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# Partition of energy in quantum systems

Rozprawa doktorska

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**Słowa kluczowe**: kwantowe układy otwarte, kwantowy ruch Browna, kwantowe uogólnione równania Langevina, twierdzenie o ekwipartycji energii, twierdzenia fluktuacyjno-dyssypacyjne, partycja energii kinetycznej w układach kwantowych

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[1] uwzględniając merytoryczny wkład i dyskusje z promotorem oraz promotorem pomocniczym (w ramach prowadzonego seminarium dyplomowego)

# Podziękowania

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# Contents

# Abstract

This dissertation is a study of some aspects of open quantum systems - phenomena that emerge in a system that is a quantum particle coupled to thermostat. The problem is once again revisited and modeled in the well known Caldeira-Leggett framework as a quantum particle (quantum system) plus quantum thermostat composed of an infinite number of harmonic oscillators. The composite system is treated as a closed quantum system. The analysis is performed using the language of quantum generalized Langevin equations which for particular cases are solved by the Laplace transformation method. This is by no means a novel problem, nonetheless, as it became apparent, even such a seemingly well-known system can conceal previously unknown properties. This, in turn, allows for deeper understanding properties of the system and formulation of new interpretations of known relations. In this dissertation, I have included the re-derivation of quantum Langevin equations for two paradigmatic and exactly solvable models: a free Brownian particle and a harmonic oscillator.

The main result of this dissertation is the formulation of the *theorem on partition of kinetic energy for quantum systems*. By virtue of this theorem both mean kinetic energy $E_k$ at the thermodynamical equilibrium state and, for the case of the harmonic oscillator, mean potential energy $E_p$ can be expressed as the relations $E_k = \langle \mathcal{E}_k \rangle$ and $E_p = \langle \mathcal{E}_p \rangle$, where $\langle \mathcal{E}_k \rangle$ and $\langle \mathcal{E}_p \rangle$ are average kinetic and potential energies per one degree of freedom of the harmonic oscillators of thermostat. Here, the symbol $\langle \ldots \rangle$ denotes a two-fold averaging:

1. over the Gibbs canonical state for the thermostat and
2. over thermostat oscillators frequencies $\omega$ which contribute to $E_k$ and $E_p$ according to the probability distributions $\mathbb{P}_k(\omega)$ and $\mathbb{P}_p(\omega)$, respectively.

This can be viewed as a long-awaited quantum counterpart of the classical *energy equipartition theorem* and is a significant contribution to fundamentals of quantum statistical physics.

# Streszczenie

Niniejsza rozprawa doktorska poświęcona jest zagadnieniu energetyki układów kwantowych oddziałujących z termostatem. Omawiany problem został opisany w oparciu o model Caldeiry-Leggetta: kwantowa cząstka (układ kwantowy) plus kwantowy termostat składający się z nieskończonej liczby niezależnych oscylatorów harmonicznych. Analiza przedstawiona w pracy jest oparta na uogólnionych równaniach Langevina, które rozwiązywałem przy użyciu metody tranformacji Laplace'a. Zagadnienie któremu poświęcona jest ta rozprawa nie jest w żadnej mierze nowym problem, niemniej jednak nawet tak dobrze poznane układy mogą skrywać w sobie ciągle nieodkryte własności. To z kolei może prowadzić do głębszego zrozumienia problemu oraz sformułowania nowych interpretacji. W rozprawie tej zawarłem analizę dwóch paradygmatycznych i analitycznie rozwiązywalnych modeli: swobodnej cząstki Browna oraz oscylatora harmonicznego. Główny rezultat tej pracy zawarty jest w zaproponowanym *twierdzeniu o partycji energii* na mocy którego zarówno średnia energia kinetyczna $E_k$ w stanie równowagi termodynamicznej, jak i w przypadku oscylatora harmonicznego jego średnia energia potencjalna $E_p$, mogą zostać wyrażone za pomocą relacji $E_k = \langle \mathcal{E}_k \rangle$ i $E_p = \langle \mathcal{E}_p \rangle$, gdzie $\langle \mathcal{E}_k \rangle$ oraz $\langle \mathcal{E}_p \rangle$ są odpowiednio średnią energią kinetyczną i potencjalną przypadającą na jeden stopień swobody oscylatorów harmonicznych wchodzących w skład termostatu. Użyty tu symbol $\langle \ldots \rangle$ oznacza podwójne średniowanie:

1. ze względu na stany zespołu kanonicznego Gibbsa dla termostatu
2. ze względu na częstości oscylatorów termostatu $\omega$, które wnoszą wkład do energii kinetycznej $E_k$ jak i potencjalnej $E_p$ określony poprzez odpowiednie rozkłady prawdopodobieństwa $\mathbb{P}_k(\omega)$ i $\mathbb{P}_p(\omega)$.

Wynik ten jest odpowiednikiem klasycznego *twierdzenia o ekwipartycji energi* dla układów kwantowych i stanowi istotny wkład do kwantowej fizyki statystycznej.

# 1 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 forces, quantum information: these are generic examples which in turn carry the potential for new applications in the near or further future. Yet, there remain new properties, behavior and phenomena to be uncovered in this world. One such an example is a theorem on equipartition of energy. It is one of the fundamental and universal laws of classical statistical physics. In this context, the quantum counterpart of this theorem still has not been formulated for quantum systems. In this PhD thesis, I attempt to take one step forward. In classical statistical physics, this theorem states that for each degree of freedom the average kinetic energy equals $E_k = k_B T/2$, where $k_B$ is the Boltzmann constant and T is temperature of the system. Already in 1845 John James Waterston, an often forgotten pioneer of the kinetic theory of gases, proposed equipartition of kinetic energy for translational motion. This idea was further extended by the fathers of modern statistical physics in the persons of James Clerk Maxwell (1859) and Ludwig Boltzmann (1876). Since that time the theorem on energy equipartition has become one of the most important and most useful relations exploited in various branches of Natural Science, including physics, chemistry and biology. Surprisingly, from the time of Max Planck (1900) and the birth of quantum mechanics, there is no quantum analogue of the energy equipartition theorem.

In literature, one can find reports on energetics of selected quantum systems [1]. In Ref. [2], an exact expression for the thermodynamic 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 the more conventional method using the fluctuation-dissipation theorem and obtained the expression for kinetic energy of the quantum oscillator [3]. At the same time, the review on quantum Brownian motion was published [4]. Formulas for the variance of position and momentum of the oscillator are presented in Table 2 therein. There are also books [5, 6, 7, 8] in which different expressions for kinetic energy of a free Brownian particle can be obtained directly or indirectly. Lately, kinetic energy of a trapped Fermi gas has been considered [9]. Many other aspects of quantum Brownian motion have been intensively studied in last few years [10, 11, 12, 13, 14, 15, 16, 17, 18]. However, the previous results have not been *directly* related to the energy equipartition theorem.

In our papers [19, 20, 21, 22], after over 150 years from its first manifestation for classical systems and after over 100 years of development of quantum theory, we try to fill this far-reaching gap, at least partially, and derive quantum law for partition of energy which seemingly has escaped from the researchers eyes for so many years. The proposed law has an appealing, transparent and simple form in which $E_k$ can be related to thermal kinetic energy per one degree of freedom of the *thermostat* consisting of quantum harmonic oscillators (bosons). It is valid for an arbitrary strength of the system-thermostat coupling. We derive it for two paradigmatic and exactly solvable models of quantum open systems: a free Brownian particle and a harmonic oscillator. Last but not least, we formulate conditions for the validity of this law for a general quantum system. To this aim we apply the Callen-Welton fluctuation-dissipation relation. However, we still cannot prove the normalization condition of an auxiliary probability density for arbitrary quantum systems.

Due to its fundamental character, the presented problem is of broad interest (for all physicists) and has significant implications across all subfields of quantum physics. Moreover, we propose a new theoretical technique with far-reaching impact in which the average value of quantum observables in equilibrium state, in particular, kinetic energy, may be directly inferred solely from the known properties of the heat bath. It is a challenge to extend our approach to other quantum systems to show that indeed our proposed law is universal and holds true for all quantum systems. One of the methods could be based on thermodynamic retarded Green functions which can be calculated for toy systems or approximately for selected systems and next to test the normalization condition.

## 1.1 Structure of the dissertation

The PhD thesis is based on four published papers:

- 1. P. Bialas and J. Łuczka, Kinetic energy of a free quantum Brownian particle, *Entropy* **20**, 123 (2018)
- 2. J. Spiechowicz, P. Bialas, and J. Łuczka, Quantum partition of energy for a free Brownian particle: Impact of dissipation, *Phys. Rev.* A **98**, 052107 (2018)
- 3. P. Bialas, J. Spiechowicz, J. Łuczka, Partition of energy for a dissipative quantum oscillator, *Scientific Reports* **8**, 16080 (2018)
- 4. P. Bialas, J. Spiechowicz, J. Łuczka, Quantum analogue of energy equipartition theorem, *Journal of Physics A: Mathematical and Theoretical* **52**, 15 (2019)

The chronology of these papers is different. In the first paper (sent to *Entropy* at the end of 2017), I started to attack the problem of calculation of kinetic energy for a free quantum particle without any attempt to relate it to the theorem on equipartition of energy. I exploited the method of the integro-differential Langevin equation and solved this equation for a special form of the integral (memory) kernel by converting this equation into a set of differential equations. Accidentally we have noticed that the expression for kinetic energy of the Brownian particle can be interpreted as a mean value of kinetic energy of the quantum oscillator over some probability distribution $\mathbb{P}$. It was a stimulus to look deeper into the universality of this expression and next the fourth paper (*J. Phys. A*) has been written. The method of solution of the Langevin equation has been radically simplified and this method allowed to reveal a relation between the probability density $\mathbb{P}$ and the response function $R(t)$ which solves the Langevin equation. The relation is extremely simple and therefore remarkable. Chronologically and historically, the fourth paper (*J. Phys. A*) was the second one (because of a long procedure in publishing this paper). The next two papers (2 and 3) have been published without any perturbations and contain a detailed analysis of the problem for selected examples of dissipation mechanisms in dynamics of selected quantum systems.

The thesis is organized in the following way: In Chapter 2, the theorem on energy equipartition for classical systems is formulated. I describe an alternative interpretation of this relation for the total system (the given system + thermostat) being in the

Gibbs canonical state. I present the method of a generalized Langevin equation for classical systems and properties of classical thermal noise. The classical version of the fluctuation-dissipation theorem is reminded. It allows to compare it with its quantum counterpart. I also show how the energy equipartition relation follows from the standard Langevin equation. Chapter 3 comprises a brief discussion on quantum Brownian motion and introduction to the theory of a generalized Langevin equation. I list properties of quantum thermal noise and quantum version of the fluctuation-dissipation relation. In Chapters 4 and 5, two exactly solved models are studied: a free Brownian particle and quantum dissipative oscillator. These two old clichéd models have been re-considered many, many times by each next generation of physicists. However, it has been difficult to find a transparent presentation of this fundamental issue of the quantum statistical physics focused on kinetic energy. Chapter 4 contains a detailed analysis of energetics for free quantum Brownian motion. This chapter contains a solution of the generalized Langevin equation. The solution method is based on the Laplace transformation. Next, I formulate the *quantum energy partition theorem* and analyze it for a broad spectrum of specific memory kernels of the generalized Langevin equation. Various forms of the memory kernels correspond to various dissipation mechanisms of energy. Moreover, the case of exponentially decaying oscillations of memory kernel is calculated by two different methods (mainly because of the pedagogical reason and to include the method used in the first paper). At the end of this chapter, some specific regimes are discussed. In Chapter 5, the quantum dissipative oscillator is analyzed. An additional aspect is analyzed, namely, potential energy of the oscillator is re-considered in the framework of the energy partition. In Chapter 6, I apply the Callen-Welton fluctuation-dissipation relation to derive the energy partition relation for arbitrary quantum systems. However, while the positivity (non-negativity) of the probability distribution $\mathbb{P}$ is proved, its normalization is still an open problem and is re-formulated to the question of the value of the corresponding generalized susceptibility $\chi(\omega)$ at zero frequency, i.e. what is the value of $\chi(0)$? In the final part of the thesis, there are five Appendices with supplemental technical materials.

# 2 Equipartition of kinetic energy for classical systems

## 2.1 Equipartition of energy - Gibbs canonical distribution approach

In 1845 John James Waterston formulated a version of equipartition of energy for translational motion [23]. In 1876 Ludwig Boltzmann proposed the following [24]:

**For a system in thermodynamic equilibrium, the mean kinetic energy is equally shared among all degrees of freedom of the system.**

We re-derive the formula for equipartition of kinetic energy in classical systems in a way that allows us to generalize it also for quantum systems.

Let the classical system $S$ of particles be in a thermodynamic equilibrium state with thermostat (environment, heat bath, surroundings) $E$ of temperature $T$. The system $S$ is characterized by the Hamiltonian:

$$H_S = H_S(\mathbf{X}, \mathbf{P}) = \sum_i \frac{P_i^2}{2M_i} + \sum_i U_S(X_i) + \sum_{i,j} V_S(X_i, X_j), \tag{2.1}$$

where $\mathbf{X}, \mathbf{P}$ are vectors of all coordinates $\{X_i\}$ and all momenta $\{P_i\}$ of the system $S$.

Let the thermostat $E$ be characterized by the Hamiltonian:

$$H_E = H_E(\mathbf{x}, \mathbf{p}) = \sum_k \frac{p_k^2}{2m_k} + \sum_k U_E(x_k) + \sum_{k,n} V_E(x_k, x_n), \tag{2.2}$$

where $\mathbf{x}, \mathbf{p}$ are vectors of all coordinates $\{x_k\}$ and all momenta $\{p_k\}$ of the thermostat $E$. The interaction between the system and thermostat is of a general form,

$$H_{S-E} = H_{S-E}(\mathbf{X}, \mathbf{x}) = \sum_{i,k} \lambda_{ik}\, V(X_i, x_k), \tag{2.3}$$

where the set of parameters $\{\lambda_{ik}\}$ characterizes the coupling strength between the system and thermostat.

We assume that the thermodynamic equilibrium state of the total system $S + E$ is described by the Gibbs canonical states $P(\mathbf{X}, \mathbf{P}, \mathbf{x}, \mathbf{p}) = (1/C_0)e^{-H/k_BT}$, where $k_B$ is the Boltzmann constant, the total Hamiltonian is the sum:

$$H = H(\mathbf{X}, \mathbf{P}, \mathbf{x}, \mathbf{p}) = H_S + H_{S-E} + H_E \tag{2.4}$$

and the normalization constant $C_0$ reads

$$C_0 = \int_{-\infty}^{\infty} \mathbf{dP} \int_{-\infty}^{\infty} \mathbf{dX} \int_{-\infty}^{\infty} \mathbf{dp} \int_{-\infty}^{\infty} \mathbf{dx} \, \exp\{-H(\mathbf{X}, \mathbf{P}, \mathbf{x}, \mathbf{p})/k_B T\}. \tag{2.5}$$

We calculate averaged kinetic energy $\mathcal{E}_k^{(S)}$ of one degree of freedom of the system $S$, namely,

$$\mathcal{E}_k^{(S)} = \frac{1}{2M_i}\langle P_i^2 \rangle = \frac{1}{C_0} \int_{-\infty}^{\infty} \mathbf{dP} \int_{-\infty}^{\infty} \mathbf{dX} \int_{-\infty}^{\infty} \mathbf{dp} \int_{-\infty}^{\infty} \mathbf{dx} \, \frac{P_i^2}{2M_i} \, \exp\{-H(\mathbf{X}, \mathbf{P}, \mathbf{x}, \mathbf{p})/k_B T\}. \tag{2.6}$$

Integration yields:

$$\mathcal{E}_k^{(S)} = \frac{1}{2M_i}\langle P_i^2 \rangle = \frac{1}{2} k_B T.$$

Next, we calculate averaged kinetic energy $\mathcal{E}_k^{(E)}$ of one degree of freedom of the thermostat $E$:

$$\mathcal{E}_k^{(E)} = \frac{1}{2m_k}\langle p_k^2 \rangle = \frac{1}{C_0} \int_{-\infty}^{\infty} \mathbf{dP} \int_{-\infty}^{\infty} \mathbf{dX} \int_{-\infty}^{\infty} \mathbf{dp} \int_{-\infty}^{\infty} \mathbf{dx} \, \frac{p_k^2}{2m_k} \, \exp\{-H(\mathbf{X}, \mathbf{P}, \mathbf{x}, \mathbf{p})/k_B T\}. \tag{2.7}$$

The result reads

$$\mathcal{E}_k^{(S)} = \frac{1}{2m_k}\langle p_k^2 \rangle = \frac{1}{2} k_B T.$$

From above consideration it follows that

$$\mathcal{E}_k^{(S)} = \frac{1}{2M_i}\langle P_i^2 \rangle = \frac{1}{2} k_B T = \frac{1}{2m_k}\langle p_k^2 \rangle = \mathcal{E}_k^{(E)} \tag{2.8}$$

Now, one can re-formulate the theorem on equipartition of kinetic energy in the following way:

**For each degree of freedom of the system $S$, its averaged kinetic energy is equal to the averaged kinetic energy of one degree of freedom of thermostat** $E$, i.e.,

$$\mathcal{E}_k^{(S)} = \mathcal{E}_k^{(E)} \tag{2.9}$$

Moreover, $\mathcal{E}_k^{(S)}$ does not depend on the number of particles, the form of the potential $U_S(X_i)$, the form of interaction $V_S(X_i, X_j)$ and the strength of coupling $\lambda_{ik}$ between the system and thermostat. It depends only on temperature $T$ of thermostat.

## 2.2 Langevin equation

Let us consider a particle (called the Brownian particle) in contact with a large amount of non-interacting particles forming thermostat. Each particle of thermostat is modeled as a harmonic oscillator. An interaction between the Brownian particle and thermostat starts at time $t = 0$. For time $t \leq 0$, thermostat is in the Gibbs canonical state. We assume the celebrated Caldeira-Leggett Hamiltonian of the total closed system [25]:

$$H = \frac{P^2}{2M} + U(X) + \sum_k \left[ \frac{p_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \left( q_k - \eta_k X \right)^2 \right]. \tag{2.10}$$

The total Hamiltonian can be divided into three parts: the Hamiltonian of the Brownian particle:

$$H_B = \frac{P^2}{2M} + U(X), \tag{2.11}$$

the Hamiltonian of thermostat:

$$H_E = \sum_k \left[ \frac{p_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} q_k^2 \right] \tag{2.12}$$

and bi-linear interaction:

$$H_I = \sum_k m_k \eta_k \omega_k^2 \, q_k X \tag{2.13}$$

The last part $\sum_k m_k \omega_k^2 \eta_k^2 X^2/2$ is a counter-term which must be included to ensure that dissipation is homogeneous in all space.

### 2.2.1 Derivation of Langevin equation

We want to construct an effective dynamics of the Brownian particle. To this aim we use the Hamilton equations of motion for all degrees of freedom, both for the particle and for thermostat. They read

$$\dot{X}(t) = \{X, H\} = \frac{P}{M}, \tag{2.14}$$

$$\dot{P}(t) = \{P, H\} = \sum_k \eta_k \omega_k^2 m_k \left(q_k - \eta_k X\right) - U'(X), \tag{2.15}$$

$$\dot{q_k}(t) = \{q_k, H\} = \frac{p_k}{m_k}, \tag{2.16}$$

$$\dot{p_k}(t) = \{p_k, H\} = \omega_k^2 m_k \left(X\eta_k - q_k\right), \tag{2.17}$$

where

$$U'(X) = \frac{d}{dX} U(X). \tag{2.18}$$

The last two Hamilton equations can be rewritten in the form of one second order differential equation:

$$m_k \frac{d^2}{dt^2} \mathrm{q_k}\,(t) = \eta_k \omega_k^2 m_k X(t) - \omega_k^2 m_k \,\mathrm{q_k}\,(t) \tag{2.19}$$

This inhomogeneous differential equation can be solved by the Green's function method:

$$q_k(t) = q_{k0} \cos(\omega_k t) + \frac{p_{k0}}{m_k \omega_k} \sin(\omega_k t) + \eta_k \omega_k \int_0^t ds \, \sin\left[\omega_k (t-s)\right] X(s), \quad t > 0, \tag{2.20}$$

where $q_{k0} = q_k(0)$ and $p_{k0} = p_k(0)$ are initial values of the coordinate and momentum of the thermostat oscillators, respectively. Next, we insert it into Eq. (2.15). From (2.14) and (2.15) we then obtain

$$\begin{aligned} M \frac{d^2}{dt^2} X(t) &= -U'(X(t)) - \eta_k^2 \omega_k^2 m_k X(t) + \eta_k \omega_k^2 m_k \,\mathrm{q_k}\,(t) \\ &= -U'(X(t)) - \sum_k \eta_k^2 \omega_k^2 m_k X(t) \\ &+ \sum_k \eta_k \omega_k^2 m_k \left\{ q_{k0} \cos(\omega_k t) + \frac{p_{k0} \sin(\omega_k t)}{m_k \omega_k} + \eta_k \omega_k \int_0^t ds \, \sin[\omega_k (t-s)] X(s) \right\} \end{aligned} \tag{2.21}$$

We integrate by parts the integral term and finally we get the effective equation in the form

$$M\ddot{X}(t) + U'(X(t)) = -\int_0^t ds\, \gamma(t-s) \dot{X}(s) - \gamma(t) X(0) + F(t), \quad t > 0, \tag{2.22}$$

where

$$\gamma(t-s) = \sum_k \frac{c_k^2}{m_k\omega_k^2} \cos\omega_k(t-s) \tag{2.23}$$

is the memory kernel or the dissipation function and

$$F(t) = \sum_k c_k \left[ q_{k0}\cos(\omega_k t) + \frac{p_{k0}\sin(\omega_k t)}{m_k\omega_k} \right] \tag{2.24}$$

is the fluctuating force - the random force or thermal noise which arise from random (or uncertain) initial conditions for positions and momenta of the thermostat particles. Moreover, we have introduced the rescaled coupling parameters

$$c_k = \eta_k m_k \omega_k^2. \tag{2.25}$$

Although we do not know precisely initial conditions for thermostat, we can assume their initial probability distribution. Eq. (2.22) is called a generalized Langevin equation and alone it does not offer the full description of the investigated problem. In order to get the full picture, we have to assume properties of classical thermal noise $F(t)$.

