Quantum partition of energy for a free Brownian particle: Impact of dissipation

J. Spiechowicz, P. Bialas, and J. Łuczka*

Institute of Physics and Silesian Center for Education and Interdisciplinary Research, University of Silesia, 41-500 Chorzów, Poland

(Received 19 August 2018; published 7 November 2018)

We study the quantum counterpart of the theorem on energy equipartition for classical systems. We consider a free quantum Brownian particle modeled in terms of the Caldeira-Leggett framework: a system plus thermostat consisting of an infinite number of harmonic oscillators. By virtue of the theorem on the averaged kinetic energy E_k of the quantum particle, it is expressed as $E_k = \langle \mathcal{E}_k \rangle$, where $\mathcal{E}_k$ is the thermal kinetic energy of the thermostat per 1 degree of freedom and $\langle \dots \rangle$ denotes averaging over the frequencies ω of thermostat oscillators which contribute to E_k according to the probability distribution $\mathbb{P}(\omega)$. We explore the impact of various dissipation mechanisms, via the Drude, Gaussian, algebraic, and Debye spectral density functions, on the characteristic features of $\mathbb{P}(\omega)$. The role of the system-thermostat coupling strength and the memory time on the most probable thermostat oscillator frequency as well as the kinetic energy E_k of the Brownian particle is analyzed.

DOI: 10.1103/PhysRevA.98.052107

I. INTRODUCTION

Quantum physics shows that its world can exhibit behavior which is radically different from its classical counterpart. Wave-particle duality, entanglement of states, decoherence, Casimir force, quantum information: these are generic examples which in turn carry the potential for new applications in the near or farther future. Yet, there remain new properties, behavior, and phenomena to be uncovered in this world. In this context, the quantum counterpart of the theorem on energy equipartition for classical systems is still not formulated in the general case. We attempt to take one step forward. In classical statistical physics, the theorem on equipartition of energy states that, for a system at thermodynamic equilibrium, its kinetic energy E_k is shared equally among all energetically accessible degrees of freedom (df). It also relates the average energy $E_k = k_B T/2$ per 1 df to the temperature T of the system (k_B is the Boltzmann constant). When the thermostat is modeled as an infinite collection of harmonic oscillators of temperature T, then the averaged kinetic energy of thermostat per 1 df is also $\mathcal{E}_k = k_B T/2$. In other words, $E_k = \mathcal{E}_k$ and all degrees of freedom of both system and thermostat have exactly the same averaged kinetic energy. This is why it is named *equipartition*. It is universal in the sense that it does not depend on the number of particles in the system, a potential force which acts on them, any interaction between particles, or the strength of coupling between system and thermostat [1,2]. For quantum systems, in the general case its counterpart is not known. In the literature, one can find reports on energetics of selected quantum systems [3]. In Ref. [4], an exact expression for the free energy of a quantum oscillator interacting, via dipole coupling, with a blackbody radiation field was derived. Next, the same authors studied a similar problem by a more conventional method using the fluctuation-dissipation theorem and obtained the expression for the kinetic energy of the quantum oscillator [5]. At the same time, the review paper on quantum Brownian motion has been published [6]. Formulas for the variance of the position and momentum of the oscillator are presented in Table 2 therein. There are also books [7–10] in which different versions of the kinetic energy of a free Brownian particle can be obtained directly or indirectly. Recently, the kinetic energy of a trappped Fermi gas has been considered [11]. Many other aspects of quantum Brownian motion have been intensively studied in the last few years [12–20]. However, the previous results have not been *directly* related to the energy equipartition theorem. Very recently, some progress has been made in the formulation of this law assuming that the thermostat is a collection of an infinite number of quantum oscillators [21,22]. Contrary to the classical case, the averaged kinetic energy of the thermostat oscillator depends on its frequency, $\mathcal{E}_k = \mathcal{E}_k(\omega)$, and as a consequence, the kinetic energy of the Brownian particle E_k depends on all $\mathcal{E}_k$ but in a nonuniform way determined by the probability distribution $\mathbb{P}(\omega)$ of the thermostat oscillator frequencies ω. In turn, $\mathbb{P}(\omega)$ depends on microscopic details of the thermostat and interactions. The latter aspect can be modeled by the spectral density of thermostat modes, which contains necessary information on the system-thermostat interaction. The aim of this work is to analyze the impact of various dissipation mechanisms on the kinetic energy E_k of the free Brownian particle.

The paper is structured as follows. The presentation starts in Sec. II, where, for the paper to be self-contained, we recapitulate very briefly some of the well-known key points on quantum Brownian motion. We apply a simple yet powerful minimal model based on the concept of the Hamiltonian for a composite quantum system: a Brownian particle plus thermostat [23]. Starting from the Heisenberg equations of motion for all position and momentum operators, an exact effective evolution equation can be derived for the coordinate and momentum operators of the Brownian particle. This integro-differential equation is called a generalized quantum Langevin equation in which an integral (damping) kernel and a thermal

*jerzy.luczka@us.edu.pl

noise term are related via the fluctuation-dissipation theorem. We recall a solution of this equation for the momentum of the free Brownian particle and present the quantum law for energy partition of the Brownian particle which is derived in Ref. [22]. In Sec. III, we comment on the energy partition theorem and discuss relations to the fluctuation-dissipation theorem derived in the linear response theory. In the main part of the paper, Sec. IV, we are interested in the impact of various dissipation mechanisms on $\mathbb{P}(\omega)$. This mechanism is modeled via the damping kernel of the Langevin equation. We consider two families of memory functions: (i) exponentially and (ii) algebraically decaying. Two subfamilies are analyzed: (a) monotonically and (b) periodically decaying functions. It covers the majority of crucial and accessible models of dissipation mechanisms. On one hand, we reveal similarities for the impact of various dissipation mechanisms, and on the other hand, there are interesting and significant differences. In Sec. V, we analyze the first two statistical moments of the frequency probability distribution. The first moment is directly related to the averaged kinetic energy at zero temperature; the second moment, to the first quantum correction to the classical result in the high-temperature regime. We summarize the results of the work in the last section, VI. In the Appendixes we present the solution of the generalized Langevin equation, derive the formula for the kinetic energy of the Brownian particle, and present the fluctuation-dissipation relation.

II. PARTITION OF ENERGY FOR A FREE BROWNIAN PARTICLE

The archetype of Brownian motion of a quantum particle is based on the Hamiltonian description of a composite system: the quantum particle plus thermostat. By way of explanation, a particle of mass M is subjected to the potential $U(x)$ and interacts with a large number of independent oscillators, which form a thermal reservoir of temperature T. The typical quantum-mechanical Hamiltonian of such a closed (and conservative) system assumes the form, à la Caldeira-Leggett ones [7,23–31],

$$H = \frac{p^2}{2M} + U(x) + \sum_i \left[\frac{p_i^2}{2m_i} + \frac{m_i\omega_i^2}{2}\left(q_i - \frac{c_i}{m_i\omega_i^2} x \right)^2 \right]. \tag{1}$$

The coordinate and momentum operators $\{x, p\}$ refer to the Brownian particle and $\{q_i, p_i\}$ are the coordinate and momentum operators of the ith heat-bath oscillator of mass m_i and the eigenfrequency ω_i. The parameter c_i characterizes the interaction strength of the particle with the ith oscillator. There is the counterterm, the last term proportional to x^2, which is included to cancel the harmonic contribution to the particle potential. All coordinate and momentum operators obey canonical equal-time commutation relations.

The next step is to write the Heisenberg equations of motion for all coordinate and momentum operators $\{x, p, q_i, p_i\}$ and solve the Heisenberg equations for the reservoir operators to obtain an effective equation of motion only for the particle coordinate $x(t)$. It is the so-called generalized quantum Langevin equation, which reads (for detailed derivation, see, e.g., [21])

$$M\ddot{x}(t) + \int_0^t \gamma(t-s)\dot{x}(s)\,ds = -U'(x(t)) - \gamma(t)x(0) + \eta(t), \tag{2}$$

where $\dot{x}(t) = p(t)/M$, $U'(x)$ denotes differentiation with respect to x, and $\gamma(t)$ is a dissipation function (damping or memory kernel),

$$\gamma(t) = \sum_i \frac{c_i^2}{m_i\omega_i^2}\cos(\omega_i t) \equiv \int_0^\infty d\omega J(\omega)\cos(\omega t), \tag{3}$$

where

$$J(\omega) = \sum_i \frac{c_i^2}{m_i\omega_i^2}\delta(\omega - \omega_i) \tag{4}$$

is the spectral function of the heat bath, which contains information on its modes and the system-heat bath interaction. The term $\eta(t)$ can be interpreted as a random force acting on the Brownian particle,

$$\eta(t) = \sum_i c_i \left[q_i(0)\cos(\omega_i t) + \frac{p_i(0)}{m_i\omega_i}\sin(\omega_i t) \right]. \tag{5}$$

It depends on the initial conditions imposed on oscillators of the thermostat. We note that effective dynamics of the quantum Brownian particle is described by an integrodifferential equation for the coordinate operator $x(t)$ and the initial condition $x(0)$ occurs in this evolution equation. This is not typical for ordinary differential equations. Usually, the initial conditions are separated from the equations of motion and independently accompanied by them. Here, for the open system, the initial conditions are an integral part of the effective dynamics and not an independent input. The initial preparation of the total system fixes the statistical properties of the thermostat and the Brownian particle.

