# Quantum Brownian Motion: A Review

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**Abstract.** We review in a pedagogic manner the topic of quantum Brownian motion, with an emphasis on its thermodynamic aspects. For the sake of completeness, we begin with the classical treatment of one-dimensional Brownian motion, discussing correlation functions and fluctuation-dissipation relations. The equation-of-motion approach, based on the Langevin equation, is mostly followed throughout the paper. A microscopic derivation of the generalized Langevin equation is outlined, based on the microscopic model of a heat bath as a collection of a large number of independent classical harmonic oscillators. We then consider a fully quantum-mechanical treatment of Brownian motion based on the quantum Langevin equation, where the bath is modelled as a collection of independent quantum harmonic oscillators. In the stationary state, we analyze the quantum counterpart of energy equipartition theorem, which has generated a considerable amount of interest in recent literature. The free energy, entropy and third law of thermodynamics are discussed for the one-dimensional quantum Brownian motion in a harmonic well. Following this, we explore some aspects of dissipative diamagnetism in the context of two-dimensional quantum Brownian motion. The role of an external magnetic field and confining potentials is discussed. We then briefly outline the path-integral approach to thermodynamics of a quantum Brownian particle. Finally, we devote a substantial part of the review to discussing stochastic thermodynamics and fluctuation theorems in the context of classical and quantum Langevin equation.

#### 1. Introduction

Coupling a system to its environment turns it into a dissipative or an open system. Open systems are ubiquitous in nature, from a cup of freshly-brewed coffee that continuously loses heat to the environment, to complex biological processes inside living cells. A paradigm of open systems is provided by the Brownian motion, named after Robert Brown. The earliest observation of the Brownian motion has been by Brown himself in 1827 in the context of pollen grains (the "Brownian" particles) suspended in a liquid in thermal equilibrium at temperature T and being constantly buffeted by the liquid molecules, resulting in a dissipative dynamics of the Brownian particles [1]. A satisfactory microscopic understanding of the Brownian motion however emerged much later, in the 20th century with the seminal work of Einstein [2]. Subsequently, many researchers made notable contributions to this field, and some significant outcomes include the Einstein-Smoluchowski relation [3], the Langevin equation [4] and the Fokker-Planck equation description of the Brownian motion [5], as well as extensions and applications of the Brownian motion, i.e., the Ornstein-Uhlenbeck process [6], the Kramers problem [7], the phenomenological stochastic model for lineshapes in spectroscopy [8], and many others. The work of Einstein is path breaking in that it provided the first formal connection between dissipative forces and thermal fluctuations, encoded in the so-called Einstein relation that relates the coefficient of diffusion D of the Brownian particles, a measure of fluctuations in its motion as a function of time, to the strength of dissipation  $\gamma$  in the dynamics of the Brownian particles and the amount of thermal fluctuations (=  $k_BT$ , with  $k_B$  the Boltzmann constant) present in the system. This connection between dissipation and related fluctuations was later put on a solid foundation by Johnson and Nyquist in the context of thermal agitation of charge carriers inside electrical conductors in equilibrium [9, 10, 11]. Relations between the dissipative and fluctuating aspects of the dynamics of an open system are clubbed together under fluctuation-dissipation relations.

Quantum mechanically, the problem is more subtle. It is natural to seek a description in terms of a quantum system (say, a single particle) in contact with a heat bath such that the overall dynamics of the system-plus-heat-bath is unitary. Then, the total Hamiltonian describing the situation will be of the form  $H = H_{\rm S} + H_{\rm B} + H_{\rm SB}$ , where  $H_{\rm S}$  and  $H_{\rm B}$  are respectively the Hamiltonian operators of the system and the bath, while  $H_{\rm SB}$  summarizes the interaction between them. In the Schrödinger picture, the time evolution of the state describing the system and the bath together is of the form

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = (H_S + H_B + H_{SB}) |\Psi(t)\rangle,$$
 (1)

where  $|\Psi(t)\rangle$  denotes the state of the composite system, and  $\hbar$  denotes the reduced Planck's constant. However, one is typically interested in the dynamics of the system alone, and it is not immediately clear from Eq. (1) as to how to appropriately eliminate or "trace out" the bath variables so that what remains is the information about the dynamics of the "open" quantum system S. In a seminal work [12], Feynman and Vernon

suggested the use of path integrals to trace out the environmental effects, i.e., the degrees of freedom constituting the bath. The procedure involves the computation of a quantity known as the "influence functional," which appropriately describes the effect of the bath on the system. Caldeira and Leggett [13] extended the Feynman-Vernon scheme to the case of a quantum particle moving in an arbitrary potential, and in contact with a bath of quantum harmonic oscillators. Utilizing the path integral formalism, Caldeira and Leggett worked with the density operator in the Schrödinger-picture representation. Following the work of Feynman and Vernon [12], it was demonstrated in a celebrated paper by Ford et al. [14] that a description of the heat bath as an infinite collection of harmonic oscillators is indeed a good one (both classically and quantum mechanically), in the sense that in the Heisenberg picture, the dynamical operators of the system S admit a Brownian motion-like dynamics when the equations of motion for the bath variables are solved and are substituted for into the former. Stochastic (noise) terms depending upon the initial conditions of the bath variables arise in the equation(s) of motion describing the system, and one assumes that these initial conditions are distributed according to some statistical distribution such as the Boltzmann distribution so as to model the situation that the bath is in equilibrium all through the time evolution of the system. In this situation, one indeed gets a quantum (operator-valued) Langevin equation describing the quantum Brownian motion of the system. Over the years, there have been several works within this framework, which are devoted to study of a quantum harmonic oscillator (consituting the system of interest S) in contact with a heat bath consisting of an infinite set of harmonic oscillators [15, 16, 17, 18, 19, 20].

The main purpose of this paper is to pedagogically introduce the active area of quantum Brownian motion. We shall primarily follow the route due to Ford et al., i.e., the approach involving the quantum Langevin equation describing the reduced dynamics of the system that is in contact with a heat bath. We shall particularly stress on stationary state and thermodynamic aspects of the dynamics [21, 22, 23, 24, 25]. Although it may come as a surprise that thermodynamics can be consistently formulated for a single Brownian particle, which is far from the thermodynamic limit that one invokes in traditional thermodynamical studies, it turns out that not only does a thermal description follow naturally from the framework of classical and quantum Brownian motion, it is also consistent with all the laws of thermodynamics, including the third law [22, 26, 27]. We will contrast the expressions of average energy between classical and quantum Brownian motion, which will lead us to the recently-proposed quantum counterpart of energy equipartition theorem [28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38]. As a condensed matter physics application of the framework of quantum Brownian motion, we shall discuss dissipative diamagnetism [38, 39] and emphasize on the role of confining potentials. Although our approach shall primarily deal with the equation-ofmotion method, which involves computing correlation functions (see Refs. [40, 41]), we shall also describe briefly an alternate approach to studying thermodynamics, based on the concept of the partition function.

The review is divided into several sections. In the next section, we shall describe

in somewhat detail the classical problem of Brownian motion. While fluctuationdissipation theorems and stationary states are particularly emphasized upon, following Ref. [14], we describe a microscopic derivation of the generalized Langevin equation. In Section 3, we introduce the quantum mechanical problem of Brownian motion, and discuss various intricate details of the formalism based on the quantum Langevin equation. Sections 4 and 5 summarize thermodynamic aspects of quantum Brownian motion, with appropriate comparisons done with the classical case. We discuss the mean energy, the free energy and the entropy of a quantum particle executing Brownian motion. The problem of dissipative diamagnetism is analyzed in Section 6 in some detail. In Section 7, we describe quantum Brownian motion with momentummomentum coupling between the system and the heat bath. Then, in Section 8, we describe an alternate route to studying the thermodynamics of quantum Brownian motion, based on path integrals and utilizing the notion of the influence functional mentioned earlier. Finally, we discuss in the context of the Brownian motion stochastic thermodynamics and fluctuation theorems of the Gallavotti-Cohen kind, respectively, in Sections 9 and 10. The review ends with some closing remarks. Some of the technical details of computation are relegated to the two appendices.

#### 2. Classical Brownian motion

As an appropriate prelude to the quantum Brownian motion, the main topic of this review, let us start with a brief discussion of the classical Brownian motion. experimental set-up is that of a collection of weakly-interacting<sup>+</sup> Brownian particles immersed in a viscous fluid. The fluid is in thermal equilibrium at a well-defined temperature  $T = 1/(k_B\beta) > 0$ . The Brownian particles, all taken to be identical with mass m, are being constantly buffeted by the fluid molecules that are in incessant motion. The Brownian particles are larger and heavier than the fluid molecules and consequently move on a much slower time scale than the fluid molecules. The fluid acts as a heat bath for the Brownian particles. Through a continual exchange of energy with the fluid (in fact, the particles on the average lose energy to the bath while wading their way through the fluid), the Brownian particles eventually come to a stationary state in which they are in thermal equilibrium (i.e., canonical equilibrium) with the surrounding fluid. When evaluating the average properties of the Brownian particles at any time t > 0, one may consider a tagged Brownian particle and compute its average properties at time t by averaging with respect to an ensemble of experimental set-ups in all of which the Brownian particle has a given position and a given velocity at the initial instant t=0, while the positions and the momenta of the fluid molecules vary across the different set-ups. Alternatively, one may consider only one experimental setup, but average with respect to the different Brownian particles in the system, with the

<sup>&</sup>lt;sup>+</sup> This is in the sense that the motion of the individual Brownian particles is predominantly dictated by the motion of the surrounding fluid molecules and less dominantly by the presence of other Brownian particles.

particles by virtue of being weakly interacting may be taken to be executing independent motion. The two approaches are expected to yield identical results; here, we will adopt the former and not the latter approach.

Throughout this paper, in order to describe the motion of the Brownian particles, we shall primarily be following the equation-of-motion approach, often attributed to Langevin [4]. In one dimension, the Langevin equation is given by (see also Refs. [42, 43, 44] and references therein)

$$m\ddot{x}(t) + m\gamma\dot{x}(t) = f(t), \tag{2}$$

where the dot indicates derivative with respect to time, and x(t) is the position of a given Brownian particle at time t. The second term on the left hand side (LHS) is a friction or a viscous drag term arising from Stokes' law, whose origin may be traced to collisions suffered by the Brownian particle with the surrounding fluid molecules; here,  $\gamma > 0$  is a suitable friction coefficient (per unit mass). The term on the right-hand side (RHS) is a noise term that is a random function of time, and which is characterized by the following statistical properties:

$$\langle f(t) \rangle = 0, \quad \langle f(t)f(t') \rangle = \Gamma \delta(t - t'),$$
 (3)

where the averages denoted by the angular brackets are over all noise realizations, and  $\Gamma$  is a positive constant standing for the strength of the noise. The first property above implies that f(t) is completely random and so has zero mean at every time instant. The second property implies that the noise values at two different time instants are completely uncorrelated. Since a Gaussian distribution can be completely characterized by its first and second moments, namely, that all moments of a Gaussian distribution may be expressed in terms of the mean and the variance, it is usual to assume the noise f(t) for every t to be distributed according to the same Gaussian distribution. It then follows that the statistical average of an odd number of factors of f(t) is zero, while that of an even number of factors is equal to the sum of products of pair averages [42].

In order to understand the equilibrium behavior of the Brownian particles, we rewrite Eq. (2) in terms of the velocity  $v(t) = \dot{x}(t)$ , as

$$\dot{v}(t) + \gamma v(t) = \frac{f(t)}{m}. (4)$$

This equation can be solved to yield

$$v(t) = v_0 e^{-\gamma t} + \frac{1}{m} \int_0^t dt' \ f(t') e^{-\gamma (t - t')}, \tag{5}$$

where  $v_0$  is the initial velocity. Thus, we obtain  $\langle v(t) \rangle = v_0 e^{-\gamma t}$ , where we have utilized the fact that  $\langle f(t) \rangle = 0$ . Therefore, at large times  $t \to \infty$  (more precisely, for times  $t \gg 1/\gamma$ ), when the system of Brownian particles attains equilibrium, the average velocity of the particle vanishes:

$$\langle v(t) \rangle_{\text{eq}} = 0,$$
 (6)

where eq stands for equilibrium. It is clear that  $\tau_{\rm ch} \equiv 1/\gamma$  is a characteristic time scale intrinsic to the dissipative dynamics (2), and will be called the relaxation time.

The result (6), however, does not obviously imply that the particle comes to rest, which it simply cannot as it is constantly being bombarded by the surrounding fluid molecules. As a result, even in equilibrium, x(t) will be a function of t. Indeed, a further integration of Eq. (5) with respect to time yields

$$x(t) = x_0 + \frac{v_0}{\gamma} (1 - e^{-\gamma t}) + \frac{1}{m\gamma} \int_0^t dt' \ f(t') \left( 1 - e^{-\gamma (t - t')} \right), \tag{7}$$

where  $x_0$  is the initial position. We thus obtain  $\langle x(t)f(t)\rangle = 0$ , and that  $\langle x(t)\rangle = x_0 + (v_0/\gamma)(1 - e^{-\gamma t})$ , yielding  $\langle x(t)\rangle_{eq} = x_0 + v_0/\gamma$ , a constant independent of time.

# 2.1. Fluctuation-dissipation relation

Let us now consider the average kinetic energy of the Brownian particle at time t:  $E_k(t) = m\langle v^2(t)\rangle/2$ . From Eq. (5), we obtain on using Eq. (3) that

$$\langle v^2(t)\rangle = v_0^2 e^{-2\gamma t} + \frac{\Gamma}{2\gamma m^2} (1 - e^{-2\gamma t}),$$
 (8)

which yields the equilibrium behavior:

$$\langle v^2(t)\rangle_{\text{eq}} = \frac{\Gamma}{2\gamma m^2},$$
 (9)

so that the equilibrium kinetic energy equals  $(E_k)_{eq} = m \langle v^2(t) \rangle_{eq}/2 = \Gamma/(4\gamma m)$ . At long times, when the system of Brownian particles comes to thermal equilibrium with the surrounding fluid, the velocity distribution of the given Brownian particle will be given by the canonical-equilibrium distribution  $\rho_{eq}(v) = \sqrt{m\beta/(2\pi)} \exp(-\beta mv^2/2)$ , which implies that one has

$$(E_k)_{\rm eq} = \frac{k_B T}{2}. (10)$$

Comparing the two obtained expressions for  $(E_k)_{eq}$  allows to fix the value of  $\Gamma$  as

$$\Gamma = 2m\gamma k_B T. \tag{11}$$

This is a remarkable result, which states that the friction (dissipation) coefficient  $\gamma$  is related to the statistical properties of the noise (fluctuations) induced into the dynamics of the Brownian particles through their interaction with the surrounding fluid. This result is a fluctuation-dissipation relation, or, more precisely, the second fluctuation-dissipation theorem (FDT) [42, 43, 45].

# 2.2. Mean-squared displacement

We have already seen that in equilibrium, the average displacement of the Brownian particle from the initial position is  $\langle x(t) \rangle_{eq} - x_0 = v_0/\gamma$ . One may ask: what is the

mean-squared displacement (MSD)  $\langle [\Delta x(t)]^2 \rangle \equiv \langle (x(t) - \langle x(t) \rangle)^2 \rangle$  as a function of time, and what is its value in equilibrium? From Eq. (7), we get

$$\langle [\Delta x(t)]^2 \rangle = \frac{2k_B T}{m\gamma} \left[ t - \frac{2}{\gamma} (1 - e^{-\gamma t}) + \frac{1}{2\gamma} (1 - e^{-2\gamma t}) \right],$$
 (12)

where we have used Eqs. (3) and (11). In equilibrium, i.e., for times  $t \gg 1/\gamma$ , we have the diffusive behavior of the MSD:

$$\langle [\Delta x(t)]^2 \rangle_{\text{eq}} = \frac{2k_B T}{m\gamma} t,$$
 (13)

which on writing as  $\langle [\Delta x(t)]^2 \rangle_{eq} = 2Dt$  gives the familiar Einstein-Stokes expression for the diffusion coefficient D as

$$D = \frac{k_B T}{m\gamma}. (14)$$

# 2.3. Velocity autocorrelation and the Kubo formula

One may use Eqs. (5) and (3) to obtain the velocity autocorrelation as

$$\langle v(t)v(t')\rangle = v_0^2 e^{-\gamma(t+t')} + \frac{\Gamma}{2\gamma m^2} \left[ e^{-\gamma|t-t'|} - e^{-\gamma(t+t')} \right], \tag{15}$$

so that the equilibrium autocorrelation, obtained by considering the simultaneous limits  $t \to \infty, t' \to \infty$ , keeping  $|t - t'| = \tau$  fixed and finite, is given by

$$\lim_{t \to \infty, t' \to \infty, \tau \equiv |t - t'| = \text{fixed and finite}} \langle v(t)v(t') \rangle = \frac{\Gamma}{2\gamma m^2} e^{-\gamma \tau}.$$
 (16)

We may rewrite the above equation as

$$\langle v(0)v(t)\rangle_{\text{eq}} = \frac{\Gamma}{2\gamma m^2} e^{-\gamma t},$$
 (17)

so that integrating both sides with respect to time, we obtain the celebrated Kubo formula [45]:

$$\Gamma = 2m^2 \gamma^2 \int_0^\infty dt \ \langle v(0)v(t)\rangle_{\text{eq}}.$$
 (18)

#### 2.4. Microscopic derivation of the Langevin equation

In this subsection, we outline a microscopic derivation of the Langevin equation (2). Our microscopic model is based on a large particle of mass m with coordinate x and momentum p (which constitutes our system of interest) and moving in an arbitrary potential V(x). The particle interacts with a collection of  $N \gg 1$  independent harmonic oscillators with masses  $\{m_j\}$ , position coordinates  $\{q_j\}$ , momenta  $\{p_j\}$  and frequencies  $\{\omega_j\}$  ( $j=1,2,\ldots,N$ ). The collection in the limit  $N\to\infty$  behaves as a heat bath [14, 46]; we have  $m\gg m_j \ \forall \ j$ . The set-up is shown schematically in Fig. 1. It

is usually assumed that the coupling between the particle and the heat-bath oscillators is bilinear and of the coordinate-coordinate type, i.e.,  $\propto xq_j$ . The total microscopic Hamiltonian of the system-plus-heat-bath is of the form  $H=H_{\rm S}+H_{\rm B}+H_{\rm SB}$ , where  $H_{\rm S}$  is the system Hamiltonian,  $H_{\rm B}$  is the Hamiltonian of the bath, while  $H_{\rm SB}$  models the interaction between the system and the bath degrees of freedom. For our model system, we have

$$H = \frac{p^2}{2m} + V(x) + \sum_{j=1}^{N} \left[ \frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left( q_j - \frac{c_j x}{m_j \omega_j^2} \right)^2 \right], \tag{19}$$

so that

$$H_{\rm S} = \frac{p^2}{2m} + V(x),$$
 (20)

$$H_{\rm B} = \sum_{j=1}^{N} \left[ \frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 q_j^2 \right],\tag{21}$$

$$H_{\rm SB} = -c_j q_j x + \frac{c_j^2 x^2}{2m_j \omega_j^2}.$$
 (22)

Here,  $c_j$  denotes the coefficient of linear coupling between the coordinate of the particle and that of the *j*-th oscillator. Let us introduce a canonical transformation  $\widetilde{q}_j \equiv m_j \omega_j^2/c_j q_j$  and  $\widetilde{p}_j \equiv c_j/(m_j \omega_j^2) p_j$ , in terms of which the Hamiltonian (19) becomes

$$\widetilde{H} = \frac{p^2}{2m} + V(x) + \sum_{j=1}^{N} \left[ \frac{\widetilde{p}_j^2}{2\widetilde{m}_j} + \frac{1}{2} \widetilde{m}_j \omega_j^2 (\widetilde{q}_j - x)^2 \right], \tag{23}$$

where the renormalized mass is defined as

$$\widetilde{m}_j \equiv \frac{c_j^2}{m_j \omega_i^4}. (24)$$

Clearly, the Hamiltonian (23) is translationally invariant, i.e., the system-bath coupling is homogeneous in the sense that the system is coupled in an identical manner to each of the bath oscillators. This explains the inclusion of the term  $\sum_{j=1}^{N} c_j^2 x^2/(2m_j\omega_j^2)$  in the Hamiltonian (19) with the purpose of making it translationally invariant.

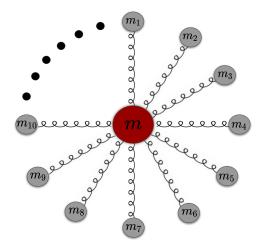
The Hamilton's equations for the system variables (x, p) and the bath variables  $(q_j, p_j)$  are

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{p}{m},\tag{25}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial V(x)}{\partial x} + \sum_{j=1}^{N} c_j \left( q_j - \frac{c_j x}{m_j \omega_j^2} \right),\tag{26}$$

$$\frac{\mathrm{d}q_j}{\mathrm{d}t} = \frac{p_j}{m_j},\tag{27}$$

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = -m_j \omega_j^2 \left( q_j - \frac{c_j x}{m_j \omega_j^2} \right). \tag{28}$$



**Figure 1.** Relevant to Section 2.4, the figure shows a large particle of mass m (the one at the centre) interacting with a set of  $N \gg 1$  independent harmonic oscillators (represented by the particles at the periphery) with masses  $\{m_j\}$  and frequencies  $\{\omega_j\}$ ;  $j=1,2,\ldots,N$ .