### 2.2.2 Classical thermal noise

We assume that at initial time $t=0$, thermostat is in the state of thermal equilibrium and is characterized by the Gibbs canonical distribution:

$$f(\bar{q},\bar{p}) = C_0 \exp\left(-\frac{H_E}{k_B T}\right) \tag{2.26}$$

where $\bar{q} = (q_1, q_2, \ldots)$ and $\bar{p} = (p_1, p_2, \ldots)$ refer to thermostat degrees of freedom. The constant $C_0$ is the normalization parameter determined by the condition

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\bar{q}d\bar{p} f(\bar{q},\bar{p}) = 1 \tag{2.27}$$

Because the Hamilton function of thermostat is a quadratic form, the distribution $f(\bar{q},\bar{p})$ is a Gaussian distribution. Taking into account properties of the Gaussian distribution, we can calculate the mean values for positions and momenta:

$$\langle x_k(0)\rangle = 0 \tag{2.28}$$

$$\langle p_k(0)\rangle = 0 \tag{2.29}$$

$$\langle p_k(0)p_j(0)\rangle = \left\langle p_k(0)^2\right\rangle \delta_{k,j} = m_k k_B T \delta_{k,j} \tag{2.30}$$

$$\langle x_k(0)x_j(0)\rangle = \left\langle q_k(0)^2\right\rangle \delta_{k,j} = \frac{k_B T}{m_k \omega_k^2}\delta_{k,j} \tag{2.31}$$

$$\langle p_k(0)x_j(0)\rangle = 0 \tag{2.32}$$

From the above relations one can deduce properties of thermal noise. It is a stochastic Gaussian process of zero-mean,

$$\langle F(t)\rangle = \sum_k c_k \left[\langle q_k(0)\rangle \cos(\omega_k t) + \frac{\langle p_k(0)\rangle \sin(\omega_k t)}{m_k \omega_k}\right] = 0 \tag{2.33}$$

and its correlation function reads

$$\langle F(t_1)F(t_2)\rangle = \sum_k c_k^2 \left[\left\langle q_k(0)^2\right\rangle \sin(\omega_k t_1)\sin(\omega_k t_2) + \frac{\left\langle p_k(0)^2\right\rangle}{m_k^2 \omega_k^2}\cos(\omega_k t_1)\cos(\omega_k t_2)\right] \tag{2.34}$$

At this point we can utilize Eqs. (2.30) and (2.31) and it allows to write down the noise correlation function as

$$\langle F(t_1)F(t_2)\rangle = k_B T \sum_k \frac{c_k^2}{m_k \omega_k^2}\cos\left(\omega_k\left(t_1 - t_2\right)\right) \tag{2.35}$$

We note that the above expression resembles a definition of the memory kernel $\gamma(t)$ in Eq. (2.23). Hence, we can write:

$$\langle F(t_1)F(t_2)\rangle = k_B T \gamma(t_1 - t_2) \tag{2.36}$$

This constitutes the fluctuation-dissipation theorem for classical systems. Previously described reasoning and utilizing properties of the noise term allows to obtain a full picture of a classical Brownian motion in the form of the effective equation - the generalized Langevin equation:

$$M\ddot{X}(t) + U'(X(t)) = -\int_0^t ds\gamma(t-s)\dot{X}(t) - \gamma(t)X(0) + F(t), \quad t > 0 \tag{2.37}$$

$$\langle F(t)\rangle = 0 \tag{2.38}$$

$$\langle F(t_1)F(t_2)\rangle = k_B T \gamma(t_1 - t_2) \tag{2.39}$$

This equation is a basis of many applications to a broad class of problems. The simplest is the case of a free Brownian particle, i.e. when $U(X(t)) \equiv 0$ and when thermal noise is the Dirac delta-correlated Gaussian force $F(t)$. In literature, it is named the ohmic damping, i.e. when $\gamma(t) = 2\gamma_0\delta(t)$, and $F(t)$ is called Gaussian white noise. In this case, the generalized Langevin equation (2.37) reduces to the form

$$M\ddot{X}(t) = -\gamma_0\dot{X}(t) + F(t) \tag{2.40}$$

$$\langle F(t)\rangle = 0 \tag{2.41}$$

$$\langle F(t_1)F(t_2)\rangle = 2\gamma_0 k_B T\,\delta(t_1 - t_2) \tag{2.42}$$

It is a Langevin equation for a free Brownian particle which correctly describes properties of its velocity $v(t) = \dot{X}(t)$. In particular, the second moment $< v^2(t) >$ is finite.

## 2.3 Equipartition of energy - Langevin equation approach

Application of the Langevin equation in classical statistical physics is diverse. This approach was proposed by Paul Langevin to analyze the simplest case of Brownian motion - the problem discussed by Smoluchowski and Einstein. Langevin in his paper proposed in his own words "infinitely more simple" approach to this issue. His method is based on rewriting the problem (2.40) in the form of the stochastic differential equation[26, 27]:

$$m\dot{v} = -\gamma v + L(t) \tag{2.43}$$

$$\langle L(t)\rangle = 0 \tag{2.44}$$

$$\langle L(t)L(s)\rangle = \zeta\delta(t-s), \quad \zeta = 2\gamma k_B T, \tag{2.45}$$

where $v$ is the velocity of the Brownian particle and $L(t)$ is noise (that arises from random collisions of the Brownian particle with particles of environment).

The solution of this inhomogeneous linear differential equation reads

$$v(t) = v_0 e^{-\gamma t/m} + \int_0^t e^{-\gamma(t-\tau)/m}\, L(\tau)\, d\tau \tag{2.46}$$

The averaged value of the velocity is

$$\langle v(t)\rangle = \langle v_0\rangle\, e^{-\gamma t/m} \tag{2.47}$$

and the second moment reads

$$\left\langle v(t)^2 \right\rangle = \left\langle v_0^2 \right\rangle e^{-2\gamma t/m} + \frac{\zeta}{2\gamma m}(1 - e^{-2\gamma t/m}) \tag{2.48}$$

For long time, when the equilibrium state is reached, one gets

$$\lim_{t \to = \infty} \left\langle v(t)^2 \right\rangle = \frac{\zeta}{2\gamma m} = \frac{kT}{m} \tag{2.49}$$

and for mean kinetic energy

$$E_k = \frac{m \left\langle v^2(t) \right\rangle}{2} = \frac{1}{2} k_B T \tag{2.50}$$

It shows how the energy equipartition relation can be obtained from the Langevin equation.

# 3 Generalized quantum Langevin equation

## 3.1 Introduction

Physical aspects of classical Brownian motion was studied at the beginning of 20th century by Einstein and Smoluchowski. The quantum Brownian motion certainly is the simplest case of a dissipative quantum system. It is a well-known problem and as such has been investigated for many decades by scientists and there are hundreds of papers published on this topic. It would seem that nowadays there is nothing more to say about such a system. I want to show that even in the simplest systems still new findings can be revealed.

## 3.2 Hamiltonian formulation of problem

Let us consider a quantum system defined in the following way:

- a quantum Brownian particle of mass $M$ is coupled to bosonic heat bath
- at time $t = 0$ thermostat is in a state of thermal equilibrium
- thermostat consists of an infinite set of non-interacting quantum oscillators
- the total system (the Brownian particle + thermostat) is a closed system evolving according to the unitary evolution determined by the total Hamiltonian

$$H = H_B + H_E + H_I \tag{3.1}$$

where $H_B$ is the Hamiltonian of the Brownian particle, $H_E$ is the Hamiltonian of thermostat and interaction between the particle and thermostat is described by the Hamiltonian $H_I$. As in the classical case, we choose the Caldeira-Legget Hamiltonian:

$$H = \frac{p^2}{2M} + U(x) + \sum_k \left[ \frac{p_k^2}{2m_k} + \frac{m_k \omega_k^2}{2} \left( q_k - \eta_k x \right)^2 \right] \tag{3.2}$$

where:

$$H_B = \frac{p^2}{2M} + U(x) \tag{3.3}$$

$$H_E = \sum_k \left[\frac{p_k^2}{2m_k} + \frac{m_k\omega_k^2}{2}q_k^2\right] \tag{3.4}$$

$$H_I = \sum_k \left[m_k\omega_k^2 q_k \eta_k x\right] \tag{3.5}$$

and the coordinate and momentum operators $\{x, p\}$ refer to the Brownian particle while $\{q_k, p_k\}$ are the coordinate and momentum operators of the $k$-th heat bath oscillator of mass $m_k$ and the eigen-frequency $\omega_k$. The parameter $\eta_k$ characterizes the interaction strength of the particle with the $k$-th oscillator. There is the counter-term, the last term proportional to $x^2$, which is included to cancel a harmonic contribution to the particle potential. All coordinate and momentum operators obey canonical equal-time commutation relations.

## 3.3 Heisenberg equations

Analogically as in the case of classical systems, we write down equations of motion which in this case are the Heisenberg equations:

$$\dot{x} = -\frac{i}{\hbar}[x, H] = \frac{p}{M} \tag{3.6}$$

$$\dot{p} = -\frac{i}{\hbar}[p, H] = -\frac{\mathrm{i}}{\hbar}[p, U(x)] + \sum_k c_k\left(q_k - \eta_k x\right) \tag{3.7}$$

$$\dot{q_k} = -\frac{i}{\hbar}[q_k, H] = \frac{p_k}{m_k} \tag{3.8}$$

$$\dot{p_k} = -\frac{i}{\hbar}[p_k, H] = -m_k\omega_k^2\left(q_k - \eta_k x\right), \quad c_k = \eta_k m_k \omega_k^2 \tag{3.9}$$

By combining equations (3.8) and (3.9) we construct the second order differential equation:

$$m_k \ddot{q_k}(t) = -m_k\omega_k^2\left[q_k(t) - \eta_k x(t)\right] \tag{3.10}$$

with the solution

$$q_k(t) = q_{k0}\cos\left(\omega_k t\right) + \frac{p_{k0}\sin\left(\omega_k t\right)}{m_k\omega_k} + \eta_k\omega_k \int_0^t ds\, \sin\left[\omega_k\left(t - s\right)\right] x(s), \tag{3.11}$$

where $x_{k0} = x_k(0)$ and $p_{k0} = p_k(0)$. It has the same form as Eq. (2.20) introduced in the previous chapter for classical Brownian motion. Nevertheless, there is a vital difference in the meaning of used symbols. Now $q_k$, $p_k$, $x$ and $p$ are operators acting on vectors of the Hilbert space. Other differences will become apparent when we proceed into deeper analysis.

Next, we can insert the previously found solution (3.11) into the equation:

$$M\ddot{x} = -\frac{\mathrm{i}}{\hbar}\left[p, U(x)\right] + \sum_k c_k\left(q_k - \eta_k x\right) \tag{3.12}$$

As a result we obtain

$$\begin{aligned} M\ddot{x}(t) &= -\frac{\mathrm{i}}{\hbar}\left[p(t), U(x(t))\right] \\ &+ \sum_k c_k\left(q_{k0}\cos\left(\omega_k t\right) + \frac{p_{k0}\sin\left(\omega_k t\right)}{m_k\omega_k} - \eta_k x + \eta_k\omega_k\int_0^t ds\,\sin\left[\omega_k\left(t-s\right)\right]x(s)\right) \end{aligned} \tag{3.13}$$

The integration by part of the integral term results in the following effective equation of motion for the particle coordinate operator $x(t)$, namely,

$$M\ddot{x}(t) + \frac{\mathrm{i}}{\hbar}\left[p(t), U(x(t))\right] = -\int_0^t ds\,\gamma(t-s)\dot{x}(s) - \gamma(t)x(0) + \eta(t) \tag{3.14}$$

$$p(t) = M\dot{x}(t) \tag{3.15}$$

where:

$$\gamma(t-s) = \sum_k \frac{c_k^2}{m_k\omega_k^2}\cos(\omega_k(t-s)) \tag{3.16}$$

$$\eta(t) = \sum_k c_k\left[q_{k0}\cos(\omega_k t) + \frac{p_{k0}}{m_k\omega_k}\sin(\omega_k t)\right] \tag{3.17}$$

The function $\gamma(t)$ is the *memory kernel* or the *dissipation function* and $\eta(t)$ is an operator which mimics thermal noise. The above formulas look like the corresponding formulas for classical systems. The function $\gamma(t)$ is a scalar function but $\eta(t)$ is an operator and its commutator at different moments is:

$$\left[\eta(t_1), \eta(t_2)\right] = \sum_k c_k^2\left[\frac{i\hbar}{m_k\omega_k}\sin(\omega_k t_1)\cos(\omega_k t_2) - \frac{i\hbar}{m_k\omega_k}\cos(\omega_k t_1)\sin(\omega_k t_2)\right] \tag{3.18}$$

$$= i\hbar\sum_k \frac{c_k^2}{m_k\omega_k}\sin\omega_k(t_1 - t_2) \tag{3.19}$$

As we can see thermal noise at different instants does not commute.

## 3.4 Quantum thermal noise

We assume that the initial state $\rho(0)$ of the composite system $S+E$ is uncorrelated, i.e.,

$$\rho(0) = \rho_S(0) \otimes \rho_E(0),$$

where $\rho_S$ is an arbitrary state of the Brownian particle and $\rho_E$ is an equilibrium Gibbs canonical state $\rho_E \propto \exp(-H_E/k_B T)$ of thermostat of temperature $T$ with the Hamiltonian $H_E$ given by Eq. (3.4). Next, the thermodynamic limit is imposed meaning that thermostat is infinitely extended and the quasi-periodic dissipation kernel $\gamma(t)$ is a decaying function of time. The bosonic thermostat in the Gibbs state is distributed according to the Bose-Einstein distribution. For the thesis to be self-contained, some useful formulas can be found in Appendix A. The correlation function of quantum thermal noise is:

$$\langle \eta(t_1)\eta(t_2)\rangle = \sum_k \frac{\hbar c_k^2}{2m_k\omega_k}\left[\coth\left(\frac{\hbar\omega_k}{2kT}\right)\cos\omega_k\,(t_1-t_2) + \frac{1}{\mathrm{i}}\sin\omega_k\,(t_1-t_2)\right] \tag{3.20}$$

We note that the correlation function is complex and its imaginary part is an odd function. It does not tend to its classical limit and therefore we have to introduce the symmetric correlation function:

$$C(t_1-t_2) = \left\langle [\eta(t_1), \eta(t_2)]_+ \right\rangle = \frac{1}{2}\left(\langle \eta(t_1)\eta(t_2)\rangle + \langle \eta(t_2)\eta(t_1)\rangle\right) \tag{3.21}$$

$$= \sum_k \frac{\hbar c_k^2}{2m_k\omega_k}\coth\left(\frac{\hbar\omega_k}{2kT}\right)\cos\omega_k\,(t_1-t_2) \tag{3.22}$$

This function is even and has only real values. In summary, the operator-valued random force $\eta(t)$ is a family of non-commuting operators whose commutators are $c$-numbers. Its mean value is zero, $\langle\eta(t)\rangle \equiv \mathrm{Tr}\,[\eta(t)\rho_E] = 0$ and the symmetrized correlation function $C(t_1-t_2)$ depends only on time difference $|t_1-t_2|$. Statistical characteristics of the operator $\eta(t)$ are similar to characteristics for a classical stationary Gaussian stochastic process, which models thermal equilibrium fluctuations in classical systems. Therefore, it is called the Gaussian operator, which represents quantum thermal equilibrium noise.

## 3.5 Quantum fluctuation-dissipation theorem

In the classical case examined in the previous chapter we have shown the relation connecting fluctuations of random force and the dissipation kernel. For classical Brownian motion these two objects are connected by the linear relation:

$$\langle \eta(t_1)\eta(t_2)\rangle = k_B T\,\gamma(t_1 - t_2) \tag{3.23}$$

For quantum Brownian motion the fluctuation-dissipation theorem can be also formulated. For the sake of latter investigation let us firstly introduce the spectral function:

$$J(\omega) = \sum_k \frac{c_k^2}{m_k\omega_k^2}\delta(\omega - \omega_k). \tag{3.24}$$

Then the damping kernel (3.16) can be expressed as

$$\gamma(\tau) = \int_0^\infty d\omega J(\omega)\cos\omega\tau \tag{3.25}$$

and the correlation function (3.21) reads

$$C(\tau) = \int_0^\infty d\omega\,\frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)J(\omega)\cos\omega\tau. \tag{3.26}$$

If we introduce the Fourier cosine transforms of the dissipation and correlation functions in the form

$$\gamma(\tau) = \int_0^\infty d\omega\,\hat{\gamma}_F(\omega)\cos\omega\tau, \quad C(\tau) = \int_0^\infty d\omega\,\hat{C}_F(\omega)\cos\omega\tau, \tag{3.27}$$

then we see that the following equality

$$\hat{C}_F(\omega) = \frac{\hbar\omega}{2}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\hat{\gamma}_F(\omega) \tag{3.28}$$

holds true. It constitutes the quantum version of the *fluctuation-dissipation theorem* [28]. In contrast to the classical world, in the quantum case this relation connects spectra $\hat{C}_F(\omega)$ of the noise correlation function and spectra $\hat{\gamma}_F(\omega)$ of dissipation. Quantumness is contained in the prefactor in the above equation which depends on the frequency $\omega$. For high temperature

$$\coth\left(\frac{\hbar\omega}{2k_BT}\right) \approx \frac{2k_BT}{\hbar\omega} \tag{3.29}$$

and then

$$\hat{C}_F(\omega) = k_BT\,\hat{\gamma}_F(\omega) \tag{3.30}$$

which is the Fourier transform of the classical relation (2.36).

## 3.6 Generalized Langevin equation

We have derived the effective evolution equation for the coordinate and momentum operators of the Brownian particle in the form

$$M\ddot{x}(t) + \frac{\mathrm{i}}{\hbar}\left[p(t), U(x(t))\right] = -\int_0^t ds \gamma(t-s)\dot{x}(s) - \gamma(t)x(0) + \eta(t) \tag{3.31}$$

$$p(t) = M\dot{x}(t) \tag{3.32}$$

together with properties of Gaussian operator-valued thermal noise:

$$\langle \eta(t) \rangle = 0 \tag{3.33}$$

$$C(t_1 - t_2) = \left\langle [\eta(t_1); \eta(t_2)]_+ \right\rangle \tag{3.34}$$

$$\hat{C}_F(\omega) = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_BT}\right) \hat{\gamma}_F(\omega) \tag{3.35}$$

Probably Magalinskij [29] was the first, in 1959, who derived the generalized Langevin equation and formulated the problem in the above way. Next, from 1966, a series of papers has been published on this topic, but a complete list of papers is too long to present here. We cite a part of them [30, 31, 32, 33, 34, 35]. Eq. (3.31) with thermal noise description defines a wide class of systems. There are two ingredients which have to be prescribed to determine a specific system - that is:

- the potential $U(x)$
- the memory kernel $\gamma(t)$ or associated with it the correlation function of thermal noise via Eq. (3.35).

The choice of the memory kernel $\gamma(t)$ models dissipation mechanism of the system.

The quantum generalized Langevin equation can be exactly solved only for two forms of the potential $U(x)$, i.e.,

1. for a free Brownian particle when $U(x) \equiv 0$
2. for a harmonic oscillator when $U(x) \propto x^2$

In other cases, approximative methods are used. However, usually they are mathematically uncontrolled. One can also use numerical analysis (which is also an approximation).

# 4 Partition of energy for free quantum Brownian particle

## 4.1 Formulation of problem

Let us start from the simplest exactly solvable case of quantum Brownian motion, i.e., the free Brownian particle. In this case the potential $U(x) \equiv 0$ and the Langevin equation reduces to the form

$$M\ddot{x}(t) = -\int_0^t ds\gamma(t-s)\dot{x}(s) - \gamma(t)x(0) + \eta(t) \tag{4.1}$$

$$p(t) = M\dot{x}(t) \tag{4.2}$$

The integro-differential equation (4.1) is a linear equation and the integral term is of a convolution form. Therefore one can apply e.g. the Laplace transform method. The use of integral transformation provides the benefits of transforming an analytical problem into algebraic ones. Moreover the problem that we are dealing with is defined on time semi-line, which makes a choice of the Laplace transformation to be natural. The main object of our interests is kinetic energy of the Brownian particle in the long-time limit, when a thermodynamic equilibrium state is reached .

## 4.2 Laplace transformation method

To construct a solution for the position operator $x = x(t)$ we apply the Laplace transformation of Eq. (4.1),

$$\begin{aligned}\mathcal{L}\left\{M\ddot{x}(t)\right\}(z) &= M\mathcal{L}\left\{x(t)\right\}(z)\, z^2 - Mzx(0) - M\dot{x}(0) \qquad (4.3)\\ &= M\left(\hat{X}_L(z)z^2 - x(0)z - \dot{x}(0)\right)\\ \mathcal{L}\left\{\int_0^t ds\gamma(t-s)\dot{x}(s)\right\}(z) &= \mathcal{L}\left\{\gamma(t)\right\}(z)\,\mathcal{L}\left\{\dot{x}(t)\right\}(z) \qquad (4.4)\\ &= \hat{\gamma}_L(z)z\hat{X}_L(z) - \hat{\gamma}_L(z)x(0)\\ \mathcal{L}\left\{-\gamma(t)x(0) + \eta(t)\right\}(z) &= -\hat{\gamma}_L(z)x(0) + \hat{\eta}_L(z) \qquad (4.5)\end{aligned}$$

where we use the following notation for the Laplace transform

$$\mathcal{L}\left\{f(t)\right\}(z) = \hat{f}_L(z) = \int_0^{+\infty} dz e^{-tz} f(t) \tag{4.6}$$

We note here that in literature one can find various notation for this transformation like $\mathcal{L}\left(f\right)(z)$, $\left[\mathcal{L}f\right](z)$ $\mathcal{L}_t\left[f\right]$ or $\mathcal{L}_t[f(t)]$ or $\mathcal{L}\left\{f(t)\right\}$. The last notation is used for instance in Ref. [36]. We apply it here with a slight modification of adding explicitly $z$ indicating the point at which the Laplace transformation is taken. For the sake of brevity and readability we use shorthand notation for the Laplace transform of the function $f$: $\hat{f}_L(z)$, where index $L$ stands for "Laplace".

We can summarize equations (4.3) together with (4.4) and (4.5) into the form:

$$\hat{x}_L(z)\left(Mz^2 + \hat{\gamma}_L(z)\right) = Mzx(0) + M\dot{x}(0) + \hat{\eta}_L(z) \tag{4.7}$$

By performing the inverse Laplace transformation for (4.7) we get the solution:

$$x(t) = R(t)x(0) + Q(t)p(0) + \int_0^t Q(t-s)\eta(s)ds \tag{4.8}$$

In a similar way one can obtain a solution for the momentum operator:

$$p(t) = \dot{R}(t)x(0) + R(t)p(0) + \int_0^t R(t-s)\eta(s)ds \tag{4.9}$$

where the functions $Q(t)$ and $R(t)$ are defined by their Laplace transforms:

$$\mathcal{L}\left\{Q(t)\right\}(z) = \hat{Q}_L(z) = \frac{1}{Mz^2 + z\hat{\gamma}_L(z)} \tag{4.10}$$

$$\mathcal{L}\left\{R(t)\right\}(z) = \hat{R}_L(z) = \frac{M}{Mz + \hat{\gamma}_L(z)} \tag{4.11}$$

Both functions are called the *response functions* for the position and momentum operators, respectively.