We consider the free Brownian particle for which $U'(x) = 0$. From Eq. (2) one obtains the equation of motion for the momentum operator,

$$\dot{p}(t) + \frac{1}{M}\int_0^t \gamma(t-s)p(s)\,ds = -\gamma(t)x(0) + \eta(t). \tag{6}$$

Its solution reads (see Appendix A)

$$p(t) = R(t)p(0) - \int_0^t du\; R(t-u)\gamma(u)x(0) + \int_0^t du\; R(t-u)\eta(u), \tag{7}$$

where $R(t)$ is a response function determined by its Laplace transform,

$$\hat{R}_L(z) = \frac{M}{Mz + \hat{\gamma}_L(z)}. \tag{8}$$

Here, $\hat{\gamma}_L(z)$ is the Laplace transform of the dissipation function $\gamma(t)$ and for any function $f(t)$ its Laplace transform is defined as

$$\hat{f}_L(z) = \int_0^\infty dt e^{-zt} f(t). \tag{9}$$

Using Eq. (7), one can calculate the averaged kinetic energy $E_k(t) = \langle p^2(t)\rangle/2M$ of the Brownian particle. In the long-time limit $t \to \infty$, when a thermal equilibrium state is reached, it has the form [see Eq. (B10) in Appendix B]

$$E_k = \langle \mathcal{E}_k \rangle = \int_0^\infty d\omega \, \mathcal{E}_k(\omega)\mathbb{P}(\omega), \tag{10}$$

where

$$\mathcal{E}_k(\omega) = \frac{\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_B T}\right) \tag{11}$$

is the thermal kinetic energy per 1 df of the thermostat consisting of free harmonic oscillators [32] and $\langle \ldots \rangle$ denotes averaging over the frequencies ω of those thermostat oscillators which contribute to E_k according to the probability distribution [see Eq. (B9) in Appendix B]

$$\mathbb{P}(\omega) = \frac{1}{\pi}[\hat{R}_L(i\omega) + \hat{R}_L(-i\omega)]. \tag{12}$$

Formula (10) together with Eq. (12) constitutes the *quantum law for partition of energy*. This means that the averaged kinetic energy E_k of the Brownian particle is the averaged kinetic energy $\mathcal{E}_k$ per 1 df of the thermostat oscillators. The averaging is twofold: (i) over the thermal equilibrium Gibbs state for the thermostat oscillators resulting in $\mathcal{E}_k(\omega)$ given by Eq. (11) and (ii) over the frequencies ω of those thermostat oscillators which contribute to E_k according to the probability distribution $\mathbb{P}(\omega) \geqslant 0$, which is normalized on the frequency half-line [22], $\int_0^\infty d\omega \, \mathbb{P}(\omega) = 1$.

We rewrite formula (12) to a form which is convenient for calculations. To this end we note that the Laplace transform can be expressed by the cosine and sine Fourier transforms. In particular,

$$\hat{\gamma}_L(i\omega) = \int_0^\infty dt \, \gamma(t) e^{-i\omega t} = A(\omega) - i B(\omega), \tag{13a}$$

$$A(\omega) = \int_0^\infty dt \, \gamma(t) \cos(\omega t), \tag{13b}$$

$$B(\omega) = \int_0^\infty dt \, \gamma(t) \sin(\omega t). \tag{13c}$$

We put it into Eqs. (8) and (12) to get the following expression:

$$\mathbb{P}(\omega) = \frac{2M}{\pi} \frac{A(\omega)}{A^2(\omega) + [B(\omega) - M\omega]^2}. \tag{14}$$

Let us observe that the function $A(\omega)$ is related to the spectral function $J(\omega)$. Indeed, from Eq. (3), Eq. (C7a) in Appendix C, and definition (13b) of $A(\omega)$ it follows that $A(\omega) = (\pi/2)J(\omega)$. Because the spectral function, (4), is nonnegative, $J(\omega) \geqslant 0$, and the denominator in (14) is positive, the function $\mathbb{P}(\omega)$ is nonnegative as required.

Representation (14) allows us to study the influence of various forms of the dissipation function $\gamma(t)$ or, equivalently, the spectral density $J(\omega)$.

III. PHYSICAL SIGNIFICANCE OF THE QUANTUM ENERGY PARTITION THEOREM

As we write in Sec. I, various expressions for the kinetic energy of a free Brownian particle can be found both in original papers and in well-known books, e.g., Eq. (83) in Ref. [3], Eq. (4.14) in Ref. [5], the equation for the second moment of the momentum in Table 2 of Ref. [6], and Eq. (3.475) in Ref. [10]. The form of E_k can also be deduced from the fluctuation-dissipation relation obtained in the framework of the linear response theory, which relates the relaxation of a weakly perturbed system to the spontaneous fluctuations in thermal equilibrium; see, e.g. Eq., (124.10) in Ref. [8], Eq. (17.19g) in Ref. [9], and Eq. (3.499) in Ref. [10]. All expressions for E_k should be equivalent, although they are written in different forms. However, our specific formula, (10), allows alternative solutions to the old problem and the formulation of new interpretations:

(i) The mean kinetic energy E_k of a free quantum particle equals the average kinetic energy $\langle \mathcal{E}_k \rangle$ of the thermostat degrees of freedom, i.e., $E_k = \langle \mathcal{E}_k \rangle$. *Mutatis mutandis*, the form of this statement is exactly the same as for classical systems: The mean kinetic energy of a free classical particle equals the average kinetic energy of the thermostat degrees of freedom.

(ii) The function $\mathbb{P}(\omega)$ is the probability density; i.e., it is nonnegative and normalized in the interval $(0, \infty)$. From the probability theory it follows that there exists a random variable ξ for which $\mathbb{P}(\omega)$ is its probability distribution. Here, this random variable is interpreted as the frequency of thermostat oscillators.

(iii) Equation (12) can be converted to the transparent form

$$\mathbb{P}(\omega) = \frac{2}{\pi} \int_0^\infty dt \, R(t) \cos(\omega t). \tag{15}$$

Thus the probability distribution $\mathbb{P}(\omega)$ is the cosine Fourier transform of the response function $R(t)$ which solves the generalized Langevin equation, (6).

(iv) Thermostat oscillators contribute to E_k in a nonuniform way according to the probability distribution $\mathbb{P}(\omega)$. The form of this distribution depends on the response function in which full information on the thermostat modes and system-thermostat interaction is contained.

(v) For high temperatures, Eq. (11) is approximated by $\mathcal{E}_k(\omega) = k_B T/2$, and from Eq. (10) we obtain the relation $E_k = k_B T/2$; i.e., Eq. (10) reduces to the energy equipartition theorem for classical systems.

The next comment concerns the relation of Eq. (10) with the fluctuation-dissipation theorem derived in the linear response theory. We adapt Eq. (124.10) from the Landau-Lifshitz book [8] in order to get the kinetic energy of the quantum particle, namely,

$$E_k = \frac{1}{2M}\langle p^2 \rangle = \frac{\hbar}{2\pi M} \int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2k_B T}\right] \alpha''(\omega), \tag{16}$$

where $\alpha''(\omega)$ is the imaginary part of the generalized susceptibility $\alpha(\omega) = \alpha'(\omega) + i\alpha''(\omega)$. By direct comparison of Eqs. (10) and (16) we find the nontrivial relation between the probability distribution and the imaginary part of the generalized susceptibility:

$$\mathbb{P}(\omega) = \frac{2}{\pi}\frac{\alpha''(\omega)}{M\omega}. \tag{17}$$

The second example is Eq. (4.14) in Ref. [5],

$$E_k = \frac{\hbar}{2\pi}\int_0^\infty d\omega \coth\left[\frac{\hbar\omega}{2k_BT}\right] M\omega^2\,\mathrm{Im}[\alpha(\omega + i0^+)], \tag{18}$$

where $\alpha(\omega)$ is also called the susceptibility, which is not the same as in Eq. (16). Again, if we compare Eqs. (10) and (18), we can find the relation between $\mathbb{P}(\omega)$ and $\mathrm{Im}[\alpha(\omega + i0^+)]$. But now we get

$$\mathbb{P}(\omega) = \frac{2}{\pi}M\omega\,\mathrm{Im}[\alpha(\omega + i0^+)]. \tag{19}$$

We have presented only two examples, and to avoid confusion the reader should be careful with such relations because they depend on the specific form of the expression for E_k. Paraphrasing, "Various authors present the same topic differently."