Combining Eqs. (27) and (28), we obtain

$$\frac{\mathrm{d}^2 q_j}{\mathrm{d}t^2} = -\omega_j^2 \left( q_j - \frac{c_j}{m_j \omega_j^2} x \right),\tag{29}$$

which may be solved to obtain

$$q_{j}(t) - \frac{c_{j}x(t)}{m_{j}\omega_{j}^{2}} = \left(q_{j}(0) - \frac{c_{j}x(0)}{m_{j}\omega_{j}^{2}}\right)\cos(\omega_{j}t)$$

$$+ \frac{p_{j}(0)}{m_{j}\omega_{j}}\sin(\omega_{j}t) + \frac{c_{j}}{m_{j}\omega_{j}^{2}}\int_{0}^{t}dt' \frac{p(t')}{m}\cos[\omega_{j}(t-t')]. \tag{30}$$

Plugging Eq. (30) into Eq. (26), one gets

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial V(x)}{\partial x} - \int_0^t \mathrm{d}t' \, \frac{p(t')}{m} \sum_{j=1}^N \frac{c_j^2}{m_j \omega_j^2} \cos[\omega_j(t - t')] 
+ \sum_{j=1}^N c_j \left( q_j(0) - \frac{c_j x(0)}{m_j \omega_j^2} \right) \cos(\omega_j t) + \sum_{j=1}^N \frac{c_j p_j(0)}{m_j \omega_j} \sin(\omega_j t).$$
(31)

The above equation may be rewritten in the form of a generalized Langevin equation:

$$m\ddot{x}(t) + \int_{-\infty}^{t} dt' \ \mu(t - t')\dot{x}(t') + \frac{\partial V(x)}{\partial x} = f(t), \tag{32}$$

where the noise term is given by

$$f(t) = \sum_{j=1}^{N} \left[ c_j \left( q_j(0) - \frac{c_j x(0)}{m_j \omega_j^2} \right) \cos(\omega_j t) + \frac{c_j p_j(0)}{m_j \omega_j} \sin(\omega_j t) \right], \tag{33}$$

which depends on the initial coordinates and momenta of the heat-bath oscillators (as well as on the initial particle position). Further, the friction kernel  $\mu(t)$  is given by

$$\mu(t) = \Theta(t) \sum_{j=1}^{N} \frac{c_j^2}{m_j \omega_j^2} \cos(\omega_j t), \tag{34}$$

where  $\Theta(t \leq 0) = 0$  and  $\Theta(t > 0) = 1$  is the Heaviside step function.

Now, we will take a vital step in order to introduce time irreversibility into the dynamics, by considering an ensemble of initial conditions in which the initial coordinate x(0) and the initial momentum p(0) of the particle have given and fixed values for the different members of the ensemble, while the joint distribution of the set  $\{q_j(0), p_j(0)\}$  of the initial coordinates and the momenta of the oscillators is given by the canonical-equilibrium distribution (implementing the fact that at the initial instant as also for subsequent times, the bath is in thermal equilibrium):

$$\mathcal{P}_{B+SB}(\{p_j(0)\}, \{q_j(0)\}) = \frac{\exp(-\beta H_{B+SB})}{\prod_{l=1}^{N} \int dq_l(0) dp_l(0) \exp(-\beta H_{B+SB})},$$
 (35)

with

$$H_{\text{B+SB}} = \sum_{j=1}^{N} \left[ \frac{p_j^2(0)}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left( q_j(0) - \frac{c_j x(0)}{m_j \omega_j^2} \right)^2 \right].$$
 (36)

Subsequently, at a time  $t \gtrsim 0$ , the particle is released, so that further evolution of the system is governed by the Hamiltonian (19). Note that this scenario of introducing an ensemble of initial conditions is consistent with choosing the retarded solution (30). Corresponding to such an ensemble, one finds that the function f(t) is a random function of time, whose statistical properties may be deduced by using  $\langle q_j(0)\rangle = \langle p_j(0)\rangle = 0$ , and that  $\langle (q_j(0) - c_j x(0)/(m_j \omega_j^2))^2 \rangle = k_B T/(m_j \omega_j^2)$ ,  $\langle p_j^2(0)\rangle = m_j k_B T$ . Here, the angular brackets denote averaging with respect to the mentioned ensemble, that is, with respect to the distribution (35). We finally obtain

$$\langle f(t) \rangle = 0, \tag{37}$$

$$\langle f(t)f(t')\rangle = k_B T \mu(t - t'), \tag{38}$$

so that Eq. (32) now has all the characteristics of a generalized Langevin equation. One may observe that Eq. (38) is an explicit expression of the fluctuation-dissipation theorem in terms of the microscopic parameters  $m_j$ ,  $\omega_j$  and  $c_j$ .

Note that, as we have already mentioned in the leading paragraph of this subsection, we should consider the collection of independent harmonic oscillators in the limit  $N \to \infty$ , when it becomes a heat bath, and only in this limit that Eq. (32) becomes a bona fide Langevin equation. Now, in the limit  $N \to \infty$ , it is reasonable to replace any occurrence of a summation over j with an integral, as in

$$\sum_{i=1}^{N} \to N \int_{0}^{\infty} d\omega \ g(\omega), \tag{39}$$

where  $g(\omega)$  denotes the density of states, that is,  $g(\omega)d\omega$  gives the probability to find a heat-bath oscillator with frequency between  $\omega$  and  $\omega + d\omega$ .

Let us now define the so-called bath spectral function  $J(\omega)$  as

$$J(\omega) \equiv \frac{\pi}{2} \sum_{j=1}^{N} \frac{c_j^2}{m_j \omega_j} \delta(\omega - \omega_j), \tag{40}$$

so that Eq. (34) yields

$$\mu(t) = \Theta(t) \frac{2}{\pi} \int_0^\infty d\omega \, \frac{J(\omega)}{\omega} \cos(\omega t). \tag{41}$$

A particularly simple example for  $J(\omega)$  is that of Ohmic dissipation, for which the bath spectral function reads as

$$J(\omega) = m\gamma\omega;$$
 Ohmic dissipation, (42)

or, equivalently,  $\mu(t) = 2m\gamma\delta(t)\Theta(t)$ , using  $\delta(x) = (1/\pi)\int_0^\infty \mathrm{d}t \cos(xt)$  (we are relegating to the following subsection a discussion on how Ohmic dissipation may arise in a physical situation.). This corresponds to a memory-less friction, i.e., the drag force represented by the second term on the LHS of Eq. (32) is instantaneous, and, on using  $\int_{-\infty}^a \mathrm{d}x \ \delta(x-a) = 1/2$ , equals  $m\gamma\dot{x}(t)$ . Moreover, we get on using Eq. (38) that

$$\langle f(t)f(t')\rangle = 2m\gamma k_B T\delta(t-t'); \quad t,t'>0.$$
(43)

This allows (for t > 0) to reduce the generalized Langevin equation (32) to the Langevin equation (2) for the Brownian particle for the choice V(x) = 0. In our microscopic derivation, the time instant t = 0 is special, as it pertains to the preparation of the initial condition mentioned in the paragraph preceding Eq. (35), and consequently, the microscopic model yields the Langevin equation (2) only for times t > 0.

2.4.1. Ohmic dissipation We take a small detour to explain how Ohmic dissipation may arise in a physical situation. To this end, let us consider the situation in which all the heat-bath oscillators have the same mass, and the coupling constants  $\{c_j\}$  are all equal and scaling as inverse square-root of the number of oscillators, i.e., we have  $m_j = \tilde{m}$  and  $c_j = \tilde{c}/\sqrt{N}$ . In this case, Eq. (34), with the replacement (39), writes as

$$\mu(t) = \Theta(t) \frac{\tilde{c}^2}{\tilde{m}} \int_0^\infty d\omega \, \frac{g(\omega)}{\omega^2} \cos(\omega t). \tag{44}$$

A comparison with Eq. (41) suggests that the bath spectral function is related, up to constant prefactors, to the density of states as  $J(\omega) \sim g(\omega)/\omega$ , for the case at hand  $(m_j = \tilde{m} \text{ and } c_j = \tilde{c}/\sqrt{N})$ .

The integral in Eq. (44) may diverge for certain choices of  $g(\omega)$ . For instance, if the high-frequency behavior of the density of states is such that  $g(\omega) \sim \omega^a$  for  $a \geq 2$ , then

the integral diverges. The Ohmic dissipation model is precisely the choice  $g(\omega) \sim \omega^2$ , with the frequencies restricted to a certain cut-off frequency, i.e., one has

$$g(\omega) = \frac{3\omega^2}{\omega_{\text{cut}}^3}; \quad \omega < \omega_{\text{cut}},$$

$$= 0; \quad \omega > \omega_{\text{cut}}.$$
(45)

We thus have  $J(\omega) \sim \omega$  for  $\omega < \omega_{\text{cut}}$ , while it is zero otherwise. Substituting the above choice in Eq. (44) gives

$$\mu(t) = \Theta(t) \frac{3\tilde{c}^2}{\tilde{m}\omega_{\text{out}}^3} \frac{\sin(\omega_{\text{cut}}t)}{t}.$$
 (46)

We now consider the limit of very large  $\omega_{\text{cut}}$ ; Using  $\delta(x) = \lim_{\omega \to \infty} \sin(\omega x)/(\pi x)$ , we get

$$\mu(t) \approx 2m\gamma\delta(t),$$
 (47)

where, provided  $\widetilde{c}$  scales as  $\omega_{\mathrm{cut}}^{3/2}$ , one has  $\gamma$  a constant given by

$$\gamma \equiv \frac{3\pi \tilde{c}^2}{2m\tilde{m}\omega_{\text{cut}}^3}.$$
 (48)

We thus obtain the friction kernel as a delta function that we have encountered in Section 2.4. Equation (48) is an explicit expression of the friction coefficient  $\gamma$  in terms of the microscopic parameters  $\tilde{m}$  and  $\tilde{c}$  characterizing the heat-bath oscillators. Throughout our subsequent discussions, while considering Ohmic dissipation, we shall be taking  $\omega_{\text{cut}}$  to be large enough that integrals involving  $\omega$  may be performed between the limits  $[0, \infty)$ .

#### 3. Quantum Brownian motion

We now turn to a discussion of the quantum Brownian motion. Similar to the classical case, here the starting point is that of a quantum particle interacting with a quantum heat bath, and the total Hamiltonian is of the generic form  $H = H_{\rm S} + H_{\rm B} + H_{\rm SB}$ . In the following subsection, we shall discuss the quantum analog of the generalized Langevin equation, which will turn out to be governed by non-white noise even when the drag force is instantaneous, as, e.g., applicable to Ohmic dissipation.

# 3.1. Quantum Langevin equation

With respect to the classical case discussed in Section 2.4, two obvious differences are to be expected: (i) All the position and momentum variables encountered therein, which were real numbers, now become operators. (ii) As regards time evolution, one has to now use instead of the classical Hamilton's equations (25)-(28) the Heisenberg equations of motion for the position and momentum operators. Although the resulting equations are identical to the analogous equations presented for the classical case, one should remember that the dynamical variables and their time derivatives are now quantum

operators that follow a prescribed commutator algebra. The total Hamiltonian is the same as in the classical case, see Eq. (19) [14, 19, 47]:

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2 x^2}{2} + \sum_{j=1}^{N} \left[ \frac{p_j^2}{2m_j} + \frac{m_j \omega_j^2}{2} \left( q_j - \frac{c_j x}{m_j \omega_j^2} \right)^2 \right],\tag{49}$$

where we have made for the potential V(x) the choice of a harmonic well potential, which will prove particularly useful in the context of dissipative diamagnetism to be discussed later in the review [39]. The relevant commutation relations for the various position and momentum operators are as follows:

$$[x, p] = i\hbar, \quad [q_i, p_k] = i\hbar\delta_{ik},$$

$$(50)$$

where  $\delta_{jk}$  is the Kronecker- $\delta$  function.

Considering the total Hamiltonian (49), one may obtain the Heisenberg equations for the system and bath variables, namely,  $i\hbar dA/dt = [A, H]$ , for  $A = x, p, q_j, p_j$ . Similar to the classical case discussed in Section 2.4, one first solves the equations of motion for the bath variables and then substitutes the solution into the equations of motion for the system variables, leading finally to the following equation

$$m\ddot{x}(t) + \int_{-\infty}^{t} dt' \ \mu(t - t')\dot{x}(t') + m\omega_0^2 x(t) = f(t),$$
 (51)

under the assumption that the state of the system at the initial instant t=0, corresponding to a correlation-free preparation, is given by the total density matrix operator

$$\rho(0) = \rho_{\rm S}(0) \otimes \rho_{\rm B+SB},\tag{52}$$

where the initial density matrix operator  $\rho_{\rm S}(0)$  of the system is given by

$$\rho_{\mathcal{S}}(0) = \delta(x - x(0))\delta(p), \tag{53}$$

while we have for the heat-bath oscillators a canonical-equilibrium distribution at temperature  $T = 1/(k_B \beta)$ :

$$\rho_{\text{B+SB}} = \frac{1}{Z_{\text{B+SB}}} \exp\left[-\beta \sum_{j=1}^{N} \left\{ \frac{p_j^2(0)}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left(q_j(0) - \frac{c_j x(0)}{m_j \omega_j^2}\right)^2 \right\} \right], \tag{54}$$

with  $Z_{\rm B+SB}$  being the normalizing factor or the canonical partition function. Similar to the classical set-up, at a time  $t \gtrsim 0$ , the particle is released, so that further evolution of the system is dictated by the Hamiltonian (49). Note that Eq. (54) is the exact quantum analogue of the classical set-up, Eq. (35), and moreover, the preparation of the initial state is done in an identical manner in the classical and the quantum case. Equation (51) is known as the quantum Langevin equation [47], and since it greatly resembles the classical Langevin equation (32) that for the case of Ohmic dissipation describes the dynamics of the Brownian motion, the quantum particle will be said to execute a quantum Brownian motion. Equation (51) is characterized by an operator-valued random force f(t) and a viscous drag force described by the friction kernel  $\mu(t)$ . Below we discuss in more detail the various terms appearing in Eq. (51).

3.1.1. Friction kernel The friction kernel  $\mu(t)$  has the same expression as in the classical case, Eq. (34) (see, for instance, Refs. [21, 40, 47]). Consequently, Eq. (41) also holds for the quantum case at hand, and for the case of Ohmic dissipation discussed in Section 2.4, for which  $\mu(t) = 2m\gamma\delta(t)\Theta(t)$ , the viscous drag force experienced by the quantum Brownian particle is instantaneous, analogous to the situation for its classical counterpart.

Employing the bath spectral function (40), we may obtain the total renormalized mass of the bath oscillators, defined in Eq. (24), as

$$\sum_{j=1}^{N} \widetilde{m}_{j} = \frac{2}{\pi} \int_{0}^{\infty} d\omega \, \frac{J(\omega)}{\omega^{3}}.$$
 (55)

If the low-frequency behavior of the bath spectral function is as  $J(\omega) \sim \omega^a$ , then for  $a \leq 2$ , the total renormalized mass of the bath oscillators is infinite. This happens for the case of Ohmic dissipation for which one has a=1, see Eq. (42). It should be noted that this divergence is an infrared divergence, and is independent of the high-frequency (ultraviolet) behavior of  $J(\omega)$ . On the other hand, let us recall that the full Hamiltonian (49) contains a term of the form  $\sum_{j=1}^{N} c_j^2 x^2 / 2m_j \omega_j^2$ , which ensures that the system-bath coupling is homogeneous in space (see the discussion following Eq. (23)). Using the bath spectral function, one may write this term as

$$\sum_{j=1}^{N} \frac{c_j^2 x^2}{2m_j \omega_j^2} = \frac{x^2}{\pi} \int_0^\infty d\omega \, \frac{J(\omega)}{\omega}.$$
 (56)

Clearly, this term is divergent for Ohmic dissipation, but is finite if a suitable high-frequency cut-off is imposed. Its divergence is therefore dictated by the high-frequency behavior of  $J(\omega)$ , in contrast to the divergence of the total renormalized mass of the bath oscillators that we have seen above to stem from the low-frequency behavior of  $J(\omega)$ .

In our subsequent analysis, we will frequently encounter the Fourier transform of  $\mu(t)$ , defined as

$$\widetilde{\mu}(\omega) \equiv \int_0^\infty dt \ \mu(t)e^{i\omega t}; \ \operatorname{Im}[\omega] > 0,$$
 (57)

where we have used the fact that  $\mu(t)$  vanishes for negative times, see Eq. (34). The above definition implies that  $\widetilde{\mu}(\omega)$  is analytic in the upper-half complex- $\omega$  plane. Further, there are two more important mathematical properties that any  $\widetilde{\mu}(\omega)$  must possess. Firstly, its real part should be positive everywhere on the real- $\omega$  axis, i.e.,

$$\operatorname{Re}[\widetilde{\mu}(\omega + i0^{+})] > 0 \ \forall \ \omega \in (-\infty, \infty).$$
 (58)

This requirement emerges from the second law of thermodynamics [47]. The second important mathematical property that has to be satisfied by any  $\tilde{\mu}(\omega)$  is the reality condition:

$$\widetilde{\mu}(\omega + i0^{+}) = \widetilde{\mu}(-\omega + i0^{+})^{*}, \tag{59}$$

where \* denotes complex conjugation. The above property follows from the fact that the factor x appearing in the quantum Langevin equation (51) is a Hermitian operator. The above-mentioned properties imply that  $\widetilde{\mu}(\omega)$  falls into a special class of functions that are known as positive real functions. Furthermore, as a positive real function in the complex- $\omega$  plane,  $\text{Re}[\widetilde{\mu}(\omega)]$  has to be positive (not just analytic!) in the upper-half complex- $\omega$  plane, i.e.,  $\text{Re}[\widetilde{\mu}(\omega)] > 0$  for  $\text{Im}[\omega] > 0$ . A few more generic properties of  $\widetilde{\mu}(\omega)$  have been discussed in Ref. [47].

3.1.2. Quantum noise In Eq. (51), f(t) is an operator-valued random noise with zero mean,

$$\langle f(t) \rangle = 0, \tag{60}$$

and with the following symmetric and anti-symmetric correlation functions [48]:

$$\langle \{f(t), f(t')\} \rangle = \frac{2}{\pi} \int_0^\infty d\omega \ \hbar\omega \ \text{Re}[\widetilde{\mu}(\omega)] \coth\left(\frac{\hbar\omega}{2k_B T}\right) \cos[\omega(t - t')], \quad (61)$$

$$\langle [f(t), f(t')] \rangle = \frac{2}{\mathrm{i}\pi} \int_0^\infty \mathrm{d}\omega \, \hbar\omega \, \mathrm{Re}[\widetilde{\mu}(\omega)] \sin[\omega(t - t')]. \tag{62}$$

Here, the angular brackets denote averaging with respect to the density operator (54). In addition to the above properties, f(t) also has the Gaussian property: the statistical average of an odd number of factors of f(t) is zero, while that of an even number of factors is equal to the sum of products of pair averages with the order of the factors preserved.

Equation (62) above is consistent with the fact that the noise operator commutes with itself at any given instant of time, i.e., for t=t'. Equation (61) points towards an important difference between the classical and the quantum Brownian motion: Consider the case of Ohmic dissipation, when we have the friction kernel becoming a delta function:  $\mu(t) = 2m\gamma\delta(t)\Theta(t)$  (implying  $\text{Re}[\tilde{\mu}(\omega)] = m\gamma$  and  $\text{Im}[\tilde{\mu}(\omega)] = 0$ ), and so the friction term in the Langevin equation is instantaneous in both the cases. For the classical set-up, the noise f(t) is delta correlated in time, see Eq. (43). However, in the corresponding quantum-mechanical case, the noise is not delta-correlated, as may be checked by substituting  $\text{Re}[\tilde{\mu}(\omega)] = m\gamma$  in Eq. (61). This is a hallmark of quantum Brownian motion. However, it may also be verified easily that as  $\hbar \to 0$ , when one expects classical behavior, Eq. (61) does reduce to a delta-function correlation, which one has in the classical case [21, 41, 47]. Indeed, as  $\hbar \to 0$ , using  $\coth x = 1/x$  for small x, we get from Eq. (61) that

$$\langle [f(t)f(t') + f(t')f(t)] \rangle = 4m\gamma k_B T \delta(t - t'), \tag{63}$$

which, on replacing f(t) and f(t') by c-numbers to result in f(t)f(t') = f(t')f(t), is the classical result (43).

#### 4. Quantum energy equipartition

In this section, we formulate and study the quantum counterpart of the energy equipartition theorem in the set-up of Section 3.1, namely, for a quantum particle in a harmonic well and in contact with a quantum heat bath modelled as a collection of independent quantum harmonic oscillators. The equipartition theorem for classical systems states that when in thermal equilibrium at temperature T, the average of the total kinetic energy, denoted by  $E_k$ , is shared equally among all the energetically-accessible degrees of freedom and which equals  $k_BT/2$  per degree of freedom. In the framework of the system-plus-heat-bath model of Section 2.4, in the limit in which the heat bath is an infinite collection of independent harmonic oscillators and is in equilibrium at temperature T, one can show that the average of the total kinetic energy per degree of freedom of the bath and the system when both are in thermal equilibrium are equal:  $\mathcal{E}_k = E_k = k_B T/2$  [49, 50, 51].

In recent times, there have been research activities aimed at the articulation of the quantum analogue of the energy equipartition theorem [28, 29, 34]. It has been observed that unlike the classical case, the average energy of an open quantum system, modelled as a system interacting with a collection of an infinite number of independent harmonic oscillators, can be understood as being the sum of contributions from individually-equilibrated oscillators distributed over the entire frequency spectrum of the heat bath. The contribution to the average energy of the system from bath oscillators lying in the frequency range between  $\omega$  and  $\omega + d\omega$  is characterized by a probability distribution function  $P(\omega)$ , which is very sensitive to the microscopic details of the heat bath and the coupling between the system and the bath. In what follows, we will derive these results, by using a form of the FDT due to Callen and Welton.