## 4.3 Kinetic energy

The solution (4.8) for the coordinate operator of the Brownian particle is needed for analysis of quantum diffusion process. It is not the aim of this thesis. The second solution given by Eq. (4.9) is needed to calculate a mean value of kinetic energy of the

Brownian particle. We do it for the regime of long time $t \to \infty$ when a thermal equilibrium state is reached. From Eq. (4.9) we can obtain the symmetrized momentum-momentum correlation function $\left\langle [p(t); p(s)]_+ \right\rangle$. For long times, $t \gg 1, s \gg 1$, due to the properties of the response function $R(t)$ ($\lim_{t\to\infty} R(t) = 0$, c.f. Appendix B) only one term in the expression for $\left\langle [p(t); p(s)]_+ \right\rangle$ survives:

$$\left\langle [p(t); p(s)]_+ \right\rangle = \int_0^t dt_1 \int_0^s dt_2 \; R(t-t_1) R(s-t_2) \left\langle [\eta(t_1); \eta(t_2)]_+ \right\rangle . \tag{4.12}$$

We can express the noise correlation function $C(t_1 - t_2) = \left\langle [\eta(t_1); \eta(t_2)]_+ \right\rangle$ by its Fourier transform to get

$$\left\langle [p(t); p(s)]_+ \right\rangle = \int_0^\infty d\omega \; \hat{C}_F(\omega) \int_0^t dt_1 \int_0^s dt_2 \; R(t-t_1) R(s-t_2) \cos\left[\omega\left(t_1 - t_2\right)\right] . \tag{4.13}$$

The special case $t = s$ corresponds to the second statistical moment of the momentum operator,

$$\langle p^2(t) \rangle = \int_0^\infty d\omega \; \hat{C}_F(\omega) \int_0^t dt_1 \int_0^t dt_2 \; R(t-t_1) R(t-t_2) \cos\left[\omega\left(t_1 - t_2\right)\right] . \tag{4.14}$$

By introducing new variables $\tau = t - t_1$ and $u = t - t_2$ we transform this equation into the following form

$$\langle p^2(t) \rangle = \int_0^\infty d\omega \; \hat{C}_F(\omega) \int_0^t d\tau \int_0^t du \; R(\tau) R(u) \cos\left[\omega\left(\tau - u\right)\right] . \tag{4.15}$$

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

$$E_k = \lim_{t\to\infty} \frac{1}{2M} \langle p^2(t) \rangle = \frac{1}{2M} \int_0^\infty d\omega \; \hat{C}_F(\omega) I(\omega), \tag{4.16}$$

where

$$\begin{aligned} I(\omega) &= \int_0^\infty d\tau \int_0^\infty du \; R(\tau) R(u) \cos\left[\omega\left(\tau - u\right)\right] \\ &= \frac{1}{2} \int_0^\infty d\tau R(\tau) e^{i\omega\tau} \int_0^\infty du R(u) e^{-i\omega u} + \frac{1}{2} \int_0^\infty d\tau R(\tau) e^{-i\omega\tau} \int_0^\infty du R(u) e^{i\omega u} \\ &= \hat{R}_L(i\omega) \hat{R}_L(-i\omega) \end{aligned} \tag{4.17}$$

is a product of the Laplace transforms of the response function $R(t)$. At this point, we can exploit the quantum fluctuation-dissipation relation (3.28), i.e.,

$$\hat{C}_F(\omega) = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_BT}\right) \hat{\gamma}_F(\omega), \tag{4.18}$$

to express the noise correlation spectrum $\hat{C}_F(\omega)$ by the dissipation spectrum $\hat{\gamma}_F(\omega)$ and convert (4.16) to the form

$$E_k = \langle \mathcal{E}_k \rangle = \int_0^\infty d\omega\ \mathcal{E}_k(\omega)\mathbb{P}(\omega), \tag{4.19}$$

where

$$\mathcal{E}_k(\omega) = \frac{\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_BT}\right) \tag{4.20}$$

is thermal kinetic energy per one degree of freedom of thermostat consisting of free harmonic oscillators [37] and

$$\mathbb{P}(\omega) = \frac{1}{M}\hat{\gamma}_F(\omega)\hat{R}_L(i\omega)\hat{R}_L(-i\omega). \tag{4.21}$$

The latter can be represented in an equivalent form as

$$\begin{aligned}\mathbb{P}(\omega) &= \frac{1}{M}\hat{\gamma}_F(\omega)\hat{R}_L(i\omega)\hat{R}_L(-i\omega)\\ &= \frac{M}{\pi}\frac{\hat{\gamma}_L(i\omega)+\hat{\gamma}_L(-i\omega)}{[\hat{\gamma}_L(i\omega)+iM\omega][\hat{\gamma}_L(-i\omega)-iM\omega]} = \frac{1}{\pi}\left[\hat{R}_L(i\omega)+\hat{R}_L(-i\omega)\right]\end{aligned} \tag{4.22}$$

It is interesting that $\mathbb{P}(\omega)$ is a probability measure.

### 4.3.1 Probability distribution $\mathbb{P}(\omega)$

**Theorem 1.**

*$\mathbb{P}(\omega)$ defined by Eq. (4.21) is a probability density, i.e.:*

- *it is non-negative, $\mathbb{P}(\omega) \geq 0$*
- *it is normalized over a half-line of real numbers, i.e., $\int_0^{+\infty} d\omega\, \mathbb{P}(\omega) = 1$*

*Proof.* Firstly, let us introduce another representation of the function $\mathbb{P}(\omega)$ as

$$\mathbb{P}(\omega) = \frac{1}{\pi}\left(\hat{R}_L(i\omega)+\hat{R}_L(-i\omega)\right) = \hat{R}_F(\omega) \tag{4.23}$$

where $\hat{R}_F(\omega)$ is the Fourier cosine transform of the function $R(t)$ defined as:

$$\hat{R}_F(\omega) = \frac{2}{\pi}\int_0^{+\infty} dt\, R(t)\cos{(\omega t)}, \tag{4.24}$$

$$R(t) = \int_0^{+\infty} d\omega\, \hat{R}_F(\omega)\cos{(\omega t)}. \tag{4.25}$$

Since $R(0) = 1$ (c.f. Appendix B) and from the above equation one obtains

$$R(0) = 1 = \int_0^{+\infty} d\omega\, \hat{R}_F(\omega) \tag{4.26}$$

and therefore for arbitrary system parameters

$$\int_0^{+\infty} \mathbb{P}(\omega) d\omega = 1. \tag{4.27}$$

This leads us to the conclusion that $\mathbb{P}(\omega)$ is normalized to unity. Now, we rewrite the formula (4.23) into the form which more convenient for later calculations. For this purpose we note that the Laplace transform can be expressed by the Fourier cosine and sine transforms. In particular,

$$\hat{\gamma}_L(i\omega) = \int_0^{\infty} dt\, \gamma(t)\mathrm{e}^{-i\omega t} = A(\omega) - iB(\omega) \tag{4.28a}$$

$$A(\omega) = \int_0^{\infty} dt\ \gamma(t)\cos{(\omega t)}, \tag{4.28b}$$

$$B(\omega) = \int_0^{\infty} dt\ \gamma(t)\sin{(\omega t)}. \tag{4.28c}$$

If we insert it into Eq. (4.21) then

$$\mathbb{P}(\omega) = \frac{2M}{\pi}\frac{A(\omega)}{A^2(\omega) + [B(\omega) - M\omega]^2}. \tag{4.29}$$

Let us note that the function $A(\omega)$ is related to the spectral function $J(\omega)$ defined as

$$J(\omega) = \frac{\pi}{2}\int_0^{+\infty} dt\gamma(t)\cos{\omega t}. \tag{4.30}$$

Indeed, from the above equation and the definition (4.28c) it follows that $A(\omega) = (\pi/2)J(\omega)$. Because the spectral function is non-negative, $J(\omega) \geq 0$, and the denominator in (4.29) is positive, the function $\mathbb{P}(\omega)$ is non-negative as required. The representation (4.29) allows to study the influence of various forms of the dissipation function $\gamma(t)$ or equivalently the spectral density $J(\omega)$. To summarize we have proven that $\mathbb{P}(\omega)$ is the properly defined probability density function. $\square$

The formula (4.19) together with Eq. (4.21) constitutes a *quantum law for partition of energy*. It means that the averaged kinetic energy $E_k$ of the Brownian particle is an averaged kinetic energy $\mathcal{E}_k$ per one degree of freedom 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. (4.20),

II. over frequencies $\omega$ of those thermostat oscillators which contribute to $E_k$ according to the probability distribution $\mathbb{P}(\omega)$.

Let us now consider specific cases of the memory kernel $\gamma(t)$ in order to analyze properties and feature of the probability density $\mathbb{P}(\omega)$. We want to know which thermostat degrees of freedom (which thermostat oscillators) maximally contribute to the average energy of the Brownian particle and how it depends on parameters of the system, in particular on the memory time of dissipation and the system-thermostat coupling constant. Note that via the expressions in Chapter 3.5, all information about the system-thermostat interaction and properties of thermostat are embodied either in the memory (dissipation) kernel $\gamma(t)$ or equivalently in the thermostat correlation function $C(t)$.

## 4.4 Drude model of dissipation

The simplest way to model the dissipation mechanism via the memory kernel $\gamma(t)$ in the integral term of the generalized Langevin equation. As a first example we consider the memory function $\gamma(t)$ in the form

$$\gamma_D(t) = \frac{\gamma_0}{2\tau_c} e^{-t/\tau_c} \tag{4.31}$$

with two non-negative parameters $\gamma_0$ and $\tau_c$. The first one $\gamma_0$ is the particle-thermostat coupling strength and has the unit $[\gamma_0] = [kg/s]$, i.e. the same as the friction coefficient in the Stokes drag. The second parameter $\tau_c$ characterizes time scale on which the system exhibits memory (non-Markovian) effects. Due to the fluctuation-dissipation theorem $\tau_c$ 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 considered frequently in the coloured noise problems. We choose the above form to ensure that if $\tau_c \to 0$ the function $\gamma_D(t)$ is proportional to the Dirac delta and consequently the integral term in the generalized Langevin equation reduces to the viscous Stokes drag. Other memory kernels considered in the later part of this section also possess this scaling property. For classical systems, in the limit $\tau_c \to 0$, we then obtain the Langevin equation (2.42). In the quantum case, we also obtain the equation which formally looks like (2.42). However, as we will discuss, the white-noise limit cannot be performed for quantum systems!

The Laplace transform of the Drude memory kernel reads

$$\hat{\gamma}_L(z) = \frac{1}{2}\frac{\gamma_0}{\tau_c z + 1} \tag{4.32}$$

and the Laplace transform of the response function is

$$\hat{R}_L(z) = \frac{M}{Mz + \hat{\gamma}_L} = \frac{2M\,(\tau_c z + 1)}{2Mz\,(\tau_c z + 1) + \gamma_0} \tag{4.33}$$

Instead of assuming the form of $\gamma(t)$ one can equivalently specify the spectral density of thermostat modes which for the Drude damping reads

$$J_D(\omega) = \frac{1}{\pi}\frac{\gamma_0}{1 + \omega^2\tau_c^2}. \tag{4.34}$$

From Eq. (4.22) we get the following expression for the probability density

$$\mathbb{P}(\omega) = \frac{1}{\pi}\,\frac{\mu_0\varepsilon^2(\omega^2 + \varepsilon^2)}{\omega^2[\omega^2 + \varepsilon(\varepsilon - \mu_0/2)]^2 + \mu_0^2\varepsilon^4/4}, \tag{4.35}$$

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

If we want to study the impact of the particle mass $M$ or the coupling $\gamma_0$ we have to use the following scaling

$$x = \omega\tau_c = \frac{\omega}{\varepsilon}, \tag{4.36}$$

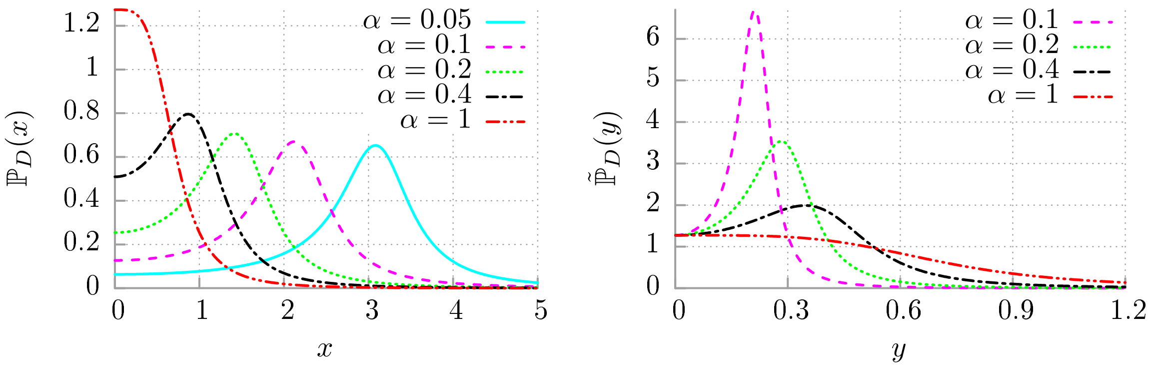

Figure 1: Exponential decay of the dissipation function $\gamma_D(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}$ known as the Drude model. The probability distribution $\mathbb{P}_D(\omega)$ and $\tilde{\mathbb{P}}_D(y)$ in two scalings are presented for different values of the dimensionless parameter $\alpha = \tau_v/\tau_c = M/(\tau_c\gamma_0)$. Left panel: $\tau_c$ is fixed and $\tau_v$ is changed. Right panel: $\tau_v$ is fixed and $\tau_c$ is changed.

which yields the expression

$$\mathbb{P}_D(x) = \varepsilon\mathbb{P}\left(\varepsilon x\right) = \frac{2}{\pi}\frac{2\alpha(x^2+1)}{x^2[2\alpha(x^2+1)-1]^2+1}, \tag{4.37}$$

where

$$\alpha = \frac{M}{\tau_c\gamma_0} = \frac{\varepsilon}{\mu_0} = \frac{\tau_v}{\tau_c} \tag{4.38}$$

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 $\alpha$ being their specific combination. We should remember that $\tau_c$ is fixed in this scaling. In Fig. 1 we present the probability distribution $\mathbb{P}_D(x)$ for different values of the parameter $\alpha$. We can observe that the thermostat oscillators contribute to kinetic energy $E_k$ in a non-homogeneous way. There is the most probable value of $\mathbb{P}_D(x)$ indicating the optimal oscillator frequency $x_M$ which brings the greatest contribution to kinetic energy of the Brownian particle. As it is illustrated in the panel, for small values of $\alpha$ mainly oscillators of high frequency contribute to $E_k$ whereas for large values of $\alpha$ primarily the thermostat oscillators low frequencies have a crucial impact on $E_k$. As $\alpha$ increases $x_M \to 0$ and $\mathbb{P}_D(x)$ becomes a monotonically decreasing function (not depicted). In other words it means that e.g. when the coupling strength between the system and thermostat $\gamma_0$ is strong then 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 $\tau_c$ on the probability distribution $\mathbb{P}(\omega)$. For this purpose we should use another scaling:

$$y = \frac{\omega}{\mu_0}. \tag{4.39}$$

It leads to the expression

$$\tilde{\mathbb{P}}_D(y) = \mu_0 \mathbb{P}(\mu_0 y) = \frac{1}{\pi} \frac{\alpha^2(y^2+\alpha^2)}{y^2[y^2+\alpha(\alpha-1/2)]^2+\alpha^4/4}, \tag{4.40}$$

with the same dimensionless parameter $\alpha$ defined in (4.38). In the right panel of Fig. 1 we present this distribution for selected values of $\alpha$. It follows that for small values of the parameter $\alpha$, or equivalently for long memory time $\tau_c$, the distribution is notably peaked in the region of low frequency modes. Then it rapidly decreases to zero. Consequently only slowly vibrating thermostat oscillators contribute significantly to kinetic energy of the particle. The situation is quite different for short memory time $\tau_c$ (large values of $\alpha$). Then the distribution is flattened meaning that much wider window of oscillators frequency contribute to $E_k$ in a similar way.

For the Drude model, the maximum of the probability density can be analytically evaluated and the result reads

$$\omega_m = \omega_0\sqrt{1-\alpha} = \omega_0\sqrt{1-\frac{M}{\tau_c\gamma_0}}, \quad \omega_0 = \sqrt{\frac{\varepsilon\mu_0}{2}} \quad \alpha < 1. \tag{4.41}$$

Hence, the distribution $\mathbb{P}(\omega)$ displays the non-monotonic character only when $\alpha < 1$. It is the case when the memory time $\tau_c$ is long enough or/and the particle-thermostat coupling constant $\gamma_0$ is sufficiently strong. In other words, the dynamics is pronouncedly non-Markovian and the thermodynamic equilibrium state is far from the Gibbs canonical one. When $\tau_c$ or/and $\gamma_0$ decreases the maximum of $\mathbb{P}(\omega)$ disappears.

In the remaining part of this chapter, we present the probability distribution $\mathbb{P}(\omega)$ for different forms of the memory kernel $\gamma(t)$ without any scaling. One can easily reproduce both scalings. For the scaling as in Eq. (4.36), one can put $\varepsilon = 1$ 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. (4.39), one can put $\mu_0 = 1$ and rescale $\varepsilon \to \varepsilon/\mu_0$

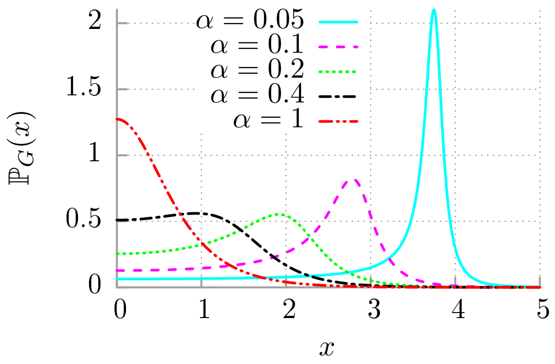

Figure 2: The case of Gaussian decay of the memory kernel $\gamma_G(t) = (\gamma_0/\sqrt{\pi}\tau_c)\,\mathrm{e}^{-t^2/\tau_c^2}$. Probability distribution $\mathbb{P}_G(x)$ is presented for different values of the dimensionless parameter $\alpha$ ($M$ and/or $\gamma_0$ is changed, $\tau_c$ is fixed).

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 $\gamma_0$. In the second scaling - the memory time $\tau_c$.

## 4.5 Gaussian memory kernel

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

$$\gamma_G(t) = \frac{\gamma_0}{\sqrt{\pi}\tau_c}\,\mathrm{e}^{-t^2/\tau_c^2}. \tag{4.42}$$

The Laplace transform of this memory kernel is:

$$\hat{\gamma}_L(\omega) = \frac{\gamma_0\left(-\operatorname{erf}\left(\frac{\omega\tau_c}{2}\right)+1\right)e^{\frac{\omega^2\tau_c^2}{4}}}{2} \tag{4.43}$$

and the Laplace transform of the response function is given by the expression

$$\hat{R}_L(\omega) = \frac{2M}{2M\omega + \gamma_0\left(-\operatorname{erf}\left(\frac{\omega\tau_c}{2}\right)+1\right)e^{\frac{\omega^2\tau_c^2}{4}}} \tag{4.44}$$

The corresponding spectral density is also Gaussian and reads

$$J_G(\omega) = \frac{\gamma_0}{\pi}\,\mathrm{e}^{-\omega^2\tau_c^2/4}. \tag{4.45}$$

The probability distribution $\mathbb{P}_G(\omega)$ has the form

$$\mathbb{P}_G(\omega) = \frac{4}{\pi\mu_0}\,\frac{e^{-(\omega/4\varepsilon)^2}}{\left[2\omega/\mu_0 + ie^{-(\omega/4\varepsilon)^2}\mathrm{Erf}\left(-i\omega/2\varepsilon\right)\right]\left[2\omega/\mu_0 - ie^{-(\omega/4\varepsilon)^2}\mathrm{Erf}\left(i\omega/2\varepsilon\right)\right]}, \tag{4.46}$$

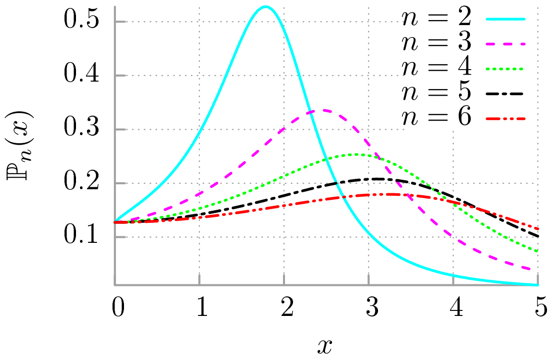

Figure 3: The probability distribution $\mathbb{P}_n(x)$ is depicted for different values of the power exponent $n$ appearing in the generalized algebraic decay of the dissipation kernel $\gamma_n(t) = [(n-1)/2]\, \gamma_0 \tau_c^{n-1}/(t+\tau_c)^n$. The dimensionless parameter $\alpha = 0.1$.

where Erf$(z)$ is the error function

$$\mathrm{Erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z dt\, e^{-t^2}. \tag{4.47}$$

In Fig. 2 we present this probability distribution $\mathbb{P}_G(x)$ [in the scaling (4.36)] for selected values of $\alpha$ ($\tau_v = M/\gamma_0$ is changed and $\tau_c$ is fixed) . Similarly as in the case of the Drude model, the oscillator frequency $x_M$ which brings the greatest contribution to kinetic energy of the particle is a decreasing function of the parameter $\alpha$. However, here we observe two differences: (i) at some interval of $\alpha$ the maximum of $\mathbb{P}_G(x)$ decreases as $\alpha$ increases and (ii) the half-width of $\mathbb{P}_G(x)$ increases as $\alpha$ increases while for the Drude model it is almost constant in a wide interval of $\alpha$. In this case, the impact of the memory time $\tau_c$ is similar to that as for the Drude dissipation, see the right panel of Fig. 1.

