pi} \int_{-\infty}^{\infty} \frac{\omega d\omega}{(\omega_0^2 - \omega^2) - i\omega\gamma} \left[1 + 2 \sum_{n=1}^{\infty} \frac{\omega^2}{\omega^2 + \nu_n^2}\right] \end{aligned} \quad (41)$$

where $\nu_n = \frac{2\pi n}{\hbar\beta}$ are the bosonic Matsubara frequencies and we have used the formula $z \coth z = 1 + 2 \sum_{n=1}^{\infty} \frac{z^2}{z^2 + (n\pi)^2}$ where z is a complex argument. Evaluating the contour integration, one finds

$$I_1 = \frac{2\gamma}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n}{\omega_0^2 + \nu_n^2 + \gamma\nu_n}. \quad (42)$$

One can immediately see that $\hbar \rightarrow 0$ which is $\beta \rightarrow \infty$ gives $I_1 \rightarrow 0$. Thus, for the classical Brownian oscillator, the time-averaged work done by the random force is exactly zero whereas it is non-zero for the quantum case. This originates from the non-Markovian nature of the quantum noise as is clear from eqns (25) and (26) where, only as $\hbar \rightarrow 0$ is the noise δ -correlated, i.e. is Markovian. Thus, the quantum virial theorem contains new bath induced effects, which are exclusively of quantum origin.

One can consider the weak-coupling limit, i.e. $\gamma \rightarrow 0$ for which it is clear from inspection that eqn (42) that $(I_1)_{\gamma \rightarrow 0} \rightarrow 0$. This implies that the terms summarized within I_1 are all environment induced and go to zero just if we decouple the system and the environment. Moreover, all the terms appearing in eqn (42) are positive definite, meaning that $I_1 > 0$ which tends to make the

time-averaged potential energy of the dissipative oscillator greater than the kinetic energy. Although for illustrative purpose and for simplicity, we have considered Ohmic dissipation, one can consider more general dissipation models such as the single relaxation model, but the general behavior and sign of the term I_1 remains unchanged in such a case.

B. Analysis of I_2

Consider now,

$$I_2 = \int_{-\infty}^t dt' \mu(t-t') C_{xv}(t-t'). \quad (43)$$

Since $\mu(t)$ signifies the friction memory, it must go to zero for $t < 0$. Thus, we can replace the upper limit in the integral above, with $+\infty$ which gives

$$\begin{aligned} I_2 &= \int_{-\infty}^{\infty} dt' \mu(t-t') C_{xv}(t-t') \\ &= \int_{-\infty}^{\infty} dt' \mu(t-t') \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{C}_{xv}(\omega) e^{-i\omega(t-t')} \end{aligned} \quad (44)$$

Let us note that $\tilde{C}_{xv}(\omega) = i\omega \tilde{C}_{xx}(\omega)$ where

$$\tilde{C}_{xx}(\omega) = \hbar \text{Im}[\alpha(\omega)] \coth\left(\frac{\hbar\omega}{2k_B T}\right) \quad (45)$$

by the fluctuation-dissipation theorem [23, 24]. Then, eqn (44) can be re-written as (see also [25])

$$\begin{aligned} I_2 &= \frac{i\hbar}{2\pi} \int_{-\infty}^{\infty} \omega \text{Im}[\alpha(\omega)] \coth\left(\frac{\hbar\omega}{2k_B T}\right) \tilde{\mu}(-\omega) d\omega \\ &= \frac{i}{\beta\pi} \int_{-\infty}^{\infty} \text{Im}[\alpha(\omega)] \left(\frac{\hbar\omega}{2k_B T}\right) \coth\left(\frac{\hbar\omega}{2k_B T}\right) \tilde{\mu}(-\omega) d\omega \\ &= \frac{i}{\beta\pi} \int_{-\infty}^{\infty} \text{Im}[\alpha(\omega)] \left[1 + 2 \sum_{n=1}^{\infty} \frac{\omega^2}{\omega^2 + \nu_n^2}\right] \tilde{\mu}(-\omega) d\omega \end{aligned} \quad (46)$$

where $\nu_n = \frac{2\pi n}{\hbar\beta}$ are the bosonic Matsubara frequencies and we have used the summation formula for $z \coth z$ for complex z . For Ohmic dissipation, i.e. $\tilde{\mu}(\omega) = m\gamma$, one has $\alpha(\omega) = [m(\omega_0^2 - \omega^2) - im\gamma\omega]^{-1}$ which gives

$$\text{Im}[\alpha(\omega)] = \frac{\gamma\omega}{m[(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2]}. \quad (47)$$