#### 4.1. Fluctuation dissipation theorem of Callen-Welton

The basic set-up and steps of analysis of the FDT à la Callen and Welton are the following [52, 53, 54]. Consider a quantum mechanical system described by a Hamiltonian H, which at an initial instant t=0 is in thermal equilibrium at temperature  $T=1/(k_B\beta)>0$ . Correspondingly, the density matrix of the system is the canonical-equilibrium distribution  $\rho=e^{-\beta H}/Z$ , where  $Z=\mathrm{Tr}[e^{-\beta H}]$  is the canonical partition function. At times t>0, the system is acted upon by a general time-dependent external force  $f_t$  (a c-number) that couples to an observable A of the system (e.g., A could be the position of a particle). Consequently, the perturbed Hamiltonian of the system for times t>0 is given by  $H'=H-f_tA$ . Let us consider another observable B of the system, which has at t=0 the thermal-equilibrium value  $\langle B \rangle_{\rm eq} \equiv \mathrm{Tr}[B\rho]$ . For times t>0, because of the application of the external force, the expectation value  $\langle B \rangle \equiv \langle B \rangle(t)$  will deviate from its thermal-equilibrium value, and will be an explicit function of time. Within a linear response theory, wherein the magnitude of  $f_t$  is assumed small for all times t>0, the deviation  $\langle \Delta B(t) \rangle \equiv \langle B \rangle(t) - \langle B \rangle_{\rm eq}$  may be related to  $f_t$  via the

response function  $\Phi_{BA}(t)$ , also called the generalized susceptibility, as

$$\langle \Delta B(t) \rangle = \int_{-\infty}^{t} ds \; \Phi_{BA}(t-s) f_s,$$
 (64)

to leading order in  $f_t$ . Consider the symmetrized, correlation function in the initial state of thermal equilibrium, given by

$$\Psi_{BA}(t - t') = \frac{1}{2} \langle (A(t)B(t') + B(t')A(t)) \rangle_{\text{eq}}, \tag{65}$$

where A(s) is the operator A in the Heisenberg picture with respect to the unperturbed Hamiltonian H, and similarly for B(s). That the symmetrized correlation is a function of the time difference t-t' follows from the fact that a state of equilibrium is invariant with respect to shift in the origin of time. The quantum fluctuation-dissipation due to Callen and Welton asserts that the Fourier transform of  $\Psi_{BA}(t)$ , given by  $\widetilde{\Psi}_{BA}(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t \ e^{\mathrm{i}\omega t} \Psi_{BA}(t)$ , is related to the Fourier transform  $\widetilde{\Phi}_{BA}(\omega)$  via

$$\widetilde{\Psi}_{BA}(\omega) = \frac{\hbar}{2i} \coth\left(\frac{\beta\hbar\omega}{2}\right) \widetilde{\Phi}_{BA}(\omega). \tag{66}$$

Let us specialize to the case when A and B are Hermitian operators. It then follows that  $\Phi_{BA}(-t) = -\Phi_{AB}(t)$ , and then one can show that

$$\widetilde{\Psi}_{BA}(\omega) = \frac{\hbar}{2i} \coth\left(\frac{\beta\hbar\omega}{2}\right) \left[\widetilde{\Phi}_{BA}(\omega + i0^{+}) - \widetilde{\Phi}_{BA}^{\star}(\omega + i0^{+})\right]. \tag{67}$$

For the case B = A, we get

$$\widetilde{\Psi}_{AA}(\omega) = \hbar \coth\left(\frac{\beta\hbar\omega}{2}\right) \operatorname{Im}\left[\widetilde{\Phi}_{AA}(\omega + i0^{+})\right]. \tag{68}$$

Now, it follows for the case at hand on using Eq. (64) that  $\Phi_{AA}(t)$  is real, which implies that  $\text{Im}[\widetilde{\Phi}_{AA}(\omega+i0^+)]$  is an odd function of  $\omega$ . Inverse Fourier transform of Eq. (68) then yields

$$\Psi_{AA}(t) = \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im} \left[ \widetilde{\Phi}_{AA}(\omega + i0^+) \right] \cos(\omega t) \coth \left( \frac{\beta \hbar \omega}{2} \right). \tag{69}$$

For the demonstration of quantum energy equipartition theorem, let us consider the set up of the quantum Langevin equation considered in Section 3.1. Next, consider a weak external force  $f_t$  to act on the particle and a set of weak external forces  $\{f_{j,t}, j=1,2,\ldots,N\}$  to act on the heat-bath oscillators. Here,  $f_t$  and  $f_{j,t}$  are c-number functions of time. We take the perturbed Hamiltonian to be of the form

$$H' = H - xf_t - \sum_{j=1}^{N} f_{j,t}q_j.$$
 (70)

Using the formalism of the Callen-Welton FDT discussed above, one may then show, by first solving the equations motion of the bath oscillators and then substituting the

solution in the equation of motion of the particle (similar to what has been done in Section 3.1), that the symmetrized correlation function of the position of the particle in the equilibrium state reads as [21, 55]:

$$C_{xx}(t_1 - t_2) \equiv \frac{1}{2} \langle x(t_1)x(t_2) + x(t_2)x(t_1) \rangle_{eq}$$

$$= \frac{\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im}[\alpha^{(0)}(\omega + i0^+)] \cos[\omega(t_1 - t_2)] \coth\left(\frac{\hbar\omega}{2k_B T}\right),$$
(71)

where the generalized susceptibility  $\alpha^{(0)}(\omega) \equiv \widetilde{\Phi}_{xx}(\omega)$  is given by

$$\alpha^{(0)}(\omega) = \frac{1}{m(\omega_0^2 - \omega^2) - i\omega\widetilde{\mu}(\omega)},\tag{72}$$

yielding

$$\operatorname{Im}[\alpha^{(0)}(\omega)] = \frac{\omega \operatorname{Re}[\widetilde{\mu}(\omega)]}{(m(\omega_0^2 - \omega^2) + \omega \operatorname{Im}[\widetilde{\mu}(\omega)])^2 + (\omega \operatorname{Re}[\widetilde{\mu}(\omega)])^2}.$$
 (73)

The result (71) is very general and holds even with  $\omega_0 = 0$ . One may also obtain the velocity autocorrelation function in equilibrium as

$$C_{vv}(t_1 - t_2) \equiv \frac{1}{2} \langle v(t_1)v(t_2) + v(t_2)v(t_1) \rangle_{eq}$$

$$= \frac{\hbar}{\pi} \int_0^\infty d\omega \ \omega^2 \text{Im}[\alpha^{(0)}(\omega + i0^+)] \cos[\omega(t_1 - t_2)] \coth\left(\frac{\hbar\omega}{2k_B T}\right). \tag{74}$$

In the same set-up, we may also compute such quantities as  $C_{q_jq_j}(t_1 - t_2) = (1/2)\langle q_j(t_1)q_j(t_2) + q_j(t_2)q_j(t_1)\rangle_{eq}$ ,  $C_{\dot{q}_j\dot{q}_j}(t_1 - t_2) = (1/2)\langle \dot{q}_j(t_1)\dot{q}_j(t_2) + \dot{q}_j(t_2)\dot{q}_j(t_1)\rangle_{eq}$  and  $C_{xq_j}(t_1 - t_2) = (1/2)\langle x(t_1)q_j(t_2) + q_j(t_2)x(t_1)\rangle_{eq}$ .

# 4.2. Partitioning of energies

Armed with the above background, we now consider our system of interest, namely, the particle that is undergoing a dissipative dynamics following the generalized Langevin equation (51), and compute its average energy in equilibrium. Let us begin with the kinetic energy. Putting  $t_1 = t_2 = t$  in Eq. (74), one obtains

$$\langle v^2(t)\rangle_{\rm eq} = \frac{\hbar}{\pi} \int_0^\infty d\omega \ \omega^2 {\rm Im}[\alpha^{(0)}(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2k_BT}\right),$$
 (75)

so that the average kinetic energy in equilibrium is

$$E_k(T) = \frac{m\hbar}{2\pi} \int_0^\infty d\omega \ \omega^2 \text{Im}[\alpha^{(0)}(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2k_B T}\right). \tag{76}$$

Let us note that every bath oscillator is an independent quantum harmonic oscillator, and that the average kinetic energy of a quantum harmonic oscillator in thermal equilibrium at temperature T equals

$$\mathcal{E}_k(\omega, T) = \frac{\hbar \omega}{4} \operatorname{coth}\left(\frac{\hbar \omega}{2k_B T}\right). \tag{77}$$

Defining

$$P_k(\omega) \equiv \frac{2m\omega}{\pi} \operatorname{Im}[\alpha^{(0)}(\omega + i0^+)], \tag{78}$$

we may identify the occurrence of the factor  $\mathcal{E}_k(\omega, T)P_k(\omega)d\omega$  in Eq. (76) and interpret it as the contribution to the average kinetic energy of the particle coming from those bath oscillators whose frequencies lie in the range between  $\omega$  and  $\omega + d\omega$ . We thus obtain

$$E_k(T) = \int_0^\infty d\omega \ \mathcal{E}_k(\omega, T) P_k(\omega), \tag{79}$$

where the factor  $P_k(\omega)$  may be interpreted as a probability density, in the sense that  $P_k(\omega)d\omega$  expresses the probability that oscillators with frequencies in the range between  $\omega$  and  $\omega+d\omega$  and with average kinetic energy equal to  $\mathcal{E}_k(\omega,T)$  contribute to the average kinetic energy of the system. It may be shown that  $P_k(\omega)$  is both positive definite and is normalized, justifying its interpretation as a bona fide probability density (see Appendix A). In recent literature, Eq. (79) has been termed as the quantum counterpart of energy equipartition theorem [28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38].

Let us turn our attention to the potential energy. In Eq. (71), putting  $t_1 = t_2 = t$ , we obtain the position autocorrelation of the system in equilibrium as

$$\langle x^2(t)\rangle_{\rm eq} = \frac{\hbar}{\pi} \int_0^\infty d\omega \, \operatorname{Im}[\alpha^{(0)}(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2k_BT}\right),$$
 (80)

yielding the average potential energy in equilibrium as

$$E_p(T) = \frac{m\omega_0^2 \hbar}{2\pi} \int_0^\infty d\omega \operatorname{Im}[\alpha^{(0)}(\omega + i0^+)] \coth\left(\frac{\hbar\omega}{2k_B T}\right). \tag{81}$$

Similar to what has been done above for the average kinetic energy, one identifies the factor

$$\mathcal{E}_p(\omega, T) \equiv \frac{\hbar \omega}{4} \coth\left(\frac{\hbar \omega}{2k_B T}\right) \tag{82}$$

as the average potential energy of a bath oscillator with frequency  $\omega$ , and the factor

$$P_p(\omega) = \frac{2m\omega_0^2}{\omega\pi} \text{Im}[\alpha^{(0)}(\omega + i0^+)]$$
(83)

as the probability density for oscillators with frequency in the range between  $\omega$  and  $\omega + d\omega$  and with average potential energy equal to  $\mathcal{E}_p(\omega, T)$  to contribute to the average potential energy of the system. Consequently, Eq. (81) writes as

$$E_p(T) = \int_0^\infty d\omega \ \mathcal{E}_p(\omega, T) P_p(\omega), \tag{84}$$

in the same vein as Eq. (79). It may be shown that similar to  $P_k(\omega)$ , the quantity  $P_p(\omega)$  is a bona fide probability density function (Appendix B).

In Figs. 2 and 3, we have plotted as a function of  $\omega/\omega_0$  the dimensionless factors  $\omega_0 P_k(\omega/\omega_0)$  and  $\omega_0 P_p(\omega/\omega_0)$ , respectively, for the case of Ohmic dissipation,

 $\operatorname{Re}[\widetilde{\mu}(\omega)] = m\gamma$ ,  $\operatorname{Im}[\widetilde{\mu}(\omega)] = 0$ , and for representative values of the relevant parameters. The data are obtained by using Eqs. (78), (83), and (73), yielding

$$P_k(\omega) = \frac{2\omega^2}{\pi} \frac{\gamma}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2},\tag{85}$$

and

$$P_p(\omega) = \frac{2\omega_0^2}{\pi} \frac{\gamma}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}.$$
 (86)

From the figures, we observe that as  $\gamma$  gets smaller, so that the system is weakly coupled to the heat bath (see Eq. (48)), the probability functions admit a sharp peak. This implies that bath oscillators whose frequencies are close to the peak frequency contribute the most to the average kinetic and potential energies of the system. Conversely, with increase of  $\gamma$ , the probability functions flatten out, meaning that a larger fraction of bath oscillators contribute appreciably to the average energy of the system. This feature has been analyzed in detail in Ref. [38]. It may be remarked that when the particle is charged and there is a magnetic field acting on it, the number of peaks increases to two or three depending on the embedding spatial dimension of the Hamiltonian [34, 38].

Combining the two cases discussed above, we may obtain the average of the total energy of the system in equilibrium, as

$$E(T) = E_k(T) + E_p(T) = \int_0^\infty d\omega \ \mathcal{E}(\omega, T) P(\omega), \tag{87}$$

where  $\mathcal{E}(\omega, T) = \mathcal{E}_k(\omega, T) + \mathcal{E}_p(\omega, T) = (\hbar \omega/2) \coth (\hbar \omega/(2k_BT))$  is the average of the total energy of a single bath oscillator in thermal equilibrium at temperature T, and we have

$$P(\omega) = \frac{P_k(\omega) + P_p(\omega)}{2} = \frac{m\omega}{\pi} \left( 1 + \frac{\omega_0^2}{\omega^2} \right) \operatorname{Im}[\alpha^{(0)}(\omega + i0^+)]. \tag{88}$$

Since  $P_k(\omega)$  and  $P_p(\omega)$  are probability density functions, their algebraic mean  $P(\omega)$  is also a probability density function, and Eq. (87) can be interpreted along the lines of Eqs. (79) and (84). Equation (87) may be interpreted as equipartition of energy, in the sense that the average energy of the system interacting with the harmonic-oscillator heat bath is the sum of contributions from individually-equilibrated oscillators distributed over the entire frequency spectrum of the heat bath.

Finally, for the case of Ohmic dissipation,  $\text{Re}[\tilde{\mu}(\omega)] = m\gamma$ ,  $\text{Im}[\tilde{\mu}(\omega)] = 0$ , we remark on the weak-dissipation limit or the weak-coupling limit  $\gamma \to 0$ . In this case, Eqs. (85) and (86) imply that the probability densities  $P_k(\omega)$  and  $P_p(\omega)$  individually approach a sum of delta-functions, i.e.,

$$P_k(\omega) = \delta(\omega - \omega_0) - \delta(\omega + \omega_0), \quad P_p(\omega) = \delta(\omega - \omega_0) - \delta(\omega + \omega_0), \tag{89}$$

and hence, Eqs. (79) and (84) yield

$$E_k|_{\gamma \to 0} = E_p|_{\gamma \to 0} = \frac{\hbar \omega_0}{4} \coth\left(\frac{\hbar \omega_0}{2k_B T}\right),$$
 (90)

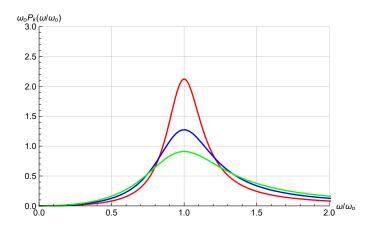


Figure 2. Plot of the dimensionles factor  $\omega_0 P_k(\omega/\omega_0)$  characterizing the average kinetic energy, Eq. (79), of the system considered in Section 3.1, as a function of  $\omega/\omega_0$ . Here, we have considered the case of Ohmic dissipation,  $\widetilde{\mu}(\omega) = \text{Re}[\widetilde{\mu}(\omega)] = m\gamma$ . The parameter values are  $\gamma = 0.3\omega_0$  (red),  $\gamma = 0.5\omega_0$  (blue) and  $\gamma = 0.7\omega_0$  (green). The data are obtained by using Eqs. (78) and (73).

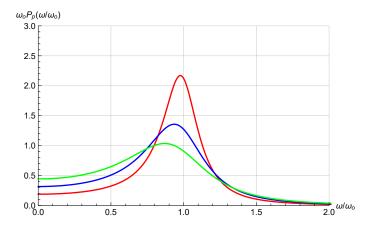


Figure 3. Plot of the dimensionles factor  $\omega_0 P_p(\omega/\omega_0)$  characterizing the average potential energy, Eq. (84), of the system considered in Section 3.1, as a function of  $\omega/\omega_0$ . Here, we have considered the case of Ohmic dissipation,  $\widetilde{\mu}(\omega) = \text{Re}[\widetilde{\mu}(\omega)] = m\gamma$ . The parameter values are  $\gamma = 0.3\omega_0$  (red),  $\gamma = 0.5\omega_0$  (blue) and  $\gamma = 0.7\omega_0$  (green). The data are obtained by using Eqs. (83) and (73).

which are just the familiar expressions for a one-dimensional quantum harmonic oscillator in equilibrium at temperature T. Physically, in this limit, only the bath oscillators whose frequencies resonate with the frequency of the system contribute to the average kinetic and potential energies of the system. Thus, Eqs. (79) and (84) should be viewed as appropriate generalizations of the undergraduate textbook result given in Eq. (90). The reader is referred to [38] for an analysis of the weak-dissipation limit in two dimensions, in presence of a magnetic field.

#### 4.3. Energy as an infinite series

Quite often, the integrals appearing in Eqs. (79) and (84), or, equivalently, in Eqs. (76) and (81), can be explicitly computed via contour integration. Utilizing the identity

$$z \coth z = 1 + 2\sum_{n=1}^{\infty} \frac{z^2}{(z^2) + (n\pi)^2},$$
(91)

for any complex argument z, one may notice that the integrand in the integrals in Eqs. (76) and (81) have poles at  $\omega = \pm i\nu_n$ , where  $\nu_n = 2\pi nk_BT/\hbar$ ; n = 1, 2, ... are known as the bosonic Matsubara frequencies. As a result, the average kinetic and potential energies of the system turn out to be an infinite series summed over the positive integer values of n. For definiteness, let us consider the case of Drude dissipation for which the bath spectral function is  $J(\omega) = m\gamma\omega/(1 + (\omega/\omega_{\rm cut})^2)$ , with  $\omega_{\rm cut}$  being the upper cut-off frequency, yielding  $\widetilde{\mu}(\omega) = m\gamma\omega_{\rm cut}^2/(\omega^2 + \omega_{\rm cut}^2) + im\gamma\omega\omega_{\rm cut}/(\omega^2 + \omega_{\rm cut}^2)$ . Following the aforementioned prescription, one obtains

$$E_k(T) = k_B T \left[ \frac{1}{2} + \sum_{n=1}^{\infty} \frac{\omega_0^2 + \frac{\nu_n \gamma \omega_{\text{cut}}}{\nu_n + \omega_{\text{cut}}}}{\nu_n^2 + \omega_0^2 + \frac{\nu_n \gamma \omega_{\text{cut}}}{\nu_n + \omega_{\text{cut}}}} \right], \tag{92}$$

$$E_p(T) = k_B T \left[ \frac{1}{2} + \sum_{n=1}^{\infty} \frac{\omega_0^2}{\nu_n^2 + \omega_0^2 + \frac{\nu_n \gamma \omega_{\text{cut}}}{\nu_n + \omega_{\text{cut}}}} \right], \tag{93}$$

where  $n = 1, 2, \ldots$  It is immediately clear that the first term in each of the above equations represents the classical result. The subsequent terms can therefore be viewed as quantum corrections. A simple inspection of Eqs. (92) and (93) tells us that the quantum corrections are always positive, implying thereby that both the average kinetic and the potential energy of the system exceed their classical counterparts. It may be verified from the above expressions that both the average kinetic and potential energies of the system are non-decreasing functions of parameters  $\gamma$ ,  $\omega_{\text{cut}}$  and  $\omega_0$  [29, 34]. One should also note that unlike in the weak-coupling limit, the average kinetic energy is not equal to the average potential energy [56].

It is interesting to consider the case of Ohmic dissipation, which is obtained by considering Drude dissipation in the limit  $\omega_{\rm cut} \to \infty$ . Then, using Eq. (93), the average kinetic energy reads as

$$E_k(T) = k_B T \left[ \frac{1}{2} + \sum_{n=1}^{\infty} \frac{\omega_0^2 + \nu_n \gamma}{\nu_n^2 + \omega_0^2 + \nu_n \gamma} \right], \tag{94}$$

which is divergent [57], since the terms in the sum scale as 1/n for large n, in contrast to Eq. (92), where the corresponding scaling is as  $\sim 1/n^2$ . Such a divergence arises due to the zero-point energy of the bath oscillators, as may be verified thus: Consider just the zero-point energy contribution, i.e.,  $\mathcal{E}_k^{(0)}(\omega) = \hbar\omega/4$ , from the bath oscillators. This gives

$$E_k^{(0)} = \int_0^\infty d\omega \ P_k(\omega) \mathcal{E}_k^{(0)}(\omega) = \frac{\hbar \gamma}{2\pi} \int_0^\infty d\omega \ \frac{\omega^3}{(\omega^2 - \omega_0^2)^2 + (\gamma \omega)^2},\tag{95}$$

which diverges! Therefore, in situations where Ohmic dissipation is considered, it is useful to re-express Eqs. (77), (78) and (79) by omitting the zero-point energy contribution:

$$E_k(T) - E_k^{(0)} = \int_0^\infty d\omega \, \frac{(\hbar\omega/2)P_k(\omega)}{e^{\hbar\omega/k_BT} - 1}.$$
 (96)

This should be viewed as a suitable renormalization scheme in which infinities have been subtracted off, leaving only the finite and physically-relevant answer. We should also remark here that the average potential energy of the particle does not suffer from a divergence when one considers the limit  $\omega_{\text{cut}} \to \infty$  in Eq. (93).

# 5. Quantum thermodynamic functions

In this section, we derive analytical expressions of various thermodynamic functions for the system described by the quantum Langevin equation (51), and for the most commonly discussed heat-bath model, namely, which is Ohmic. Our objective is to examine the effects of the heat bath on various thermodynamic functions, such as the internal energy, the free energy, and the entropy of the system.

Equation (87) gives the average energy of the system when in thermal equilibrium at temperature T while in interaction with the heat bath. There exists an alternate, inequivalent definition of energy ascribed to the system, along the lines of Refs. [19, 22, 35, 55, 58, 59]. This energy function U(T), which we shall refer to as internal energy of the system, can be derived as follows.

(i) Consider first the situation in which there is no system, but only the heat bath described by the Hamiltonian  $H_{\rm B}$ , given by the quantum version of Eq. (21). Because the bath is in thermal equilibrium at temperature T for all times  $t \geq 0$ , it is described by the canonical-equilibrium density operator  $\rho_{H_{\rm B}} \propto e^{-H_{\rm B}/k_BT}$ . We then define

$$U_{\rm B}(T) \equiv \langle H_{\rm B} \rangle_{\rho_{H_{\rm B}}} = \frac{\text{Tr} \left[ H_{\rm B} e^{-H_{\rm B}/k_{\rm B}T} \right]}{Z_{\rm B}} \tag{97}$$

as the internal energy of the free bath in its thermal-equilibrium state, with  $Z_{\rm B}$  being the canonical partition function. Since  $H_{\rm B}$  models a collection of N independent quantum harmonic oscillators, we have

$$U_{\rm B}(T) = \sum_{j=1}^{N} \frac{\hbar \omega_j}{2} \coth\left(\frac{\hbar \omega_j}{2k_B T}\right),\tag{98}$$

where the index j running from 1 to N labels the bath oscillators. Here, we have used the well-known result that the average energy of a single quantum harmonic oscillator with frequency  $\omega$  and in equilibrium at temperature T equals  $(\hbar\omega/2) \coth(\hbar\omega/(2k_BT))$ .

(ii) Next, consider a parallel situation, in which the bath is interacting with the system, so that the full Hamiltonian H, given by Eq. (49), models the composite system.