Overall, taking into account the nontrivial relation between the probability distribution $\mathbb{P}(\omega)$ and the imaginary part of the generalized susceptibility $\alpha''(\omega)$, we may say that our principle for quantum partition of energy, (10), can be seen as a specific form of the fluctuation-dissipation theorem of the Callen-Welton type, although it would be rather difficult to guess the form of $\mathbb{P}(\omega)$ knowing only the formula for fluctuation-dissipation theorem. Finally, we note that Eq. (17) establishes the relation between the probability distribution $\mathbb{P}(\omega)$ and the generalized susceptibility $\alpha''(\omega)$. This means that features of the quantum environment described by $\mathbb{P}(\omega)$ may be experimentally inferred from the measurement of the linear response of the system to an applied perturbation given as the corresponding classical susceptibility, e.g., electrical or magnetic. Consequently, according to our results the latter quantity may open a new pathway to study quantum open systems.

IV. ANALYSIS OF THE PROBABILITY DISTRIBUTION $\mathbb{P}(\omega)$

In the case of classical systems the averaged kinetic energy of the Brownian particle equals $E_k = k_BT/2$ and all thermostat oscillators have the same averaged kinetic energy $\mathcal{E}_k = k_BT/2$, which does not depend on the frequency of a single oscillator. In the quantum case, $\mathcal{E}_k = \mathcal{E}_k(\omega)$ depends on the oscillator frequency ω and oscillators of various frequencies contribute to E_k with various probabilities. Therefore it is interesting to reveal which frequencies are more or less probable depending on the dissipation mechanism. The impact of various dissipation mechanisms can be analyzed via one of three quantities: the dissipation kernel $\gamma(t)$, the correlation function $C(t)$ of the random force $\eta(t)$, or the spectral density $J(\omega)$. In our view, this mechanism can be intuitively modeled by various forms of the damping kernel $\gamma(t)$. Therefore in the following section we examine the properties of the probability distribution $\mathbb{P}(\omega)$ for several classes of $\gamma(t)$.

A. Drude model

As the first step we assume the dissipation function $\gamma(t)$ to be in the form

$$\gamma_D(t) = \frac{\gamma_0}{2\tau_c}e^{-t/\tau_c}, \tag{20}$$

with two nonnegative parameters, γ_0 and τ_c. The first one γ_0 is the particle-thermostat coupling strength and has units of $[\gamma_0] = [\mathrm{kg/s}]$, i.e., the same as the friction coefficient in the Stokes force. The second parameter τ_c characterizes the time scale on which the system exhibits memory (non-Markovian) effects. Due to the fluctuation-dissipation theorem τ_c can be also viewed as the primary correlation time of quantum thermal fluctuations. This exponential form of the memory function is known as the Drude model and it has been frequently considered in colored noise problems. We choose the above scaling to ensure that if $\tau_c \to 0$, the function $\gamma_D(t)$ is proportional to the Dirac delta and the integral term in the generalized Langevin equation reduces to the frictional force of the Stokes form. Other damping kernels considered in the latter part of this section also possess this scaling property. With (3), instead of determining $\gamma(t)$, one can equivalently specify the spectral density of thermostat modes, which for the Drude damping reads

$$J_D(\omega) = \frac{1}{\pi}\frac{\gamma_0}{1 + \omega^2\tau_c^2}. \tag{21}$$

From Eq. (14) we get the expression for the probability density

$$\mathbb{P}(\omega) = \frac{1}{\pi}\frac{\mu_0\varepsilon^2(\omega^2 + \varepsilon^2)}{\omega^2[\omega^2 + \varepsilon(\varepsilon - \mu_0/2)]^2 + \mu_0^2\varepsilon^4/4}, \tag{22}$$

where $\mu_0 = \gamma_0/M$ defines the rescaled coupling strength of the Brownian particle to the thermostat and $\varepsilon = 1/\tau_c$ is the Drude frequency. There are two control parameters, ε and μ_0, which have units of frequency or, equivalently, two time scales: the memory time τ_c and $\tau_v = M/\gamma_0 = 1/\mu_0$, which in the case of a classical free Brownian particle defines the velocity relaxation time.

If we want to analyze the impact of the particle mass M or the coupling γ_0, we should use the scaling

$$x = \omega\tau_c = \frac{\omega}{\varepsilon}, \tag{23}$$

which yields the expression

$$\mathbb{P}_D(x) = \varepsilon\mathbb{P}(\varepsilon x) = \frac{2}{\pi}\frac{2\alpha(x^2 + 1)}{x^2[2\alpha(x^2 + 1) - 1]^2 + 1}, \tag{24}$$

where

$$\alpha = \frac{M}{\tau_c\gamma_0} = \frac{\varepsilon}{\mu_0} = \frac{\tau_v}{\tau_c} \tag{25}$$

is the ratio of two characteristic times. It is remarkable that this probability distribution does not depend on these three parameters separately but only on one parameter, α, being their specific combination. We should remember that τ_c is fixed in this scaling. In Fig. 1 (left) we present the probability distribution $\mathbb{P}_D(x)$ for different values of the parameter α. We can observe that the thermostat oscillators contribute to the kinetic energy E_k in a nonhomogeneous way. There is

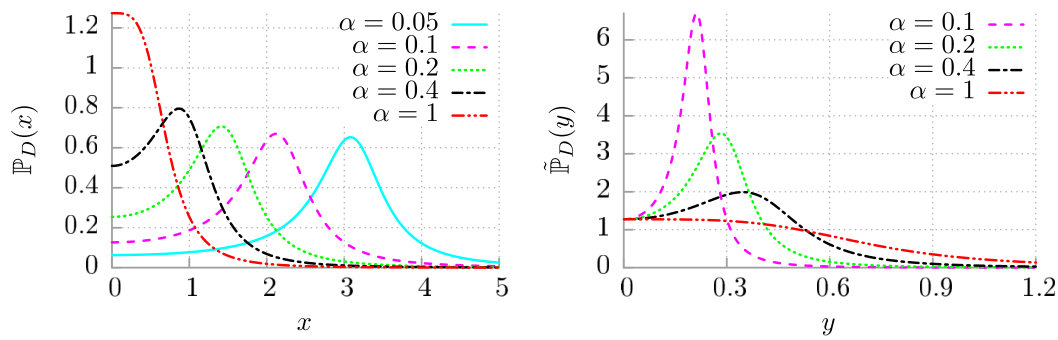

FIG. 1. Exponential decay of the dissipation function $\gamma_D(t) = (\gamma_0/2\tau_c)e^{-t/\tau_c}$, known as the Drude model. Probability distributions $\mathbb{P}_D(x)$ and $\tilde{\mathbb{P}}_D(y)$ in two scalings are shown for selected values of the dimensionless parameter $\alpha = \tau_v/\tau_c$. Left: τ_c is fixed and τ_v is changed. Right: τ_v is fixed and τ_c is changed.

the most probable value of $\mathbb{P}_D(x)$, indicating the optimal oscillator frequency x_M which makes the greatest contribution to the kinetic energy of the Brownian particle. As illustrated in the figure, x_M is inversely proportional to α: for small values of α, mainly oscillators of high frequency contribute to E_k; for large values of α, primarily low frequencies. As α increases $x_M \to 0$ and $\mathbb{P}_D(x)$ becomes a monotonically decreasing function (not depicted). In other words this means that, e.g., when the coupling strength between the system and the thermostat γ_0 is strong then the contribution of high-frequency oscillators to E_k is most pronounced; if the particle mass M increases, the optimal frequency x_M decreases.

Next we analyze the influence of the memory time τ_c on the probability distribution $\mathbb{P}(\omega)$. For this purpose we should use another scaling:

$$y = \frac{\omega}{\mu_0}. \tag{26}$$

It leads to the expression

$$\tilde{\mathbb{P}}_D(y) = \mu_0 \mathbb{P}(\mu_0 y) = \frac{1}{\pi} \frac{\alpha^2(y^2+\alpha^2)}{y^2[y^2+\alpha(\alpha-1/2)]^2+\alpha^4/4}, \tag{27}$$

with the same dimensionless parameter α defined in (25). In the right panel in Fig. 1 we present this distribution for selected values of α. It follows that for small values of the parameter α, or equivalently for long memory times τ_c, the distribution is notably peaked in the region of low-frequency modes. Then it rapidly decreases to 0. Consequently only slowly vibrating thermostat oscillators contribute significantly to the kinetic energy of the particle. The situation is quite different for short memory times τ_c (large values of α). Then the distribution is flattened, meaning that a much wider window of oscillator frequencies contributes to E_k in a similar way.