Therefore,

$$I_2 = \frac{i\gamma^2}{\beta\pi} \int_{-\infty}^{\infty} \frac{\omega d\omega}{[(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2]} \left[1 + 2 \sum_{n=1}^{\infty} \frac{\omega^2}{\omega^2 + \nu_n^2}\right] \quad (48)$$

and the integral can be evaluated with some straightforward steps giving the following expression:

$$\begin{aligned} I_2 &= \frac{\gamma^2}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n^2}{(\omega_0^2 + \nu_n^2 - \frac{\gamma^2}{2})^2 + (\Omega\gamma)^2} \\ &+ \frac{\gamma^2}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n^2}{(\omega_0^2 + \nu_n^2)^2 - (\gamma\nu_n)^2} \end{aligned} \quad (49)$$

where,

$$\Omega = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}. \quad (50)$$

Let us look at two important limiting cases. First, as one puts $\hbar \rightarrow 0$, one has $\nu_n \rightarrow \infty$ for all values of n . Thus, the series converges to $I_2 = 0$ which is the correct classical limit. Next, we take the limit $\gamma \rightarrow 0$ which is the weak-coupling regime. Clearly, the n th term of the series gives a δ -function, i.e. $\delta(\omega_0^2 + \nu_n^2)$. Since the argument of the δ -function is positive definite and is never zero for any value of n (even if we put $\omega_0 = 0$), we obtain $(I_2)_{\gamma \rightarrow 0} = 0$. This is once again consistent with eqn (4) because I_2 is an environment induced term in the virial theorem and goes away if we remove the environment. Below, we study the generalized virial theorem for an electrical circuit with non-Markovian thermal noise.

IV. ELECTRICAL CIRCUIT WITH JOHNSON-NYQUIST NOISE

In this section, we will consider an LCR -circuit in the presence of thermal voltage (noise) originating from the thermal motion of electrons. Such a thermal noise is called Johnson-Nyquist noise [26–28] and is present at all non-zero temperatures. For a circuit with no active or non-linear elements where the L , C and R elements are placed in series, Kirchhoff's voltage rule gives

$$L \frac{d^2 Q(t)}{dt^2} + R \frac{dQ(t)}{dt} + \frac{Q(t)}{C} = \mathcal{V}(t) \quad (51)$$

where $Q(t)$ is the time-varying electric charge and $\mathcal{V}(t)$ is the time-varying voltage. The time-varying current in the circuit is $I(t) = \frac{dQ(t)}{dt}$. Typically, $\mathcal{V}(t) = V(t) + F(t)$ where $V(t)$ is the applied voltage (from the source) while $F(t)$ is the Johnson-Nyquist (thermal) noise arising due to the random motion of electrons at finite temperature. Thus, eqn (51) takes the form of a Langevin equation. For simplicity, we take a situation where $V(t) = 0$ and therefore, any small time-varying currents in the circuit is entirely due to the thermal voltage. Taking into account the quantum mechanical nature of the thermal modes, the noise is not white but is associated with the power spectrum [26–28] (see also [29, 30])

$$S_F(\omega) d\omega = \frac{(2/\pi) R(\omega) \hbar \omega d\omega}{e^{\hbar\omega/k_B T} - 1} \quad (52)$$

where $R(\omega)$ is the transfer resistance which is often independent of frequency, i.e. we will put $R(\omega) = R$. Thus, the thermal modes are distributed according to the black body distribution and since the power spectrum explicitly depends upon ω , the noise is non-Markovian.

Let us note that eqn (51) is not a quantum Langevin equation in the usual sense [eqn (22)] because $Q(t)$ is not an operator and there is no microscopic Hamiltonian such as eqn (21) from which it can be derived. On the other hand, the problem is inherently quantum mechanical due to the noise not being white, but rather depending upon the frequency. Therefore, this problem deserves separate attention in the context of the virial theorem. It is easy to check that as $\hbar \rightarrow 0$, the power spectrum becomes a constant, independent of the frequency, i.e. $S_F(\omega)|_{\hbar \rightarrow 0} = 2Rk_B T/\pi$.

In [30], the mean energies in the capacitor C and the inductor L were computed, and it was demonstrated that they are consistent with the quantum counterpart of energy equipartition theorem [11–16]. We refer the reader to [30] for the detailed calculation of the mean energies using spectral analysis, and quote the final expressions below:

$$\langle E_L \rangle = \int_{-\infty}^{\infty} \frac{(R\omega^2/\pi L)}{(\omega^2 - \omega_0^2)^2 + \omega^2(R/L)^2} \epsilon(\omega, T) d\omega, \quad (53)$$

$$\langle E_C \rangle = \int_{-\infty}^{\infty} \frac{(R\omega_0^2/\pi L)}{(\omega^2 - \omega_0^2)^2 + \omega^2(R/L)^2} \epsilon(\omega, T) d\omega \quad (54)$$

where $\omega_0 = 1/\sqrt{LC}$ and for convenience, we will include the zero-point energy contribution in $S_F(\omega)d\omega$ which implies that

$$\epsilon(\omega, T) = \frac{\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_B T}\right). \quad (55)$$