Given that the bath involves N degrees of freedom (with  $N \gg 1$ ), H describes a system with (N+1) degrees of freedom, which at thermal equilibrium is described by the canonical-equilibrium density operator  $\rho_H = e^{-H/k_BT}$ . Then, we may define the internal energy of this system with (N+1) degrees of freedom as

$$\widetilde{U}(T) = \langle H \rangle_{\rho_H} = \frac{\text{Tr}\left[He^{-H/k_BT}\right]}{Z},$$
(99)

where Z is as usual the canonical partition function. Now, we may introduce normal-mode coordinates, such that the Hamiltonian H, describing a coupled (N+1)-oscillator system, can be transformed into an uncoupled (N+1)-oscillator system (see Ref. [19] for details). Consequently,  $\widetilde{U}(T)$  will be given by

$$\widetilde{U}(T) = \sum_{k=0}^{N} \frac{\hbar \Omega_k}{2} \coth\left(\frac{\hbar \Omega_k}{2k_B T}\right),\tag{100}$$

where the index k runs from 0 to N (taking into account the particle in the harmonic well), and where  $\Omega_k$ 's are the normal-mode frequencies.

Now that we have described what the quantities  $U_{\rm B}(T)$  and  $\widetilde{U}(T)$  are, we form their difference, i.e., define

$$U(T) \equiv \widetilde{U}(T) - U_{\rm B}(T),\tag{101}$$

which can be interpreted as the internal energy of our system of particle in a harmonic well, in the sense of Ref. [19]. One finally obtains

$$U(T) = \frac{1}{\pi} \int_0^\infty d\omega \ \mathcal{E}(\omega, T) \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln[\alpha^{(0)}(\omega + \mathrm{i}0^+)] \right], \tag{102}$$

where  $\mathcal{E}(\omega, T)$  is the equilibrium average of the total energy of a bath oscillator of frequency  $\omega$ :

$$\mathcal{E}(\omega, T) = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_B T}\right). \tag{103}$$

For our system of interest, we may now obtain the free energy in the same spirit as above. With  $f(\omega, T) = 2 \ln[\sinh(\hbar \omega/(2k_B T))]$  being the free energy of a quantum harmonic oscillator of frequency  $\omega$  in canonical equilibrium at temperature T, and following the discussions that we have had so far, we can write

$$F_{\rm B}(T) = \sum_{j=1}^{N} f(\omega_j, T), \qquad \widetilde{F}(T) = \sum_{k=0}^{N} f(\Omega_k, T), \qquad (104)$$

which are respectively the free energy corresponding to the situations (i) and (ii) described above. Consequently, the free energy for our system of particle in a harmonic well is just their difference [19]:  $F_U(T) = \tilde{F}(T) - F_B(T)$ , i.e.,

$$F_U(T) = \sum_{k=0}^{N} f(\Omega_k, T) - \sum_{j=1}^{N} f(\omega_j, T),$$
(105)

where the subscript 'U' reminds the reader that it is related to the internal energy function U(T) via

$$F_U(T) = U(T) + T \frac{\partial F_U(T)}{\partial T}.$$
 (106)

Consequently, we get

$$F_U(T) = \frac{1}{\pi} \int_0^\infty d\omega \ f(\omega, T) \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln[\alpha^{(0)}(\omega + \mathrm{i}0^+)] \right]. \tag{107}$$

We may alternatively discard the zero-point energy contribution in the factor  $\mathcal{E}(\omega, T)$  appearing in Eq. (102) and in the factor  $f(\omega, T)$  appearing in Eq. (107), i.e., we can consider instead the expressions

$$\mathcal{E}(\omega, T) = \frac{\hbar \omega}{e^{\hbar \omega / k_B T} - 1}, \qquad f(\omega, T) = k_B T \ln \left[ 1 - e^{-\hbar \omega / k_B T} \right]. \tag{108}$$

Then, the free energy function  $F_U(T)$  can be expressed in terms of the so-called Stieltjes J-function [22, 59].

Now, it may be shown that  $\alpha^{(0)}(\omega)$  has poles on the real axis at the normal-mode frequencies  $\Omega_k$  of the interacting system (49) and zeroes at the frequencies  $\omega_j$  of the bath oscillators, and may be written as [19]:

$$\alpha^{(0)}(\omega) = -\frac{1}{m} \frac{\prod_{j=1}^{N} (\omega^2 - \omega_j^2)}{\prod_{k=0}^{N} (\omega^2 - \Omega_k^2)}.$$
 (109)

From the well-known formula  $1/(x+i0^+) = P(1/x) - i\pi\delta(x)$ , with P denoting the principal part, it follows that

$$\frac{1}{\pi} \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln \alpha^{(0)}(\omega) \right] 
= \sum_{k=0}^{N} \left[ \delta(\omega - \Omega_k) + \delta(\omega + \Omega_k) \right] + \sum_{j=1}^{N} \left[ \delta(\omega - \omega_j) + \delta(\omega + \omega_j) \right], \tag{110}$$

inserting which into Eq. (107) gives Eq. (105).

For Ohmic dissipation, one has [22, 35]

$$\operatorname{Im}\left[\frac{\mathrm{d}}{\mathrm{d}\omega}\ln[\alpha^{(0)}(\omega)]\right] = \frac{z_{+}}{z_{+}^{2} + \omega^{2}} + \frac{z_{-}}{z_{-}^{2} + \omega^{2}},\tag{111}$$

with  $z_{\pm} = \gamma/2 \pm \sqrt{\gamma^2/4 - \omega_0^2}$ . Then, from Eq. (107), after one has subtracted off the zero-point energy contribution, we get

$$F_{U}(T) = \frac{k_{B}T}{\pi} \int_{0}^{\infty} d\omega \ln \left[ 1 - e^{-\hbar\omega/k_{B}T} \right] \left( \frac{z_{+}}{z_{+}^{2} + \omega^{2}} + \frac{z_{-}}{z_{-}^{2} + \omega^{2}} \right)$$

$$= -k_{B}T \left[ J \left( \frac{\hbar z_{+}}{2\pi k_{B}T} \right) + J \left( \frac{\hbar z_{-}}{2\pi k_{B}T} \right) \right], \tag{112}$$

where  $J(\zeta)$  is the Stieltjes *J*-function:

$$J(\zeta) = -\frac{1}{\pi} \int_0^\infty d\xi \ln\left[1 - e^{2\pi\xi}\right] \left(\frac{\zeta}{\zeta^2 + \xi^2}\right). \tag{113}$$

Using Eq. (112), one can obtain the behavior of various thermodynamic quantities at both low and high temperatures by utilizing expansion properties of the Stieltjes J-function.

#### 5.1. Behavior of internal energy

We may define the function [35]

$$\mathfrak{P}(\omega) \equiv \frac{1}{\pi} \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln[\alpha^{(0)}(\omega)] \right],\tag{114}$$

which not only satisfies  $\mathfrak{P}(\omega) > 0$  for  $\omega \in [0, \infty)$ , but is also normalized, i.e.,

$$\int_0^\infty d\omega \, \mathfrak{P}(\omega) = 1,\tag{115}$$

as can be verified from Eq. (110). In other words, the function  $\mathfrak{P}(\omega)$  may be interpreted as a probability density function [35]. Let us then rewrite Eq. (102) as

$$U(T) = \int_0^\infty d\omega \ \mathcal{E}(\omega, T) \mathfrak{P}(\omega), \tag{116}$$

which suggests that  $\mathfrak{P}(\omega)d\omega$  is the probability for oscillators with frequency in the range between  $\omega$  and  $\omega + d\omega$  and with average equilibrium energy equal to  $\mathcal{E}(\omega, T)$  to contribute to the internal energy of the system. This suggests that the quantity U(T) satisfies a quantum counterpart of energy equipartition theorem analogous to the one satisfied by the quantity E(T) that we have studied earlier. However, the probability density functions  $P(\omega)$  and  $\mathfrak{P}(\omega)$  differ, because E(T) and U(T) are different quantities, as we have already explained [60]. It may be shown that in the weak-coupling limit,  $\mathfrak{P}(\omega)$  and  $P(\omega)$  have the same behavior, as given in Eq. (89) [60], i.e.,

$$P(\omega) \approx \mathfrak{P}(\omega) \approx \delta(\omega - \omega_0) + \delta(\omega + \omega_0).$$
 (117)

As a result, E(T) and U(T) are equal in this limit. Moreover, since  $\mathfrak{P}(\omega)$  appears in the integrand of Eq. (107) for the free energy, we find that in the weak-coupling limit, we have

$$F_U(T)|_{\gamma \to 0} \approx f(\omega_0, T),$$
 (118)

which is the familiar result for the free energy of a quantum oscillator at temperature T and eigenfrequency  $\omega_0$ . Knowing the free energy of the system, one can obtain its entropy as  $S(T) = -\partial F_U(T)/\partial T$ .

#### 5.2. Entropy and third law

The third law of thermodynamics implies that thermodynamic functions such as entropy, specific heat, isobaric coefficient of expansion, isochoric coefficient of tension, etc. all approach zero as  $T \to 0$  [61]. Recent developments in nanotechnology have led to the development of the subject of quantum thermodynamics and low temperature physics of small quantum systems [62, 63] and people have asked about the validity of the third law of thermodynamics in the quantum regime and what role does dissipation play. Ford and O'Connell discussed about the third law of thermodynamics in connection with a quantum harmonic oscillator [64, 65]. Hanggi and Ingold have shown that finite dissipation actually helps to ensure that the third law of thermodynamics holds [23, 26]. Further investigations have been made in the case of dissipative cyclotron motion of a charged oscillator with different heat-bath schemes [27, 59, 66], and it was found that dissipative quantum systems indeed respect the third law of thermodynamics.

In order to obtain the low-temperature behavior of entropy, one can make use of the low-temperature expansion of the free energy based on an asymptotic expansion of the J-function [22, 27, 59]. For Ohmic dissipation, this expansion gives [22]:

$$F_U(T)|_{T\to 0} = -\frac{\pi\gamma}{6\hbar\omega_0^2}(k_B T)^2 + \mathcal{O}(T^4),$$
 (119)

implying that at low temperatures, we have on using  $S(T) = -\partial F_U(T)/\partial T$  that

$$S(T)\Big|_{T\to 0} = \frac{\pi\gamma k_B^2 T}{3\hbar\omega_0^2} + \cdots$$
 (120)

We thus see that at low temperatures, to leading order, the entropy of our system goes to zero linearly. The same behavior is obtained even for the Drude dissipation model [22], and an identical low-temperature behavior was observed for a three-dimensional Brownian oscillator placed in a magnetic field [27].

Let us note that from Eq. (107), we have  $F_U(T) = \int_0^\infty d\omega \ f(\omega, T) \mathfrak{P}(\omega)$ . This means in the weak-coupling limit (i.e., in the limit  $\gamma \to 0$ ), where we have  $\mathfrak{P}(\omega) \approx \delta(\omega - \omega_0) + \delta(\omega + \omega_0)$ , we get the entropy to be

$$S(T)\Big|_{\gamma \to 0, T \to 0} \approx -\frac{\partial}{\partial T} \int_0^\infty d\omega \ f(\omega, T) \left[ \delta(\omega - \omega_0) + \delta(\omega + \omega_0) \right]. \tag{121}$$

Using the result  $s(\omega, T) = -\partial f(\omega, T)/\partial T$ , where  $s(\omega, T)$  is the entropy of a quantum harmonic oscillator, we get

$$S(T)\Big|_{\gamma\to 0, T\to 0} \approx \int_0^\infty d\omega \ s(\omega, T) \left[\delta(\omega - \omega_0) + \delta(\omega + \omega_0)\right] = s(\omega_0, T). \tag{122}$$

Since the entropy of a quantum harmonic oscillator at low temperatures goes to zero exponentially, the entropy of our system also has the same behavior in the weak-coupling limit.

#### 6. Dissipative diamagnetism

The quantum-mechanical problem of a charged particle in presence of a magnetic field and interacting with a heat bath serves as a paradigmatic model for the well-known Landau theory of diamagnetism. In this section, we study Landau diamagnetism in the context of dissipative quantum mechanics. Diamagnetism is a material property that arises from the response of a collection of non-interacting charged particles (e.g., electrons) to an applied magnetic field. The orbital magnetic moment created by the cyclotron motion of each particle exhibits a negative magnetic susceptibility, which is characteristic of diamagnetism. The celebrated Bohr-van Leeuwen (BVL) theorem demonstrates that in the classical setting, the diamagnetic susceptibility is identically zero as the bulk contribution to diamagnetic moment exactly cancels the contribution arising from the so-called skipping orbits of electrons (see, for example, Ref. [67]). However, Landau's calculation suggests that the bulk and surface contributions are different in quantum mechanics [68], and hence, the cancellation of the two terms is incomplete, unlike in the classical case. This result is unusual in the sense that boundary effects, which generally do not affect thermodynamic properties, seem to play a crucial role in determining diamagnetism.

The problem of diamagnetism raises many fascinating issues concerning the inherent quantum nature of the problem, the role played by boundaries and by dissipation, the meaning of the thermodynamic limit, and above all, the quantum–classical crossover occasioned by environment-induced decoherence. Landau diamagnetism provides us with a unique paradigm for discussing these relevant issues. Another issue of relevance is to be able to connect the mean orbital magnetic moment, a thermodynamic property, with electrical resistivity, which characterizes transport properties of materials [69].

With the motivation outlined in the preceding paragraph, we consider a particle with charge e in the presence of an external magnetic field and in a confining harmonic potential. This system is linearly coupled to a quantum bath (modelled as a collection of independent quantum harmonic oscillators) through coordinate variables. Thus, the Hamiltonian of the composite system is a generalization of Eq. (49), and which reads as

$$H = \frac{(\mathbf{p} - \frac{e}{c}\mathbf{A})^2}{2m} + \frac{m\omega_0^2\mathbf{r}^2}{2} + \sum_{j=1}^{N} \left[ \frac{\mathbf{p}_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2 \left( \mathbf{q}_j - \frac{c_j}{m_j\omega_j^2}\mathbf{r} \right)^2 \right], \quad (123)$$

where  $\mathbf{p} = (p_x, p_y)$  and  $\mathbf{r} = (x, y)$  are the two-dimensional momentum and position operators of the charged particle,  $\mathbf{p}_j$  and  $\mathbf{q}_j$  are the corresponding variables for the j-th heat-bath oscillator, and  $\mathbf{A}$  is the vector potential. The usual commutation relations between coordinates and momenta, a generalization of Eq. (50) to two dimensions, hold. Integrating out the reservoir variables from the Heisenberg equations of motion of the particle, and following the set-up and the computation identical to the one employed to derive Eq. (51), one obtains the generalized quantum Langevin equation:

$$m\ddot{\mathbf{r}}(t) + \int_{-\infty}^{t} dt' \ \mu(t - t') \ \dot{\mathbf{r}}(t') + m\omega_0^2 \mathbf{r}(t) - \frac{e}{c}(\dot{\mathbf{r}}(t) \times \mathbf{B}) = \mathbf{f}(t), \tag{124}$$

where  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$  is the magnetic field, and  $\mu(t)$  is defined as in Eq. (34). We will consider the magnetic field  $\mathbf{B}$  to be uniform in space, with components  $B_x, B_y, B_z$ , and magnitude  $B = \sqrt{B_x^2 + B_y^2 + B_z^2}$ . The operator-valued random force  $\mathbf{f}(t)$  is defined in a manner analogous to the one-dimensional case (see Section 3.1.2), and hence, satisfies the following relations:

$$\langle \{ f_{\alpha}(t), f_{\beta}(t') \} \rangle = \delta_{\alpha\beta} \frac{2}{\pi} \int_{0}^{\infty} d\omega \, \, \hbar\omega \, \operatorname{Re}[\widetilde{\mu}(\omega)] \coth\left(\frac{\hbar\omega}{2k_{B}T}\right) \cos[\omega(t - t')],$$
(125)

$$\langle [f_{\alpha}(t), f_{\beta}(t')] \rangle = \delta_{\alpha\beta} \frac{2}{\mathrm{i}\pi} \int_{0}^{\infty} \mathrm{d}\omega \, \, \hbar\omega \, \, \mathrm{Re}[\widetilde{\mu}(\omega)] \sin[\omega(t - t')],$$
 (126)

where the indices  $\alpha$  and  $\beta$  stand for the Cartesian coordinates x and y.

# 6.1. Magnetic moment

The magnetic moment of the charged particle can be computed from the following correlation function [39]:

$$M_z(t) = \frac{|e|}{2c} \langle x(t)\dot{y}(t) - y(t)\dot{x}(t) \rangle, \tag{127}$$

involving operators in the Heisenberg picture. With a few straightforward manipulations, it follows that in the stationary state (i.e., when the charged particle comes to equilibrium with the heat bath that is always in equilibrium), one has [38] (see also Ref. [48]):

$$M_z = -\frac{e\hbar}{2\pi mc} \int_{-\infty}^{\infty} d\omega \ \omega^2 \coth\left(\frac{\beta\hbar\omega}{2}\right) \Phi(\omega), \tag{128}$$

where the function  $\Phi(\omega)$  is defined as

$$\Phi(\omega) \equiv \frac{\operatorname{Re}[\widetilde{\gamma}(\omega)]}{\left[\left(\omega^2 - \omega_0^2 - \omega\omega_c + \omega\operatorname{Im}[\widetilde{\gamma}(\omega)]\right)^2 + (\omega\operatorname{Re}[\widetilde{\gamma}(\omega)])^2\right]},$$
(129)

and we have  $\widetilde{\gamma}(\omega) = \widetilde{\mu}(\omega)/m$ . Here,  $\omega_c = eB/(mc)$  is the usual cyclotron frequency, while c is the speed of light in vacuum.

Let us now consider the case of Ohmic dissipation, for which we have  $\text{Re}[\tilde{\gamma}(\omega)] = \gamma$  and  $\text{Im}[\tilde{\gamma}(\omega)] = 0$ , which yields on using Eq. (128) that [39, 48]

$$M_z = -\frac{e\gamma\hbar}{2\pi mc} \int_{-\infty}^{\infty} d\omega \frac{\omega^2 \coth(\hbar\omega/(2k_B T))}{\left[(\omega^2 - \omega_0^2 - \omega\omega_c)^2 + (\gamma\omega)^2\right]}.$$
 (130)

We may now choose to switch off the harmonic potential, i.e., take  $\omega_0 \to 0$  and expect that the resulting expression would correspond to the magnetic moment of a free (quantum) Brownian particle (i.e., the charged particle in the absence of the confining harmonic potential, which is interacting with the heat bath of quantum harmonic

oscillators). Then, in the weak-coupling limit, i.e. for  $\gamma \to 0$ , one has

$$M_z = -\frac{e\hbar}{2mc} \int_{-\infty}^{\infty} d\omega \, \delta(\omega - \omega_c) \coth\left(\frac{\hbar\omega}{2k_B T}\right)$$
$$= -\frac{e\hbar}{2mc} \coth\left(\frac{\hbar\omega_c}{2k_B T}\right), \tag{131}$$

which is only a part of the result one gets from Landau diamagnetism. Thus, the limit  $\omega_0 \to 0$  applied to Eq. (128) does not consistently give the correct expression for magnetic moment consistent with Landau's final answer, which is derived by computing the partition function in a weak-coupling limit. Indeed, such an error creeps in if one is not careful with the role of the boundary [70]. It has been elaborated by Peierls [67] that it is the boundary electrons which have the so-called 'skipping orbits' that lead to the 'edge currents', and this makes a crucial contribution to the diamagnetism.

In order to incorporate confinement effects correctly, it is important to first evaluate the integral appearing in Eq. (130) and then take the limit  $\omega_0 \to 0$  [39, 71]. Performing the integration in Eq. (130), we find [38, 39]

$$M_z = -\frac{2ek_BT}{mc} \sum_{n=1}^{\infty} \frac{\nu_n^2 \omega_c}{[\nu_n^2 + \omega_0^2 + \gamma \nu_n]^2 + (\nu_n \omega_c)^2},$$
(132)

where  $\nu_n$  are the bosonic Matsubara frequences with  $n=0,1,2,\cdots$ . The zero-dissipation ( $\gamma=0$ ) case can be recovered rather straightforwardly from the above result, and we obtain [24, 38]

$$M_z|_{\gamma \to 0} = -2Bk_B T \left(\frac{e}{mc}\right)^2 \sum_{n=1}^{\infty} \frac{\nu_n^2}{(\nu_n^2 + \omega_0^2)^2 + (\nu_n \omega_c)^2}.$$
 (133)

Finally, if we now switch off the harmonic trap by taking the limit  $\omega_0 \to 0$  in Eq. (133), we can recover the famous Landau diamagnetism result [39]:

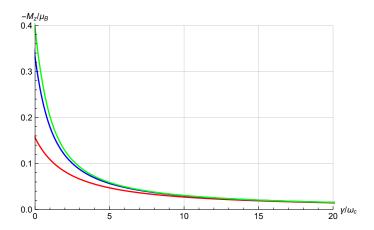
$$M_z|_{\gamma,\omega_0\to 0} = \frac{e\hbar}{2mc} \left[ \frac{2k_B T}{\hbar\omega_c} - \coth\left(\frac{\hbar\omega_c}{2k_B T}\right) \right].$$
 (134)

We emphasize that the limits  $t \to \infty$  and  $\omega_0 \to 0$  do not commute. For obtaining the above result, we have first considered the limit  $t \to \infty$  in Eq. (127) to obtain Eq. (133), followed by the limit  $\omega_0 \to 0$  in the latter equation. Reversing the order of the two limits leads to an incorrect expression. Moreover, even if we take the limit  $t \to \infty$  first to obtain Eq. (128), putting  $\omega_0 \to 0$  at this stage only leads to a part of the Landau's expression [Eq. (134)]. This demonstrates the crucial role of confining boundaries in the context of dissipative diamagnetism.

Finally, one can recast Eq. (132) in the following form:

$$M_z = -\frac{e\hbar}{mc} \times \frac{1}{\nu} \sum_{n=1}^{\infty} \frac{1}{\left(\widetilde{\mu}_n + \frac{\mu_0^2}{\widetilde{\mu}_n} + \widetilde{\rho}\right)^2 + 1},$$
 (135)

where the renormalized Drude resistivity  $\tilde{\rho} = \gamma/\omega_c$  is defined as the ratio of the Drude resistivity  $\rho \equiv m\gamma/(pe^2)$  (p is number density of the charge carrier) to the Hall resistivity



**Figure 4.** Plot of the (negative) magnetic moment in units of Bohr magneton and as a function of the Drude resistivity  $\gamma/\omega_c$  taking  $\omega_0 = 0.5\omega_c$ , and for  $\hbar\omega_c/2k_BT = 1$  (red),  $\hbar\omega_c/2k_BT = 3$  (blue) and  $\hbar\omega_c/2k_BT = 5$  (green).