In the remainder of the paper, we present the probability distribution $\mathbb{P}(\omega)$ without any scaling. The reader can easily reproduce both scalings. For the scaling as in Eq. (23), one can put $\epsilon = 1$ and rescale $\mu_0 \to \mu_0/\varepsilon$ to get the distribution $\mathbb{P}_i(x)$ (the index i indicates the form of the memory function). For the scaling as in Eq. (26), one can put $\mu_0 = 1$ and rescale $\varepsilon \to \varepsilon/\mu_0$ to get the distribution $\mathbb{P}_i(y)$. In the first scaling, one can analyze the influence of the particle mass M and the particle-thermostat coupling γ_0; in the second scaling, of the memory time τ_c.

B. Gaussian decay

Another possible choice of the dissipation kernel $\gamma(t)$ is the rapidly decreasing Gaussian function, namely,

$$\gamma_G(t) = \frac{\gamma_0}{\sqrt{\pi}\,\tau_c} e^{-t^2/\tau_c^2}, \tag{28}$$

for which the corresponding spectral density is also Gaussian and reads

$$J_G(\omega) = \frac{\gamma_0}{\pi} e^{-\omega^2\tau_c^2/4}. \tag{29}$$

In order to have notation identical to that in the previous case, we present the probability distribution in the form ($\varepsilon = 1/\tau_c$)

$$\mathbb{P}_G(\omega) = \frac{4}{\pi\mu_0} \frac{e^{-(\omega/4\varepsilon)^2}}{[2\omega/\mu_0 + ie^{-(\omega/4\varepsilon)^2}\mathrm{Erf}(-i\omega/2\varepsilon)][2\omega/\mu_0 - ie^{-(\omega/4\varepsilon)^2}\mathrm{Erf}(i\omega/2\varepsilon)]}, \tag{30}$$

where $\mathrm{Erf}(z)$ is the error function

$$\mathrm{Erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z dt e^{-t^2}. \tag{31}$$

In Fig. 2 we present this probability distribution $\mathbb{P}_G(x)$ [in the scaling, (23)] for selected values of α ($\tau_v = M/\gamma_0$ is changed and τ_c is fixed). Similarly to the case of the Drude model, the oscillator frequency x_M which makes the greatest contribution to the kinetic energy of the particle is inversely proportional to the parameter α. However, here we observe two differences: (i) at some interval of α the maximum of $\mathbb{P}_G(x)$ decreases as α increases, and (ii) the half-width of $\mathbb{P}_G(x)$ increases as α increases, while for the Drude model it is almost constant in a wide interval of α. In this case, the impact of the memory time τ_c is similar to that for the Drude dissipation (see Fig. 1, right).

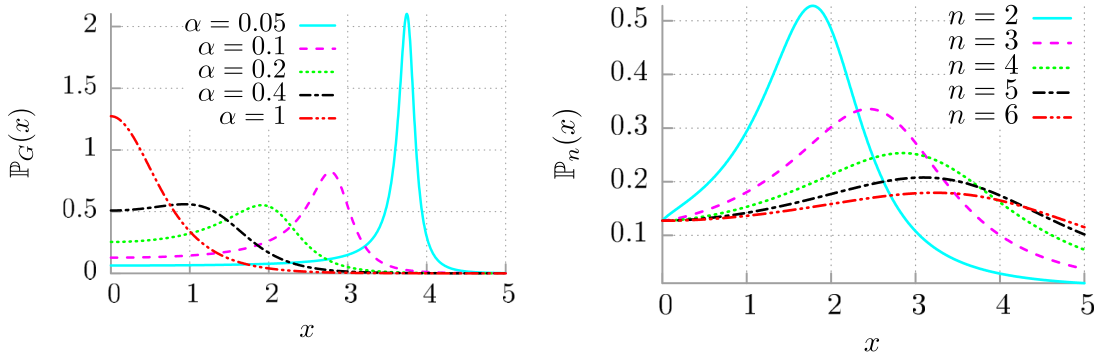

FIG. 2. Left: The case of Gaussian decay of the memory kernel $\gamma_G(t) = (\gamma_0/\sqrt{\pi}\tau_c)e^{-t^2/\tau_c^2}$. The probability distribution $\mathbb{P}_G(x)$ is presented for different values of the dimensionless parameter α (M and/or γ_0 is changed, τ_c is fixed). Right: The probability distribution $\mathbb{P}_n(x)$ is depicted for different values of the power exponent n appearing in the generalized algebraic decay of the dissipation kernel $\gamma_n(t) = [(n-1)/2]\,\gamma_0\tau_c^{n-1}/(t+\tau_c)^n$. The dimensionless parameter $\alpha = 0.1$.

C. n-Algebraic decay

Apart from the two exponential forms of the memory functions presented above, one could model the dissipation function $\gamma(t)$ with algebraic decay. It is noteworthy that the power-law decay of the memory functions has been considered as a model of anomalous transport processes [33,34]. Here, we consider the class of functions

$$\gamma_n(t) = \frac{n-1}{2}\frac{\gamma_0\tau_c^{n-1}}{(t+\tau_c)^n}, \tag{32}$$

where $n \in \mathbb{N}$ and $n \geqslant 2$. It has the same limiting Dirac delta form for $\tau_c \to 0$ as in two previous cases. The corresponding spectral density reads

$$J_n(\omega) = \frac{(n-1)\gamma_0}{2\pi}\left[e^{-i\omega\tau_c}E_n(-i\omega\tau_c) + e^{i\omega\tau_c}E_n(i\omega\tau_c)\right] \tag{33}$$

and $E_n(z)$ is the exponential integral,

$$E_n(z) = \int_1^\infty dt\,\frac{e^{-zt}}{t^n}. \tag{34}$$

The probability distribution takes the form

$$\mathbb{P}_n(\omega) = \frac{2(n-1)}{\pi\mu_0}\frac{e^{-i\omega/\varepsilon}E_n(-i\omega/\varepsilon) + e^{i\omega/\varepsilon}E_n(i\omega/\varepsilon)}{[(n-1)e^{-i\omega/\varepsilon}E_n(-i\omega/\varepsilon) - 2i\omega/\mu_0][(n-1)e^{i\omega/\varepsilon}E_n(i\omega/\varepsilon) + 2i\omega/\mu_0]}. \tag{35}$$

In Fig. 2 we present the influence of the power exponent n appearing in the dissipation function $\gamma_n(t)$ on the probability distribution $\mathbb{P}_n(x)$ for fixed $\alpha = 0.1$. The conclusion is that an increase in the exponent n causes progressive flattening of the probability density function. In other words, if the memory function decreases to 0 more and more rapidly, the wider spectrum of frequencies of the thermostat oscillators contributes to E_k.

D. Lorentzian decay

It is interesting to compare the algebraic case for $n = 2$ with the Lorentzian memory function, which reads

$$\gamma_L(t) = \frac{\gamma_0}{\pi}\frac{\tau_c}{t^2+\tau_c^2}. \tag{36}$$

In the probability theory it is termed the Cauchy distribution. Alternatively, it may be imposed by the following spectral density of thermostat modes:

$$J_L(\omega) = \frac{\gamma_0}{\pi}e^{-\omega\tau_c}. \tag{37}$$

Such a choice of the dissipation kernel leads to the probability distribution ($\varepsilon = 1/\tau_c$)

$$\mathbb{P}_L(\omega) = \frac{4\pi}{\mu_0}\frac{e^{-\omega/\varepsilon}}{\pi^2 e^{-2\omega/\varepsilon} + c^2(\omega)}, \tag{38}$$

where

$$c(\omega) = e^{-\omega/\varepsilon}\mathrm{Ei}(\omega/\varepsilon) - e^{\omega/\varepsilon}\mathrm{Ei}(-\omega/\varepsilon) - \frac{2\pi}{\mu_0}\omega \tag{39}$$

and $\mathrm{Ei}(z)$ is the exponential integral, defined as

$$\mathrm{Ei}(z) = \int_{-\infty}^{z}\frac{e^t}{t}\,dt. \tag{40}$$

We illustrate this probability distribution in Fig. 3 for different values of the dimensionless parameter $\alpha = M/\tau_c\gamma_0$. The oscillator frequency x which makes the greatest contribution to the kinetic energy of the particle is inversely proportional to the parameter α. Again, as in the previous cases, the magnitude of the maxima in the probability distribution $\mathbb{P}_L(x)$ also depends on α. For very small values of α one can note