## 4.6 n-Algebraic decay of memory kernel

Apart from two exponential forms of the memory functions which we presented above one could model the dissipation function $\gamma(t)$ with algebraic decay. It is worth noting that the power-law decay of the memory functions has been considered as a model of anomalous transport processes [38, 39]. Here, we consider the class of functions

$$\gamma_n(t) = \frac{n-1}{2} \frac{\gamma_0 \tau_c^{n-1}}{(t+\tau_c)^n}, \tag{4.48}$$

where $n \in \mathbb{N}$ and $n \geq 2$. It has the same limiting Dirac delta form for $\tau_c \to 0$ as in two previous cases. The Laplace transform of the dissipation kernel is the following:

$$\hat{\gamma}_L(t) = \frac{\gamma_0 \left(\omega\tau_c\right)^{-n+1} \left(\omega\tau_c\right)^{n-1} (n-1)\, e^{\omega\tau_c}\, \mathrm{E}_n\left(\omega\tau_c\right)}{2} \tag{4.49}$$

and the response function assumes the form

$$\hat{R}_L(\omega) = \frac{2M}{2M\omega + \gamma_0 \left(\omega\tau_c\right)^{-n+1} \left(\omega\tau_c\right)^{n-1} (n-1)\, e^{\omega\tau_c}\, \mathrm{E}_n\left(\omega\tau_c\right)} \tag{4.50}$$

The corresponding spectral density reads

$$J_n(\omega) = \frac{(n-1)\gamma_0}{2\pi} \left[e^{-i\omega\tau_c} E_n(-i\omega\tau_c) + e^{i\omega\tau_c} E_n(i\omega\tau_c)\right] \tag{4.51}$$

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

$$E_n(z) = \int_1^\infty dt\, \frac{e^{-zt}}{t^n}. \tag{4.52}$$

The probability distribution takes the form

$$\mathbb{P}_n(\omega) = \frac{2(n-1)}{\pi\mu_0} \frac{e^{-i\omega/\varepsilon} E_n(-i\omega/\varepsilon) + e^{i\omega/\varepsilon} E_n(i\omega/\varepsilon)}{\left[(n-1)e^{-i\omega/\varepsilon} E_n(-i\omega/\varepsilon) - 2i\omega/\mu_0\right]\left[(n-1)e^{i\omega/\varepsilon} E_n(i\omega/\varepsilon) + 2i\omega/\mu_0\right]}. \tag{4.53}$$

In Fig. 3 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: an increase of the exponent $n$ causes progressive flattening of the probability density function. In other words, if the memory function decreases faster and faster to zero the wider spectrum of frequencies of the thermostat oscillators contribute to $E_k$.

## 4.7 Lorentzian decay of memory kernel

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

$$\gamma_L(t) = \frac{\gamma_0}{\pi} \frac{\tau_c}{t^2 + \tau_c^2}. \tag{4.54}$$

In the probability theory it is termed as the Cauchy distribution. The Laplace transform of this function is

$$\hat{\gamma}_F(\omega) = -\frac{\gamma_0 \left(\left(2\,\mathrm{Si}\left(\omega\tau_c\right) - \pi\right)\cos\left(\omega\tau_c\right) - 2\sin\left(\omega\tau_c\right)\mathrm{Ci}\left(\omega\tau_c\right)\right)}{2\pi} \tag{4.55}$$

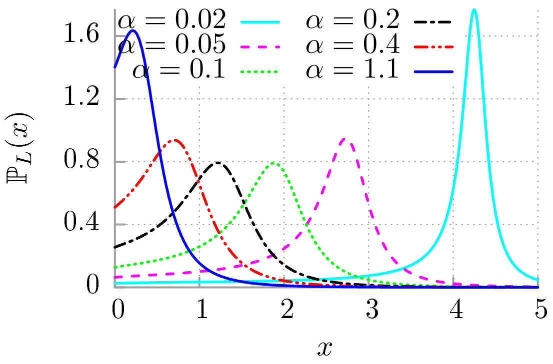

Figure 4: The probability distribution $\mathbb{P}_L(x)$ is depicted for the Lorentzian dissipation kernel $\gamma_L(t) = \gamma_0 \tau_c / \pi(t^2 + \tau_c^2)$ and selected values of the dimensionless parameter $\alpha$ ($M$ or $\gamma_0$ can be changed and $\tau_c$ is fixed).

where Si and Ci are trigonometric integrals defined as:

$$\mathrm{Si}(x) = \int_0^x \frac{\sin(t)}{t} dx \tag{4.56}$$

$$\mathrm{Ci}(x) = \int_0^x \frac{\cos(t)}{t} dx \tag{4.57}$$

and the Laplace transform of the response function can be presented in the form

$$\hat{R}_L(\omega) = \frac{2\pi M}{2\pi M\omega - \gamma_0 \left( (2\,\mathrm{Si}\,(\omega\tau_c) - \pi) \cos(\omega\tau_c) - 2\sin(\omega\tau_c)\,\mathrm{Ci}\,(\omega\tau_c) \right)} \tag{4.58}$$

Alternatively, it may be imposed by the following spectral density of thermostat modes,

$$J_L(\omega) = \frac{\gamma_0}{\pi} e^{-\omega\tau_c}. \tag{4.59}$$

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

$$\mathbb{P}_L(\omega) = \frac{4\pi}{\mu_0} \frac{e^{-\omega/\varepsilon}}{\pi^2 e^{-2\omega/\varepsilon} + c^2(\omega)}, \tag{4.60}$$

where

$$c(\omega) = e^{-\omega/\varepsilon}\mathrm{Ei}(\omega/\varepsilon) - e^{\omega/\varepsilon}\mathrm{Ei}(-\omega/\varepsilon) - \frac{2\pi}{\mu_0}\omega \tag{4.61}$$

and Ei($z$) is the exponential integral defined as

$$\mathrm{Ei}(z) = \int_{-\infty}^{z} \frac{e^t}{t}\, dt. \tag{4.62}$$

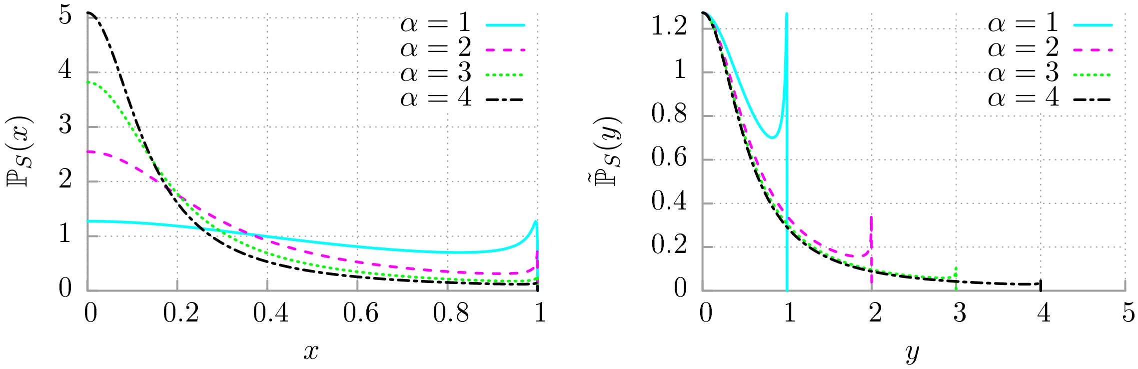

Figure 5: The probability distribution $\mathbb{P}_S(x)$ is presented for the oscillatory decay $\gamma_S(t) = (\gamma_0/\pi)\sin(t/\tau_c)/t$ (the Debye type model) and selected values of the dimensionless parameter $\alpha = \tau_v/\tau_c$. In the left panel $\tau_c$ is fixed and $\tau_v = M/\gamma_0$ is changed. In the right panel $\tau_v$ is fixed and $\tau_c$ is changed.

We illustrate this probability distribution in Fig. 4 for different values of the dimensionless parameter $\alpha = M/(\tau_c\gamma_0)$. The oscillator frequency $x$ which brings the greatest contribution to kinetic energy of the particle is a decreasing function of the parameter $\alpha$. Again, as it was in the previous cases, the magnitude of the maxima in the probability distribution $\mathbb{P}_L(x)$ also depends on $\alpha$. For very small values of $\alpha$ one can note that high frequency modes almost exclusively contribute to kinetic energy of the particle.

## 4.8 Debye type model: algebraically decaying oscillations

The next example of a damping kernel is the oscillatory memory function [40]

$$\gamma_S(t) = \frac{\gamma_0}{\pi}\frac{\sin(t/\tau_c)}{t}. \tag{4.63}$$

which takes both positive and negative values. One can show, via the fluctuation-dissipation relation, that quantum noise $\eta(t)$ exhibits anti-correlations. The Laplace transform of the memory kernel is

$$\hat{\gamma}_F(\omega) = -\frac{\gamma_0 \arctan(\omega\tau_c)}{\pi} + \frac{\gamma_0}{2} \tag{4.64}$$

and the Laplace transform of the response function reads

$$\hat{R}_L(\omega) = \frac{2\pi M}{2\pi M\omega - \gamma_0\left(2\arctan(\omega\tau_c) - \pi\right)} \tag{4.65}$$

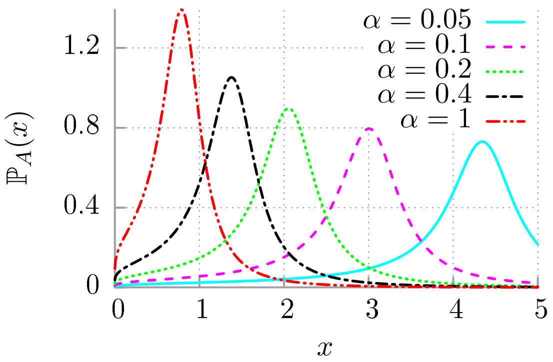

Figure 6: Algebraic decay of the dissipation function $\gamma_A(t) = \gamma_0/(t + \tau_c)$. Probability distribution $\mathbb{P}_A(x)$ is presented for different values of the dimensionless parameter $\alpha = \tau_v/\tau_c$ ($\tau_c$ is fixed and $\tau_v = M/\gamma_0$ is changed).

The spectral density is of the Debye type [40]

$$J_S(\omega) = \frac{\gamma_0}{\pi}\, \theta\left(\frac{1}{\tau_c} - \omega\right), \tag{4.66}$$

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

$$\mathbb{P}_S(\omega) = \frac{4\pi}{\mu_0}\, \frac{\theta(\varepsilon - \omega)}{\pi^2(1 + 4\omega^2/\mu_0^2) + 4\mathrm{arctanh}(\omega/\varepsilon)[\mathrm{arctanh}(\omega/\varepsilon) - 2\pi\omega/\mu_0]} \tag{4.67}$$

and has the same support as $J(\omega)$ in the interval $[0, \varepsilon]$. In Fig. 5 we present the probability density $\mathbb{P}_S(x)$ for selected values of the dimensionless parameter $\alpha$ in two various scalings. In the left panel, the memory time is fixed and the coupling $\gamma_0$ or the mass $M$ is changed. Again, when e.g. $\gamma_0$ decreases (i.e. $\alpha$ increases) more and more oscillators of low frequency contribute to $E_k$. It is the only one founded case for which the probability density has a support on finite interval. It means that the thermostat oscillators of frequencies below some threshold frequency contribute to energy of the Brownian particle. The high-frequency oscillators do not contribute at all to $E_k$. One has to stress that this feature is not related to anti-correlations of thermal noise as shown in Sec. 4.10.

## 4.9 Slow algebraic decay of memory kernel

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

$$\gamma_A(t) = \frac{\gamma_0}{t+\tau_c}. \tag{4.68}$$

The Laplace transform of the memory kernel is found to be

$$\hat{\gamma}_L(t) = \gamma_0 e^{\tau_c z}\,\mathrm{E}_1\left(\tau_c z\right) \tag{4.69}$$

and the Laplace transform of the response function can be expressed as

$$\hat{R}_L(z) = \frac{M}{Mz + \gamma_0 e^{\tau_c z}\,\mathrm{E}_1\left(\tau_c z\right)} \tag{4.70}$$

This dissipation function does not tend to the Dirac delta when $\tau_c \to 0$ (the limit does not exist at all) and therefore this case should be clearly distinguished from the previous cases. The corresponding spectral density has the form

$$J_A(\omega) = \frac{2\gamma_0}{\pi}\,a(\omega). \tag{4.71}$$

The probability distribution reads

$$\mathbb{P}_A(\omega) = \frac{2}{\pi\mu_0}\,\frac{a(\omega)}{a^2(\omega) + [b(\omega) - \omega/\mu_0]^2}, \tag{4.72}$$

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

$$a(\omega) = -\mathrm{ci}(\omega/\varepsilon)\cos(\omega/\varepsilon) - \mathrm{si}(\omega/\varepsilon)\sin(\omega/\varepsilon), \tag{4.73}$$

$$b(\omega) = \mathrm{ci}(\omega/\varepsilon)\sin(\omega/\varepsilon) - \mathrm{si}(\omega/\varepsilon)\cos(\omega/\varepsilon). \tag{4.74}$$

The functions ci($z$) and si($z$) are cosine and sine integrals defined as

$$\mathrm{ci}(z) = -\int_z^\infty \frac{\cos t}{t}\,dt, \tag{4.75}$$

$$\mathrm{si}(z) = -\int_z^\infty \frac{\sin t}{t}\,dt. \tag{4.76}$$

In Fig. 6 we depict $\mathbb{P}_A(x)$ for different values of the dimensionless parameter $\alpha$. The same as before, the optimal frequency of the thermostat oscillators which has the largest impact on kinetic energy is a decreasing function of $\alpha$. Qualitatively, it looks similar to

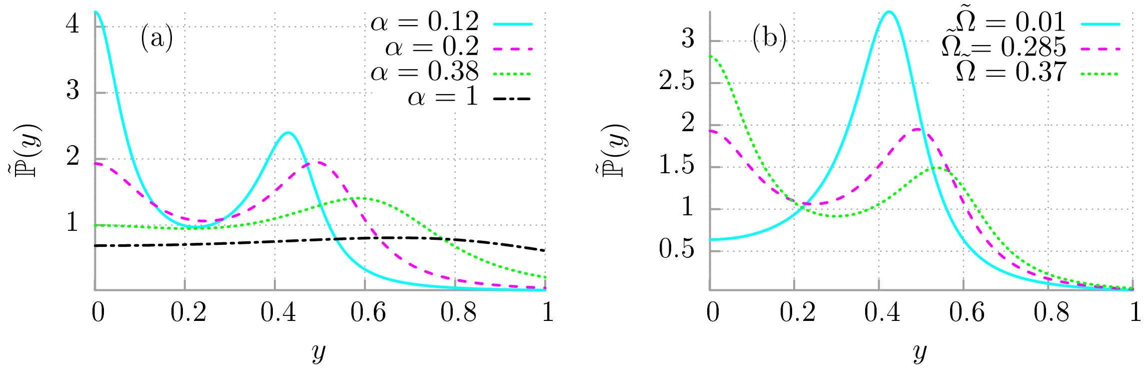

Figure 7: Panel (a): The probability distribution $\tilde{\mathbb{P}}(y)$ scaled according to Eq. (4.39) is depicted for exponentially decaying oscillations with $\gamma_E(t) = (\gamma_1/\tau_c)e^{-t/\tau_c}\cos(\Omega t)$ and different values of $\alpha = \tau_v/\tau_c$ with fixed $\tilde{\Omega} = \tau_v\Omega = 0.285, \tau_v = M/\gamma_1$. Panel (b): The same $\tilde{\mathbb{P}}(y)$ is presented for selected dimensionless frequencies $\tilde{\Omega}$ of the memory function and fixed $\alpha = 0.2$.

the case of the Drude model, c.f. Fig. 1. However, only for large value of $\alpha$ contribution of harmonic modes of lowest frequency differs significantly from zero.

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

## 4.10 Exponentially decaying oscillations - generalization of Drude model

As the last example, we consider a generalization of the Drude model in the form of exponentially decaying oscillations [19],

$$\gamma_E(t) = \frac{\gamma_1}{\tau_c}e^{-t/\tau_c}\cos(\Omega t), \tag{4.77}$$

where the parameter $\Omega$ can be related to frequency in the relaxation process of the particle momentum. Also in this case, quantum noise $\eta(t)$ exhibits anti-correlations. The limiting case $\Omega = 0$ corresponds to the Drude model of dissipation (4.31) with the rescaled parameter $\gamma_1 = \gamma_0/2$. Such a choice of the damping kernel leads to the following spectral density

$$J_E(\omega) = \frac{2}{\pi} \frac{\gamma_1 \varepsilon^2(\varepsilon^2 + \omega^2 + \Omega^2)}{(\varepsilon^2 + \omega^2)^2 + 2\Omega^2(\varepsilon^2 - \omega^2) + \Omega^2}, \tag{4.78}$$

where $\varepsilon = 1/\tau_c$. The Laplace transform of the memory kernel is

$$\hat{\gamma}_L(z) = \frac{\gamma_1 \left(\tau_c z + 1\right)}{\Omega^2 \tau_c^2 + \left(\tau_c z + 1\right)^2} \tag{4.79}$$

and the Laplace transform of the response function is given by the expression

$$\hat{R}_L(z) = \frac{M\left(\Omega^2 \tau_c^2 + \left(\tau_c z + 1\right)^2\right)}{Mz\left(\Omega^2 \tau_c^2 + \left(\tau_c z + 1\right)^2\right) + \gamma_1 \left(\tau_c z + 1\right)} \tag{4.80}$$

In this case, the probability distribution has the form [19]

$$\mathbb{P}(\omega) = \frac{2}{\pi} \frac{\mu_0 \varepsilon^2 \left(\omega^2 + \varepsilon^2 + \Omega^2\right)}{\omega^2 \left[(\omega^2 + \varepsilon^2 - \Omega^2 - \mu_0 \varepsilon)^2 + 4\varepsilon^2 \Omega^2\right] + \mu_0^2 \varepsilon^4}. \tag{4.81}$$

The parameter $\mu_0 = \gamma_1/M$ defines the rescaled coupling strength of the Brownian particle to thermostat. We note that in the considered case there are three characteristic frequencies $\mu_0$, $\varepsilon$ and $\Omega$ 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. Kinetic energy of the free Brownian particle with the exponentially decaying oscillations of the dissipation function was analyzed in detail in Ref. [19]. Now, we focus on properties of the probability density occurring in the quantum energy partition theorem. The influence of the coupling strength $\mu_0$ 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 $\mu_0$. For larger values of the latter it is shifted to the right indicating that oscillators of the higher frequency bring the greatest contribution to kinetic energy of the particle.

The influence of the reciprocal of the correlation time $\varepsilon = 1/\tau_c$ is depicted in Fig. 7(a). In this case, we scale Eq. (4.81) as in (4.39), namely $y = \omega/\mu_0$. The dimensionless parameters are $\alpha = \varepsilon/\mu_0 = M/(\tau_c\gamma_1)$ and $\tilde{\Omega} = \Omega/\mu_0, \mu_0 = \gamma_1/M$. Due to the interplay of two characteristic time scales associated with the parameters $\alpha$ 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 thermostat contribute equally to kinetic energy of the system. When the characteristic frequency $\alpha$ is slightly larger 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. It means that both oscillators of low and moderate frequency play important role. Further decrease of $\alpha$ extinguishes the contribution of higher frequencies at the favour of the near zero frequency modes which are then the most pronounced ones.

Last but not least, we elaborate on the impact of the oscillation frequency $\Omega$. We keep the scaling with respect to the system-thermostat coupling strength $\mu_0 = \gamma_1/M$. In Fig. 7(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 $\alpha = 0.2$. 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 magnitude of $\tilde{\Omega}$ and $\alpha$ is 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 $y$.

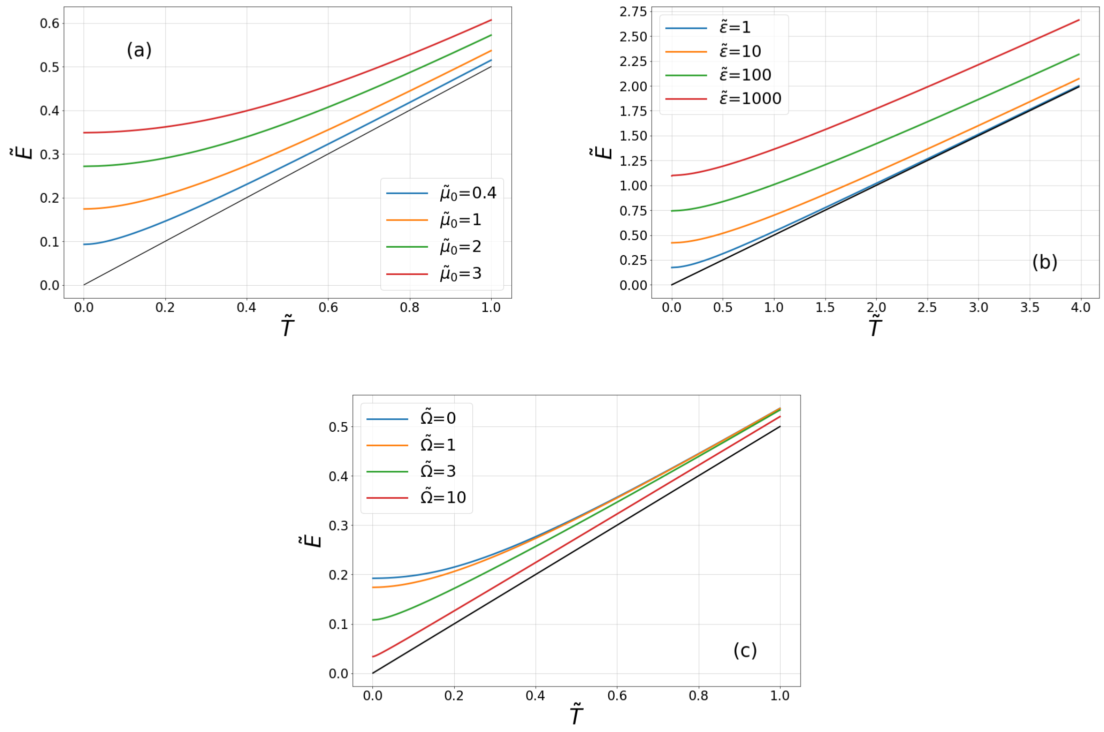

Figure 8: The generalized Drude model of dissipation: Average kinetic energy of the free Brownian particle as a function of rescaled temperature. (a) The influence of the rescaled particle-thermostat coupling strength $\tilde{\mu}_0 = \mu_0/\varepsilon$, where $\mu_0 = \gamma_1/M$ and $\varepsilon = 1/\tau_c$. The rescaled energy is $\tilde{E} = E_k/\hbar\varepsilon$ and the rescaled temperature is $\tilde{T} = k_B T/\hbar\varepsilon$. The rescaled $\tilde{\Omega} = \Omega/\varepsilon = 1$. (b) The influence of the rescaled inverse decay time $\tilde{\varepsilon} = \varepsilon/\mu_0$. The rescaled energy is $\tilde{E} = E_k/\hbar\mu_0$ and the rescaled temperature is $\tilde{T} = k_B T/\hbar\mu_0$. The rescaled $\tilde{\Omega} = \Omega/\mu_0 = 1$. (c) The influence of the rescaled frequency $\tilde{\Omega} = \Omega/\mu_0$. The rescaled energy is $\tilde{E} = E_k/\hbar\mu_0$ and the rescaled temperature is $\tilde{T} = k_B T/\hbar\mu_0$. The rescaled $\tilde{\varepsilon} = \varepsilon/\mu_0 = 1$.