 $R \equiv B/(pec)$ ; the renormalized Matsubara frequency is  $\tilde{\mu}_n = \nu_n/\omega_c = (\pi n)\nu$  with  $\nu \equiv \hbar \omega_c/(2k_BT)$ ; the renormalized confining frequency is  $\mu_0 = \omega_0/\omega_c$ . Thus, Eq. (135) is a novel result in the sense that it connects an equilibrium thermodynamic property, i.e., the orbital diamagnetic moment to a transport property of the material, i.e., the Drude resistivity  $\tilde{\rho}$ . We know that Landau diamagnetism is a result of the coherent motion of the electrons. On the other hand, as one increases Drude resistivity, the decoherence effect becomes dominant and the orbital dissipative diamagnetic moment in Eq. (135) becomes smaller [38, 69]. This ensures the validity of the Bohr-van Leeuwen theorem. As an illustration, we have plotted the magnetic moment as a function of the Drude resistivity in Fig. 4, from which it is clear that increasing the level of dissipation reduces the value of the magnetic moment. This is consistent with the fact that dissipation is associated with decoherence, which acts against diamagnetism.

#### 7. Momentum-momentum coupling

In the case of bilinear coordinate-coordinate coupling between a system and a heat bath, as discussed in the preceding sections, the coordinate of the system is coupled to the coordinate of each bath oscillator, and we obtained a reduced description of the particle motion in the form of a quantum Langevin equation that is satisfied by the coordinate operator of the particle. In this equation, coupling to the bath is described by (i) an operator-valued random force, and (ii) a friction force characterized by a friction kernel. As a relevant variation of the set-up, we consider in this section the complementary possibility of coupling of a quantum system to a quantum-mechanical heat bath through the momentum variables. The resulting dissipation appearing in the reduced dynamics of the system has been termed by Leggett as anomalous dissipation [72]. Such a scenario has been considered previously by many authors [66, 72, 73, 74, 75]. To describe our set-

up, we consider a gauge-invariant system-plus-reservoir model. The system comprises a charged quantum particle moving in a harmonic potential in the presence of a magnetic field. The particle is linearly coupled via the momentum variables to a quantum heat bath consisting of independent quantum harmonic oscillators. Although there are other velocity-dependent coupling schemes (see, for example, Refs. [55, 58]), they can be shown to be equivalent to the standard coordinate-coordinate coupling approach via suitable transformations of the variables appearing in the total Hamiltonian [47]. However, to our knowledge, this is not the case with the gauge-invariant model of momentum-momentum coupling that we consider, and therefore this situation deserves special attention. The work we review here is reported in Refs. [66] and [73].

The Hamiltonian of our gauge invariant system-plus-reservoir model has the generic form  $H = H_{\rm S} + H_{\rm B} + H_{\rm SB}$  that we have considered previously in the review, and is given in three spatial dimensions by

$$H = \frac{1}{2m} \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2 + \frac{1}{2} m \omega_0^2 \mathbf{r}^2$$

$$+ \sum_{j=1}^{N} \left[ \frac{1}{2m_j} \left( \mathbf{p}_j - g_j \mathbf{p} + \frac{g_j e}{c} \mathbf{A} \right)^2 + \frac{1}{2} m_j \omega_j^2 \mathbf{q}_j^2 \right],$$

$$(136)$$

where  $e, m, \mathbf{p}, \mathbf{r}$  are respectively the charge, the mass, the momentum operator and the coordinate operator of the particle, while  $\omega_0$  is the frequency characterizing its motion in the harmonic potential. We take the j-th heat-bath oscillator to have mass  $m_j$ , frequency  $\omega_j$ , coordinate operator  $\mathbf{q}_j$ , and momentum operator  $\mathbf{p}_j$ . The dimensionless parameter  $g_j$  describes the coupling between the particle and the j-th oscillator. The vector potential  $\mathbf{A}(\mathbf{r})$  is related to the external magnetic field  $\mathbf{B}(\mathbf{r})$  through  $\mathbf{B}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$ . The various coordinate and momentum operators follow the usual commutation relations (three-dimensional generalization of Eq. (50)). Here, as before, we will use Greek indices  $(\alpha, \beta, \ldots)$  to refer to the three spatial directions, while Roman indices  $(i, j, k, \ldots)$  will refer to the heat-bath oscillators.

Let us first demonstrate that our system of interest is gauge invariant. For this purpose, we consider the gauge transformation  $\mathbf{A}(\mathbf{r}) \to \mathbf{A}'(\mathbf{r}) = \mathbf{A}(\mathbf{r}) + \nabla f(\mathbf{r})$ , with  $f(\mathbf{r})$  an arbitrary function of coordinate  $\mathbf{r}$ , and also a unitary transformation of the state vectors of the system,  $|\psi(t)\rangle \to |\psi'(t)\rangle = U|\psi(t)\rangle$ ;  $U^{\dagger} = U^{-1}$ , with the choice  $U = \exp\left(\mathrm{i}e/(\hbar c)f(\mathbf{r})\right)$ . Using the Hadamard formula  $e^XYe^{-X} = Y + [X,Y] + (1/2!)[X,[X,Y]] + \ldots$ , and the commutation relations between the coordinate and the momentum operators, one may easily check that  $H'(\mathbf{A}') = UH(\mathbf{A})U^{\dagger}$  and hence, all physical observables remain invariant, as required.

# 7.1. Quantum Langevin equation

The Heisenberg equations of motion for the charged particle may be straightforwradly obtained from the Hamiltonian (136), and which reads as

$$m_{\rm r}\ddot{\mathbf{r}} = -m\omega_0^2 \mathbf{r} + \frac{e}{c}(\mathbf{v} \times \mathbf{B}) + \frac{i\hbar e}{2m_{\rm r}c} \Big(\nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}\Big) - \sum_{j=1}^N \frac{g_j m_{\rm r}}{m_j} \dot{\mathbf{p}}_j,$$
(137)

where the renormalized mass is

$$m_{\rm r} = \frac{m}{1 + \sum_{j=1}^{N} \frac{g_j^2 m}{m_j}}.$$
 (138)

On noting that  $\nabla(\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} = \nabla \times (\nabla \times \mathbf{A}) = \nabla \times \mathbf{B} = (4\pi/c)\mathbf{j}$ , where  $\mathbf{j}$  is the current producing the external magnetic field, and also the fact that in practice this current source lies outside the region where the charged particle moves, we get

$$m_{\rm r}\ddot{\mathbf{r}} = -m\omega_0^2 \mathbf{r} + \frac{e}{c}(\mathbf{v} \times \mathbf{B}) - \sum_{j=1}^N \frac{g_j m_{\rm r}}{m_j} \dot{\mathbf{p}}_j.$$
(139)

For the heat-bath oscillators, the Heisenberg equations of motion are

$$\dot{\mathbf{q}}_j = \frac{1}{m_j} \Big( \mathbf{p}_j - g_j \mathbf{p} + \frac{g_j e}{c} \mathbf{A} \Big), \tag{140}$$

$$\dot{\mathbf{p}}_j = -m_j \omega_j^2 \mathbf{q}_j. \tag{141}$$

Combining the above two equations and with the reasoning given in the sentence following Eq. (138), we finally obtain

$$m_j \ddot{\mathbf{q}}_j = -m_j \omega_j^2 \ \mathbf{q}_j + g_j m \omega_0^2 \mathbf{r} - \frac{g_j e}{c} (\mathbf{v} \times \mathbf{B}).$$
 (142)

Then, using  $\dot{\mathbf{p}}_j = -m_j \omega_j^2 \mathbf{q}_j$  in Eq. (139) leads to

$$m_{\mathbf{r}}\ddot{\mathbf{r}} = -m\omega_0^2 \mathbf{r} + \frac{e}{c}(\mathbf{v} \times \mathbf{B}) + \sum_{j=1}^{N} g_j m_{\mathbf{r}} \omega_j^2 \mathbf{q}_j.$$
 (143)

Let us consider the magnetic field **B** to be uniform in space, with components  $B_x, B_y, B_z$ , and magnitude  $B = \sqrt{B_x^2 + B_y^2 + B_z^2}$ . We now derive a quantum Langevin equation for the charged particle. To this end, as was done in Section 3.1, we first solve the equations of motion for the bath variables. In this case, Eq. (142) has the retarded solution

$$\mathbf{q}_{j}(t) = \mathbf{q}_{j}^{h}(t) + \frac{g_{j}m\omega_{0}^{2}}{m_{j}\omega_{j}^{2}}\mathbf{r}(t) - \frac{g_{j}m\omega_{0}^{2}}{m_{j}\omega_{j}^{2}}\mathbf{r}(0)\cos(\omega_{j}t) - \frac{g_{j}m\omega_{0}^{2}}{m_{j}\omega_{j}^{2}} \int_{0}^{t} dt' \, \dot{\mathbf{r}}(t')\cos(\omega_{j}(t-t')) - \frac{g_{j}m\omega_{c}}{m_{j}\omega_{j}B}\Gamma \int_{0}^{t} dt' \, \dot{\mathbf{r}}(t')\sin(\omega_{j}(t-t')),$$

$$(144)$$

where we have

$$\mathbf{q}_{j}^{h}(t) \equiv \mathbf{q}_{j}(0)\cos(\omega_{j}t) + \frac{\mathbf{p}_{j}(0)}{m_{j}\omega_{j}}\sin(\omega_{j}t)$$
(145)

as the contribution from the initial condition, while  $\omega_c = eB/(mc)$  is as usual the cyclotron frequency of precessional motion of the charged particle in the magnetic field, and we have

$$\Gamma \equiv \begin{bmatrix} 0 & B_z & -B_y \\ -B_z & 0 & B_x \\ B_y & -B_x & 0 \end{bmatrix}. \tag{146}$$

Substituting Eq. (144) into Eq. (143), we get

$$m_{\mathrm{r}}\ddot{\mathbf{r}} + \int_{0}^{t} \mathrm{d}t' \, \dot{\mathbf{r}}(t')\mu(t-t') + m_{\mathrm{r}}\omega_{0}^{2}\mathbf{r} + \mu_{\mathrm{d}}(t)\mathbf{r}(0) - \frac{e}{c}(\mathbf{v} \times \mathbf{B}) = \mathbf{F}(t), \tag{147}$$

where we have the operator-valued random force and the friction kernel given respectively by

$$\mathbf{F}(t) = \sum_{j=1}^{N} g_j m_r \omega_j^2 \mathbf{q}_j^h(t) \Theta(t), \tag{148}$$

$$\mu(t - t') = \mu_{\rm d}(t - t') + \Gamma \mu_{\rm od}(t - t'), \tag{149}$$

with  $\mu_d$ , the diagonal part of the friction kernel  $\mu$ , and  $\mu_{od}$ , its off-diagonal part, given by

$$\mu_{\rm d}(t-t') \equiv \Theta(t-t') \sum_{j=1}^{N} \frac{g_j^2 m m_{\rm r} \omega_0^2}{m_j} \cos(\omega_j(t-t')), \tag{150}$$

$$\mu_{\rm od}(t-t') \equiv \Theta(t-t') \sum_{j=1}^{N} \frac{g_j^2 m m_{\rm r} \omega_j \omega_c}{m_j B} \sin(\omega_j (t-t')). \tag{151}$$

Now, we want to demonstrate that the coordinate operator of the charged particle satisfies a quantum Langevin equation. To this end, let us assume that at time t = 0, there was no magnetic field, and the charged particle was held fixed at  $\mathbf{r}(0)$ , while the heat-bath oscillators were in canonical equilibrium at temperature T with respect to the free oscillator Hamiltonian

$$H_{\rm B} = \sum_{j=1}^{N} \left[ \frac{\mathbf{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \mathbf{q}_j^2 \right]. \tag{152}$$

The state of the system at the initial instant t = 0, corresponding to a correlation-free preparation, is given by the total density matrix operator

$$\rho(0) = \rho_{\rm S}(0) \otimes \rho_{\rm B},\tag{153}$$

where the initial density matrix operator  $\rho_{\rm S}(0)$  of the system is given by

$$\rho_{\rm S}(0) = \delta(\mathbf{r} - \mathbf{r}(0))\delta(\mathbf{p}), \tag{154}$$

while we have for the heat-bath oscillators a canonical-equilibrium distribution at temperature  $T = 1/(k_B\beta)$  with respect to the Hamiltonian  $H_B$ :

$$\rho_{\rm B} = \frac{e^{-\beta H_{\rm B}}}{Z_{\rm B}},\tag{155}$$

with  $Z_{\rm B}$  being the normalizing factor or the canonical partition function. At a time  $t \geq 0$ , the particle is released, and the magnetic field is turned on, so that subsequent evolution of the system is controlled by Hamiltonian (136). One may note that the preparation of the initial state is similar to the one done for the case of the coordinate-coordinate coupling in Section 3.1. Averaging with respect to the density operator (155), one obtains

$$\langle q_{j\alpha}(0)\rangle = 0,$$

$$\langle p_{j\alpha}(0)\rangle = 0,$$

$$\langle q_{j\alpha}(0)q_{k\beta}(0)\rangle = \frac{\hbar}{2m_{j}\omega_{j}}\coth\left(\frac{\hbar\omega_{j}}{2k_{B}T}\right)\delta_{jk}\delta_{\alpha\beta},$$

$$\langle p_{j\alpha}(0)p_{k\beta}(0)\rangle = \frac{\hbar m_{j}\omega_{j}}{2}\coth\left(\frac{\hbar\omega_{j}}{2k_{B}T}\right)\delta_{jk}\delta_{\alpha\beta},$$

$$\langle q_{j\alpha}(0)p_{k\beta}(0)\rangle = -\langle p_{j\alpha}(0)q_{k\beta}(0)\rangle = \frac{1}{2}i\hbar\delta_{jk}\delta_{\alpha\beta}.$$
(156)

Additionally, one has the Gaussian properties of  $q_{j\alpha}(0)$  and  $p_{j\alpha}(0)$ , i.e., the statistical average of odd number of factors is zero, while the same for an even number of factors is equal to the sum of products of pair averages with the order of the factors preserved. Using the results in Eq. (156), one finds that the force operator  $\mathbf{F}(t)$ , Eq. (148), has zero mean,  $\langle \mathbf{F}(t) \rangle = 0$ , and a symmetric correlation given by

$$\frac{1}{2}\langle F_{\alpha}(t)F_{\beta}(t') + F_{\beta}(t')F_{\alpha}(t)\rangle = \frac{\hbar\delta_{\alpha,\beta}}{2}\sum_{j=1}^{N}\frac{g_{j}^{2}m_{r}^{2}\omega_{j}^{3}}{m_{j}}\coth\left(\frac{\hbar\omega_{j}}{2k_{B}T}\right)\cos(\omega_{j}(t-t')). \quad (157)$$

Moreover,  $\mathbf{F}(t)$  has the Gaussian property, which follows from the same property of the  $\mathbf{q}_{j}(0)$  and  $\mathbf{p}_{j}(0)$ . On using the canonical commutation rules between the coordinate and the momentum operators, one can further show that  $\mathbf{F}(t)$  has the unequal-time commutator given by

$$[F_{\alpha}(t), F_{\beta}(t')] = -i\hbar \delta_{\alpha,\beta} \sum_{j=1}^{N} \frac{g_j^2 m_r^2 \omega_j^3}{m_j} \sin(\omega_j(t-t')). \tag{158}$$

Now, we can interpret Eq. (147) with  $t \geq 0$  as a quantum Langevin equation for the particle coordinate operator with  $\mathbf{F}(t)$  a random force with correlation and unequal time commutator given by Eqs. (157) and (158), respectively. The friction is as usual characterized by the friction kernel  $\mu(t)$ . Note that the initial value term that depends explicitly on the initial coordinate of the particle and the diagonal part of the

memory function can be absorbed into the definition of the random force by defining  $\mathbf{f}(t) \equiv \mathbf{F}(t) - \mu_{\rm d}(t)\mathbf{r}(0)$ , and then consider the initial state (153), with particle density operator (154) and bath density operator  $\rho_{\rm B} = e^{-H_{\rm B}^{\rm Shifted}/k_BT}/Z_{\rm B}$ , where the "shifted" bath Hamiltonian is

$$H_{\rm B}^{\rm Shifted} = \sum_{j=1}^{N} \left[ \frac{\mathbf{p}_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 \left[ \mathbf{q}_j - \frac{g_j m \omega_0^2}{m_j \omega_j^2} \mathbf{r}(0) \right]^2 \right]. \tag{159}$$

As a result, the redefined random force  $\mathbf{f}(t)$  has the same statistical properties as  $\mathbf{F}(t)$ .

Finally, one may identify certain interesting features of the quantum Langevin equation (147), which are not present in the corresponding for the case of coordinate-coordinate coupling, Eq. (124). These are: (i) the coupling with the bath renormalizes both the inertial mass as well as the harmonic potential term; (ii) the friction kernel characterizing the drag force has an explicit magnetic-field dependence; (iii) The random force has a modified form, and its symmetric correlation and unequal time commutator have different form than those in the case of coordinate-coordinate coupling. However, one may find a few resemblances as well. Similar to the coordinate-coordinate coupling case, the magnetic field appears in the quantum Langevin equation as a quantum-generalized classical Lorentz force term, and the random force itself has a form that is independent of the magnetic field.

#### 7.2. Quantum thermodynamic functions

In this subsection, we derive an exact formula for the internal energy, and hence the free energy of the charged particle in thermal equilibrium with the heat bath. Our result shows important differences in the form of the free energy with respect to that for the coordinate-coordinate coupling. For an illustrative heat-bath spectrum, we evaluate the free energy in the low-temperature limit, thereby showing that the entropy of the charged particle vanishes at zero temperature, in conformity with the third law of thermodynamics.

The free energy of the system is computed in exactly the same way as the one employed in obtaining the free energy (107) for the case of coordinate-coordinate coupling. The final expression reads as

$$F_U(T,B) = \frac{1}{\pi} \int_0^\infty d\omega \ f(\omega,T) \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln[\operatorname{Det} \alpha(\omega + \mathrm{i}0^+)] \right]$$
  
+  $\lambda(\omega) \left( \frac{\omega e B}{c} \right)^2 \left( \frac{\mathrm{d}(G(\omega))^2}{\mathrm{d}\omega} \right) \operatorname{Det} \alpha(\omega + \mathrm{i}0^+) ,$  (160)

where "Det" denotes determinant,  $f(\omega, T)$  is the free energy of a bath oscillator of frequency  $\omega$  (here we include the zero-point energy contribution):

$$f(\omega, T) = \frac{\hbar\omega}{2} + k_B T \ln\left[1 - e^{-\hbar\omega/k_B T}\right],\tag{161}$$

while  $G(\omega)$  is defined as

$$G(\omega) \equiv 1 - \sum_{j=1}^{N} \frac{g_j^2 m_r \omega_j^2}{m_j (\omega_j^2 - \omega^2)}.$$
 (162)

The quantity  $\lambda(\omega)$  is defined as

$$\lambda(\omega) \equiv -m_{\rm r}\omega^2 + m\omega_0^2 G(\omega). \tag{163}$$

With these definitions, one has

$$\alpha_{\rho\gamma}(\omega) \equiv \frac{\left[ (\lambda(\omega))^2 \delta_{\rho\gamma} - \left( \frac{\omega e G(\omega)}{c} \right)^2 B_{\rho} B_{\gamma} - \frac{i\omega\lambda(\omega)G(\omega)}{c} \epsilon_{\rho\gamma\eta} B_{\eta} \right]}{\text{Det } D(\omega)}, \tag{164}$$

and

Det 
$$D(\omega) = \lambda(\omega) \left[ (\lambda(\omega))^2 - \left( \frac{\omega e B G(\omega)}{c} \right)^2 \right],$$
 (165)

where  $\epsilon_{\rho\sigma\eta}$  is the Levi-Civita symbol.

In order to make the role of magnetic field explicit, we write

Det 
$$\alpha(\omega) = \left[\alpha^{(0)}(\omega)\right]^3 \left[1 - \left(\frac{\omega BeG(\omega)}{c}\right)^2 \left[\alpha^{(0)}(\omega)\right]^2\right]^{-1},$$
 (166)

where

$$\alpha^{(0)}(\omega) = \frac{1}{m_{\rm r}(\omega_0^2 - \omega^2) - i\omega\widetilde{\mu}_{\rm d}(\omega)}$$
(167)

is the susceptibility in the absence of the magnetic field and  $\widetilde{\mu}_{d}(\omega)$  is the diagonal part of memory function. Using Eq. (166) in Eq. (160), we get

$$F_U(T,B) = F_U(T,0) + \Delta_1 F_U(T,B) + \Delta_2 F_U(T,B), \tag{168}$$

where

$$F_U(T,0) = \frac{3}{\pi} \int_0^\infty d\omega \ f(\omega, T) \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln \left[ \alpha^{(0)}(\omega + \mathrm{i}0^+) \right] \right]$$
 (169)

is the free energy of the charged particle in the absence of the magnetic field, which is just 3 times that given in Eq. (107). The contribution from the field is contained in the two terms  $\Delta_1 F_U(T, B)$  and  $\Delta_2 F_U(T, B)$ , given by

$$\Delta_1 F_U(T, B) = -\frac{1}{\pi} \int_0^\infty d\omega \ f(\omega, T) \operatorname{Im} \left[ \frac{\mathrm{d}}{\mathrm{d}\omega} \ln \left\{ 1 - (G(\omega))^2 \left( \frac{\omega B e}{c} \right)^2 \left[ \alpha^{(0)} (\omega + \mathrm{i}0^+) \right]^2 \right\} \right], \tag{170}$$

and

$$\Delta_2 F_U(T, B) = \frac{1}{\pi} \int_0^\infty d\omega \ f(\omega, T) \operatorname{Im} \left[ \left[ \alpha^{(0)}(\omega + i0^+) \right]^2 \left( \frac{\omega e B}{c} \right)^2 \right] \times \left( \frac{d(G(\omega))^2}{d\omega} \right) \left\{ 1 - \left( \frac{\omega B e G(\omega)}{c} \right)^2 \left[ \alpha^{(0)}(\omega + i0^+) \right]^2 \right\}^{-1} \right].$$
(171)

Let us now consider a concrete example of a heat bath spectrum and find the low temperature characteristics of the free energy. We consider the case

$$\widetilde{\mu}_{\mathbf{d}}(\omega) = m_{\mathbf{r}} \gamma^{1-\nu} (-i\omega)^{\nu}, \quad -1 < \nu < 1, \tag{172}$$

where  $\gamma$  is a positive constant with the dimensions of frequency and  $\nu$  is within the indicated range so that  $\widetilde{\mu}(\omega)$  is a positive real function [66]. The Ohmic, sub-Ohmic and super-Ohmic heat baths are defined by the conditions  $\nu=0$ ,  $-1<\nu<0$  and  $0<\nu<1$ , respectively. For this case, one may show that one has the leading low-temperature behavior

$$F_U(T) = -3\Gamma(\nu+2)\zeta(\nu+2)\cos\left(\frac{\nu\pi}{2}\right)\frac{\hbar\gamma^3}{\pi\omega_0^2}\left(\frac{k_BT}{\hbar\gamma}\right)^{\nu+2},\tag{173}$$

where  $\Gamma(z)$  is the gamma function, while  $\zeta(z)$  is the Riemann zeta function. Thus, the free energy at low temperatures is  $F_U(T) \sim T^{\nu+2}$ , meaning that one has the entropy  $S = -\partial F_U(T)/\partial T \to 0$  as  $T \to 0$ , in agreement with the third law. For Ohmic dissipation  $(\nu = 0)$ , we have the power-law behavior  $S(T) \sim T$ , which matches with that discussed in Section 5.2 for the case of coordinate-coordinate coupling.