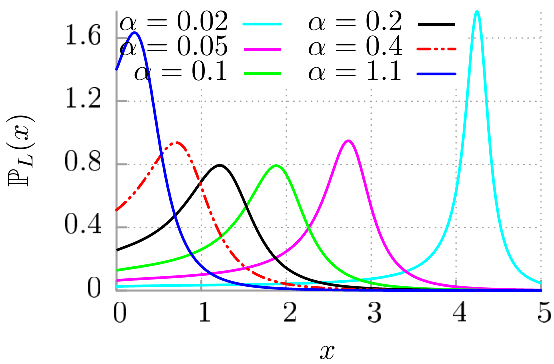

FIG. 3. The probability distribution $\mathbb{P}_L(x)$ is depicted for the Lorentzian dissipation kernel $\gamma_L(t) = \gamma_0\tau_c/\pi(t^2 + \tau_c^2)$ and selected values of the dimensionless parameter α (M or γ_0 can be changed and τ_c is fixed).

that high-frequency modes almost exclusively contribute to the kinetic energy of the particle.

E. Debye-type model: Algebraically decaying oscillations

The next example of this series is the oscillatory memory function [35]

$$\gamma_S(t) = \frac{\gamma_0}{\pi}\frac{\sin(t/\tau_c)}{t}, \tag{41}$$

which takes both positive and negative values. One can show that, via the fluctuation-dissipation relation, the quantum noise $\eta(t)$ exhibits anticorrelations. The spectral density is of the Debye type [35],

$$J_S(\omega) = \frac{\gamma_0}{\pi}\,\theta\left(\frac{1}{\tau_c} - \omega\right), \tag{42}$$

where $\theta(x)$ denotes the Heaviside step function. This spectral density is constant, $J(\omega) = \gamma_0/\pi$, on the *compact* support $[0, 1/\tau_c]$ determined by the memory time τ_c or the cutoff frequency $\varepsilon = 1/\tau_c$. Under this assumption the probability density $\mathbb{P}_S(\omega)$ reads

$$\mathbb{P}_S(\omega) = \frac{4\pi}{\mu_0}\,\frac{\theta(\varepsilon - \omega)}{\pi^2\left(1 + 4\omega^2/\mu_0^2\right) + 4\mathrm{arctanh}(\omega/\varepsilon)[\mathrm{arctanh}(\omega/\varepsilon) - 2\pi\omega/\mu_0]} \tag{43}$$

and has the same support as $J(\omega)$ in the interval $[0, \varepsilon]$. In Fig. 4 we present the probability density $\mathbb{P}_S(x)$ for selected values of the dimensionless parameter α in two various scalings. In the left panel, the memory time is fixed and the coupling γ_0 or the mass M is changed. Again, when, e.g., γ_0 decreases (i.e., α increases), more and more oscillators of low frequency contribute to E_k.

F. Slow algebraic decay

In this subsection we consider slow algebraic decay of the memory kernel assuming

$$\gamma_A(t) = \frac{\gamma_0}{t + \tau_c}. \tag{44}$$

This dissipation function does not tend to the Dirac delta when $\tau_c \to 0$ (the limit does not exist) and therefore is not placed in Sec. IV C. The corresponding spectral density has the form

$$J_A(\omega) = \frac{2\gamma_0}{\pi}\,a(\omega). \tag{45}$$

The probability distribution reads

$$\mathbb{P}_A(\omega) = \frac{2}{\pi\mu_0}\,\frac{a(\omega)}{a^2(\omega) + [b(\omega) - \omega/\mu_0]^2}, \tag{46}$$

where ($\varepsilon = 1/\tau_c$)

$$a(\omega) = -\mathrm{ci}(\omega/\varepsilon)\cos(\omega/\varepsilon) - \mathrm{si}(\omega/\varepsilon)\sin(\omega/\varepsilon), \tag{47}$$

$$b(\omega) = \mathrm{ci}(\omega/\varepsilon)\sin(\omega/\varepsilon) - \mathrm{si}(\omega/\varepsilon)\cos(\omega/\varepsilon). \tag{48}$$

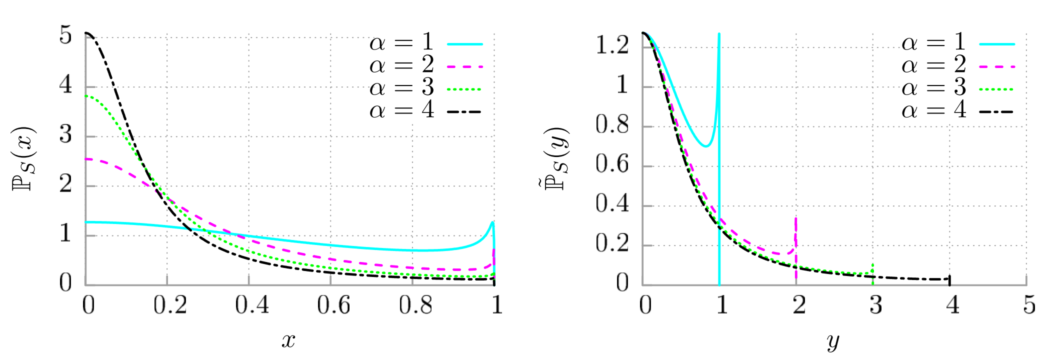

FIG. 4. The probability distribution $\mathbb{P}_S(x)$ is presented for the oscillatory decay $\gamma_S(t) = (\gamma_0/\pi)\sin(t/\tau_c)/t$ (the Debye-type model) and selected values of the dimensionless parameter $\alpha = \tau_v/\tau_c$. Left: τ_c is fixed and $\tau_v = M/\gamma_0$ is changed. Right: τ_v is fixed and τ_c is changed.

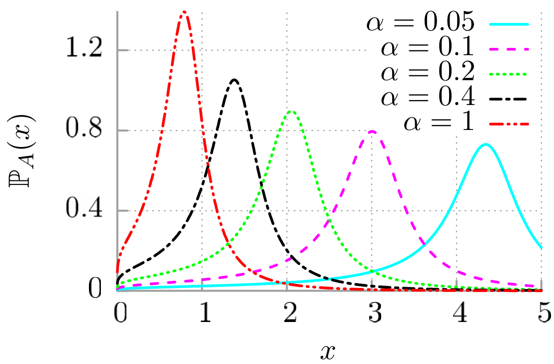

FIG. 5. Algebraic decay of the dissipation function $\gamma_A(t) = \gamma_0/(t + \tau_c)$. The probability distribution $\mathbb{P}_A(x)$ is presented for different values of the dimensionless parameter α.

The functions $\mathrm{ci}(z)$ and $\mathrm{si}(z)$ are cosine and sine integrals defined as

$$\mathrm{ci}(z) = -\int_z^\infty \frac{\cos t}{t} dt, \tag{49}$$

$$\mathrm{si}(z) = -\int_z^\infty \frac{\sin t}{t} dt. \tag{50}$$

In Fig. 5 we depict $\mathbb{P}_A(x)$ for different values of the dimensionless parameter α. As before, the optimal frequency of the oscillator which has the largest impact on the kinetic energy is inversely proportional to α. Qualitatively, this looks similar to the case of the Drude model (cf. Fig. 1). However, only for large values of α does the contribution of harmonic modes of the lowest frequency $x \to 0$ differ significantly from 0.

Overall, the common characteristic of all the cases presented above is that the probability distribution $\mathbb{P}(x)$ occurring in the quantum law for energy equipartition depends on only one dimensionless parameter, $\alpha = M/\tau_c\gamma_0$. Moreover, for a small value of this parameter (strong particle-thermostat coupling) one typically finds a bell-shaped probability density with a pronounced maximum for high frequency x_M which is inversely proportional to the magnitude of α. For large values of α, thermostat oscillators of low frequency dominate the contributions to the kinetic energy of the Brownian particle.