### 4.10.1 Average kinetic energy in terms of series

From the relation

$$E_k = \langle \mathcal{E}_k \rangle = \int_0^\infty d\omega \; \mathcal{E}_k(\omega)\mathbb{P}(\omega), \tag{4.82}$$

it is difficult to draw conclusions on dependence of the average kinetic energy on the system parameters. However, for the exponentially decaying oscillations (4.77) we can present another form of $E_k$. For this purpose we exploit the series expansion [36]

$$x \coth\left(\frac{x}{2}\right) = 2 + 4 \sum_{n=1}^{\infty} \frac{x^2}{x^2 + 4\pi^2 n^2} \tag{4.83}$$

that allows us to calculate the integral in (4.19). Details on this procedure are presented in Appendix E. From Eq. (E.8) shown there we get the expression

$$E_k = \frac{k_B T}{2} \left[ 1 + 2 \sum_{n=1}^{\infty} \frac{\hbar\mu_0 \, \hbar\varepsilon \left(\hbar\varepsilon + 2\pi n k_B T\right)}{\hbar\mu_0 \, \hbar\varepsilon \left(\hbar\varepsilon + 2\pi n k_B T\right) + 2\pi n k_B T \left(\hbar\varepsilon + 2\pi n k_B T\right)^2 + 2\pi n k_B T (\hbar\Omega)^2} \right], \tag{4.84}$$

where $\mu_0 = \gamma_1/M$ is related to the coupling constant and $\varepsilon = 1/\tau_c$ is related to the memory time. Here, the average kinetic energy is represented by an infinite series and some information on $E_k$ can be inferred from this form. Since for $n \geq 1$ all terms under the sum are non-negative, hence $k_B T/2$ is a lower bound for the energy $E_k$. Therefore energy of a quantum Brownian particle is always greater than for classical one. The term under the sum is a rational function of four characteristic energies $k_B T$, $\hbar\mu_0$, $\hbar\varepsilon$, $\hbar\Omega$. The numerator and denominator are the products of energy to power three like e.g. $(\hbar\mu_0)$ $(\hbar\varepsilon)$ $(k_B T)$. It is easy to observe that each term under the sum is a non-increasing function with respect to $\Omega$ because it occurs only in the denominator. Moreover, it can be shown that partial derivatives of each term with respect to $\mu_0$ and $\varepsilon$ are non-negative and it follows that all terms are non-decreasing with respect to $\mu_0$ and $\varepsilon$, respectively. In consequence, $E_k$ is a non-increasing function of $\Omega$ and a non-decreasing function of $\mu_0$ and $\varepsilon$. All these properties are illustrated in Fig. (8).

### 4.10.2 Regime of long memory time

The damping kernel $\gamma(t)$ in the Langevin Eq. (4.1), i.e.,

$$M\ddot{x}(t) = -\int_0^t ds \gamma(t-s)\dot{x}(s) - \gamma(t)x(0) + \eta(t) \tag{4.85}$$

$$p(t) = M\dot{x}(t) \tag{4.86}$$

describes memory effects determined by the relaxation (decay) time $\tau_c$. For the time scales shorter than $\tau_c$, memory effects may play an important role. For times longer than $\tau_c$ memory effects can be neglected. Now, we consider the generalized Drude model and the case of long decay time $\tau_c$. More precisely, we assume that $\tau_c$ is much longer than the thermal Matsubara time $\hbar/k_BT$, namely,

$$\tau_c = \frac{1}{\varepsilon} \gg \frac{\hbar}{2\pi k_B T}. \tag{4.87}$$

In other words, $\hbar\varepsilon \ll 2\pi k_BT$ and then $\hbar\varepsilon + 2\pi n k_BT \approx 2\pi n k_BT$ in Eq. (4.84). In this regime, Eq. (4.84) takes the form

$$E_k = \frac{k_BT}{2}\left[1 + 2\sum_{n=1}^{\infty} \frac{\hbar^2\mu_0\,\varepsilon}{\hbar^2(\mu_0\varepsilon + \Omega^2) + (2\pi n k_BT)^2}\right]. \tag{4.88}$$

We can use the formula (4.83) to rewrite the above equation in a more compact form as

$$E_k = \frac{k_BT}{2}\left[\frac{\Omega^2}{\varepsilon\mu_0 + \Omega^2} + \frac{\hbar\varepsilon\mu_0}{2k_BT\sqrt{\varepsilon\mu_0 + \Omega^2}}\coth\left(\frac{\hbar\sqrt{\varepsilon\mu_0 + \Omega^2}}{2k_BT}\right)\right]. \tag{4.89}$$

For the Drude model, when $\Omega = 0$, it reduces to the following equation

$$E_k = \frac{\hbar\sqrt{\varepsilon\mu_0}}{4}\coth\left(\frac{\hbar\sqrt{\varepsilon\mu_0}}{2k_BT}\right). \tag{4.90}$$

It is an interesting result because it looks like Eq. (4.20) for averaged kinetic energy of the oscillator with its redefined eigenfrequency $\omega_0 = \sqrt{\varepsilon\mu_0} = \sqrt{\gamma_1/(M\tau_c)}$. Remember that the relation (4.87) should be satisfied and it means that

$$\tau_c >> 1.21 \times 10^{-12}\frac{1}{T}\ \text{sec. K}. \tag{4.91}$$

E.g., for temperature 1 Kelvin, $\tau_c \gg 10^{-12}$ sec. while for $10^{-4}$ Kelvin, $\tau_c \gg 10^{-8}$ sec. Therefore for higher temperatures it is easier to fulfil this condition.

### 4.10.3 Method of differential equations

The integral part of the generalized Langevin Eq. (4.1) is convolution of $\gamma(t)$ and $\dot{x}(t)$. It suggests to apply integral transforms like Laplace or Fourier ones to solve it. Here we want to demonstrate another method which is based on the observation that:
if $\gamma(t)$ fulfils a linear ordinary differential equation with constant coefficients then Eq. (4.1) can be converted to a set of ordinary differential equations.

It is a case of the generalized Drude model. Note that the function $\gamma(t)$ in the form (4.77) fulfils a differential equation of second order which is similar to the Newton equation for a damped harmonic oscillator. We introduce auxiliary variables (in fact, operators) $u(t)$ and $v(t)$ by the relations

$$u(t) = \mu \int_0^t e^{-\varepsilon(t-s)} \cos[\Omega(t-s)]\, p(s) ds, \tag{4.92}$$

$$v(t) = \mu \int_0^t e^{-\varepsilon(t-s)} \sin[\Omega(t-s)]\, p(s) ds, \tag{4.93}$$

$$\mu = \mu_0\, \varepsilon, \quad \mu_0 = \frac{\gamma_1}{M}, \quad \varepsilon = \frac{1}{\tau_c}. \tag{4.94}$$

Then Eq. (4.1) for $\gamma(t)$ defined in Eq. (4.77) is converted to the following set of four differential equations

$$\begin{aligned} \dot{x}(t) &= \frac{1}{M} p(t), \\ \dot{p}(t) &= -u(t) - \gamma(t)x(0) + \eta(t), \\ \dot{u}(t) &= \mu p(t) - \varepsilon u(t) - \Omega v(t), \\ \dot{v}(t) &= \Omega u(t) - \varepsilon v(t). \end{aligned} \tag{4.95}$$

In such a case, in order to calculate averaged kinetic energy, it is sufficient to consider the reduced set of three equations

$$\begin{aligned} \dot{p}(t) &= -u(t) - \gamma(t)x(0) + F(t), \\ \dot{u}(t) &= \mu p(t) - \varepsilon u(t) - \Omega v(t), \\ \dot{v}(t) &= \Omega u(t) - \varepsilon v(t). \end{aligned} \tag{4.96}$$

It can be rewritten in the matrix form

$$\frac{d}{dt}\mathbf{X}(t) = \mathbf{A}\mathbf{X}(t) + \mathbf{B}(t), \tag{4.97}$$

where

$$\mathbf{X}(t) = [p(t), u(t), v(t)]^{\mathsf{T}}, \tag{4.98}$$

$$\mathbf{B}(t) = (-\gamma(t)x(0) + \eta(t)) \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}^{\mathsf{T}} \tag{4.99}$$

and $\mathsf{T}$ denotes the transpose of a matrix which switches the row into the column. The matrix $\mathbf{A}$ has the form

$$\mathbf{A} = \begin{bmatrix} 0 & -1 & 0 \\ \mu & -\varepsilon & -\Omega \\ 0 & \Omega & -\varepsilon \end{bmatrix}. \tag{4.100}$$

The solution of the non-homogeneous linear differential Eq. (4.97) reads

$$\mathbf{X}(t) = \mathbf{R}(t)\mathbf{X}(0) + \int_0^t \mathbf{R}(t-s)\mathbf{B}(s)ds, \quad \mathbf{R}(t) = e^{\mathbf{A}t}, \tag{4.101}$$

where

$$\mathbf{X}(0) = [p(0), 0, 0]^{\mathsf{T}}. \tag{4.102}$$

The spectrum of the matrix $\mathbf{A}$ and its invariant subspaces determine the time dependence of (4.101). Now, the only problem is to determine the exponential of the matrix $\mathbf{A}t$, i.e. the matrix $\mathbf{R}(t)$, which can be computed in many ways. The authors of the paper [41] say about 19 ways. As they write: "In practice, consideration of computational stability and efficiency indicates that some of the methods are preferable to others, but that none are completely satisfactory". The traditional way is to transform $\mathbf{A}$ to its Jordan canonical form. Here we will use a less traditional method, namely, the Putzer algorithm [42], in which the exponential of the matrix $\mathbf{A}t$ can be computed knowing nothing more than the eigenvalues of the matrix $\mathbf{A}$. Moreover, the algorithm does not require that the matrix $\mathbf{A}$ is diagonalizable. We think that this method is simple, elegant and suitable for presentation to students and younger researchers. It is described in Appendix C.

The operator of kinetic energy $H_k(t) = p^2(t)/2M$ is expressed by the momentum $p(t)$ which is the first component of the vector $\mathbf{X}(t)$ determined by Eq. (4.101). We calculate its average in the long time limit $t \to \infty$ when a stationary state is approached. The first component of $\mathbf{X}(t)$ is

$$p(t) = R_{11}(t)p(0) + \int_0^t R_{11}(t-s)\gamma(s)x(0)ds + \int_0^t R_{11}(t-s)F(s)ds, \tag{4.103}$$

where $R_{11}(t)$ is the first element of the matrix $\mathbf{R}(t)$. As is shown in Appendix C, elements of this matrix are exponentially decreasing functions of time. It means that the average value of the momentum $\langle p(t)\rangle \to 0$ as $t \to \infty$. To evaluate the average kinetic energy, we consider the symmetrized momentum-momentum correlation function $\left\langle [p(t);p(u)]_+\right\rangle$. In the long time limit, the first two terms of Eq. (4.103) do not contribute to it and only the last term contributes yielding

$$\left\langle [p(t);p(s)]_+\right\rangle = \int_0^t dt_1 \int_0^s dt_2 \; R_{11}(t-t_1)R_{11}(s-t_2)\left\langle [\eta(t_1);\eta(t_2)]_+\right\rangle . \tag{4.104}$$

This corresponds to the earlier result (4.12) with $R_{11}$ corresponding to the response function $R$. Furthermore using Eq. (4.104) we can construct energy in the long time limit:

$$E_k = \lim_{t\to\infty} \frac{1}{2M}\langle p^2(t)\rangle = \frac{1}{2M}\int_0^\infty d\omega \; \hat{C}_F(\omega) I^1(\omega), \tag{4.105}$$

where:

$$I^1(\omega) = \int_0^\infty d\tau \int_0^\infty du \; R_{11}(\tau)R_{11}(u)\cos\left[\omega\left(\tau - u\right)\right] \tag{4.106}$$

which corresponds to equations (4.16) and (4.17). In Appendix D, this function is alternatively calculated using the explicit form of the function $R_{11}(t)$ given by equation (C.11) in Appendix C.

## 4.11 Discussion and remarks

As we wrote in the Introduction, various expressions for kinetic energy of a free Brownian particle can be found both in original papers and the well-known books, e.g. Eq. (83) in Ref. [1], Eq. (4.14) in Ref. [3], equation for the second moment of momentum in Table 2 of Ref. [4] and Eq. (3.475) in Ref. [8]. 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 relaxation of a weakly perturbed system to the spontaneous fluctuations in thermal equilibrium, see e.g. Eq. (124.10) in Ref. [6], Eq. (17.19g) in Ref. [7] and Eq. (3.499) in Ref. [8]. All expressions for $E_k$ should be equivalent although they are written in different forms. However, our specific formula (4.19) allows to reveal a new face of the old problem and formulate 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 degree 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, see Eq. (2.9): The mean kinetic energy of a free classical particle equals the average kinetic energy of the thermostat degree of freedom.

II. The function $\mathbb{P}(\omega)$ is a probability density, i.e. it is non-negative and normalized on the interval $(0, \infty)$. From the probability theory it follows that there exists a random variable $\xi$ for which $\mathbb{P}(\omega)$ is its probability distribution. Here, this random variable is interpreted as eigen-frequency of thermostat oscillators. In the thermodynamic limit for thermostat, there are infinitely many oscillators of various eigen-frequencies $\omega$ which contribute to $E_k$ according to $\mathbb{P}(\omega)$.

III. The last expression in Eq. (4.23) can be converted to the transparent form

$$\mathbb{P}(\omega) = \frac{2}{\pi} \int_0^\infty dt R(t) \cos(\omega t). \tag{4.107}$$

Thus the probability distribution $\mathbb{P}(\omega)$ is a cosine transform of the response function $R(t)$ which solves the generalized Langevin Eq. (4.1). It is amazing that for so many years nobody has revealed this simple relation!

IV. Thermostat oscillators contribute to $E_k$ in a non-uniform 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 comprised.

V. The probability density function $\mathbb{P}(\omega)$ does not depend on temperature $T$. However, it depends on coupling between the Brownian particle and thermostat. There is no restriction on the value of this coupling - it means that strong coupling is included as well. It also depends on the memory time - it means that non-Markovian regime is included as well. And finally it depends on mass $M$ of the Brownian particle. Note that for classical systems, there in no mass-dependence.

### 4.11.1 High temperature regime

We focus now on the regime of high temperatures. In this case $T \to \infty$ and we use the approximation

$$\coth\left(\frac{\hbar\omega}{2k_BT}\right) \approx \frac{2k_BT}{\hbar\omega}. \tag{4.108}$$

Then Eq. (4.19) can be approximated as follows

$$\begin{aligned} E_k = \langle \mathcal{E}_k \rangle &= \int_0^\infty d\omega\ \mathcal{E}_k(\omega)\mathbb{P}(\omega) = \int_0^\infty d\omega\ \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\mathbb{P}(\omega) \\ &\approx \frac{1}{2}k_BT\int_0^\infty d\omega\ \mathbb{P}(\omega) = \frac{1}{2}k_BT, \end{aligned} \tag{4.109}$$

that is it takes the form for classical systems,

$$E_k = \frac{1}{2}k_BT \tag{4.110}$$

Note that (4.110) holds true for weak as well as strong system-thermostat interaction.

### 4.11.2 Low temperature regime

When temperature is low, $T \to 0$, the following approximation may be applied

$$\coth(x) = 1 + 2\,\frac{\mathrm{e}^{-2x}}{1-\mathrm{e}^{-2x}} \approx 1 + 2\mathrm{e}^{-2x}, \quad x = \frac{\hbar\omega}{2k_BT}. \tag{4.111}$$

We insert this expression into Eq. (4.19) and obtain

$$E_k = E_0 + E_1(T), \tag{4.112}$$

where

$$E_0 = \frac{1}{4}\int_0^\infty d\omega\ \hbar\omega\,\mathbb{P}(\omega) \tag{4.113}$$

is the average kinetic energy at temperature $T = 0$, i.e. when the thermostat is in the vacuum state and

$$E_1(T) = \frac{1}{2}\int_0^\infty d\omega\ \hbar\omega\,\mathbb{P}(\omega)\exp\left[-\frac{\hbar\omega}{k_BT}\right] \tag{4.114}$$

is the first correction for small temperature $T > 0$.

From Fig. 8 one infers that the energy $E_0$ is finite for all finite values of parameters and behaves in the following way:

(i) $E_0$ increases monotonically from zero to infinity when the coupling strength $\mu_0$ grows from zero to infinity.

(ii) When the decay rate $\varepsilon = 1/\tau_c$ increases from zero to infinity $E_0$ grows from zero to infinity. It means that when the memory function tends to the Dirac delta function, i.e. for quantum white noise, the average energy tends to infinity! It is not physical. One can conclude that the white noise limit cannot be performed. In other words, the Markovian limit does not exist and the process is non-Markovian.

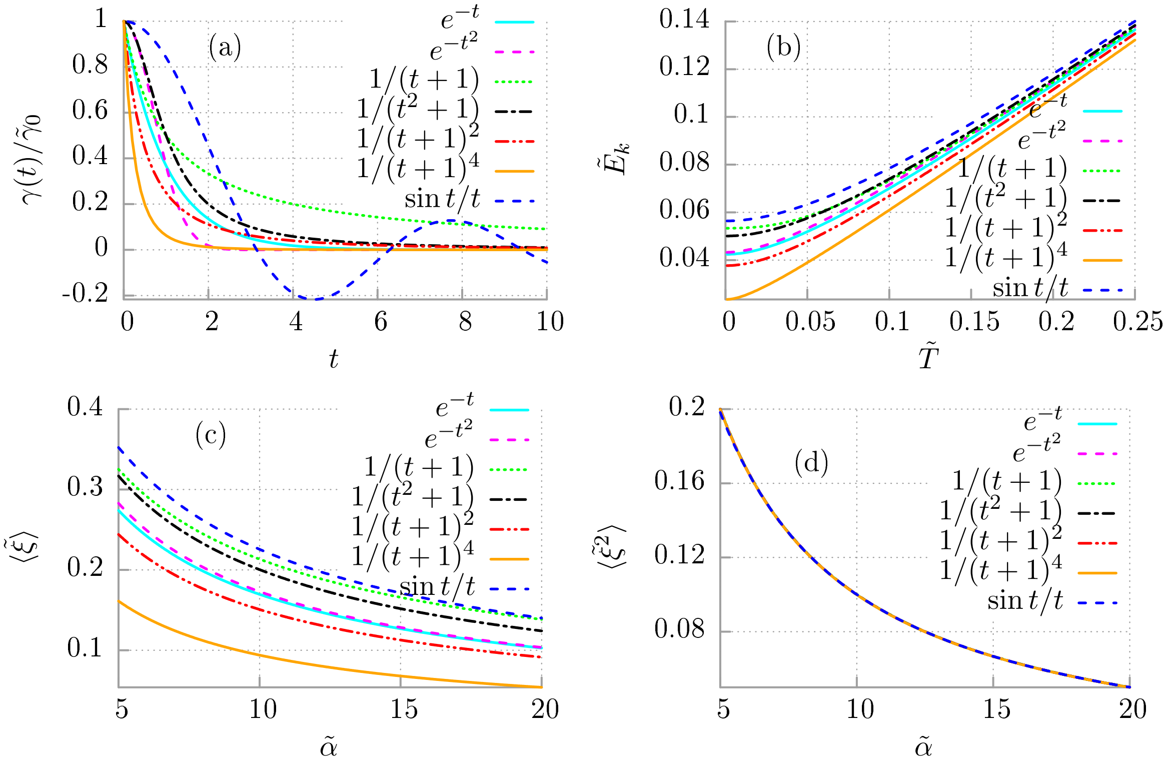

Figure 9: Panel (a): The normalized memory functions $\gamma(t)/\tilde{\gamma}_0$ representing various dissipation mechanisms. Panel (b): The dimensionless kinetic energy $\tilde{E}_k = \tau_c E_k/\hbar$ of the free Brownian particle presented versus dimensionless temperature $\tilde{T} = \tau_c k_B T/\hbar$ and various forms of $\gamma(t)$. Panel (c): The first moment $\langle\tilde{\xi}\rangle = \tau_c\langle\xi\rangle$ and panel (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 $\gamma(t)$.

### 4.11.3 Statistical moments of probability distribution $\mathbb{P}(\omega)$

Let us now discuss statistical moments of the random variable $\xi$ distributed according to the probability density $\mathbb{P}(\omega)$:

$$\langle\xi^n\rangle = \int_0^\infty d\omega\, \omega^n \mathbb{P}(\omega). \tag{4.115}$$

A caution is needed since not all moments may exist, e.g. for the distribution (4.35). The first two of them have a clear physical interpretation. The first moment, i.e. the mean value $\langle\xi\rangle$ of the random variable $\xi$ is proportional to kinetic energy $E_k$ of the

Brownian particle at zero temperature $T = 0$, namely,

$$E_0 = E_k(T=0) = \frac{\hbar}{4}\,\langle \xi \rangle. \tag{4.116}$$

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

$$E_k = \frac{1}{2} k_B T + \frac{\hbar^2}{24 k_B T}\,\langle \xi^2 \rangle. \tag{4.117}$$

We note that averaged kinetic energy $E_0$ at zero temperature $T = 0$ is non-zero for all values of the system parameters. It is so because of intrinsic quantum vacuum fluctuations. Moreover, $E_k$ monotonically increases from some non-zero value to infinity when temperature goes to infinity.

### 4.11.4 Comparison of mean energy for various dissipation mechanisms

If we want to compare impact of various dissipation mechanisms on $E_k$ we have to change the scaling of all dissipation functions $\gamma(t)$. Now, we re-define $\gamma(t)$ in such a way that for all memory functions $\gamma(0) = \tilde{\gamma}_0$, where $\tilde{\gamma}_0$ still characterizes the particle-thermostat coupling but now it has the unit $[\tilde{\gamma}_0] = [kg/s^2]$. E.g. 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 panel (a) of Fig. 9, where all $\gamma(t)$ assume the same value for $t = 0$. In the classical case, it would correspond to the fixing of the second moment of the random force $\eta(t)$. In our previous considerations, we define $\gamma(t)$ in such a way that it 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 $\eta(t)$. Now, the scaling is different.