# 8. Path-integral approach to thermodynamics

In this section, we will very briefly outline an approach aimed at studying equilibrium thermodynamics of the quantum Brownian motion in a harmonic well, which is different from the one discussed in the preceding sections. In the previous sections, our starting point was a microscopic Hamiltonian describing the dynamics of the system and the bath, together with their interactions. Subsequently, the equations of motion for the bath variables were solved and substituted into that of the system to yield the quantum Langevin equation given in Eqs. (51) and (124). Thermodynamic quantities were then obtained primarily from equilibrium correlation functions computed using the quantum Langevin equation.

A rather different approach to describing the thermodynamics of the system at hand (quantum Brownian motion in a harmonic well) is to construct a consistent Gibbs distribution (and hence a partition function) by tracing over the degrees of freedom of the heat bath. In order to do so, we shall use the imaginary-time path integral formalism. While we are going to be very brief here and shall skip most of the details, the reader is referred to Refs. [12, 13, 76, 77] (see also Refs. [25, 78]) for a rather detailed treatment. The reader is also encouraged to look at Refs. [79, 80] (see also Ref. [57]) for a general introduction to path integrals.

We begin by recalling that when a system described by some generic Hamiltonian H is in equilibrium with temperature  $T = 1/k_B\beta$ , the density matrix  $\rho$  describing the equilibrium state of the system is given by

$$\rho(x, x') = \frac{\langle x | e^{-\beta H} | x' \rangle}{Z}; \quad Z = \int dx \, \langle x | e^{-\beta H} | x \rangle, \tag{174}$$

in the position representation, and where the normalization Z is the partition function. Let us compare the above expression with that of the quantum-mechanical propagator K(x,t;x',0) in the position representation, which gives the probability amplitude to be in state  $|x\rangle$  at time t>0 while starting from the state  $|x'\rangle$  at time t=0:

$$K(x,t;x',0) = \langle x|e^{-iHt/\hbar}|x'\rangle. \tag{175}$$

On comparison, we may make the identification  $it = \beta \hbar$ , or, in other words, we obtain a correspondence between inverse temperature and imaginary time! In what follows, we will set  $\hbar = 1$  for the sake of convenience, so that inverse temperature may be identified with  $\beta = \sigma \equiv it$ .

Let us recall that the propagator K(x, t; x', 0) can also be expressed as the path integral, that is, we have [79, 80]

$$K(x,t;x',0) = \int_{\bar{x}(0)=x'}^{\bar{x}(t)=x} \mathcal{D}[\bar{x}]e^{i\mathcal{S}[\bar{x}]},$$
(176)

where  $S[\bar{x}]$  is the action functional, and the integration is over all possible paths joining the two end points. Here, a path is denoted as  $\bar{x}(t)$ . For a Hamiltonian of the form  $H = p^2/2m + V(x)$ , the action is

$$S = \int_0^{-i\beta} dt \left[ \frac{m}{2} \left( \frac{dx}{dt} \right)^2 - V(x) \right]. \tag{177}$$

The classical path between an initial and a final point is one that extremizes this action. Now, if we put  $t = -i\sigma$ , then we get

$$S \to iS^{(E)} = i \int_0^\beta d\sigma \left[ \frac{m}{2} \left( \frac{dx}{d\sigma} \right)^2 + V(x) \right],$$
 (178)

where  $\mathcal{S}^{(E)}$  is called the Euclidean action. Thus, the dynamics of the system in real time t with potential V(x) is equivalent to the dynamics of the system in imaginary time  $\sigma$  with an inverted potential -V(x), with  $x = x(\sigma)$ . Using the Euclidean action, one may then obtain the density matrix (up to a normalization) as

$$\langle x|e^{-\beta H}|x'\rangle = \int_{\bar{x}(0)=x'}^{\bar{x}(\beta)=x} \mathcal{D}[\bar{x}]e^{-\mathcal{S}^{E[\bar{x}]}}.$$
 (179)

Thus, computing the partition function requires evaluation of an imaginary time path integral. Once the quantity  $\langle x|e^{-\beta H}|x'\rangle$  has been calculated using the path integral, the partition function is straightforwardly calculated using the second equation in Eq. (174).

For the our system of quantum Brownian motion in a harmonic well, whose Hamiltonian summarizing the dynamics of the system, the heat bath and the interactions among them is given by Eq. (49), one may check that the Euclidean action reads as

 $\mathcal{S}^{(E)} = \mathcal{S}_{\mathrm{S}}^{(E)} + \mathcal{S}_{\mathrm{B}}^{(E)} + \mathcal{S}_{\mathrm{SB}}^{(E)}$ , where

$$S_{\rm S}^{(E)} = \int_0^\beta d\sigma \left[ \frac{m}{2} \left( \frac{d\bar{x}}{d\sigma} \right)^2 + \frac{m\omega^2 \bar{x}^2}{2} \right], \tag{180}$$

$$S_{\rm B}^{(E)} = \int_0^\beta d\sigma \sum_{j=1}^N \left[ \frac{m_j}{2} \left( \frac{d\bar{q}_j}{d\sigma} \right)^2 + \frac{m_j \omega_j^2 \bar{q}_j^2}{2} \right], \tag{181}$$

$$S_{SB}^{(E)} = \int_0^\beta d\sigma \left[ -\bar{x} \sum_{j=1}^N c_j \bar{q}_j + \bar{x}^2 \sum_{j=1}^N \frac{c_j^2}{2m_j \omega_j^2} \right].$$
 (182)

Let us define  $\mathcal{S}_{B+SB}^{(E)}$  as  $\mathcal{S}_{B+SB}^{(E)} \equiv \mathcal{S}_{B}^{(E)} + \mathcal{S}_{SB}^{(E)}$ . The reduced density matrix  $\rho_{S}$  for our system can be obtained by taking a trace over the bath degrees of freedom. It turns out that we may express  $\rho_{S}$  as

$$\rho_{\rm S} = \frac{1}{Z_{\rm S}} \int \mathcal{D}[\bar{x}] e^{-\mathcal{S}_{\rm S}^{(E)}[\bar{x}]} \mathcal{F}[\bar{x}], \tag{183}$$

where  $\mathcal{F}[\bar{x}]$  is known as the influence functional [12, 77], and the function  $Z_{\rm S}$  is the reduced partition function which differs from the full partition function Z that normalizes the full density matrix  $\rho$ . The influence functional is given by

$$\mathcal{F}[\bar{x}] = \prod_{j} \frac{\mathcal{F}_{j}[\bar{x}]}{Z_{j}},\tag{184}$$

with  $Z_j \equiv [2\sinh(\beta\omega_j/2)]^{-1}$  being the well known canonical partition function of an isolated bath oscillator. The form of  $\mathcal{F}_j[\bar{x}]$  is

$$\mathcal{F}_{j}[\bar{x}] \equiv \int dq_{j} \oint \mathcal{D}[\bar{q}_{j}] e^{-\mathcal{S}_{B+SB}^{(E)}[\bar{x},\bar{q}_{j}]}.$$
 (185)

In Eqs. (183) and (185) above, the paths run from  $\bar{x}(0) = x'$  and  $\bar{q}_j(0) = q'_j$  to  $\bar{x}(\beta) = x$  and  $\bar{q}_j(\beta) = q_j$ , and the closed integration symbol appearing in Eq. (185) implies that we need to integrate over closed paths  $\bar{q}_j(0) = \bar{q}_j(\beta) = q_j$  while performing the trace over the bath degrees of freedom. Since the paths  $\bar{x}(\sigma)$  and  $\bar{q}_j(\sigma)$  are associated with a periodicity  $\beta$ , let us consider their Fourier mode expansions:

$$\bar{x}(\sigma) = \sum_{n=1}^{\infty} \tilde{x}(\nu_n) e^{-i\nu_n \sigma}, \quad \bar{q}_j(\sigma) = \sum_{n=1}^{\infty} \tilde{q}_j(\nu_n) e^{-i\nu_n \sigma}, \quad (186)$$

where  $\nu_n = 2\pi n/\beta$  are the bosonic Matsubara frequencies that we have encountered earlier. Substituting these into Eqs. (183) and (185), one finds the following expression for the partition function  $Z_{\rm S}$  that normalizes  $\rho_{\rm S}$  (see Ref. [77] for the detailed calculation):

$$Z_{\rm S} = \frac{1}{\beta \omega_0} \prod_{n=1}^{\infty} \frac{\nu_n^2}{\nu_n^2 + \omega_0^2 + \nu_n \hat{\gamma}(\nu_n)},$$
 (187)

where

$$\hat{\gamma}(\nu_n) = \frac{2}{m\pi} \int_0^\infty d\omega \, \frac{J(\omega)}{\omega} \frac{\nu_n^2}{\nu_n^2 + \omega^2}$$
(188)

specifies the particular dissipation mechanism. The free energy  $F_{\rm S}(T) = -\beta^{-1} \ln Z_{\rm S}$  is then easily obtained as

$$F_{\rm S}(T) = \frac{1}{\beta} \ln(\beta \omega_0) - \frac{1}{\beta} \sum_{n=0}^{\infty} \ln\left[\frac{\nu_n^2}{\nu_n^2 + \omega_0^2 + \nu_n \hat{\gamma}(\nu_n)}\right]. \tag{189}$$

Thermodynamic quantities can now be computed straightforwardly. For instance, the mean energy can be computed as

$$E_{\rm S}(T) = -\frac{\partial}{\partial \beta} \ln Z_{\rm S}. \tag{190}$$

A similar treatment can be performed with the two-dimensional quantum Brownian oscillator in the presence of a magnetic field [78]. The equilibrium magnetization obtained from the partition function reported in [78] is

$$M_z = -\frac{4}{\beta B} \sum_{n=1}^{\infty} \frac{\omega_c^2 \nu_n^2}{(\nu_n^2 + \omega_0^2 + \nu_n \widetilde{\gamma}(\nu_n))^2 + \omega_c^2 \nu_n^2},$$
(191)

which for Ohmic dissipation agrees exactly with Eq. (130) that has been obtained via the equation-of-motion approach [81]. We refer the reader to Refs. [24, 25, 26, 38, 78] for thermodynamic results for the quantum Brownian oscillator. We conclude this section by mentioning that the computation of the influence functional and the corresponding partition function in the case of momentum-momentum coupling [Section 7] is still an open problem.

#### 9. Stochastic thermodynamics

Until now we have discussed equilibrium phenomena within the paradigm of quantum Brownian motion. The method of calculation has hinged on a quantum Langevin equation that is based on equations of motion of dynamical variables, much as in the Heisenberg picture of quantum mechanics. This is in contrast to the Schrödinger picture that applies to the path integral formulation of the density operator, briefly touched upon in Section 8. The Langevin equation constitutes a convenient and physically motivated theoretical machinery to handle nonequilibrium phenomena. Additionally, it provides a different way of doing equilibrium statistical mechanics than the usual ensemble approach, as physical quantities in equilibrium, such as the internal energy, the free energy, etc. can be retrieved from the asymptotic solutions when the time approaches infinity  $(t \to \infty)$ , with the proviso that consistency conditions, e.g., fluctuation-dissipation theorems, are built-in, at the outset. This fact was exemplified in Sections 4 – 7. The underlying principle of recovering equilibrium statistical mechanics from a time-dependent set of equations that models quantum Brownian motion had prompted Kadanoff to dub the aforesaid method as the "Einstein approach," distinct from the "Gibbs approach" to doing statistical mechanics [82].

Standard thermodynamics, considered as the mother of all sciences – physics, chemistry and biology – pertains to a system in equilibrium. The underlying import of the cliche "equilibrium" is that all fields such as the temperature, the pressure, the magnetic field, the electric field, etc., are held fixed and the system is allowed sufficient time so that all dynamical variables, e.g., position, momentum and their functions, attain values that are on the average constant in time. If any of the above- mentioned fields is changed to another value, the system in general is expected to come to a new equilibrium after a time much longer than what is known as the "relaxation time," akin to the inverse of the friction coefficient  $\gamma$  appearing in a Langevin equation for Brownian motion, as discussed before. Standard thermodynamics, however, does not touch upon the origin of the relaxation time or the time evolution of the system. On the other hand, when we come to systems that are so tiny that they are hardly ever in equilibrium, there is a need to go beyond standard thermodynamics and treat fluctuating, time-dependent effects.

Given this background, and also the axiom that (microscopic) statistical mechanics provides the base for (macroscopic) thermodynamics, a natural question may arise: Can the time-dependent Langevin equations be effectively utilized to formulate a theory for a "time-dependent thermodynamics"? Such time-dependencies would evidently encompass fluctuations in thermodynamic quantities when the system is far from equilibrium. Thus, these fluctuations are very distinct from fluctuations around an equilibrium, which can be probed through "linear response". Usually, fluctuations in thermodynamic variables are considered "small" for macroscopic objects. However, recently, there has been an upsurge of interest in observing the behavior of nanoscale systems, especially in biology, comprising cell motion, biopolymers, colloidal suspensions, molecular motors, "active" matter, nano engines, and so on. While the aforesaid systems belong to the realm of classical thermodynamics, there are issues in solid state systems of nano junctions, q-bits etc., classified as mesoscopics, that require generalization of equilibrium thermodynamics to the nonequilibrium regime.

The above considerations then motivated, first Sekimoto [83] and subsequently, Seifert [84] (see also Refs. [85, 86, 87, 88, 89, 90, 91]), to put forward what they called "stochastic thermodynamics". Because the Langevin equations subsume the stochastic fluctuations induced by the environment, they are omnipresent in the basic building blocks of stochastic thermodynamics. Therefore, we will employ much of what we already discussed in presenting this new approach to thermodynamics, first in the realm of classical physics in Sections 9.1 and 9.2, and then extend the analysis to the quantum domain in Section 9.3. For illustrative purposes, we will use the already-familiar model of the one-dimensional harmonic oscillator, treated extensively earlier in the review.

#### 9.1. Classical stochastic thermodynamics

Recall that the first two laws of thermodynamics can be combined to write the incremental work, specified by the symbol  $\Delta$  prefixing the work W, as

$$\Delta W = T dS - dE = -dF - S dT, \tag{192}$$

where T is the temperature, S is the entropy, E is the internal energy and F is the Helmholtz free energy. In contrast to  $\Delta$ , the symbol 'd' indicates perfect (exact) differentials. Note that all the thermodynamic quantities on the right of Eq. (192) have microscopic meaning in terms of statistical mechanics, as in

$$k_B T \sim \langle K. E. \rangle, \quad S = k_B \ln \Omega,$$
 (193)

$$F = -k_B T \ln Z, \quad E = k_B T^2 \frac{\partial}{\partial T} \ln Z, \tag{194}$$

where  $\langle K. E. \rangle$  denotes the statistical average of the kinetic energy (abbreviated as K.E.),  $\Omega$  is the number of accessible microstates, and Z is the canonical partition function. Interestingly, the Boltzmann constant  $k_B$  occurs in all the equalities above, underscoring the towering and pioneering presence of Boltzmann in the formulation of thermodynamics, kinetic theory and statistical mechanics. The meaning of the partial derivative with respect to T is that in the process, all other variables such as volume, pressure, etc., are kept fixed. It is evident that the quantities E and F contain the complete (and essential) link via the partition function Z between thermodynamics and statistical mechanics.

If we examine Eq. (192), it is evident that the work done by, say an engine, can be computed by simply integrating E over an iso-entropic process or by integrating F over an isothermal process. On the other hand, E and F can be independently calculated in equilibrium via Z. It should be added that  $\Delta W$  itself is determined by P dV (for mechanical work) or -B dM (for magnetic work) or  $\mathcal{E} d\Pi$  (for electrical work). Here P is the pressure, V is the volume, B is the magnetic field, M is the magnetization,  $\mathcal{E}$  is the electrical field, and  $\Pi$  is the electric polarization.

With this brief summary of standard thermodynamics and its connection to statistical mechanics, we revisit the classical memory-less Langevin equation with constant friction  $\gamma$ , Eq. (2), with an additional potential term, i.e.,

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = -\frac{\mathrm{d}V(x)}{\mathrm{d}x} - \gamma p(t) + f(t),\tag{195}$$

where all symbols have their usual meaning. The Sekimoto stratagem is to assume that the state of the system is altered by a small amount dx. Multiplying the forces in Eq. (195) by (-dx) would then represent the energy balance:

$$-\left(\frac{\mathrm{d}p(t)}{\mathrm{d}t}\right)\mathrm{d}x = \left(\frac{\mathrm{d}V(x)}{\mathrm{d}x}\right)\mathrm{d}x - \left[-\gamma p(t) + f(t)\right]\mathrm{d}x. \tag{196}$$

Here the terms within the square brackets represent the forces due to the interaction between the system and the heat bath, with  $-\gamma p(t)$  being the systematic damping force and f(t) the remainder of the fluctuating force.

We may now manipulate the LHS of Eq. (196) and rewrite it for incremental changes as

$$-\Delta p \left(\frac{\Delta x}{\Delta t}\right) = -\mathrm{d}(p^2/2m). \tag{197}$$

Imagine at this stage that the potential energy V(x) depends on not just the coordinate of the system but also on another parameter 'a' that can be independently varied. An explicit example of 'a' will be given in the next subsection. Thus, we write

$$dV(x,a) = \left(\frac{\partial V(x,a)}{\partial x}\right)_{a} dx + \left(\frac{\partial V(x,a)}{\partial a}\right)_{x} da, \tag{198}$$

which implies that the first term on the RHS of Eq. (196) will have to be modified to  $dV(x, a) - (\partial V(x, a)/\partial a))_x da$ , thus yielding from Eqs. (196) and (197) that

$$0 = dH - \left(\frac{\partial V(x, a)}{\partial a}\right)_x da - \left[-\gamma p(t) + f(t)\right] dx, \tag{199}$$

where H is the Hamiltonian given by

$$H = \frac{p^2}{2m} + V(x, a). {(200)}$$

Given that the internal energy E connotes to the "statistical" average of H, i.e.,  $\langle H \rangle$ , Eq. (199) can be re-interpreted as the law of thermodynamics vis à vis Eq. (192), if we recognize that  $-(\partial V(x,a)/\partial a)_x da$  is the incremental work done by the system. Thus, we reach the following identification as far as stochastic thermodynamics is concerned:

$$\Delta W = \Delta Q - dE, \tag{201}$$

where we have

$$dE = d(p^2/2m + V(x, a)), (202)$$

$$\Delta W = -\left(\frac{\partial V(x,a)}{\partial a}\right)_x da,\tag{203}$$

$$\Delta Q = \left[ -\gamma p(t) + f(t) \right] dx. \tag{204}$$

The basic thermodynamic principle is thus nicely encapsulated under Eq. (201); the useful work done by the system is the heat dumped into it by the external bath minus the increase in its internal energy. It must be underscored, however, that unlike standard thermodynamics, all the quantities appearing on the right hand sides of Eqs. (202) – (204) are fluctuating stochastic processes, which would have to be treated with the aid of the underlying probability distributions. We shall illustrate this novel formulation by means of the familiar example of a harmonic oscillator, in the subsection below.

#### 9.2. Harmonic oscillator as a classical nano engine

We envisage our system to be a nano harmonic oscillator of mass m and with frequency  $\omega_0$  that can be varied with time. The potential energy is given by

$$V(x,a) = \frac{ax^2}{2} = \frac{m\omega_0^2 x^2}{2},\tag{205}$$

where we have  $a = m\omega_0^2$ . The standard thermodynamic scenario is that the particle endowed with a constant frequency  $\omega_0$  is kept in contact with a heat bath comprising a large system of many degrees of freedom and in equilibrium at a constant temperature T. In stochastic thermodynamics, however, we will take T, just as  $\omega_0$ , to be also time-dependent. The scales on which these variations take place would yield different results in different regimes of experimental timescales at hand. Before proceeding further, we summarize the well-known results for the thermodynamic potentials, which can be derived from the underlying classical partition function Z. Thus, we have

$$E = k_B T, \quad F = k_B T \ln\left(\frac{\hbar\omega_0}{k_B T}\right), \quad S = k_B \left[1 - \ln\left(\frac{\hbar\omega_0}{k_B T}\right)\right].$$
 (206)

The expression for the internal energy is just the statement of the equipartition theorem, indicated cryptically in the first equality of Eq. (194). Next, we observe that in the classical formulae for F and S, the Planck constant  $\hbar$  still shows up, merely though as a normalization constant in the phase space integrals as far as the partition function Z is concerned. Evidently, S depends on the temperature only though the dimensionless ratio  $\alpha = \hbar \omega_0/k_B T$ , which must be kept fixed for an isoentropic process; hence, if  $\omega_0$  has a time variation so must have T. Further, in standard thermodynamics, we have

$$dF = -SdT - PdV, (207)$$

which signifies that F should be regarded as a function of two variables T and V. It is then appropriate to say that a variation in  $\omega_0$  is tantamount to a change in V; conversely, an isochoric process is the one in which  $\omega_0$  is kept fixed.