G. Exponentially decaying oscillations

As the last example, we consider a generalization of the Drude model in the form of exponentially decaying oscillations [21],

$$\gamma_E(t) = \frac{\gamma_0}{\tau_c} e^{-t/\tau_c} \cos{(\Omega t)}, \tag{51}$$

where, in addition to the previously defined parameters γ_0 and τ_c, now Ω is the frequency in the relaxation process of the particle momentum. Also in this case, the quantum noise $\eta(t)$ exhibits anticorrelations. The limiting case $\Omega = 0$ corresponds to the Drude model of dissipation. This choice of damping kernel leads to the spectral density

$$J_E(\omega) = \frac{2}{\pi} \frac{\gamma_0 \varepsilon^2(\varepsilon^2 + \omega^2 + \Omega^2)}{(\varepsilon^2 + \omega^2)^2 + 2\Omega^2(\varepsilon^2 - \omega^2) + \Omega^2}, \tag{52}$$

where $\varepsilon = 1/\tau_c$. From the quantum law for the partition of energy we obtain the probability distribution in the form [21]

$$\mathbb{P}(\omega) = \frac{2}{\pi} \frac{\mu_0 \varepsilon^2(\omega^2 + \varepsilon^2 + \Omega^2)}{\omega^2[(\omega^2 + \varepsilon^2 - \Omega^2 - \mu_0\varepsilon)^2 + 4\varepsilon^2\Omega^2] + \mu_0^2\varepsilon^4}. \tag{53}$$

The parameter $\mu_0 = \gamma_0/M$ defines the rescaled coupling strength of the Brownian particle to the thermostat. We note that in the considered case there are three characteristic frequencies, μ_0, ε, and Ω, or, equivalently, three time scales which are equal to the reciprocals of these frequencies. This observation must be contrasted with all previously considered damping kernels leading to two characteristic time scales. The kinetic energy of the free Brownian particle with exponentially decaying oscillations in the dissipation function was analyzed in detail in Ref. [21]. Instead, here we focus on the properties of the probability density occurring in the quantum energy partition theorem. The influence of the coupling strength μ_0 on $\mathbb{P}(\omega)$ is similar to that of the Drude model: there is only one maximum for a fixed value of the coupling strength μ_0. For larger values of the latter it is shifted to the right, indicating that oscillators of higher frequency make the greatest contribution to the kinetic energy of the particle.

The influence of the reciprocal of the correlation time $\varepsilon = 1/\tau_c$ is depicted in Fig. 6(a). In this case, we scale Eq. (53) as in (26), namely, $y = \omega/\mu_0$. The dimensionless parameters are $\alpha = \varepsilon/\mu_0$ and $\tilde{\Omega} = \Omega/\mu_0$. Due to the interplay of two characteristic time scales associated with the parameters α and $\tilde{\Omega}$ we observe here qualitatively new features. For large values of $\alpha \gg \tilde{\Omega}$ the distribution is almost flat, indicating that all oscillators of the thermostat contribute equally to the kinetic energy of the system. When the characteristic frequency α is slightly higher than the other one, $\alpha > \tilde{\Omega}$, a single maximum is born. When the opposite situation occurs, i.e., $\alpha < \tilde{\Omega}$, then the distribution $\tilde{\mathbb{P}}(y)$ exhibits a clear bimodal character. This means that oscillators of both low and moderate frequency play an important role. A further decrease in α extinguishes the contribution of higher frequencies in favor of near-zero frequency modes, which are then the most pronounced ones.

Last but not least, we elaborate on the impact of the oscillation frequency Ω. We keep the scaling with respect to the system-thermostat coupling strength μ_0. In Fig. 6(b) we present the probability distribution $\tilde{\mathbb{P}}(y)$ for a few values of the dimensionless frequency $\tilde{\Omega} = \Omega/\mu_0$ and fixed $\alpha = \varepsilon/\tau_c = 0.2$. The result confirms our earlier observation that, due to interplay of two characteristic time scales, the probability density may be bimodal. It is realized when the magnitudes of $\tilde{\Omega}$ and α are comparable. For very small $\tilde{\Omega}$ the distribution $\tilde{\mathbb{P}}(y)$ possesses one very pronounced maximum, whereas for large $\tilde{\Omega}$ it becomes a monotonically decreasing function of the dimensionless frequency y.

V. STATISTICAL MOMENTS OF THE PROBABILITY DISTRIBUTION $\mathbb{P}(\omega)$

Let us now discuss statistical moments of the random variable ξ distributed according to the probability

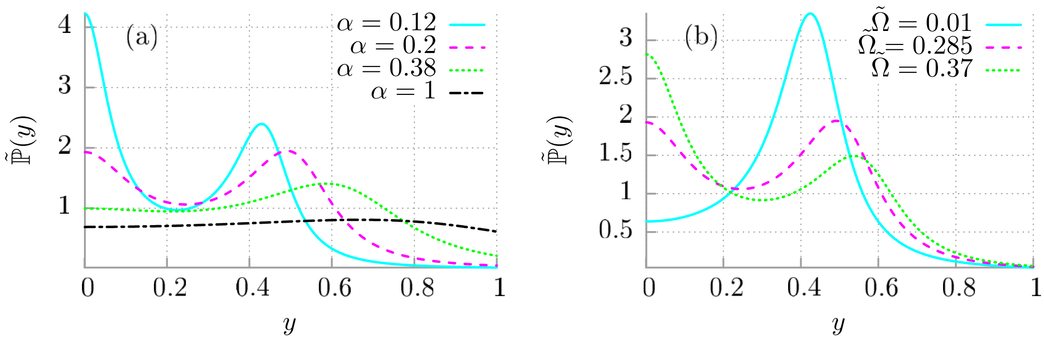

FIG. 6. (a) The probability distribution $\tilde{\mathbb{P}}(y)$ scaled according to Eq. (26) is depicted for exponentially decaying oscillations with $\gamma_E(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}\cos(\Omega t)$ and different values of $\alpha = \varepsilon/\mu_0$ and fixed $\tilde{\Omega} = \Omega/\mu_0 = 0.285$. (b) The same $\tilde{\mathbb{P}}(y)$ is presented for selected dimensionless frequencies $\tilde{\Omega}$ of the memory function and fixed $\alpha = 0.2$.

density $\mathbb{P}(\omega)$,

$$\langle \xi^n \rangle = \int_0^\infty d\omega\, \omega^n \mathbb{P}(\omega). \tag{54}$$

Caution is needed since not all moments may exist, e.g., for distribution (22). The first two moments have a clear physical interpretation [22]. The first moment, i.e., the mean value $\langle \xi \rangle$ of the random variable ξ, is proportional to the kinetic energy E_k of the Brownian particle at zero temperature, $T = 0$, namely,

$$E_0 = E_k(T = 0) = \frac{\hbar}{4}\langle \xi \rangle. \tag{55}$$

The second moment $\langle \xi^2 \rangle$ is proportional to the first correction of the kinetic energy E_k in the high-temperature regime,

$$E_k = \frac{1}{2}k_B T + \frac{\hbar^2}{24 k_B T}\langle \xi^2 \rangle. \tag{56}$$

We note that the averaged kinetic energy E_0 at zero temperature $T = 0$ is nonzero for all values of the system parameters. This is so because of intrinsic quantum vacuum fluctuations. Moreover, E_k monotonically increases from some nonzero value to ∞ when the temperature goes to ∞. If we want to compare the impacts of various dissipation mechanisms on E_k, we have to change the scaling of all dissipation functions $\gamma(t)$. Now, we redefine $\gamma(t)$ in such a way that for all memory functions $\gamma(0) = \tilde{\gamma}_0$, where $\tilde{\gamma}_0$ still characterizes the particle-