In Fig. 9(b) we compare 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. 9(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 $\omega = x/\tau_c$ like in (4.36) with fixed $\tau_c$. 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) increase of the particle mass $M$ or (ii) decrease of the coupling strength $\tilde{\gamma}_0$. Moreover, we can see that for the n-algebraic decay ($n = 2$ and $n = 4$ for red and orange curve, respectively) kinetic energy at zero temperature $E_0$ is smaller than for other memory functions. The negligible difference is observed for the Drude and Gaussian decay. The largest kinetic energy is induced by the Debye type dissipation (anti-correlation and the compact support of the probability density). In the high temperature regime (panel (d) of Fig. 9), 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 zero for $\tau_c \to 0$ (it is not a limit to the Dirac delta!) and saturates to a finite value as $\tau_c$ is longer and longer (not depicted).

# 5 Partition of energy for quantum oscillator

## 5.1 Formulation of problem

The second (and the last) exactly solvable case of the Langevin equation defined by the formula (3.14), i.e.,

$$M\ddot{x}(t) + \frac{\mathrm{i}}{\hbar}\left[p, U(x)\right] = -\int_0^t ds\gamma(t-s)\dot{x}(s) - \gamma(t)x(0) + \eta(t) \tag{5.1}$$

$$p(t) = M\dot{x}(t) \tag{5.2}$$

is the case of a harmonic oscillator for which the potential $U(x) \propto x^2$. The corresponding dynamics is determined by the linear integro-differential equation:

$$M\ddot{x}(t) + M\omega_0^2 x(t) = -\int_0^t \gamma(t-s)\dot{x}(s)ds - \gamma(t)x(0) + \eta(t) \tag{5.3}$$

$$\dot{x}(t) = \frac{1}{M}p(t) \tag{5.4}$$

Sometimes we will refer to this oscillator as a central oscillator to discriminate it from the thermostat oscillators. Our goal is to find the solution of the above Langevin equation. To this aim we use the Laplace transformation method and our interest is to investigate the second moment of both the position $\langle x^2(t)\rangle$ and the momentum $\langle p^2(t)\rangle$ operators in the long time limit, when the stationary stated is reached. This procedure allows to study both the potential and kinetic energy of the central oscillator, respectively.

## 5.2 Laplace transformation of Langevin equation

Applying the Laplace transformation to Eq. (5.3) we obtain for the left hand side

$$\mathcal{L}\left\{M\ddot{x}(t) + M\omega_0^2 x(t)\right\}(z) = Mz^2\mathcal{L}\left\{x(t)\right\}(z) - Mx(0) - M\dot{x}(0) + M\omega_0^2\mathcal{L}\left\{x(t)\right\}(z)\,, \tag{5.5}$$

and for the right hand side

$$\mathcal{L}\left\{-\int_0^t \gamma(t-s)\dot{x}(s)ds - \gamma(t)x(0) + \eta(t)\right\}(z) = -z\mathcal{L}\left\{\gamma(t)\right\}(z)\,\mathcal{L}\left\{x(t)\right\}(z) \tag{5.6}$$

$$+\,x(0)\mathcal{L}\left\{\gamma(t)\right\}(z) - x(0)\mathcal{L}\left\{\gamma(t)\right\}(z) \tag{5.7}$$

$$+\,\mathcal{L}\left\{\eta(t)\right\}(z)\,. \tag{5.8}$$

Using the shorthand notation we sumarize them as

$$\left(Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2\right)\hat{x}_L(z) = M\dot{x}(0) + Mx(0)z + \hat{\eta}_L(z). \tag{5.9}$$

We introduce two *response functions* defined by their Laplace transforms

$$\mathcal{L}\left\{Q(t)\right\}(z) = \hat{Q}_L(z) = \frac{1}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} \tag{5.10}$$

$$\mathcal{L}\left\{R(t)\right\}(z) = \hat{R}_L(z) = \frac{Mz}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} \tag{5.11}$$

Rewriting Eq. (5.9) in terms of these response functions we obtain the solution for the position operator

$$\mathcal{L}\left\{x(t)\right\}(z) = x(0)\hat{R}_L(z) + M\dot{x}(0)\hat{Q}_L(z) + \hat{Q}_L(z)\hat{\eta}_L(z) \tag{5.12}$$

$$x(t) = x(0)R(t) + p(0)Q(t) + \int_0^t ds\, Q(t-s)\eta(s) \tag{5.13}$$

Analogous calculations can be performed for the momentum operator with the results:

$$\mathcal{L}\left\{p(t)\right\}(z) = M\dot{x}(0)\hat{R}_L(z) + Mx(0)z\hat{R}_L(z) + \hat{R}_L(z)\hat{\eta}_L(z) \tag{5.14}$$

$$p(t) = Mx(0)\dot{R}(t) + p(0)R(t) + \int_0^t ds\, R(t-s)\eta(s) \tag{5.15}$$

We note that here the free particle case analyzed in the previous chapter can be retrieved by putting $\omega_0 = 0$. Therefore we can interpret these calculations as a generalisation of the specific case which we have dealt before with.

## 5.3 Potential energy

In Chapter 4, we have derived the relation for kinetic energy of a free quantum Brownian particle in the long time-limit. For the quantum harmonic oscillator studied here analogous expression can also be derived for potential energy of the oscillator. The latter is defined by the operator

$$E_p(x(t)) = \frac{1}{2} M \omega_0^2 x^2(t) \tag{5.16}$$

By using the solution for the position operator (5.13) we can write down formula for potential energy explicitly. However, due to the properties of response functions $R$ and $Q$, which are discussed in detail in Appendix B, only a part of all terms for $\left\langle [x(t); x(t)]_+ \right\rangle$ is non-zero in the long time limit. Hence, for such a limit the expression is simplified to the form:

$$\lim_{t\to+\infty} \left\langle [x(t); x(t)]_+ \right\rangle = \lim_{t\to+\infty} \int_0^t \int_0^t Q(t-\tau_1)Q(t-\tau_2) \left\langle [\eta(\tau_1); \eta(\tau_2)]_+ \right\rangle d\tau_1 d\tau_2 \tag{5.17}$$

In the next step we present the noise correlation function $\left\langle [\eta(\tau_1); \eta(\tau_2)]_+ \right\rangle$ by its Fourier cosine transform (3.27) and next utilise the fluctuation-dissipation relation (3.28), i.e.,

$$\hat{C}_F(\omega) = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_B T}\right) \hat{\gamma}_F(\omega) \tag{5.18}$$

By changing the integration variables $\tau = t - \tau_1$ and $u = t - \tau_2$ we obtain the expression

$$\left\langle x^2(t) \right\rangle = \int_0^\infty d\omega\, \hat{C}_F(\omega) \int_0^t d\tau \int_0^t du\, Q(\tau)Q(u) \cos\left[\omega\left(\tau - u\right)\right] \tag{5.19}$$

Now, we have to perform the limit $t \to \infty$ to get

$$\begin{aligned} E_p &= \lim_{t\to+\infty} \frac{1}{2} M\omega_0^2 \left\langle x^2(t) \right\rangle \\ &= \frac{M\omega_0^2}{2} \int_0^\infty d\omega\, \hat{C}_F(\omega) \left\{ \int_0^{+\infty} d\tau \int_0^{+\infty} du\, Q(\tau)Q(u) \cos\left[\omega\left(\tau - u\right)\right] \right\} \\ &\equiv \frac{M\omega_0^2}{2} \int_0^{+\infty} d\omega\, \hat{C}_F(\omega) I_p(\omega). \end{aligned} \tag{5.20}$$

which has a similar form as Eq. (4.15) and therefore

$$E_p = \int_0^{+\infty} d\omega\, \mathcal{E}_p(\omega) \mathbb{P}_p(\omega) \tag{5.21}$$

where

$$\mathbb{P}_p(\omega) = M\omega_0^2 \hat{\gamma}_F(\omega) \hat{Q}_L(i\omega) \hat{Q}_L(-i\omega) \tag{5.22}$$

and

$$\mathcal{E}_p(\omega) = \frac{\hbar\omega}{4} \coth\left(\frac{\hbar\omega}{2k_B T}\right) \tag{5.23}$$

or in the equivalent form

$$\mathbb{P}_p(\omega) = \frac{iM\omega_0^2}{\pi\omega}\left(\hat{Q}_L(i\omega) - \hat{Q}_L(-i\omega)\right). \tag{5.24}$$

**Theorem 2.**

*The function $\mathbb{P}_p(\omega)$ is a properly defined probability density function, i.e.,*

*I. it it non-negative, $\mathbb{P}_p(\omega) \geq 0$*

*II. it is normalized, $\int_0^{+\infty} d\omega\, \mathbb{P}_p(\omega) = 1$*

*Proof.* We start with the normalization condition

$$\mathbb{P}_p(\omega) = \frac{iM\omega_0^2}{\pi\omega}\left[\hat{Q}_L(i\omega) - \hat{Q}_L(-i\omega)\right] = \frac{M\omega_0^2}{\omega}\tilde{Q}_S(\omega) \tag{5.25}$$

where $\tilde{Q}_S(\omega)$ is a sine transform, i.e.

$$\tilde{Q}_S(\omega) = \frac{2}{\pi}\int_0^{\infty} dt\, Q(t)\sin(\omega t). \tag{5.26}$$

Let us define an auxiliary function

$$\Theta(t) = \int_t^{+\infty} d\tau\ Q(\tau) \tag{5.27}$$

obeying the equation

$$\frac{d}{dt}\Theta(t) = -Q(t). \tag{5.28}$$

The cosine transform of $\Theta(t)$ reads

$$\tilde{\Theta}_C(\omega) = \frac{2}{\pi}\int_0^{+\infty} dt\, \Theta(t)\cos(\omega t) \tag{5.29}$$

Integrating it by parts yields

$$\tilde{\Theta}_C(\omega) = \frac{2}{\pi}\int_0^{+\infty} dt\, \Theta(t)\cos(\omega t) = \left|\begin{array}{cc} u = \Theta(t) & v' = \cos(\omega t) \\ u' = -Q(t) & v = \frac{1}{\omega}\sin(\omega t) \end{array}\right| \tag{5.30}$$

$$= \underbrace{\frac{2}{\pi}\frac{1}{\omega}\sin(\omega t)\Theta(t)\Big|_0^{+\infty}}_{=0} + \frac{2}{\pi}\int_0^{+\infty} dt\, Q(t)\frac{\sin(\omega t)}{\omega} = \frac{1}{\omega}\tilde{Q}_S(\omega). \tag{5.31}$$

Using Eq. (5.25) we immediately notice that

$$\mathbb{P}_p(\omega) = M\omega_0^2\tilde{\Theta}_C(\omega). \tag{5.32}$$

Moreover, we calculate (see Appendix B)

$$\Theta(0) = \int_0^{+\infty} dt\, Q(t) = \hat{Q}_L(0) = \frac{1}{M\omega_0^2}. \tag{5.33}$$

On the other hand

$$\Theta(0) = \int_0^{+\infty} d\omega\, \tilde{\Theta}_C(\omega) = \frac{1}{M\omega_0^2}, \tag{5.34}$$

and therefore finally we obtain

$$\int_0^{+\infty} d\omega\, \mathbb{P}(\omega) = M\omega_0^2 \int_0^{+\infty} d\omega\, \tilde{\Theta}_C(\omega) = M\omega_0^2 \Theta(0) = 1. \tag{5.35}$$

In order to prove the non-negativity condition it will be easier to use another equivalent form of $\mathbb{P}_p(\omega)$, i.e.,

$$\mathbb{P}_p(\omega) = \frac{2M}{\pi} \frac{\omega_0^2 A(\omega)}{\omega^2 A^2(\omega) + \left[M(\omega_0^2 - \omega^2) + \omega B(\omega)\right]^2} \tag{5.36}$$

where (cf. Sec. 4.3.1)

$$A(\omega) = \int_0^{\infty} dt\; \gamma(t) \cos(\omega t), \tag{5.37}$$

$$B(\omega) = \int_0^{\infty} dt\; \gamma(t) \sin(\omega t). \tag{5.38}$$

The denominator in (5.36) is always positive and it is sufficient to show that the numerator $A(\omega) \geq 0$. From the definition of $A(\omega)$ it follows that $A(\omega) = (\pi/2)J(\omega)$. Since the spectral function $J(\omega)$ is non-negative the same holds true for $A(\omega)$ and therefore $\mathbb{P}_p(\omega) \geq 0$. □

This result is very similar to the previous one for kinetic energy of a free Brownian particle. Note that in the numerator the eigen-frequency $\omega_0$ of the oscillator occurs and for $\omega_0 \to 0$ also $\mathbb{P}_p(\omega) \to 0$ (as it should be). Potential energy of the harmonic oscillator in long time limit can be represented as an average of potential energy of the thermostat particles. The averaging is two-fold:

I. over the thermal equilibrium Gibbs state for the thermostat oscillators resulting in $\mathcal{E}_p(\omega)$,

II. over frequencies $\omega$ of those thermostat oscillators which contribute to $E_p$ according to the probability distribution $\mathbb{P}_p(\omega)$.

## 5.4 Kinetic energy and total energy of quantum oscillator

The above reasoning can be repeated also for kinetic energy of the harmonic oscillator leading to the previously introduced representation

$$E_k = \int_0^{+\infty} d\omega\, \mathcal{E}_k(\omega)\mathbb{P}_k(\omega) \tag{5.39}$$

where formula for $\mathbb{P}_k$ is identical to Eq. (4.21), i.e.

$$\mathbb{P}_k(\omega) = \frac{1}{M}\hat{\gamma}_F(\omega)\hat{R}_L(i\omega)\hat{R}_L(-i\omega) = \frac{1}{\pi}\left[\hat{R}_L(i\omega) + \hat{R}_L(-i\omega)\right], \tag{5.40}$$

The only difference is the form of the response function $R(t)$ which now is given by Eq. (5.11).

Thermal averages over the Gibbs state of kinetic and potential energy of the thermostat oscillators are the same, i.e.,

$$\mathcal{E}_k = \mathcal{E}_p = \frac{\hbar\omega}{4}\coth\frac{\hbar\omega}{2k_BT} = \frac{1}{2}\mathcal{E}_T, \tag{5.41}$$

where $\mathcal{E}_T$ is total energy of the thermostat oscillator. Therefore total energy of the central oscillator can be represented as

$$\begin{aligned} E = E_k + E_p &= \int_0^{+\infty} d\omega\, \frac{1}{2}\mathcal{E}_T(\omega)\left(\mathbb{P}_k(\omega) + \mathbb{P}_p(\omega)\right) \\ &= \int_0^{+\infty} d\omega\, \mathcal{E}_T(\omega)\mathbb{P}_T(\omega) \end{aligned} \tag{5.42}$$

where $\mathbb{P}_T(\omega)$ reads

$$\mathbb{P}_T(\omega) = \frac{\mathbb{P}_k(\omega) + \mathbb{P}_p(\omega)}{2}. \tag{5.43}$$

Thus the total averaged energy of the dissipative quantum oscillator is thermally averaged energy of the thermostat oscillators additionally averaged over the distribution (5.43). In the next sections we present explicit expressions for both probability densities and analyze their properties. The aim of this detailed and tedious presentation is three-fold. First, to compare properties of both distributions $\mathbb{P}_k(\omega)$ and $\mathbb{P}_p(\omega)$ to reveal differences and similarities. Second, the potential readers can use these formulas. Third, in the future, one can test approximations for models which are not exactly soluble.

## 5.5 Drude model of dissipation

We recall the dissipation kernel $\gamma(t)$ for this model,

$$\gamma(t) = \frac{\gamma_0}{\tau_c} e^{-\frac{t}{\tau_c}} \tag{5.44}$$

parametrized by two non-negative constants $\gamma_0$ and $\tau_c$. We again remind that $\gamma_0$ is the particle-thermostat coupling strength and $\tau_c$ is the characteristic time of system - it characterizes memory of the system. The Laplace transform of the memory kernel is:

$$\hat{\gamma}_L(\omega) = \frac{\gamma_0}{\omega\tau_c + 1} \tag{5.45}$$

and the response function for this memory kernel reads

$$\hat{Q}_L(\omega) = \frac{(\omega\tau_c + 1)}{M\left(\omega^2 + \omega_0^2\right)(\omega\tau_c + 1) + \gamma_0\omega} \tag{5.46}$$

The probability density for potential energy is

$$\mathbb{P}_p(\omega) = \frac{2M\gamma_0\omega_0^2\left(\omega^2\tau_c^2 + 1\right)}{\pi\left(\gamma_0^2\omega^2 + \left(M\left(\omega^2 - \omega_0^2\right)\left(\omega^2\tau_c^2 + 1\right) - \gamma_0\omega^2\tau_c\right)^2\right)} \tag{5.47}$$

The probability density for kinetic energy takes the form

$$\mathbb{P}_k(\omega) = \frac{2M\gamma_0\omega^2\left(\omega^2\tau_c^2 + 1\right)}{\pi\left(\gamma_0^2\omega^2 + \left(M\left(\omega^2 - \omega_0^2\right)\left(\omega^2\tau_c^2 + 1\right) - \gamma_0\omega^2\tau_c\right)^2\right)} \tag{5.48}$$

Note that difference between $\mathbb{P}_p(\omega)$ and $\mathbb{P}_k(\omega)$ is in the nominators: $\omega_0^2 \leftrightarrow \omega^2$. We should rewrite this probability density functions in the rescaled, dimensionless form. As in the previous case of the free Brownian particle, we could distinguish two characteristic time scales defined by characteristic time $\tau_c$ and $\tau_v = 1/\mu_0 = M/\gamma_0$. We introduce the notation

$$x = \omega\tau_c \tag{5.49}$$

$$x_0 = \omega_0\tau_c \tag{5.50}$$

and then the probability density can be presented in the form

$$\mathbb{P}_p^D(x) = \frac{1}{\tau_c}\mathbb{P}_p\left(\frac{x}{\tau_c}\right) = \frac{2\alpha x_0^2\left(x^2 + 1\right)}{\pi\left(x^2 + \left(\alpha\left(x^2 + 1\right)\left(x^2 - x_0^2\right) - x^2\right)^2\right)} \tag{5.51}$$

and

$$\mathbb{P}_k^D(x) = \frac{1}{\tau_c}\mathbb{P}_k\left(\frac{x}{\tau_c}\right)\frac{2\alpha x^2\left(x^2+1\right)}{\pi\left(x^2+\left(\alpha\left(x^2+1\right)\left(x^2-x_0^2\right)-x^2\right)^2\right)} \tag{5.52}$$

where

$$\alpha = \frac{M}{\tau_c\gamma_0} = \frac{1}{\mu_0\tau_c} = \frac{\tau_v}{\tau_c}, \tag{5.53}$$

is the only dimensionless parameter on which the probability density functions depend. This scaling can be used to examine impact of the characteristic frequency $\mu_0 = \gamma_0/M$ while the second characteristic time scale $\tau_c$ is fixed in this scaling.

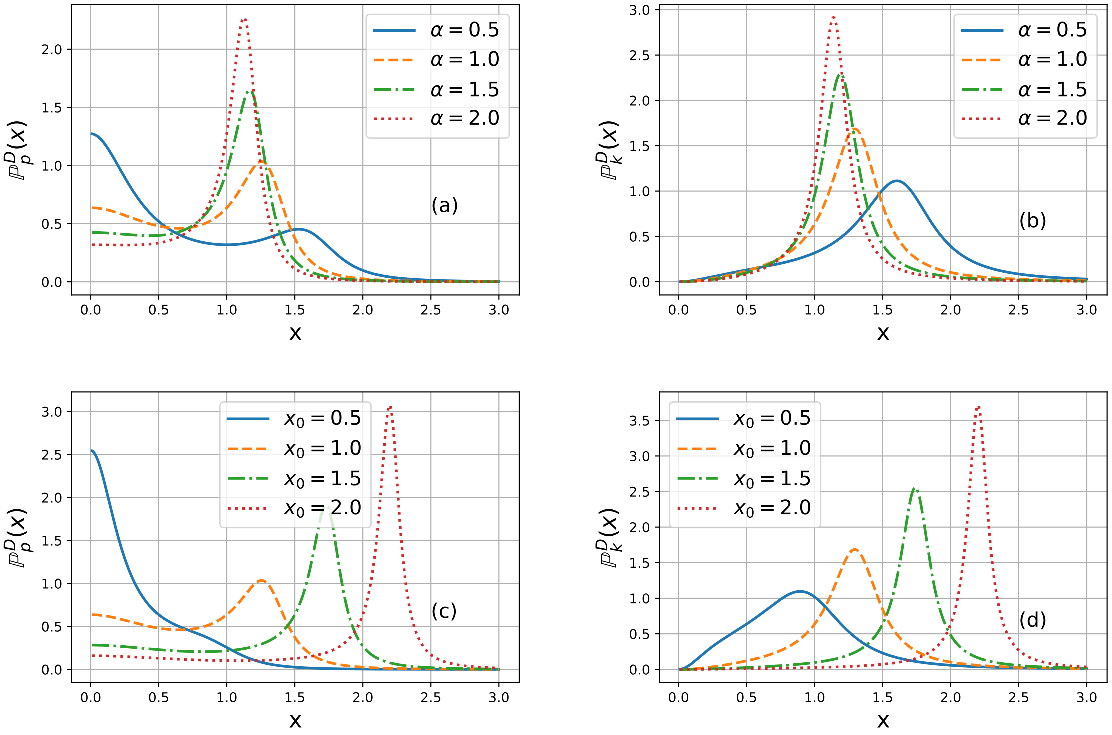

Figure 10: The probability density functions for the Drude model of dissipation. The memory kernel is $\gamma(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}$. In panels (a) and (b) the dimensionless oscillator eigen-frequency is fixed $x_0 = \omega_0\tau_c = 1.0$ and impact of $\alpha = \tau_v/\tau_c$ is depicted ($\tau_c$ is fixed and $\tau_v = M/\gamma_0$ is changed). In panels (c) and (d) the parameter $\alpha = 1.0$ and impact of $x_0$ is shown.