Clearly, the mean energies $\langle E_L \rangle$ and $\langle E_C \rangle$ of the inductive and capacitive elements are not equal, because the integrands in eqns (53) and (54) are different. However, as $\hbar \rightarrow 0$, it is easy to verify that $\langle E_L \rangle = \langle E_C \rangle = \frac{k_B T}{2}$ which is the genuine classical limit for which the noise is white, i.e. Markovian. The fact that in general $\langle E_L \rangle \neq \langle E_C \rangle$ is the electrical analogue of the statement that the mean kinetic and potential energies of the dissipative oscillator are unequal which we studied in the previous section. Since at present, there is no microscopic Hamiltonian for the electrical problem from where we can compute a virial theorem, let us analyze the difference

$$\begin{aligned} \langle E_L \rangle - \langle E_C \rangle &= \frac{R}{\pi L} \int_{-\infty}^{\infty} \frac{(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + \omega^2(R/L)^2} \epsilon(\omega, T) d\omega \\ &= \frac{\gamma}{2\pi\beta} \int_{-\infty}^{\infty} \frac{(\omega^2 - \omega_0^2) d\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2} \left[1 + 2 \sum_{n=1}^{\infty} \frac{\omega^2}{\omega^2 + \nu_n^2} \right]. \end{aligned} \quad (56)$$

where we have put $\gamma = R/L$ and have used the summation formula for the coth function. This difference would then be analogous to the combined contributions of I_1 and I_2 computed for the quantum Brownian oscillator in the previous section. In eqn (56), the first term inside the parenthesis ($n = 0$ contribution) integrates to zero. The remaining terms give non-trivial contributions which are computed to be

$$\langle E_L \rangle - \langle E_C \rangle = \frac{\gamma}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n(\nu_n^2 + \omega_0^2)}{(\nu_n^2 + \omega_0^2)^2 - (\gamma\nu_n)^2} - \frac{2\gamma^2}{\beta} \sum_{n=1}^{\infty} \frac{\nu_n^2}{(\omega_0^2 + \nu_n^2 - \frac{\gamma^2}{2})^2 + (\gamma\Omega)^2} \quad (57)$$

where Ω is defined in eqn (50).

A careful inspection reveals that this difference is positive, meaning that the mean magnetic energy in the inductor exceeds the mean electrical energy stored in the capacitor. This demonstrates the fact that the mean energies in the inductive and capacitive elements are unequal in the quantum regime, analogous to the mean kinetic and potential energies of the dissipative oscillator considered in the previous section. In the classical limit, i.e. for $\nu_n \rightarrow \infty$ for all n , all the terms in the series appearing in eqn (57) become zero meaning that the mean

energies are equal, i.e. $\langle E_L \rangle = \langle E_C \rangle = \frac{k_B T}{2}$. The same conclusions are obtained in the high temperature limit, for which $\beta \rightarrow 0$. It is noteworthy that we had considered the Johnson-Nyquist noise to be a non-Markovian quantum noise with power spectrum given in eqn (52). If instead, one considered a Markovian noise, such as that which arises from eqn (52) as $\hbar \rightarrow 0$, one would obtain $\langle E_L \rangle = \langle E_C \rangle$. Thus, we have demonstrated the validity of the generalized virial theorem in the case of a linear circuit with thermal noise.

V. DISCUSSION

In this paper, we have discussed the virial theorem in the context of both classical and quantum dissipative systems. For classical systems, we demonstrated the crucial role played by noise in this context. The presence of noise not only leads to a thermal interpretation to the time-averages, i.e. the time-averaged quantities coincide with their thermal averages, the Markovian nature of the classical noise makes the averaged kinetic and potential energies of an oscillator equal. On the other hand, for a quantum system noise is non-Markovian and thus, apart from lending a thermal nature to the averages, it leads to novel dissipation induced terms in the virial theorem. The kinetic and potential energies are no longer equal, except in the classical limit or the zero-dissipation case, where bath induced terms obviously vanish.

For the dissipative oscillator, the generalized virial theorem acquires two additional contributions due to the bath. The first one, which is summarized by I_1 in section-(III) is the time-averaged work done on the system due to the non-Markovian quantum noise. It should perhaps be noted that the series appearing in eqn (42) diverges. This happens due to the zero point energy contribution from the bath degrees of freedom (see for instance [31]) and can be regularized by imposing a suitable cut-off such as choosing a single-relaxation dissipation model, or by explicitly subtracting the zero-point contribution, say I_1^0 (which is infinite). Thus, one may interpret $\tilde{I}_1 - I_1 - I_1^0$ to be the meaningful contribution to the generalized virial theorem leading to a suitable renormalization. The same arguments go through for the first series in eqn (57)

in the electrical problem [section-(IV)]. Now, the other contribution to the generalized virial theorem discussed in section-(III) is given by I_2 whose final expression in the form of an infinite series has been given in eqn (49). Following the analysis presented in [25], we believe it is related to the time-averaged rate of power transfer due to dissipation. It is noteworthy that the series in I_2 does not diverge, since for large n the terms go as $1/n^2$.

Finally, we considered an electrical circuit, experiencing thermal noise with a power spectrum given by eqn (52), i.e. the noise is of quantum origin and is non-Markovian. We found that the mean energies in the inductor and capacitor are unequal, and the their difference was computed in eqn (57) where $\gamma = R/L$ and $\omega_0 = 1/\sqrt{LC}$. Thus, even in the non-mechanical problem, the non-Markovian nature of the noise plays a crucial role in controlling the averaged energies. In the Markovian limit however, the energies are equal, as with the classical Brownian oscillator considered in subsection-(IIB).

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