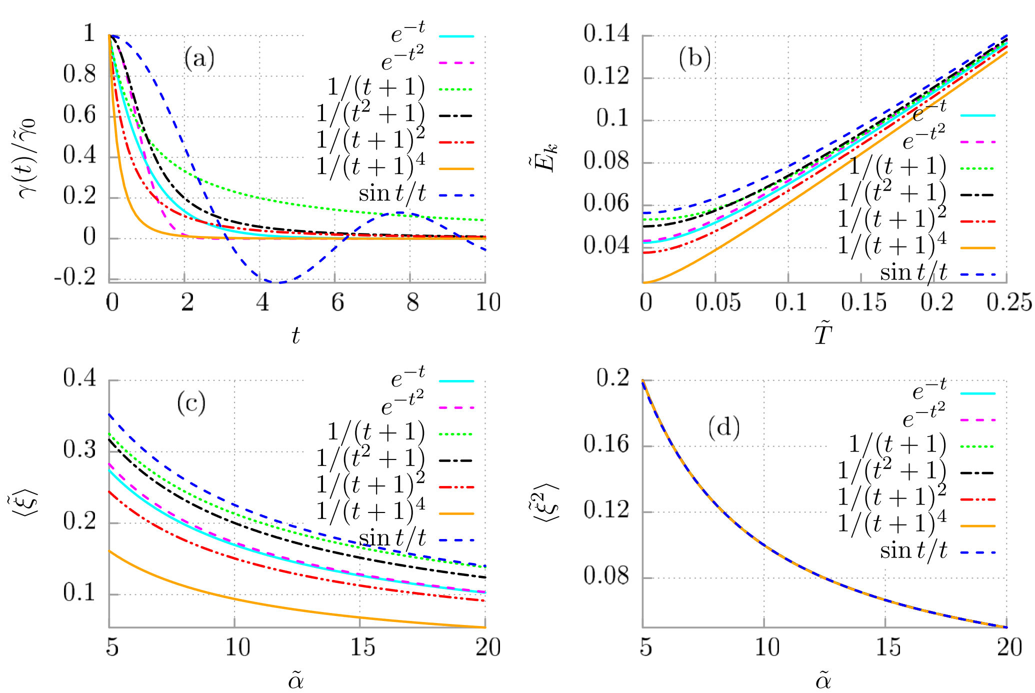

FIG. 7. (a) The normalized memory functions $\gamma(t)/\tilde{\gamma}_0$ representing various dissipation mechanisms. (b) The dimensionless kinetic energy $\tilde{E}_k = \tau_c E_k/\hbar$ of the free Brownian particle presented versus the dimensionless temperature $\tilde{T} = \tau_c k_B T/\hbar$ and various forms of $\gamma(t)$. (c) The first moment $\langle \tilde{\xi} \rangle = \tau_c \langle \xi \rangle$ and (d) the second moment $\langle \tilde{\xi}^2 \rangle = \tau_c^2 \langle \xi^2 \rangle$ depicted versus the dimensionless parameter $\tilde{\alpha} = M/\tilde{\gamma}_0 \tau_c^2$ for different variants of the damping kernel $\gamma(t)$.

thermostat coupling but now has the units $[\tilde{\gamma}_0] = [\mathrm{kg/s}^2]$. For example, for the Drude model $\gamma_D(t) = \tilde{\gamma}_0 \exp(-t/\tau_c)$ or for the Lorenzian shape $\gamma_L(t) = \tilde{\gamma}_0/[(t/\tau_c)^2 + 1]$ [see Fig. 7(a)], where all $\gamma(t)$ assume the same value for $t = 0$. In the classical case, this would correspond to the fixing of the second moment of the random force $\eta(t)$. In Sec. IV, we define $\gamma(t)$ in such a way that $\gamma(t)$ tends to the Dirac delta when the memory time $\tau_c \to 0$, which in the classical case corresponds to Gaussian white noise of the random force $\eta(t)$.

In Fig. 7(b) we compare the kinetic energy E_k for different forms of the memory function $\gamma(t)$. The various curves E_k versus temperature never intersect each other for the same set of parameters. Therefore it is sufficient to analyze the energy only at zero temperature $E_0 \propto \langle \xi \rangle$. We present this characteristic in Fig. 7(c), where we depict the dimensionless first moment $\langle \tilde{\xi} \rangle = \tau_c \langle \xi \rangle$ of the probability density $\mathbb{P}(\omega)$ versus the dimensionless parameter $\tilde{\alpha} = M/\tilde{\gamma}_0\tau_c^2$. In calculations we scale $\omega = x/\tau_c$ as in (23) with fixed τ_c. First, we note that in all cases the averaged kinetic energy at zero temperature decreases when the parameter $\tilde{\alpha}$ increases. We recall that it translates to either (i) an increase in the particle mass M or (ii) a decrease in the coupling strength $\tilde{\gamma}_0$. Moreover, we can see that for the n-algebraic decay ($n = 4$ for green and $n = 2$ for red curves, respectively) the kinetic energy at zero temperature E_0 is lower than for other memory functions. A negligible difference is observed for Drude and Gaussian decay. The highest kinetic energy is induced by the Debye-type dissipation. In the high-temperature regime [Fig. 7(d)], the correction $\langle \tilde{\xi}^2 \rangle = \tau_c^2 \langle \xi^2 \rangle$ depends very weakly on the form of $\gamma(t)$ and the differences are indistinguishable. Finally, at $T = 0$, the energy E_0 increases starting from 0 for $\tau_c \to 0$ and saturates to a finite value as τ_c is longer and longer (not depicted).

VI. SUMMARY

In this work we have revisited an archetype model of quantum Brownian motion formulated in terms of the generalized quantum Langevin equation for a free particle interacting with a large number of independent oscillators that form a thermal reservoir. In particular, we have analyzed the impact of various dissipation mechanisms on the averaged kinetic energy E_k of the Brownian particle. For this purpose we harvested the recently formulated quantum law for partition of energy. It expresses the kinetic energy E_k of the particle as the mean kinetic energy per 1 df of the thermostat oscillators $E_k = \langle \mathcal{E}_k \rangle$. Averaging over the frequencies ω of those oscillators is performed according to the probability distribution $\mathbb{P}(\omega)$, which is related to the dissipation kernel $\gamma(t)$ via the quantum partition theorem. We focused mainly on the influence of the form of the dissipation function on the characteristic features of the probability density $\mathbb{P}(\omega)$.

We have analyzed a multitude of dissipation mechanisms, which are grouped into two classes: algebraic and exponential decay. Within each of these we have considered monotonic as well as oscillating decay. For dissipation functions possessing two characteristic time scales associated with the relaxation time of the particle momentum M/γ_0 and the correlation time of quantum thermal fluctuations τ_c, typically we observed a bell-shaped probability distribution $\mathbb{P}(\omega)$. This means that there is an optimal oscillator frequency which makes the greatest contribution to the kinetic energy of the particle. The magnitude of this optimum is inversely proportional to the system-thermostat coupling strength γ_0. For large values of the latter the contribution of high-frequency oscillators is most pronounced. We have studied also the impact of the memory time τ_c on the shape of the distribution $\mathbb{P}(\omega)$. For a long memory time τ_c the probability density is noticeably peaked, whereas for a short τ_c the distribution is almost flat. Consequently, a decrease in the memory time τ_c causes flattening of the probability density $\mathbb{P}(\omega)$. In this class of dissipation functions we have considered the peculiar case of algebraically decaying oscillations $\gamma(t) \propto \sin t/t$. This choice leads to the distribution $\mathbb{P}(\omega)$'s possessing a finite cutoff frequency which curiously depends on the correlation time of quantum fluctuations τ_c. For a dissipation mechanism with an additional characteristic time scale associated with the period of oscillations $2\pi/\Omega$, qualitatively new features emerge in the density $\mathbb{P}(\omega)$. We exemplify this observation for the case of exponentially decaying oscillations. When the magnitudes of τ_c and $2\pi/\Omega$ are similar then the probability distribution displays a bimodal character. This means that there are two characteristic frequencies of the thermostat oscillators which make a significant contribution to the kinetic energy of the system.

We have demonstrated that the quantum law for energy partition in the present formulation is a conceptually simple yet very powerful tool for analysis of quantum open systems. We hope that our work will stimulate further successful applications.

ACKNOWLEDGMENTS

J.S. was supported by a Foundation for Polish Science (FNP) START fellowship and NCN Grant No. 2017/26/D/ST2/00543. P.B. and J.Ł. were supported by NCN Grant No. 2015/19/B/ST2/02856.

APPENDIX A: SOLUTION OF THE LANGEVIN EQUATION (6)

Equation (6) is a linear integrodifferential equation for the momentum operator $p(t)$. Because its integral part is a convolution, it can be solved by the Laplace transform method, yielding

$$z\hat{p}_L(z) - p(0) + \frac{1}{M}\hat{\gamma}_L(z)\hat{p}_L(z) = -\hat{\gamma}_L(z)x(0) + \hat{\eta}_L(z), \tag{A1}$$

where $\hat{p}_L(z)$, $\hat{\gamma}_L(z)$, and $\hat{\eta}_L(z)$ are the Laplace transforms of $p(t)$, $\gamma(t)$, and $\eta(t)$, respectively [see Eq. (9)]. The operators $p(0)$ and $x(0)$ are the momentum and coordinate operators of the Brownian particle at time $t = 0$. From this equation it follows that

$$\hat{p}_L(z) = \hat{R}_L(z)p(0) - \hat{R}_L(z)\hat{\gamma}_L(z)x(0) + \hat{R}_L(z)\hat{\eta}_L(z), \tag{A2}$$

where

$$\hat{R}_L(z) = \frac{M}{Mz + \hat{\gamma}_L(z)}. \tag{A3}$$

The inverse Laplace transform of (A2) gives the solution $p(t)$ for the momentum of the Brownian particle, namely,

$$p(t) = R(t)p(0) - \int_0^t du\ R(t-u)\gamma(u)x(0) + \int_0^t du\ R(t-u)\eta(u), \tag{A4}$$

where the response function $R(t)$ is the inverse Laplace transform of the function $\hat{R}_L(z)$ in Eq. (A3). Because the statistical properties of thermal noise $\eta(t)$ are specified, all statistical characteristics of the particle momentum $p(t)$ can be calculated, in particular, its kinetic energy.