In what follows, we will apply the formalism developed here to calculate the efficiency of a Stirling engine, first from standard thermodynamics and then from stochastic thermodynamics in the stationary state, in order to have a consistency check. We choose the Stirling engine in preference to the more familiar Carnot cycle because for the former, the efficiency is different in the classical and quantum situations, even in the stationary state. A schematic of the Stirling cycle is shown below.

$$\omega_1, T_c$$
 Isothermal  $\omega_2, T_c$ 

$$3 \longrightarrow 4$$
Isochoric  $\uparrow \qquad \downarrow \qquad$  Isochoric
$$2 \longleftarrow 1$$

$$\omega_1, T_h \qquad \text{Isothermal} \qquad \omega_2, T_h$$

$$\omega_2 > \omega_1, T_h > T_c$$

In the calculations involving the Stirling cycle, while referring to specific values of the trap frequency  $\omega_0$  at points '1' and '2', we will drop the subscript '0' and use the notation  $\omega_1$  and  $\omega_2$  respectively. Now, the net work done is given by

$$W = W_{1\to 2} + W_{3\to 4}. (208)$$

Referring to the discussion below Eq. (192), it is clear that

$$W = -\left[F(\omega_1, T_h) - F(\omega_2, T_h)\right] - \left[F(\omega_2, T_c) - F(\omega_1, T_c)\right]$$
$$= k_B(T_h - T_c) \ln\left(\frac{\omega_2}{\omega_1}\right). \tag{209}$$

On the other hand, the heat transferred from the hot source is given by

$$Q = [E_{1\to 2} + E_{4\to 1}] + W_{1\to 2}$$
  
=  $0 + k_B \left(\frac{T_h - T_c}{2}\right) + k_B T_h \ln\left(\frac{\omega_2}{\omega_1}\right).$  (210)

There is the presence of an apparently mysterious factor of one-half in the internal energy-change  $E_{4\to 1}$ , the justification for which only emanates post facto from stochastic considerations (see below). Combining Eqs. (209) and (210), we obtain for the efficiency of the Stirling cycle the result

$$\eta_{\rm S}^{\rm (cl)} = \frac{W}{Q} = \eta_C \left[ 1 + \frac{\eta_C}{\ln(\omega_2/\omega_1)} \right]^{-1},$$
(211)

where  $\eta_C = 1 - T_c/T_h$  is the Carnot efficiency.

We now turn to the efficiency computation from stochastic thermodynamics and demonstrate that in the stationary state, the answer matches with Eq. (211). The incremental work operator is now given by

$$\Delta W = -m\omega_0 x^2 d\omega_0. \tag{212}$$

From Eq. (208), we have

$$W = -\int_{\omega_1}^{\omega_2} d\omega \frac{\langle m\omega^2 x^2 \rangle_{T_c}}{\omega} + \int_{\omega_1}^{\omega_2} d\omega \frac{\langle m\omega^2 x^2 \rangle_{T_h}}{\omega}$$
$$= k_B (T_h - T_c) \ln \left(\frac{\omega_2}{\omega_1}\right), \tag{213}$$

where in the last step, we have employed the classical equipartition theorem in extracting the angular bracketed quantities in the integrands. As expected, this result agrees with Eq. (209). Next, in computing the heat gained from the hot source in the stationary state, we need  $E_{1\to 2} + E_{4\to 1}$  (cf., Eq. (210)). We have

$$E_{1\to 2} = \int_{1}^{2} d(p^2/2m + m\omega_0^2 x^2/2) = 0, \tag{214}$$

having used the equipartition theorem again and the fact that the temperature is the same at points '1' and '2'. However, in  $E_{4\rightarrow 1}$ , we use only the input from the kinetic

energy, again goaded by considerations behind the factor of half, alluded to in the sentence following Eq. (210):

$$E_{4\to 1} = \int_4^1 d(p^2/2m) = \frac{k_B(T_h - T_c)}{2}.$$
 (215)

Thus, we have

$$Q = [E_{1\to 2} + E_{4\to 1}] + W_{1\to 2}$$
  
=  $\frac{k_B(T_h - T_c)}{2} + k_B T_h \ln\left(\frac{\omega_2}{\omega_1}\right),$  (216)

where  $W_{1\to 2}$  has already been calculated in the second integral in Eq. (213). Once again, this agrees with the expression in Eq. (210), confirming that the stationary-state result for the efficiency in stochastic thermodynamics must conform to standard thermodynamics.

Summing up, the subject of stochastic thermodynamics takes us beyond standard thermodynamics and hence incorporates in a natural manner the dissipative parameters. *Inter alia*, it provides a framework in which thermodynamic potentials like the internal energy and the free energy are given new meaning in terms of dynamics. The appropriate dynamical equation is the Langevin equation, which is at the heart of the Brownian motion. Though fluctuations in thermodynamic variables are not explicitly treated in the example in this section, as we have restricted our analysis to the stationary state, we will return to these nonequilibrium features when we take up the quantum case in the next subsection.

#### 9.3. Quantum stochasticity beyond stationary state

First of all, we intend to rewrite the classical thermodynamic potentials in their quantal forms, i.e.,

$$E = \hbar\omega_0 \left[ n(\omega_0, T) + \frac{1}{2} \right],\tag{217}$$

$$F = k_B T \ln \left[ 2 \sinh \left( \frac{\hbar \omega_0}{2k_B T} \right) \right], \tag{218}$$

$$S = k_B \left\{ [n(\omega_0, T) + 1] \ln[n(\omega_0, T) + 1] - n(\omega_0, T) \ln n(\omega_0, T) \right\}.$$
 (219)

In the above equations,  $n(\omega_0, T)$  is the Bose factor, defined as

$$n(\omega_0, T) \equiv \frac{1}{e^{\hbar \omega_0 / k_B T} - 1}.$$
 (220)

The quantum-mechanical calculation for the efficiency of the Stirling engine in standard thermodynamics follows exactly the same route as in the classical case. We will have to simply substitute the internal energy and free energy results, i.e., Eqs. (217) and (217),

into our earlier expressions for the work done and heat transfer, in Eqs. (209) and (210) respectively. We find

$$\eta_{\rm S}^{({\rm qu})} = \left(1 - \frac{T_c}{T_h}\right) \left[1 + \frac{X}{Y}\right]^{-1},$$
(221)

with

$$X = \frac{\beta_h}{2} \left\{ \hbar \omega_1 \coth\left(\frac{\beta_h \hbar \omega_1}{2}\right) - \frac{\hbar \omega_2}{2} \left[ \coth\left(\frac{\beta_h \hbar \omega_2}{2}\right) + \coth\left(\frac{\beta_c \hbar \omega_1}{2}\right) \right] \right\}, \quad (222)$$

and that

$$Y = \ln \left\{ \frac{\sinh\left(\frac{\beta_h \hbar \omega_1}{2}\right)}{\sinh\left(\frac{\beta_h \hbar \omega_2}{2}\right)} \right\},\tag{223}$$

where we have  $\beta_h = 1/k_B T_h$  and  $\beta_c = 1/k_B T_c$ . Evidently, in the classical limit, i.e.  $\beta\hbar\omega \ll 1$ , the efficiency defined above approaches  $\eta_{\rm S}^{\rm (cl)}$  defined in Eq. (211).

We now turn our attention to time-dependent effects à la the quantum Langevin equation appropriate to the stochastic thermodynamics of a quantum harmonic oscillator. This equation has the same structure as its classical counterpart in Eq. (195), supplemented by the constitutive relations dx(t)/dt = p(t) and  $V(x) = (1/2)ax^2$ , with however the important proviso that the quantities p, x, f(t) are all quantum operators with prescribed commutation properties. Further, the noise force is also an operator f(t) with the following autocorrelation:

$$\langle f(t)f(t')\rangle = 2D\delta(t-t'),$$
 (224)

where we have  $D = m\gamma\hbar\omega_0 \coth{(\beta\hbar\omega_0/2)}$ . Two distinct remarks are in order with regard to the form of the systematic damping term  $-\gamma p(t)$  as well as the noise correlation. First of all, as we have seen earlier, the fact that the damping is constant emanates from a memory-less Langevin equation, which emerges from a specific choice of the spectral properties of the bath called the Ohmic dissipation. Second, it may be reiterated that our earlier derivation of the quantum Langevin equation, based on a microscopic system-plus-bath approach, was in some way exact in that it made no assertion about the strength of the system-bath coupling. Thus, "strong dissipation" has already been incorporated in our earlier treatment. While such strong coupling results are of crucial consequences such as for the validity of the third law of thermodynamics, as alluded to in Section 5.2, the present quantum Langevin equation (as in Eq. (195)) is, on the other hand, based on "weak dissipation". It is pertinent to observe that in many applications to nonequilibrium phenomena, e.g., in quantum optics, it suffices to consider weak interaction between the system and the bath so that the latter can be treated in the Born approximation of the underlying master equation for the density operator. In addition, a Markovian assumption is made, which physically stipulates that the system timescales are much longer than those related to bath fluctuations. In the present instance, the system timescale is governed by the inverse of the harmonic oscillator frequency  $\omega_0$ , and hence, the Markovian assumption amounts to the neglect of

off-resonant terms. That is to say, only those frequencies of the bath fluctuations that are in resonance with  $\omega_0$  are considered relevant, justifying what is referred to as the "rotating wave approximation" (RWA). That is why the diffusion coefficient D, defined in terms of  $\omega_0$ , can be extricated out of the integrand in Eq. (61) in which it appears as a cotangent function of  $\beta\hbar\omega$ , with  $\omega$  being a typical bath frequency. For our present discussion on efficiencies of quantum engines, Eq. (195) turns out to be quite adequate and therefore, is investigated here in detail.

The Sekimoto scheme of writing the Langevin equation as in Eq. (199) still works, except that care has to be taken in maintaining the order of terms like pdx. The equation is rewritten here to set the ball rolling for further analysis of quantum stochasticity:

$$0 = dH - \left(\frac{\partial V(x, a)}{\partial a}\right)_x da - \left[-\gamma p(t) + f(t)\right] dx, \qquad (225)$$

leading to energy balance concomitant with thermodynamic interpretation of the energy, work and heat operators. Formally, the solution of the Langevin equation can be written as

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = M(t) \begin{pmatrix} x(0) \\ p(0) \end{pmatrix} + \int_0^t dt' \ M(t) M^{-1}(t') \begin{pmatrix} 0 \\ f(t')\sqrt{2}D(t') \end{pmatrix}, \tag{226}$$

where, in the spirit of stochastic thermodynamics, the diffusion coefficient D has been endowed with explicit time-dependence. Here the matrix M(t) solves the set of homogeneous equations  $\mathrm{d}x(t)/\mathrm{d}t = p(t)/m$  and  $\mathrm{d}p(t)/\mathrm{d}t = -m\omega_0^2x(t) - \gamma p(t)$ , or equivalently,

$$\frac{\mathrm{d}}{\mathrm{d}t} \begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 & 1/m \\ -m\omega_0^2 & -\gamma \end{pmatrix} \begin{pmatrix} x(t) \\ p(t) \end{pmatrix}. \tag{227}$$

When  $\omega_0$  is constant, the matrix M(t) can be obtained by exponentiating the  $2 \times 2$  matrix in Eq. (227). We find

$$M(t) = \begin{pmatrix} P & R \\ m \frac{\mathrm{d}P}{\mathrm{d}t} & m \frac{\mathrm{d}R}{\mathrm{d}t} \end{pmatrix},\tag{228}$$

where we have

$$P(t) = (\lambda_{+} - \lambda_{-})^{-1} [\lambda_{+} e^{-\lambda_{-}t} - \lambda_{-} e^{-\lambda_{+}t}], \tag{229}$$

while we have

$$R(t) = [m(\lambda_{+} - \lambda_{-})]^{-1} [e^{-\lambda_{-}t} - e^{-\lambda_{+}t}].$$
 (230)

In the above equations,  $\lambda_{\pm}$  are the eigenvalues of the  $2 \times 2$  matrix, given by (these were denoted  $z_{\pm}$  in Section 5)

$$\lambda_{\pm} = \frac{\gamma}{2} \pm \sqrt{\omega_0^2 - \frac{\gamma^2}{4}} i. \tag{231}$$

At this stage, it is important to clarify, upon looking at the eigenvalues, the nomenclature of under-damping ( $\gamma \ll \omega_0$ ) when the eigenvalues have an imaginary component, implying coherent quantum evolution), and over-damping ( $\gamma \gg \omega_0$ ). These different

regimes of damping are still treatable within the present weak-dissipation approach inherent in the Born approximation to the master equation.

While we have presented above the in-principle solutions of the quantum Langevin equations for a constant  $\omega_0$ , the full impact of stochastic thermodynamics can be assessed by delving into the transient domain in which timescale effects can be investigated. For this, it is interesting to follow a protocol in which the diffusion coefficient D is taken to vary with time as in

$$D(t) = D_0 + (D_1 - D_0)\frac{t}{\tau}, \quad 0 \le t \le \tau$$
  
=  $D_1, \quad t > \tau.$  (232)

Considering that the frequency  $\omega_0$  is held fixed, the protocol implies that we are dealing with an isochoric process of a Brownian engine when the latter is first (at t=0) put in contact with a heat bath at one fixed temperature corresponding to a diffusion constant  $D_0$  and then, the temperature is altered such that the diffusion coefficient linearly changes to a new value  $D_1$  without further change. In addition, in order to simplify the algebra, we go up to the time  $t=\tau$ , starting from t=0 and then stop the process. It is found that

$$\langle x^2(\tau) \rangle = \xi(\tau) \langle x^2 \rangle_0 + (1 - \xi(\tau)) \langle x^2 \rangle_1, \tag{233}$$

$$\langle p^2(\tau) \rangle = \zeta(\tau) \langle p^2 \rangle_0 + (1 - \zeta(\tau)) \langle p^2 \rangle_1, \tag{234}$$

where the subscripts 0 and 1 refer to the two diffusion constant values  $D_1$  and  $D_1$  respectively. If the time  $\tau$  is taken to  $\infty$ , both  $\xi(\tau)$  and  $\zeta(\tau)$  vanish and  $\langle x^2(\tau) \rangle$  and  $\langle p^2(\tau) \rangle$  reach their respective asymptotic values appropriate to  $D_1$ .

Furthermore, the parameters  $\xi(\tau)$  and  $\zeta(\tau)$  (at their fixed values at time  $t = \tau$ ) help allay the apparent ad-hoc prescription in computing  $E_{4\to 1}$ , first in the context of standard thermodynamics where we had an elusive factor of half, and then with regard to stochastic thermodynamics in the stationary state when we had dropped the contribution of  $m\omega_0^2\langle x^2\rangle/2$ . The point gets clarified when we compute  $E_{4\to 1}$  anew in the nonequilibrium situation depicted by Eq. (232), when we observe that

$$E_{4\to 1} = (1-\zeta)\frac{\langle p^2 \rangle_1 - \langle p^2 \rangle_4}{2m} + (1-\xi)\frac{m\omega_0^2}{2}(\langle x^2 \rangle_1 - \langle x^2 \rangle_4), \tag{235}$$

in which  $\xi$  and  $\zeta$  are their respective (constant) values at the time  $\tau$ . It is clear then that the second term disappears in the over-damped limit when we have  $\xi \to 1$  and  $\zeta \to 0$ . Thus, the apparent mystery alluded to at the beginning of this paragraph is resolved.

Because for a harmonic oscillator, in the weak-dissipation regime, we have  $\langle p^2 \rangle/2m = m\omega_0^2 \langle x^2 \rangle/2$ , and so Eq. (235) can be written in a more compact form as

$$E_{4\to 1} = 2\mu \frac{\langle p^2 \rangle_1 - \langle p^2 \rangle_4}{2m},\tag{236}$$

where  $\mu = 1 - \frac{\xi + \zeta}{2}$  parametrizes the emergence of nonequilibrium behavior in a phenomenological way, as the system transits from being decoupled from one bath to

being recoupled to another bath. While in the process of re-coupling, the bath remains in equilibrium at a temperature appropriate to  $D_2$ , the system has not had the time to equilibrate to the new situation. This is quite in contrast to standard thermodynamics, where it is assumed that the parameters at hand (such as the diffusion coefficient that subsumes the temperature and the frequency of the oscillator) is changed so slowly that at every stage of the transformation, the system comes to equilibrium with the bath. The nonequilibrium effect then generalizes Eqs. (211) and (221) for the efficiency of the Stirling engine, in the classical and quantal cases, respectively to

$$\eta_{\rm S}^{\rm (cl)} = \eta_C \left[ 1 + \frac{\mu \eta_C}{\ln(\omega_2/\omega_1)} \right]^{-1},$$
(237)

$$\eta_{\rm S}^{({\rm qu})} = \eta_C \left[ 1 + \frac{X^{({\rm qu})}}{Y} \right]^{-1},$$
(238)

where  $\eta_C$  is the Carnot efficiency, Y is given by Eq. (223), while  $X^{\mathrm{qu}}$  takes the form

$$X^{(\text{qu})} = \frac{\beta_h}{2} \left\{ \hbar \omega_1 \coth\left(\frac{\beta_h \hbar \omega_1}{2}\right) - \frac{\hbar \omega_2}{2} \left[ (1 - \mu) \coth\left(\frac{\beta_h \hbar \omega_2}{2}\right) + \mu \coth\left(\frac{\beta_c \hbar \omega_1}{2}\right) \right] \right\}. \tag{239}$$

In conclusion, our model of a Stirling engine as a nano quantum harmonic oscillator has enabled us to analytically calculate the efficiency, in standard thermodynamics and also in stochastic thermodynamics. The latter considerations have allowed us to go beyond stationary, equilibrium effects to transient, nonequilibrium domain, which throw light on the important role of a damping parameter that helps elucidate the computation of the internal energy with regard to dynamical evolution of the underlying system. Although we have treated here the Brownian motion of a quantum harmonic oscillator which was discussed earlier (Section 3), the analysis can be extended to the case of dissipative quantum cyclotron motion (Section 6), for the efficiency-computation of a corresponding Stirling engine in which, in addition to the frequency  $\omega_0$  of the trap, the external magnetic field emerges as a new parameter that can be independently varied. The cyclotron case paves the path for a natural extension of the one-dimensional treatment of the harmonic oscillator to two dimensions.

# 10. Fluctuation theorems

An important attribute of a quantum solid is its transport properties, as can be measured by subjecting it to a time-dependent external force field and examining the asymptotic, stationary-state response. Because of the omnipresent field, there is constant infusion of energy into the system so that even in the stationary state, the system is not in equilibrium. Thus, we are dealing here with an "open," out-of-equilibrium system. A case in point is the celebrated Drude-Ohm geometry, in which the system concerned is an electron subjected to a monochromatic frequency-dependent electrical conductivity. When the magnitude of the electric field is weak, as in the so-called "linear response" regime, the stationary-state electrical conductivity is given by the famous Kubo formula

that generalizes Eq. (18) to the frequency-dependent case:

$$\sigma(\omega) = e^2 \int_0^\infty dt \ e^{i\omega t} \langle v(0)v(t)\rangle_0, \tag{240}$$

where, e is the electron's charge,  $\omega$  is the frequency of the applied field  $E\cos(\omega t)$ , v(t) is the velocity of the electron at time t, and the angular brackets imply an autocorrelation of the velocity in the absence of the field, indicated by the subscript '0'.

Our classical Langevin treatment in Section 2 yields

$$\langle v(0)v(t)\rangle_0 = \frac{k_B T}{m} e^{-t/\tau},\tag{241}$$

with  $\tau$  being the Drude relaxation time and the pre-factor is the equipartition result. Equation (241) then leads to the complex conductivity

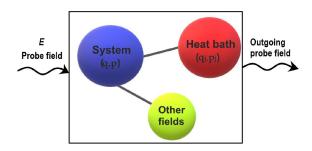
$$\sigma(\omega) = \frac{e^2 k_B T}{m} \frac{\tau (1 + i\omega \tau)}{1 + (\omega \tau)^2},$$
(242)

where the imaginary component is responsible for dissipation.

The question that we address now is: What happens when we go far beyond the linear response domain, and are there general relations akin to the Kubo formula for such nonlinear, nonequilibrium systems? Keeping the electron paradigm in mind the work done over a time t can be expressed as

$$W(t) = -e \int_0^t dt' \ E(t')v(t'), \tag{243}$$

where E(t) is an applied electric field (notation not be be confused with energy). Therefore, what we propose to study in this section is the statistical property of the stochastic process W(t) within the Brownian motion picture adopted in this review. Recall that we have already discussed the fluctuating properties of W(t) within stochastic thermodynamics in Section 9. However, as we underscored earlier, stochastic thermodynamics is based on the first and second laws of thermodynamics, which hinge on energy balance: the heat infused is distributed between the internal energy and the work done. For a driven system as depicted in Fig. 5, there is evidently no such (total) energy conservation. Thus, albeit the poser here is in the spirit of stochastic thermodynamics, we need to go beyond energy balance considerations, for driven/open thermodynamic systems. Interestingly, there have been important developments in recent years, primarily due to the efforts of Gallavoti, Cohen and Jarzynski [92, 93] in devising fluctuation theorems for the aforesaid systems, and we intend to provide here an overview. Once again, our model system is a Brownian particle, especially in the context of cyclotron motion – both classical (Section 10.1) and quantal (Section 10.2). As emphasized earlier, the cyclotron case is like that of a two-dimensional harmonic oscillator, and the presence of an extra dimension gives rise to possible "isometric" effects [94, 95, 96] in the context of fluctuation theorems.



**Figure 5.** Schematics of a typical (experimental) set-up. In the present model, the probe field is the electric field, and other fields include the magnetic field and a possible parabolic trap.

The Gallavoti-Cohen statement of the fluctuation theorem reads

$$\frac{p(-W)}{p(W)} = e^{-\alpha W},\tag{244}$$

where p(W) refers to the probability distribution of W. While in most thermodynamic applications, the constant  $\alpha$  does have the universal value of  $1/k_BT$ , we will assess below if there is any deviation from this, due to the two-dimensionality of cyclotron motion, which may involve an asymmetry in the diffusivity. For a one-dimensional process in which

$$W(t) = m \int_0^t dt' \ F(t')v(t'), \tag{245}$$

the theorem is easily proven as follows. Because v(t) for a Brownian particle is a Gaussian process [44] (see Section 2), so is W(t) and hence, the characteristic function C(h) defined by

$$C(h) = \langle e^{ihW} \rangle, \tag{246}$$

can be decomposed as

$$C(h) = e^{\mathrm{i}h\langle W \rangle} \langle e^{\mathrm{i}hm \int_0^t \mathrm{d}t' \ F(t')[v(t') - \langle v(t') \rangle]} \rangle$$

$$= e^{\mathrm{i}h\langle W \rangle} e^{-\frac{h^2 m^2}{2} \int_0^t \mathrm{d}t' \ \int_0^t \mathrm{d}t'' \ F(t')F(t')[\langle v(t')v(t'') \rangle - \langle v(t') \rangle \langle v(t'') \rangle]}, \tag{247}$$

where, in the last step, we have used the property of Gaussian processes as far as their cumulants are concerned [44], and have written

$$\langle W \rangle = m \int_0^t dt' \ F(t') \langle v(t') \rangle.$$
 (248)

Defining then the variance  $\sigma^2$  by the exponent in the second term in Eq. (247) we have

$$C(h) = e^{\mathrm{i}h\langle W\rangle} e^{\frac{-h^2\sigma^2}{2}}.$$
 (249)

Hence, p(W), which is the Fourier transform of C(h), is also Gaussian:

$$p(W) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{(W - \langle W \rangle)^2}{2\sigma^2}},$$
(250)

from which follows Eq. (244) if we identify

$$\alpha = \frac{2\langle W \rangle}{\sigma^2}.\tag{251}$$

It remains then to enquire into the structure of  $\alpha$ , as done in the next two subsections.