In Fig. 10 we depict the probability density as function of $x = \omega\tau_c$ for the Drude model of dissipation. In the left panels ,i.e, (a) and (c) we present the probability density for potential energy and in the right panels we show probability density for kinetic energy. In particular, in panel (a) and (b) we present the influence of $\tau_v = M/\gamma_0$ via the parameter $\alpha = \tau_v/\tau_c$ - the memory time $\tau_c$ is fixed in this scaling - and the rescaled oscillator eigen-frequency $x_0 = \omega_0\tau_c = 1$ for all cases. We can see in (a) that for all shown parameters $\mathbb{P}_p^D(x)$ is non-zero for $x = 0$, in contrary to $\mathbb{P}_k^D(x)$ for which $\mathbb{P}_k^D(0) = 0$. We can observe that the thermostat oscillators contribute to $E_p$ as well as to $E_k$ in a non-homogeneous way. There is the optimal thermostat oscillator frequency $x_M$ which makes the greatest contribution to $E_p$. The similar observation is also for $E_k$ but in general these two optimal frequencies are different. Moreover the values $x_M$ for $E_p$ and $E_k$ depend on the system parameters $\alpha$ and $x_0$. One can easily note that in all cases depicted in panels (a) and (b) the contribution is peaked in the region of low-frequency modes and then it rapidly decreases to 0. In panels (c) and (d) we illustrate the influence of the rescaled eigen-frequency $x_0 = \omega_0\tau_c$ for the fixed parameter $\alpha = 1$. We can see here that the frequency of the local maximum $x_M$ depends strongly on $x_0$ and for higher values of $x_0$ it is shifted to the higher frequency modes of thermostat.

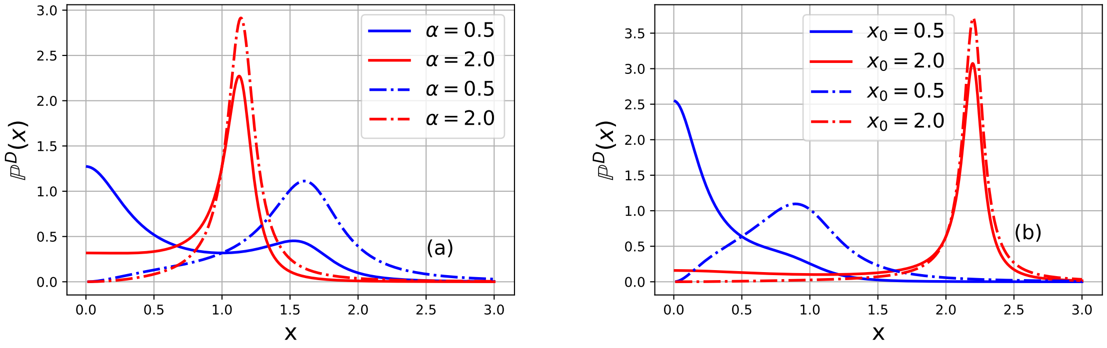

Figure 11: A comparison of probability density functions for potential energy (solid line) and kinetic energy (dash-dot line) for the Drude model of dissipation. Panel (a): fixed $x_0 = 1.0$ and different values of $\alpha = \tau_v/\tau_c$ ($\tau_c$ is fixed and $\tau_v$ is changed). Panel (b): fixed $\alpha = 1.0$ and selected values of $x_0 = \omega_0\tau_c$

In Fig. 11 we compare the probability densities $\mathbb{P}_p^D(x)$ and $\mathbb{P}_k^D(x)$. The functions with the same values of parameters are drawn using the same color. The solid line depicts $\mathbb{P}_p^D(x)$ while the dash-dot line depicts $\mathbb{P}_k^D(x)$.

Now, we analyze impact of the memory time $\tau_c$ and use the scaling:

$$y = \frac{\omega}{\mu_0} \tag{5.54}$$

$$y_0 = \frac{\omega_0}{\mu_0} \tag{5.55}$$

which yields

$$\tilde{\mathbb{P}}_p^D(y) = \mu_0 \mathbb{P}_p(\mu_0 y) = \frac{2\alpha^2 y_0^2 \left(\alpha^2 + y^2\right)}{\pi \left(\alpha^4 y^2 + \left(\alpha y^2 - \left(\alpha^2 + y^2\right)\left(y^2 - y_0^2\right)\right)^2\right)} \tag{5.56}$$

$$\tilde{\mathbb{P}}_k^D(y) = \mu_0 \mathbb{P}_k(\mu_0 y) = \frac{2\alpha^2 y^2 \left(\alpha^2 + y^2\right)}{\pi \left(\alpha^4 y^2 + \left(\alpha y^2 - \left(\alpha^2 + y^2\right)\left(y^2 - y_0^2\right)\right)^2\right)} \tag{5.57}$$

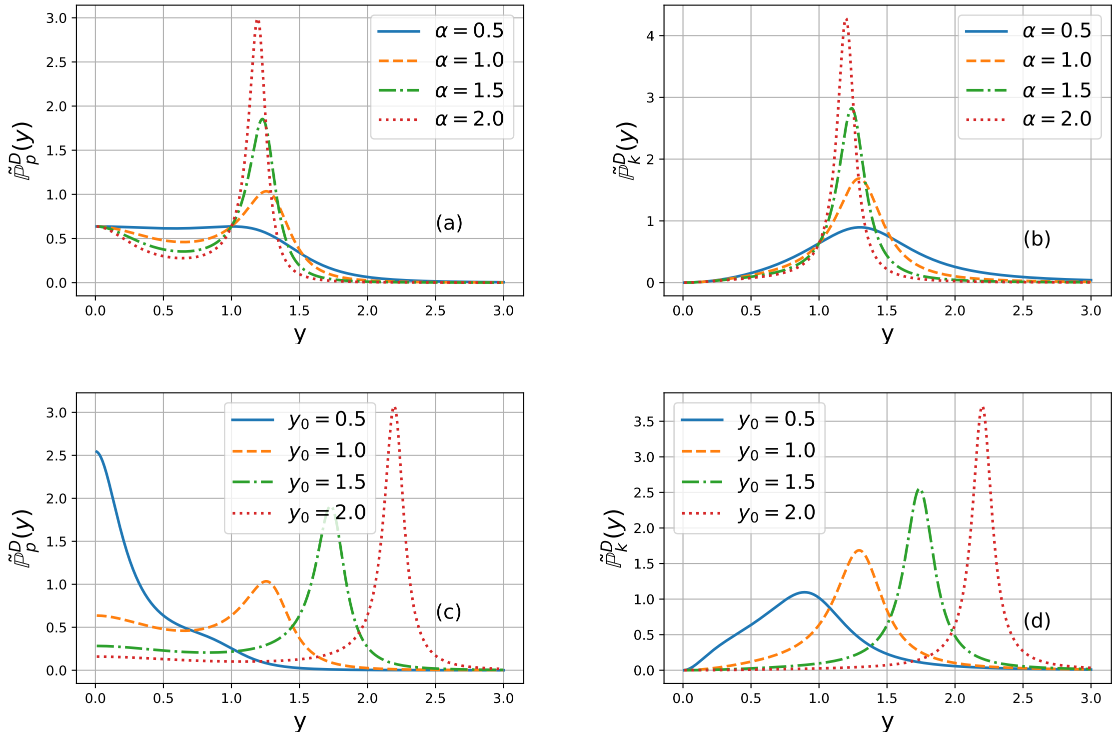

Figure 12: Probability density functions for the Drude model of dissipation. The memory kernel is $\gamma(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}$. In panels (a) and (b): the eigen-frequency is fixed $y_0 = \omega_0\tau_v = 1$ and impact of $\alpha = \tau_v/\tau_c$ is shown ($\tau_v$ is fixed and $\tau_c$ is changed). In panels (c) and (d): $\alpha = 1.0$ and the dimensionless eigen-frequency $y_0 = \omega_0\tau_v$ varies. Note that in panels (c) and (d) there are the same probability distributions as in Fig. 10. We repeat them to compare with other panels.

In Fig. 12 the probability density functions for potential and kinetic energy are shown. In left panels (a) and (c), the function $\tilde{\mathbb{P}}_p^D(y)$ defined in (5.56) is presented and in panels (b) and (d) the function $\tilde{\mathbb{P}}_k^D(y)$ defined in (5.57) is shown. We use here scaling $y = \tau_v\omega$. In upper panels (a) and (b) we present influence of the memory time $\tau_c$ via the parameter $\alpha = \tau_v/\tau_c$. In lower panels (c) and (d) we present influence of the rescaled eigen-frequency $y_0 = \tau_v\omega_0$. We observe that with increasing $y_0$ the frequency $y_M$ of maximal contribution to energy is shifted to the higher frequency modes.

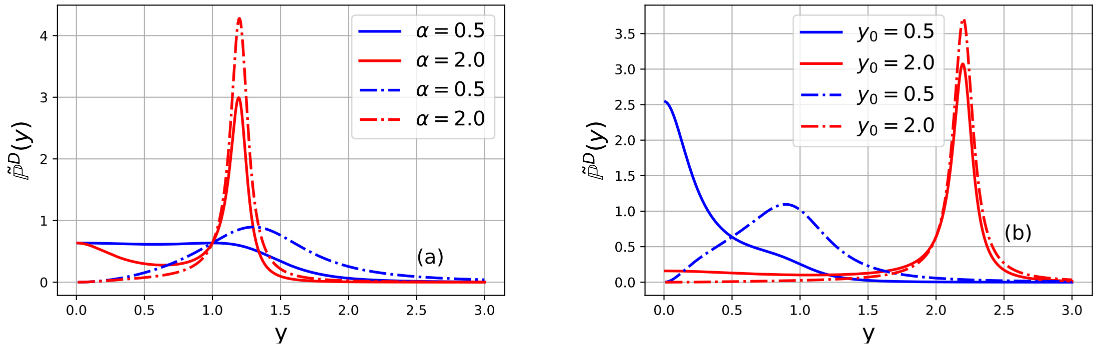

Figure 13: A comparison of probability density functions for potential energy (solid line) and kinetic energy (dash-dot line) for the Drude model of dissipation. Panel (a): fixed $y_0 = \omega_0 \tau_v = 1.0$ and different values of $\alpha = \tau_v/\tau_c$ ($\tau_v$ is fixed and $\tau_c$ is changed). Panel (b): fixed $\alpha = 1.0$ and selected values of $y_0$.

Comparison of the probability density functions $\tilde{\mathbb{P}}_p^D(y)$ and $\tilde{\mathbb{P}}_k^D(y)$ is presented in Fig. 13. In panel (a), the parameter $y_0$ is fixed, $y_0 = 1$, and influence of the parameter $\alpha$ is depicted. We can see that $\tilde{\mathbb{P}}_p^D(y)$ (solid line) has the non-zero value for $y = 0$ and $\tilde{\mathbb{P}}_k^D(y)$ drawn by dash-dot line has zero value for this argument. For both functions we note that after reaching local maximum both functions rapidly decrease to 0.

## 5.6 Generalized Drude model of dissipation

The memory kernel for this model is reminded to be

$$\gamma(t) = \frac{\gamma_0}{\tau_c} e^{-\frac{t}{\tau_c}} \cos(\Omega t) \tag{5.58}$$

The Laplace transform of it reads

$$\hat{\gamma}_L(\omega) = \frac{\gamma_0 (\omega \tau_c + 1)}{\Omega^2 \tau_c^2 + (\omega \tau_c + 1)^2} \tag{5.59}$$

Due to complexity we use functions $A(\omega)$ and $B(\omega)$ to represent probability density functions for energies:

$$A(\omega) = \frac{\gamma_0 (\Omega^2 \tau_c^2 + \omega^2 \tau_c^2 + 1)}{(\Omega^2 \tau_c^2 - 2\Omega\omega\tau_c^2 + \omega^2 \tau_c^2 + 1)(\Omega^2 \tau_c^2 + 2\Omega\omega\tau_c^2 + \omega^2 \tau_c^2 + 1)} \tag{5.60}$$

$$B(\omega) = -\frac{\gamma_0 \omega \tau_c (\Omega^2 \tau_c^2 - \omega^2 \tau_c^2 - 1)}{(\Omega^2 \tau_c^2 - 2\Omega\omega\tau_c^2 + \omega^2 \tau_c^2 + 1)(\Omega^2 \tau_c^2 + 2\Omega\omega\tau_c^2 + \omega^2 \tau_c^2 + 1)} \tag{5.61}$$

The probability density functions for energies are

$$\mathbb{P}_p(\omega) = \frac{2M}{\pi} \frac{\omega_0^2 A(\omega)}{\omega^2 A^2(\omega) + \left[M(\omega_0^2 - \omega^2) + \omega B(\omega)\right]^2} \tag{5.62}$$

$$\mathbb{P}_k(\omega) = \frac{2M}{\pi} \frac{\omega^2 A(\omega)}{\omega^2 A^2(\omega) + \left[M(\omega_0^2 - \omega^2) + \omega B(\omega)\right]^2} \tag{5.63}$$

There are four parameters $\Omega, \tau_c, \mu_0$ and the characteristic frequency $\omega_0$. Using appropriate scaling one can reduce a number of parameters. Let us introduce at this point the following scaling:

$$x = \omega \tau_c \tag{5.64}$$

$$x_0 = \omega_0 \tau_c \tag{5.65}$$

The corresponding probability density functions can be rewritten in the following way:

$$\mathbb{P}_p^E(x) = \frac{2\alpha x_0^2\left(\hat{\Omega}^2+x^2+1\right)\left(\hat{\Omega}^2-2\hat{\Omega}x+x^2+1\right)\left(\hat{\Omega}^2+2\hat{\Omega}x+x^2+1\right)}{\pi\left(x^2\left(\hat{\Omega}^2+x^2+1\right)^2+\left(\alpha\left(x^2-x_0^2\right)\left(\hat{\Omega}^2-2\hat{\Omega}x+x^2+1\right)\left(\hat{\Omega}^2+2\hat{\Omega}x+x^2+1\right)-x^2\left(-\hat{\Omega}^2+x^2+1\right)\right)^2\right)} \tag{5.66}$$

$$\mathbb{P}_k^E(x) = \frac{2\alpha x^2\left(\hat{\Omega}^2+x^2+1\right)\left(\hat{\Omega}^2-2\hat{\Omega}x+x^2+1\right)\left(\hat{\Omega}^2+2\hat{\Omega}x+x^2+1\right)}{\pi\left(x^2\left(\hat{\Omega}^2+x^2+1\right)^2+\left(\alpha\left(x^2-x_0^2\right)\left(\hat{\Omega}^2-2\hat{\Omega}x+x^2+1\right)\left(\hat{\Omega}^2+2\hat{\Omega}x+x^2+1\right)-x^2\left(-\hat{\Omega}^2+x^2+1\right)\right)^2\right)} \tag{5.67}$$

where:

$$\hat{\Omega} = \Omega \tau_c \tag{5.68}$$

$$\alpha = \frac{M}{\tau_c \gamma_0} = \frac{1}{\mu_0 \tau_c} \tag{5.69}$$

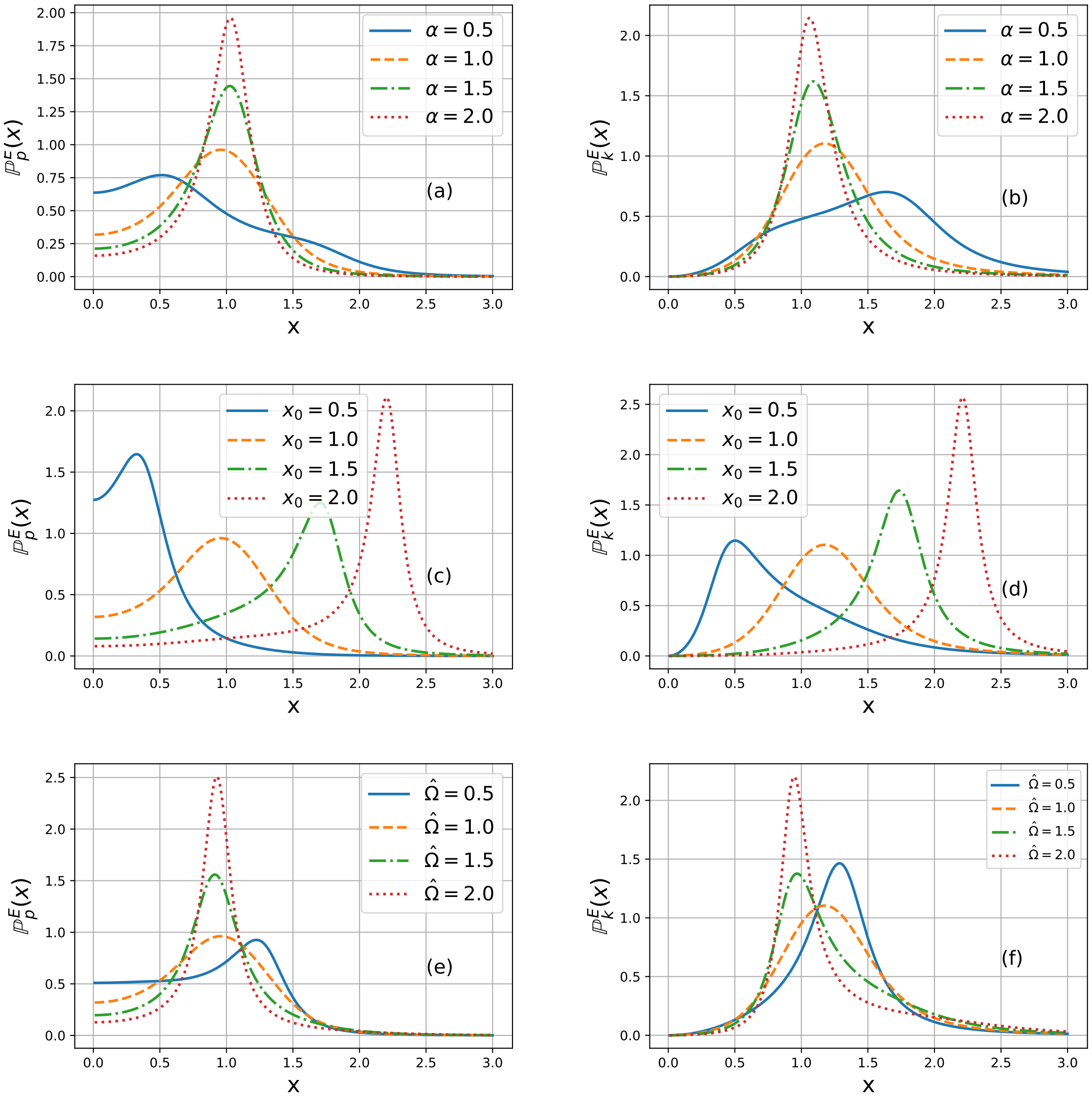

Figure 14: Probability density functions for the generalized Drude model of dissipation. The memory kernel is $\gamma(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}\cos(\Omega t)$. Panels (a), (c) and (e) present the probability density functions for potential energy. Panels (b), (d) and (f) are for kinetic energy. Probability functions are scaled as functions of the dimensionless parameter $x = \omega\tau_c$. In panels (a) and (b): $\hat{\Omega} = \Omega\tau_c = 1$, $x_0 = \omega_0\tau_c = 1$ and lines are drawn for different values of the parameter $\alpha = \tau_v/\tau_c$ ($\tau_v = M/\gamma_0$ is changed). In panels (c) and (d): $\hat{\Omega} = 1$, $\alpha = 1$ and $x_0$ varies. In panels (e) and (f): $\alpha = 1$, $y_0 = 1$ and $\hat{\Omega}$ varies. In all panels $\tau_c$ is fixed.

Fig. 14 shows the probability density functions for the generalized Drude model of dissipation. In left panels we present $\mathbb{P}_p^E(x)$ defined in (5.66), in right panels $\mathbb{P}_k^E(x)$ defined in (5.67) is shown. In all panels we use scaling $x = \tau_c \omega$. The functions depend on three parameters $\alpha = \tau_v/\tau_c$, $x_0 = \tau_c \omega_0$ and $\hat{\Omega} = \Omega \tau_c$. To show influence of all relevant parameters we use here six panels with every row depicting influence of different parameters and fixed parameters are assumed to be 1.

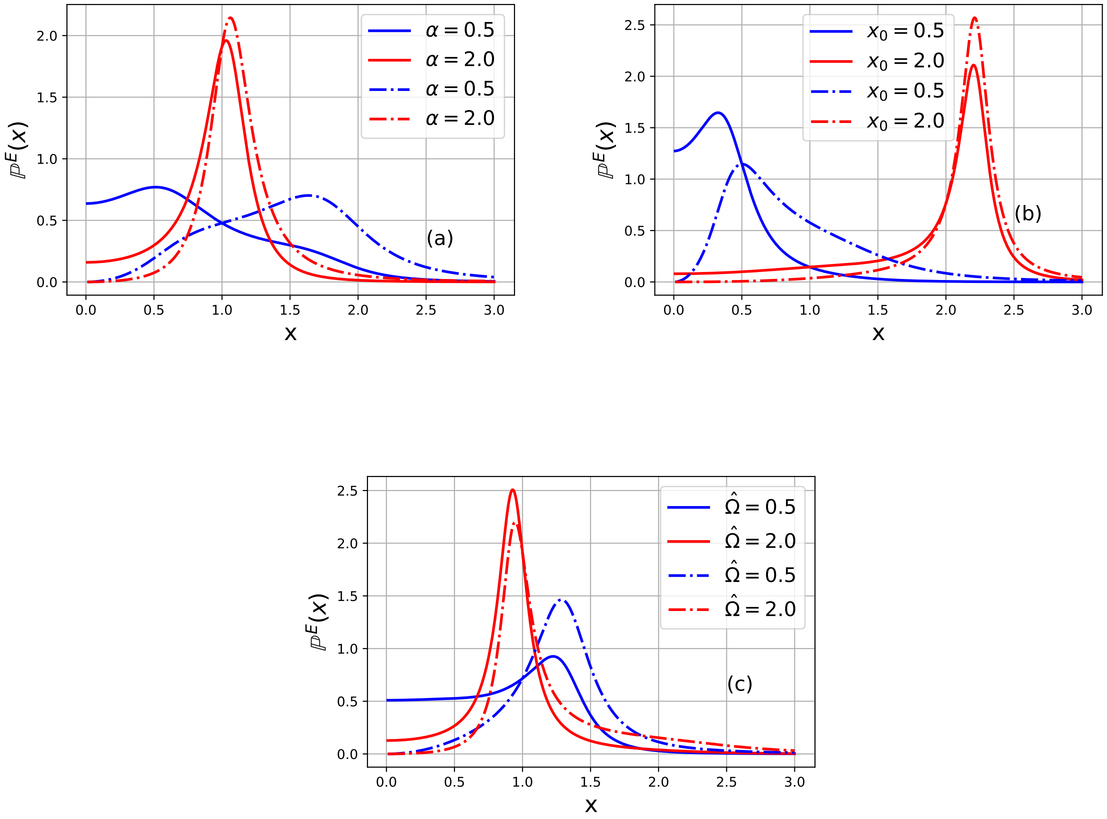

Figure 15: A comparison of probability density functions for potential energy (solid line) and kinetic energy (dash-dot line) for the generalized Drude model of dissipation. Panel (a): fixed $x_0 = \hat{\Omega} = 1.0$ and different values of $\alpha = \tau_v/\tau_c$ ($\tau_c$ is fixed and $\tau_v$ is changed). Panel (b): fixed $\alpha = \hat{\Omega} = 1.0$ and selected values of $x_0 = \omega_0 \tau_c$. Panel (c): fixed $\alpha = x_0 = 1.0$ and selected values of Panel (b): fixed $\alpha = \hat{\Omega} = 1.0$ and selected values of $\hat{\Omega} = \Omega \tau_c$.