APPENDIX B: KINETIC ENERGY IN THE EQUILIBRIUM STATE

In order to derive the averaged kinetic energy of the Brownian particle in the equilibrium state, we first calculate the symmetrized momentum-momentum correlation function $\langle [p(t); p(s)]_+\rangle$. For long times, $t \gg 1$, $s \gg 1$, only the last term in (A4) contributes and then

$$\langle [p(t); p(s)]_+\rangle = \int_0^t dt_1 \int_0^s dt_2\ R(t-t_1)R(s-t_2) \times \langle [\eta(t_1); \eta(t_2)]_+\rangle. \tag{B1}$$

Now, we express the correlation function $C(t_1 - t_2) = \langle [\eta(t_1); \eta(t_2)]_+\rangle$ of quantum thermal noise by its Fourier transform [see Eq. (C6b) in Appendix C],

$$\langle [p(t); p(s)]_+\rangle = \int_0^\infty d\omega\ \hat{C}_F(\omega) \int_0^t dt_1 \int_0^s dt_2\ R(t-t_1) \times R(s-t_2)\cos[\omega(t_1-t_2)]. \tag{B2}$$

In particular, for $t = s$, it is the second statistical moment of the momentum,

$$\langle p^2(t)\rangle = \int_0^\infty d\omega\ \hat{C}_F(\omega) \int_0^t dt_1 \int_0^t dt_2\ R(t-t_1) \times R(t-t_2)\cos[\omega(t_1-t_2)]. \tag{B3}$$

We introduce new integration variables, $\tau = t - t_1$ and $u = t - t_2$, and convert Eq. (B3) to the form

$$\langle p^2(t)\rangle = \int_0^\infty d\omega\ \hat{C}_F(\omega) \int_0^t d\tau \int_0^t du\ R(\tau)R(u) \times \cos[\omega(\tau-u)]. \tag{B4}$$

We perform the limit $t \to \infty$ to derive an expression for the average kinetic energy in the equilibrium state, namely,

$$E_k = \lim_{t\to\infty} \frac{1}{2M}\langle p^2(t)\rangle = \frac{1}{2M}\int_0^\infty d\omega\ \hat{C}_F(\omega)I(\omega), \tag{B5}$$

where

$$I(\omega) = \int_0^\infty d\tau \int_0^\infty du\ R(\tau)R(u)\cos[\omega(\tau-u)] = \hat{R}_L(i\omega)\hat{R}_L(-i\omega) \tag{B6}$$

is the product of the Laplace transform of the response function $R(t)$. At this point, we can exploit the fluctuation-dissipation relation, (C8) (Appendix C), to express the noise correlation spectrum $\hat{C}_F(\omega)$ by the dissipation spectrum $\hat{\gamma}_F(\omega)$ and convert (B5) to the form

$$E_k = \int_0^\infty d\omega\ \frac{\hbar\omega}{4M}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\hat{\gamma}_F(\omega)\hat{R}_L(i\omega)\hat{R}_L(-i\omega). \tag{B7}$$

We observe that

$$\mathcal{E}_k(\omega) = \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_BT}\right) \tag{B8}$$

is the averaged (thermal) kinetic energy per 1 df of the thermostat consisting of free harmonic oscillators [32]. The remaining part of the integrand in Eq. (B7) reads

$$\begin{aligned}\mathbb{P}(\omega) &= \frac{1}{M}\hat{\gamma}_F(\omega)\hat{R}_L(i\omega)\hat{R}_L(-i\omega)\\ &= \frac{M}{\pi}\frac{\hat{\gamma}_L(i\omega)+\hat{\gamma}_L(-i\omega)}{[\hat{\gamma}_L(i\omega)+iM\omega][\hat{\gamma}_L(-i\omega)-iM\omega]}\\ &= \frac{1}{\pi}[\hat{R}_L(i\omega)+\hat{R}_L(-i\omega)],\end{aligned} \tag{B9}$$

where we have used Eq. (A3) for $\hat{R}_L(z)$ and the relation between the Laplace and the cosine Fourier transforms. With these two expressions for $\mathcal{E}_k(\omega)$ and $\mathbb{P}(\omega)$, the final form of the averaged kinetic energy E_k of the Brownian particle reads

$$E_k = \int_0^\infty d\omega\ \mathcal{E}_k(\omega)\mathbb{P}(\omega). \tag{B10}$$

APPENDIX C: FLUCTUATION-DISSIPATION RELATION

We assume a factorized initial state of the composite system, i.e., $\rho(0) = \rho_S \otimes \rho_E$, where ρ_S is an arbitrary state of the Brownian particle and ρ_E is an equilibrium canonical state of the thermostat of temperature T, namely,

$$\rho_E = \exp(-H_E/k_BT)/\mathrm{Tr}[\exp(-H_E/k_BT)], \tag{C1}$$

where

$$H_E = \sum_i\left[\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2q_i^2\right] \tag{C2}$$

is the Hamiltonian of the thermostat. The factorization means that there are no initial correlations between the particle and the thermostat. The initial preparation turns the force $\eta(t)$ into the operator-valued quantum thermal noise, which in fact is a family of noncommuting operators whose commutators are c numbers. This noise is unbiased and its mean value is 0:

$$\langle\eta(t)\rangle \equiv \mathrm{Tr}[\eta(t)\rho_E] = 0. \tag{C3}$$

Its symmetrized correlation function

$$C(t,u) = \langle[\eta(t);\eta(u)]_+\rangle = \tfrac{1}{2}\langle\eta(t)\eta(u)+\eta(u)\eta(t)\rangle \tag{C4}$$

depends on the time difference

$$C(t,u) = C(t-u) = \sum_i \frac{\hbar c_i^2}{2m_i\omega_i}\coth\left(\frac{\hbar\omega_i}{2k_BT}\right)\cos[\omega_i(t-u)] = \int_0^\infty d\omega\,\frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)J(\omega)\cos[\omega(t-u)], \tag{C5}$$

where the spectral function $J(\omega)$ is given by Eq. (4). The higher-order correlation functions are expressed by $C(t_i - t_j)$ and have the same form as the statistical characteristics for classical stationary Gaussian stochastic processes. Therefore $\eta(t)$ defines a quantum stationary Gaussian process with time homogeneous correlations.

The dissipation and correlation functions can be presented as cosine Fourier transforms,

$$\gamma(t) = \int_0^\infty d\omega\,\hat{\gamma}_F(\omega)\cos(\omega t), \tag{C6a}$$

$$C(t) = \int_0^\infty d\omega\,\hat{C}_F(\omega)\cos(\omega t), \tag{C6b}$$

with their inverses,

$$\hat{\gamma}_F(\omega) = \frac{2}{\pi}\int_0^\infty dt\,\gamma(t)\cos(\omega t), \tag{C7a}$$

$$\hat{C}_F(\omega) = \frac{2}{\pi}\int_0^\infty dt\,C(t)\cos(\omega t). \tag{C7b}$$

If we compare Eqs. (3) and (C5)–(C6b), we observe that

$$\hat{C}_F(\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\hat{\gamma}_F(\omega). \tag{C8}$$

This relation between the spectrum $\hat{\gamma}_F(\omega)$ of dissipation and the spectrum $\hat{C}_F(\omega)$ of thermal noise correlations is the body of the fluctuation-dissipation theorem [36,37] in which quantum effects are incorporated via the prefactor on the right-hand side of Eq. (C8). We want to stress that definition (4) of the spectral density $J(\omega)$ differs from another frequently used form, $\tilde{J}(\omega) = \omega J(\omega)$. We prefer definition (4) because of the direct relation to the Fourier transforms of (3) and (C6a), i.e., $J(\omega) = \hat{\gamma}_F(\omega)$. Here, the ohmic case corresponds to $J(\omega) = \text{const}$.

For a finite number of thermostat oscillators, all dynamical quantities are almost-periodic functions of time, in particular, the dissipation function $\gamma(t)$ and the correlation function $C(t)$. In the thermodynamic limit, when the number of oscillators tends to ∞, the dissipation function $\gamma(t)$ decays to 0 as $t \to \infty$ and the singular spectral function $J(\omega)$ defined by Eq. (4) tends to a (piecewise) continuous function. From this point of view, the dissipation mechanism is determined by the memory kernel $\gamma(t)$ or, equivalently, by the spectral density of thermostat modes $J(\omega)$, which contains necessary information on the particle-thermostat interaction.

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