# 10.1. Fluctuation theorem for classical cyclotron motion

The Hamiltonian of an electron subject to a magnetic field  $\bf B$  along the z-axis is given by

$$H = \frac{(\mathbf{p} - \frac{e\mathbf{A}}{c})^2}{2m}.\tag{252}$$

In the symmetric gauge, the vector potential **A** has components

$$\mathbf{A} = \left(\frac{By}{2}, -\frac{Bx}{2}, 0\right). \tag{253}$$

The Langevin equations are given by [48]

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = v_j, \quad v_j = \frac{\left(p_j - \frac{eA_j}{c}\right)}{m},\tag{254}$$

$$\frac{\mathrm{d}v_j}{\mathrm{d}t} = -\gamma v_j - \omega_c \sum_k v_k S_{kj} + f_j, \tag{255}$$

where j = x, y, the quantity  $\gamma$  is the damping coefficient,  $\omega_c = eB/mc$  is the cyclotron frequency, and  $S = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ . The  $f_j$ 's are Gaussian processes with

$$\langle f_j(t)\rangle = 0, \quad \langle f_j(t)f_k(t')\rangle = 2m\gamma k_B T \delta_{j,k} \delta(t - t').$$
 (256)

In the stationary state, the Boltzmann distribution is proportional to  $e^{\frac{-m(v_x^2+v_y^2)}{2k_BT}}$  and hence, we have

$$\langle v_x^2 \rangle = \langle v_y^2 \rangle = \frac{k_B T}{m},\tag{257}$$

while  $\langle v_x v_y \rangle = 0$ . At this stage, we make a special assumption that the external force (an electric field in the present instance) is applied along the x-axis, as in the usual Drude geometry. As it turns out, the value of  $\alpha$  in the Gallavoti-Cohen fluctuation relation is contingent upon this stipulation and also that the damping  $\gamma$  has been chosen to be independent of the index j. The mean of the work variable then is

$$\langle W \rangle = m \int_0^t dt' \ F(t') \langle v_x(t') \rangle,$$
 (258)

where the average of  $\langle v_x(t') \rangle$  is to be obtained by solving the two-dimensional Langevin equations. The explicit solution for  $v_x(t)$  reads

$$v_x(t) = e^{-\gamma t} \int_0^t dt' \ e^{\gamma t} \left\{ \left( f_x(t') \cos[\omega_c(t - t')] - f_y(t') \sin[\omega_c(t - t')] \right) + F(t') \cos[\omega_c(t - t')] \right\}. \tag{259}$$

Hence, we have

$$\langle v_x(t)\rangle = e^{-\gamma t} \int_0^t dt' e^{\gamma t} F(t') \cos[\omega_c(t - t')], \tag{260}$$

and substituting this into Eq. (258) gives

$$\langle W \rangle = m \int_0^t dt'' \int_0^t dt'' F(t') F(t'') e^{-\gamma(t'-t'')} \cos[\omega_c(t-t')]. \tag{261}$$

On the other hand, the fluctuation in W is given by

$$\langle \sigma(t)^2 \rangle = m^2 \int_0^t dt' \int_0^t dt'' F(t') F(t'') \langle v_x(t') v_x(t'') \rangle. \tag{262}$$

We first write this double integral in a time ordered form by replacing the upper limit t of the second integral by t' and concomitantly introduce a pre-factor of 2. We then evaluate the velocity correlation from Eq. (259) by utilizing the noise correlation from Eq. (256), and compute the stationary state result as  $t', t'' \to \infty$ , while keeping t' - t'' finite. We thus find

$$\langle \sigma(t)^2 \rangle = 2mk_B T \int_0^t dt' \int_0^{t'} dt'' F(t') F(t'') e^{-\gamma(t'-t'')} \cos[\omega_c(t-t')], \qquad (263)$$

which, upon comparison with Eq. (258), gives

$$\langle \sigma(t)^2 \rangle = 2k_B T \langle W(t) \rangle.$$
 (264)

Finally, then the parameter  $\alpha$  turns out to be

$$\alpha = \frac{1}{k_B T},\tag{265}$$

validating the Gallavoti-Cohen fluctuation theorem in the present instance, even though the dissipative dynamics is in a four-dimensional space - two coordinates and two velocities. However, as emphasized earlier, if the friction coefficients are taken to be distinct for the motion along x and y, leading to anisotropic diffusion, the parameter  $\alpha$  would deviate from its universal value in Eq. (265), as is the case for isometric fluctuations [94, 95, 96].

#### 10.2. Fluctuation theorem for quantum cyclotron motion

In this section, we exemplify the application of the Gallavoti-Cohen fluctuation theorem to quantum phenomena with the aid of cyclotron motion. As our objective is limited to quantum Brownian motion, we begin the discussion with the corresponding quantum Langevin equations, which have the same structure as their classical counterparts in Eqs. (254) and (255):

$$\frac{\mathrm{d}x_j}{\mathrm{d}t} = v_j, \quad v_j = \frac{\left(p_j - \frac{eA_j}{c}\right)}{m},\tag{266}$$

$$\frac{\mathrm{d}v_j}{\mathrm{d}t} = -\gamma v_j - \omega_c \sum_k v_k S_{kj} + f_j, \tag{267}$$

with however the crucial proviso that the underlying variables are non-commuting quantum operators and that  $f_j$ 's are also quantum operators with the following correlation properties (see Eq. (256), for comparison):

$$\langle f_j(t)\rangle = 0, \quad \langle f_j(t)f_k(t')\rangle = 2m\gamma\hbar\omega_c \coth\left(\frac{\hbar\omega_c}{k_BT}\right)\delta_{j,k}\delta(t-t').$$
 (268)

The reader is referred to Eq. (224) for the corresponding relation for the noise correlation for a quantum harmonic oscillator (in which the oscillator frequency  $\omega_0$  occurs in place of the cyclotron frequency  $\omega_c$ ) and the detailed discussion thereafter. We have explained below Eq. (224) the reason for the appearance of the pre-factor in Eq. (224) that is based on the weak coupling (with the bath) and the RWA, prevalent in quantum optics. Evidently, this approximation is limited to the regime of large magnetic field  $\omega_c \gg \gamma$ . Incidentally, this is the regime in which quantum Hall measurements are carried out wherein the electrons predominantly occupy the lowest Landau levels.

Now comes the important issue of defining the work operator in quantum mechanics, the ambiguity of which has been discussed in the literature threadbare, as it is linked with the "measurement" problem. Here we follow the path of how quantum mechanics itself had evolved from classical mechanics wherein dynamical variables were replaced by operators with commutation relations emanating from the underlying Poisson brackets and so on [97]. Thus, assuming the Drude geometry in which the electric field E(t) (a classical field) is applied in the x-direction, we adopt the usual electrodynamics prescription of writing the work operator as

$$W(t) = -e \int_0^t dt' \ E(t')v_x(t'), \tag{269}$$

where, however, we have to remember the significant aspect that  $v_x(t)$  is a quantum operator which does not commute with itself at different times, and hence its proper time ordering is essential.

Interestingly, it is only the assumption of constant damping (arising from Ohmic dissipation) and not the RWA that needs to be invoked in calculating the mean work. Since the Langevin equations describing the dissipative cyclotron motion, i.e., Eqs. (266) and (267) have the same structure as the corresponding classical equations, i.e. Eqs. (254) and (255), the solution for  $v_x(t)$  in the quantum mechanical case is of the same form as given in Eq. (259) with F(t) = -eE(t)/m. Because even in the quantum case, the noise average is zero, the mean work is

$$\langle W(t) \rangle = m \int_0^t dt' \int_0^{t'} dt'' e^{-\gamma(t'-t'')} F(t') F(t'') \cos[\omega_c(t'-t'')],$$
 (270)

which is the same result as in the classical case.

On the other hand, the calculation for the fluctuation of W will in general be much more complicated [97] in the light of the generalized quantum Langevin equations discussed earlier, because of the non-Markovian nature of the noise correlations,

notwithstanding Ohmic dissipation. However, the application of RWA and willy-nilly the assumption of weak coupling leads to a rather straightforward extension of the classical result given in Eq. (264). We find

$$\langle \sigma^2(t) \rangle = \hbar \omega_c \coth\left(\frac{\hbar \omega_c}{2k_B T}\right) \langle W(t) \rangle.$$
 (271)

Therefore, the fluctuation theorem retains the Gallavoti-Cohen structure of Eq. (244) where the constant  $\alpha$  is

$$\alpha = \left[\hbar\omega_c \coth\left(\frac{\hbar\omega_c}{2k_B T}\right)\right]^{-1}.$$
 (272)

In order to delve a bit deeper into the *modus operandi* of low-temperature quantum features, it is instructive to examine a specific form for the applied electric field [97]. We assume that the latter is endowed with a frequency  $\Omega$  as also a decay parameter  $\Gamma$ :

$$F(t) = F_0 e^{-\Gamma t} \cos(\Omega t). \tag{273}$$

The choice is dictated to, by two reasons: (a) the presence of  $\Gamma$  precludes the divergence of  $\langle W \rangle$  at long times, and (b) the frequency  $\Omega$  provides a handle to tune it vis à vis the cyclotron frequency  $\omega_c$ . We find that in the long-time limit, i.e.,  $t \to \infty$ , we have

$$\langle W \rangle \to \frac{F_0^2}{m\Gamma} \frac{\gamma + \Gamma}{(\gamma + \Gamma)^2 + \omega^2}, \qquad \Omega = 0,$$
 (274)

$$\langle W \rangle \to \frac{F_0^2}{m\Gamma} \frac{\gamma + \Gamma}{(\gamma + \Gamma)^2 + (\Omega - \omega_c)^2}, \quad \Omega \to \omega_c.$$
 (275)

For these two limiting values of  $\Omega$ , we find for the fluctuations of W(t) the expressions

$$\langle \sigma^2 \rangle = 2k_B T \langle W(t) \rangle, \qquad \Omega = 0,$$
 (276)

$$\langle \sigma^2 \rangle = \hbar \omega_c \coth\left(\frac{\hbar \omega_c}{2k_B T}\right) \langle W(t) \rangle, \quad \Omega \to \omega_c.$$
 (277)

While Eq. (277) merges with Eq. (276) in the high- temperature limit, quantum effects prominently show up at zero temperature when

$$\langle \sigma^2 \rangle = \hbar \omega_c \langle W(t) \rangle, \text{ for } \Omega \to \omega_c, T \to 0,$$
 (278)

implying that the thermal energy  $2k_BT$  gets replaced by the zero-point energy  $\hbar\omega_c$  in this extreme limit.

To summarize, the prototype of cyclotron motion in the quantum domain, which necessarily elevates the one-dimensional quantum harmonic oscillator to two dimensions, throws additional light on the validity of the fluctuation theorems, though we have not addressed here the occurrence of isometric fluctuations. Furthermore, the rotating wave approximation, which is tantamount to assuming the system to be in weak interaction with the surrounding heat bath, seems to be able to circumvent the ticklish conundrum in defining the quantum work operator. We then end by raising the tantalizing question: Are quantum measurement issues in devising an appropriate definition of the quantum

work operator incumbent on the system being strongly coupled to the heat bath? Recall that the validity of our quantum Langevin equations in the weak coupling limit under the RWA entirely hinge on a factorization approximation for the initial density matrix wherein the system begins from a nonequilibrium state while the bath is kept fixed at a definite temperature in equilibrium. In the strong coupling situation, on the other hand, the system is never decoupled from the bath, even initially.

# 11. Closing remarks

In this review, we have presented a comprehensive overview of quantum Brownian motion in a pedagogic style, which we hope would be useful to a new entrant to the field. The study of quantum Brownian motion, inseparably linked to quantum Langevin equation, is basic to the emerging topics of nonequilibrium statistical mechanics, dissipative quantum phenomena and open quantum systems. Many of the themes, especially in the first few chapters, have been widely investigated over the last four decades. As such, these concepts have found their way, if not in textbooks, but surely in more specialized monographs, cited here. Naturally, the bibliography in this review reflects this feature of quantum Brownian motion being a much-studied problem. However, a cursory browsing through the reference section, containing new contributions to the field, would reveal that the subject is quite alive and of active contemporary interest. Keeping this in view, the review attempts to put together a slew of topics, old and new, in order to project a complete understanding of the underlying ideas, in a logical and connected manner. Thus, classical Brownian motion appears as an obvious prelude to quantum Brownian motion just as the derivation of the quantum Langevin equation follows the same steps as employed in obtaining the classical Langevin equation. Concomitantly however, new notions of non-Markov behavior, "non-white"-ness of noise, strong coupling effects, a re-look at the third law of thermodynamics, etc., emerge in this article.

Along with the (recent) historical perspective of the subject of quantum Brownian motion we have pieced together, in Sections 9 and 10, the novel topics of stochastic thermodynamics and fluctuation theorems. The latter areas deal with open quantum systems characterized by the absence of the fluctuation-dissipation theorem, deviation from standard thermodynamics to regimes that need incorporation of 'strong coupling' between the system and the heat bath, occurrence of non-Born-Markov effects in the master equation methods, and so on. These nuances of stochastic thermodynamics and quantum fluctuation theorems have profound implications in the currently pursued research topics of nano and mesoscopic structures, especially nano-Brownian engines, in both biology and condensed matter materials. We hope therefore that the presented review will prove to be relevantly useful in the analysis of coherence-to-decoherence phenomena, quantum fluctuations, and consequent influences on the storage of quantum information, which have a bearing on quantum devices on miniature scale.

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#### Appendix A. Proof of normalization of $P_k(\omega)$

In this appendix, we shall explicitly prove that the function  $P_k(\omega)$  in Eq. (78) is indeed positive definite and normalized. We have

$$P_k(\omega) = \frac{2m\omega}{\pi} \operatorname{Im}[\alpha^{(0)}(\omega)], \tag{A.1}$$

or equivalently,

$$P_k(\omega) = \frac{2\omega^2}{\pi} \frac{\operatorname{Re}[\tilde{\gamma}(\omega)]}{\left[\left(\omega^2 - \omega_0^2 + \omega \operatorname{Im}[\tilde{\gamma}(\omega)]\right)^2 + (\omega \operatorname{Re}[\tilde{\gamma}(\omega)])^2\right]},$$
(A.2)

which is positive definite owing to the positivity of  $\text{Re}[\tilde{\gamma}(\omega)]$ .

In order to prove that  $P_k(\omega)$  is normalized, let us first note the following two properties of the Laplace transform operator:

$$\mathcal{L}[\dot{x}(t)] = s\mathcal{L}[x(t)] - x(0), \tag{A.3}$$

$$\mathcal{L}[\ddot{x}(t)] = s^2 \mathcal{L}[x(t)] - sx(0) - \dot{x}(0). \tag{A.4}$$

Denoting  $\mathcal{L}[x(t)] = \hat{x}(s)$ , the quantum Langevin equation can be expressed as

$$(ms^{2} + s\hat{\gamma}(s) + m\omega_{0}^{2})\hat{x}(s) = m\dot{x}(0) + mx(0) + \hat{f}(s).$$
(A.5)

Let us denote

t us denote 
$$\mathcal{L}[Q(t)] = \hat{Q}(s) = \frac{1}{ms^2 + s\hat{\mu}(s) + m\omega_0^2}, \qquad \mathcal{L}[R(t)] = \hat{R}(s) = \frac{ms}{ms^2 + s\hat{\mu}(s) + m\omega_0^2}. \tag{A.6}$$

Then, Eq. (A.5) can be written as

$$\hat{x}(s) = m\dot{x}(0)\hat{Q}(s) + x(0)\hat{R}(s) + \hat{Q}(s)\hat{f}(s). \tag{A.7}$$

Equivalently, we have

$$x(t) = p(0)Q(t) + x(0)R(t) + \int_0^t dz \ Q(t-z)f(z), \tag{A.8}$$

where we have  $p(0) = m\dot{x}(0)$ . Similarly, one can show that the momentum operator can be expressed as

$$p(t) = p(0)R(t) + mx(0)\dot{R}(t) + \int_0^t dz \ R(t-z)f(z).$$
 (A.9)

Equation (A.9) will allow us to determine the mean kinetic energy of the system. Now, the symmetrized momentum-momentum correlation function reads

$$\langle \{p(t), p(t')\} \rangle = \int_0^t dt_1 \int_0^{t'} dt_2 \ R(t - t_1) R(t' - t_2) \langle \{f(t_1), f(t_2)\} \rangle. \tag{A.10}$$

Using the fluctuation-dissipation theorem, this can be expressed as

$$\langle \{p(t), p(t')\} \rangle = \int_0^\infty d\omega \ \widetilde{C}_{ff}(\omega) \int_0^t dt_1 \int_0^{t'} dt_2 \ R(t - t_1) R(t' - t_2) \cos[\omega(t_1 - t_2)], \ (A.11)$$

where  $\widetilde{C}_{ff}(\omega) = (\hbar \omega/2) \coth (\hbar \omega/(2k_BT)) \operatorname{Re}[\widetilde{\mu}(\omega)]$  is the cosine transform of the noise autocorrelation function. Next, we put t = t', giving us

$$\langle p^2(t) \rangle = \int_0^\infty d\omega \ \widetilde{C}_{ff}(\omega) \int_0^t d\tau \int_0^t du \ R(\tau) R(u) \cos[\omega(\tau - u)], \tag{A.12}$$

where we have put  $\tau = t - t_1$  and  $u = t - t_2$ . For the stationary state, we now take the limit  $t \to \infty$ , which gives

$$E_k = \lim_{t \to \infty} \frac{\langle p(t)^2 \rangle}{2m} = \frac{1}{2m} \int_0^\infty d\omega \ \widetilde{C}_{ff}(\omega) I(\omega), \tag{A.13}$$

with

$$I(\omega) = \int_0^\infty d\tau \int_0^\infty du \ R(\tau)R(u)\cos[\omega(\tau - u)]$$

$$= \frac{1}{2} \int_0^\infty d\tau \ R(\tau)e^{i\omega\tau} \int_0^\infty du \ R(u)e^{-i\omega u}$$

$$+ \frac{1}{2} \int_0^\infty d\tau \ R(\tau)e^{-i\omega\tau} \int_0^\infty du \ R(u)e^{i\omega u}$$

$$= \hat{R}(i\omega)\hat{R}(-i\omega). \tag{A.14}$$

Substituting this into Eq. (A.13), we find

$$E_k = \frac{1}{2m} \int_0^\infty d\omega \ \widetilde{C}_{ff}(\omega) \hat{R}(i\omega) \hat{R}(-i\omega). \tag{A.15}$$

This means that we can identify

$$P_k(\omega) = \frac{1}{m} \text{Re}[\widetilde{\mu}(\omega)] \hat{R}(i\omega) \hat{R}(-i\omega)$$
$$= [\hat{R}(i\omega) + \hat{R}(-i\omega)] := R_F(\omega). \tag{A.16}$$

It turns out that  $R_F(\omega)$  is the cosine transform of R(t), i.e.,

$$R_F(\omega) = \frac{2}{\pi} \int_0^\infty dt \ R(t) \cos(\omega t), \tag{A.17}$$

implying

$$R(t) = \int_0^\infty d\omega \ R_F(\omega) \cos(\omega t). \tag{A.18}$$

Putting t = 0, we find

$$R(0) = \int_0^\infty d\omega \ R_F(\omega). \tag{A.19}$$

We now use the initial-value theorem of the Laplace transform to give

$$R(0) = \lim_{s \to \infty} s\hat{R}(s) = 1, \tag{A.20}$$

thereby giving

$$\int_0^\infty d\omega \ R_F(\omega) = \int_0^\infty d\omega \ P_k(\omega) = 1. \tag{A.21}$$

# Appendix B. Proof of normalization of $P_p(\omega)$

In this appendix, we will prove that the function  $P_p(\omega)$  in Eq. (83) is positive definite and normalized. We have

$$P_p(\omega) = \frac{2m\omega_0^2}{\pi\omega} \operatorname{Im}[\alpha^{(0)}(\omega)], \tag{B.1}$$

or equivalently,

$$P_p(\omega) = \frac{2\omega_0^2}{\pi} \frac{\text{Re}[\tilde{\gamma}(\omega)]}{\left[\left(\omega^2 - \omega_0^2 + \omega \text{Im}[\tilde{\gamma}(\omega)]\right)^2 + (\omega \text{Re}[\tilde{\gamma}(\omega)])^2\right]},$$
(B.2)

which is positive definite owing to the positivity of  $\text{Re}[\tilde{\gamma}(\omega)]$ . In order to verify that  $P_p(\omega)$  is normalized, consider the integral

$$\int_0^\infty d\omega \ P_p(\omega) = \frac{2m\omega_0^2}{\pi} \int_0^\infty d\omega \ \frac{\operatorname{Im}[\alpha^{(0)}(\omega)]}{\omega}.$$
 (B.3)

Next, we recall the following relationship from [98]:

$$\alpha^{(0)}(i\omega) = \frac{2}{\pi} \int_0^\infty ds \, \frac{\text{Im}[\alpha^{(0)}(s)]}{\omega^2 + s^2} s, \tag{B.4}$$

which means putting  $\omega = 0$  gives us

$$\alpha^{(0)}(0) = \frac{2}{\pi} \int_0^\infty d\omega \, \frac{\text{Im}[\alpha^{(0)}(s)]}{s}.$$
 (B.5)

Therefore, if we combine Eqs. (B.3) and (B.5), we obtain

$$\int_0^\infty d\omega \ P_p(\omega) = m\omega_0^2 \alpha^{(0)}(0). \tag{B.6}$$

From Eq. (72), it directly follows that putting  $\omega = 0$  gives  $\alpha^{(0)}(0) = [m\omega_0^2]^{-1}$  which means  $P_p(\omega)$  is normalized. We refer the reader to [34], where the positivity and normalization of both  $P_k(\omega)$  and  $P_p(\omega)$  have been demonstrated in a more general setting where the number of spatial dimensions is three and there is an externally applied magnetic field.

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