In Fig. 15 functions $\mathbb{P}_p^E$ and $\mathbb{P}_k^E$ are compared. In panel (a) impact of the system-thermostat coupling $\gamma_0$ is shown via the parameter $\alpha = M/(\tau_c \gamma_0)$. We can see that with increasing value of $\alpha$ (the weaker coupling) the half-with of the probability density functions decreases. In panel (b) one can see the influence of rescaled eigen-frequency $x_0 = \tau_c \omega_0$. We can see that for all values $x_0$ the equality $\mathbb{P}_p^E(x_0) = \mathbb{P}_k^E(x_0)$ holds true.

To study impact of the memory time $\tau_c$ it is suitable to use the scaling:

$$y = \frac{\omega}{\mu_0} \tag{5.70}$$

$$y_0 = \frac{\omega_0}{\mu_0} \tag{5.71}$$

In this scaling, the probability density functions have the representation:

$$\tilde{\mathbb{P}}_p^E(y) = \frac{2\alpha^2 y_0^2 \left(\alpha^2+\tilde{\Omega}^2+y^2\right)\left(\alpha^2+\tilde{\Omega}^2-2\tilde{\Omega}y+y^2\right)\left(\alpha^2+\tilde{\Omega}^2+2\tilde{\Omega}y+y^2\right)}{\pi\left(\alpha^4 y^2\left(\alpha^2+\tilde{\Omega}^2+y^2\right)^2+\left(-\alpha y^2\left(\alpha^2-\tilde{\Omega}^2+y^2\right)+\left(y^2-y_0^2\right)\left(\alpha^2+\tilde{\Omega}^2-2\tilde{\Omega}y+y^2\right)\left(\alpha^2+\tilde{\Omega}^2+2\tilde{\Omega}y+y^2\right)\right)^2\right)} \tag{5.72}$$

$$\tilde{\mathbb{P}}_k^E(y) = \frac{2\alpha^2 y^2 \left(\alpha^2+\tilde{\Omega}^2+y^2\right)\left(\alpha^2+\tilde{\Omega}^2-2\tilde{\Omega}y+y^2\right)\left(\alpha^2+\tilde{\Omega}^2+2\tilde{\Omega}y+y^2\right)}{\pi\left(\alpha^4 y^2\left(\alpha^2+\tilde{\Omega}^2+y^2\right)^2+\left(-\alpha y^2\left(\alpha^2-\tilde{\Omega}^2+y^2\right)+\left(y^2-y_0^2\right)\left(\alpha^2+\tilde{\Omega}^2-2\tilde{\Omega}y+y^2\right)\left(\alpha^2+\tilde{\Omega}^2+2\tilde{\Omega}y+y^2\right)\right)^2\right)} \tag{5.73}$$

where:

$$\tilde{\Omega} = \frac{\Omega}{\mu_0} \tag{5.74}$$

$$\alpha = \frac{M}{\tau_c \gamma_0} = \frac{1}{\mu_0 \tau_c} \tag{5.75}$$

Their dependence on the system parameters is depicted in Figs. 16 and 17.

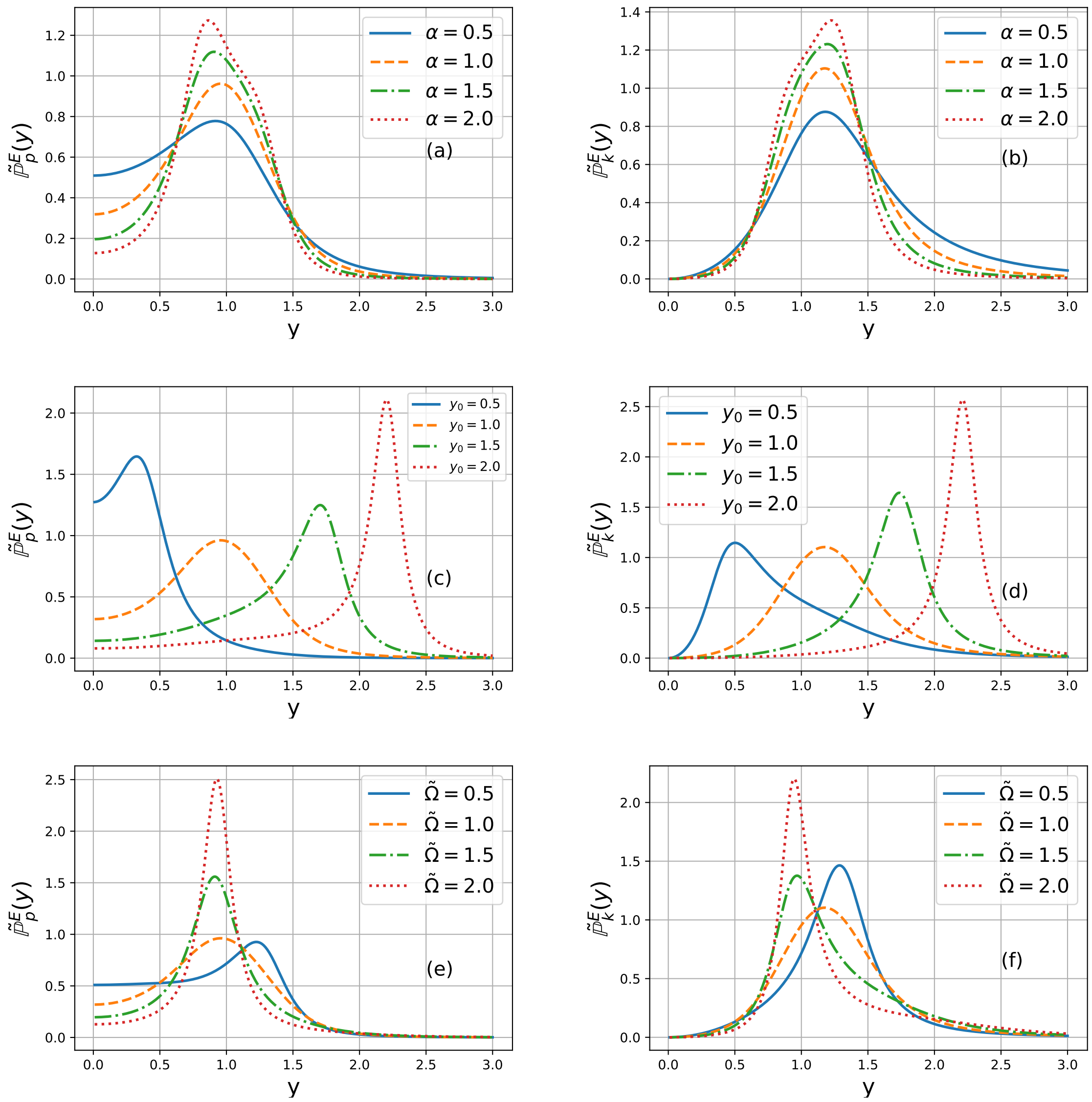

Figure 16: Probability density functions for the generalized Drude model of dissipation with the memory kernel defined as $\gamma(t) = (\gamma_0/\tau_c)e^{-t/\tau_c}\cos(\Omega t)$. Panels: (a), (c) and (e) present probability density functions for potential energy. Panels: (b), (d) and (f) are for kinetic energy. In panels (a) and (b) two parameter $\tilde{\Omega}$ and $y_0$ are fixed and equal to 1 and impact of $\alpha = \tau_v/\tau_c$ is shown ($\tau_v$ is fixed and $\tau_c$ is changed). In panels (c) and (d): $\tilde{\Omega}$ and $\alpha$ are fixed and equal to 1 with selected values of $y_0 = \omega_0\tau_v$. Panels (e) and (f): for different $\tilde{\Omega} = \Omega\tau_v$ with fixed parameters $y_0 = 1$ and $\alpha = 1$. Note that again there is a part of common distributions as in Fig. 14. We repeat them to compare with other panels.

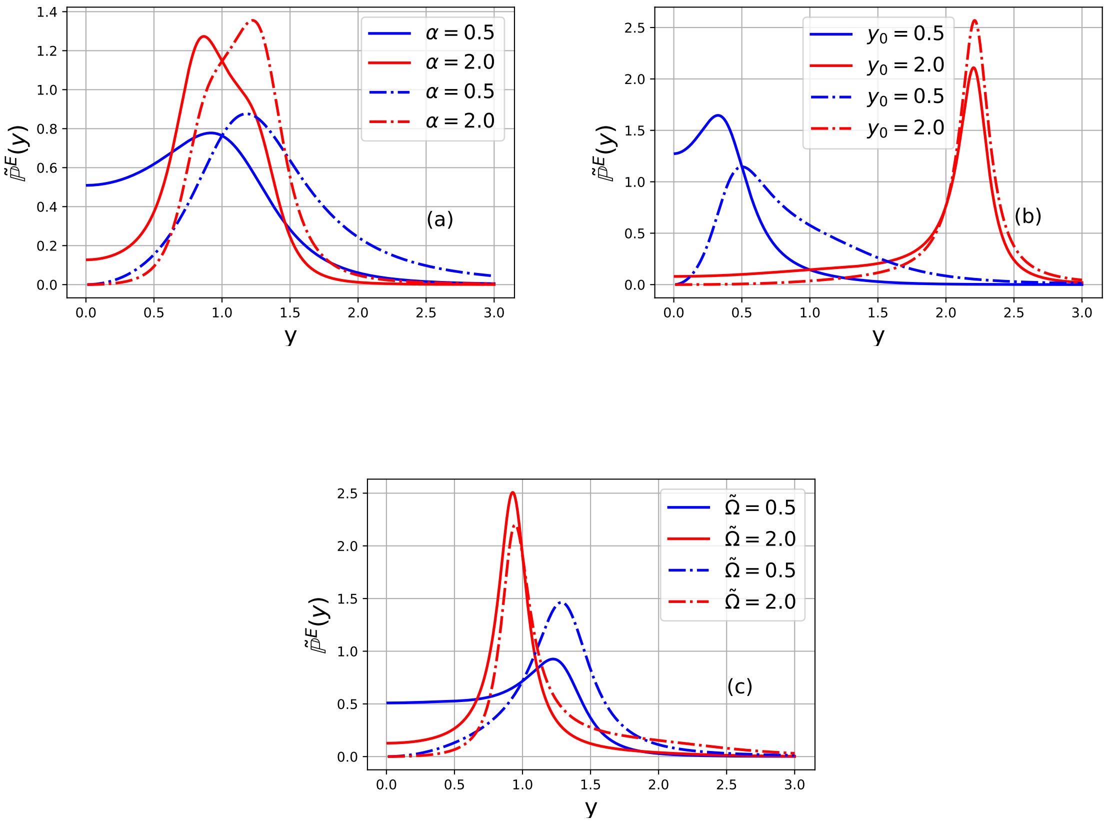

Figure 17: A comparison of probability density functions for potential energy (solid line) and kinetic energy (dash-dot line) for the generalized Drude model of dissipation. In all panels the parameter $\tau_v$ is fixed. The remaining is the same as in the previous figure.

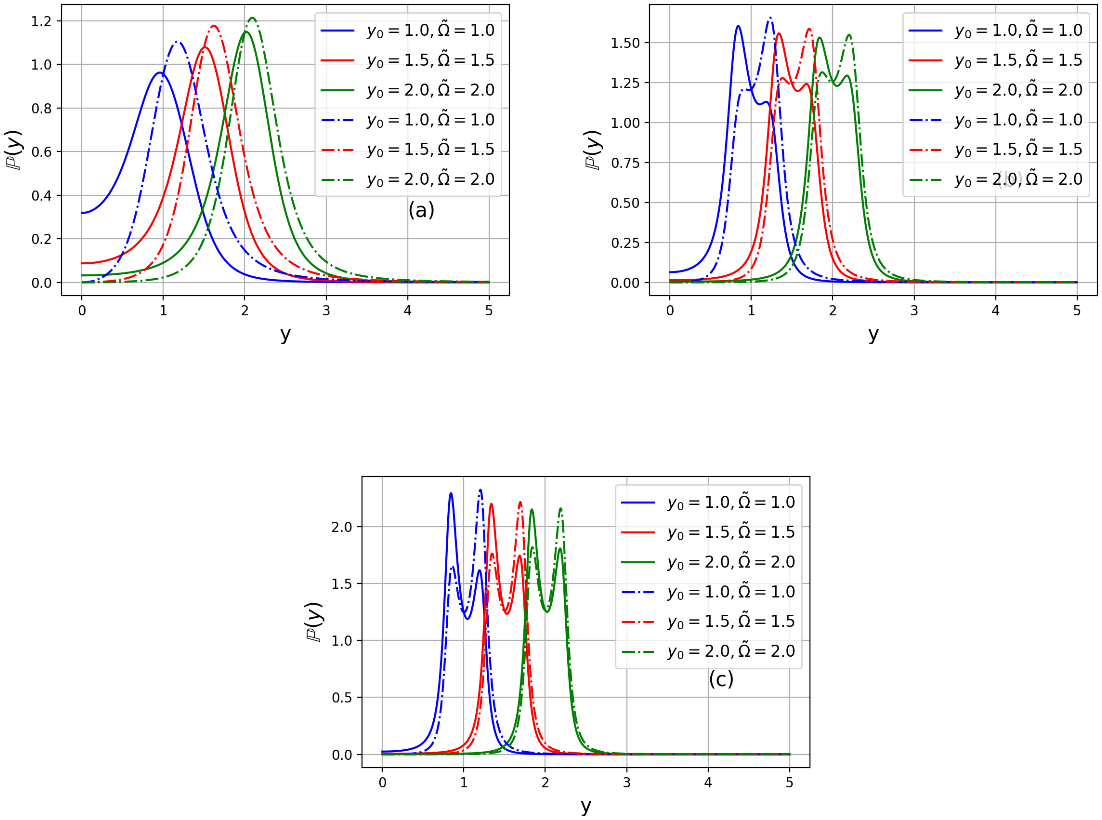

Figure 18: A comparison of probability density functions for potential energy (solid line) and kinetic energy (dash-dot line) for the generalized Drude model of dissipation. In this scaling, the parameter $\tau_c$ is fixed. Selected values of the special case $y_0 = \tilde{\Omega}$ is depicted. In panels: (a) $\alpha = 1$, (b) $\alpha = 3$, (c) $\alpha = 5$

In Fig. 18 we present interesting behavior for selected values of $y_0$ and $\tilde{\Omega}$ but for the special case when both characteristic frequencies are the same, i.e. when $y_0 = \tilde{\Omega}$. We can see that lines seemingly shifts to the higher frequency modes with increasing values of the parameters $y_0$ and $\tilde{\Omega}$. In panel (a) for which parameter $\alpha = 1$, the probability density functions exhibit only one local maximum with the some optimal frequency $y_M$ for $\tilde{\mathbb{P}}_k^E$ higher than the optimal frequency for potential energy. In panel (b) for which $\alpha = 3$ and in panel (c) for which $\alpha = 5$ the probability density functions exhibit two local maxima. This behavior becomes more apparent for higher values of $\alpha$.

## 5.7 Algebralic decay of memory kernel

The algebraic memory decay is characterized by the function

$$\gamma(t) = \frac{\gamma_0}{t+\tau_c} \tag{5.76}$$

Its Laplace transform is

$$\hat{\gamma}_L(\omega) = \gamma_0 e^{\omega\tau_c}\,\mathrm{E}_1\left(\omega\tau_c\right) \tag{5.77}$$

The functions $A(\omega)$ and $B(\omega)$ which enter to the probability densities take the form:

$$A(\omega) = \frac{\gamma_0}{2}\left(e^{2i\omega\tau_c}\,\mathrm{E}_1\left(i\omega\tau_c\right) + \mathrm{E}_1\left(-i\omega\tau_c\right)\right)e^{-i\omega\tau_c} \tag{5.78}$$

$$B(\omega) = \frac{i\gamma_0}{2}\left(e^{2i\omega\tau_c}\,\mathrm{E}_1\left(i\omega\tau_c\right) - \mathrm{E}_1\left(-i\omega\tau_c\right)\right)e^{-i\omega\tau_c} \tag{5.79}$$

Again, we introduce the scaling:

$$x = \omega\tau_c \tag{5.80}$$

$$x_0 = \omega_0\tau_c \tag{5.81}$$

in which the probability densities have the form

$$\mathbb{P}_p^A(x) = \frac{4\alpha x_0^2\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)+\mathrm{E}_1\left(-ix\right)\right)e^{ix}}{\pi\left(x^2\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)+\mathrm{E}_1\left(-ix\right)\right)^2+\left(2\alpha\left(x^2-x_0^2\right)e^{ix}-ix\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)-\mathrm{E}_1\left(-ix\right)\right)\right)^2\right)} \tag{5.82}$$

$$\mathbb{P}_k^A(x) = \frac{4\alpha x^2\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)+\mathrm{E}_1\left(-ix\right)\right)e^{ix}}{\pi\left(x^2\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)+\mathrm{E}_1\left(-ix\right)\right)^2+\left(2\alpha\left(x^2-x_0^2\right)e^{ix}-ix\left(e^{2ix}\,\mathrm{E}_1\left(ix\right)-\mathrm{E}_1\left(-ix\right)\right)\right)^2\right)} \tag{5.83}$$

where:

$$\alpha = \frac{M}{\tau_c\gamma_0} = \frac{1}{\mu_0\tau_c} \tag{5.84}$$

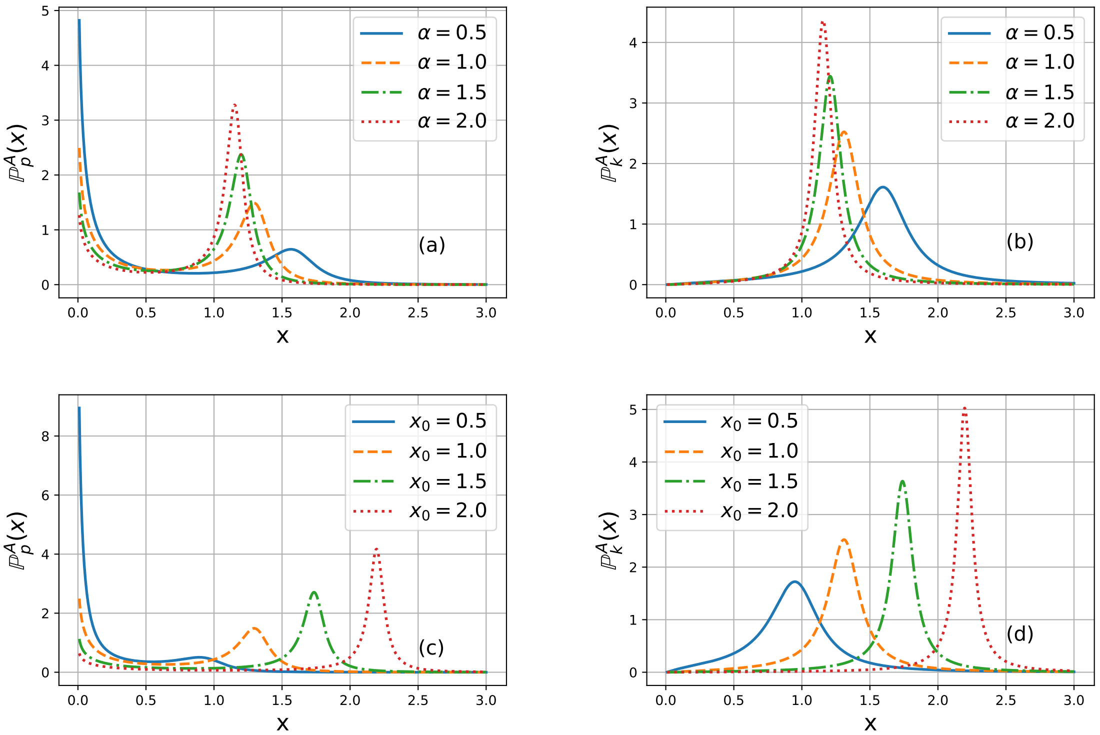

Figure 19: Probability density functions for the algebraically decaying memory function defined as $\gamma(t) = \gamma_0/(t + \tau_c)$. Panels (a) and (c) depict probability density functions for potential energy. Panels (b) and (d) are for kinetic energy. In panels (a) and (b): $x_0 = 1$ with selected values of $\alpha = \tau_v/\tau_c$ ($\tau_c$ is fixed and $\tau_v = M/\gamma_0$ is changed). In panels (c) and (b): $\alpha = 1$ and different values of $x_0 = \omega_0\tau_c$.

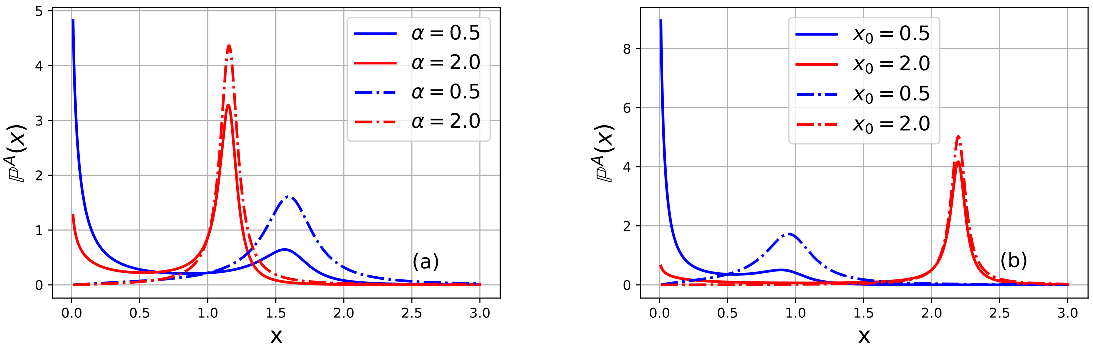

Figure 20: A comparison of probability density functions for potential energy (with solid line) and kinetic energy (dash-dot line) in the case of the algebraically decaying memory. Panel (a) is for fixed $x_0 = 1.0$ and different values of $\alpha = \tau_v/\tau_c$. Panel (b) is for fixed $\alpha = 1.0$ and different $x_0 = \omega_0 \tau_c$

For the second scaling

$$y = \frac{\omega}{\mu_0} \tag{5.85}$$

$$y_0 = \frac{\omega_0}{\mu_0} \tag{5.86}$$

the probability density functions read

$$\tilde{\mathbb{P}}_p^A(y) = \frac{4y_0^2\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) + \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right)e^{\frac{iy}{\alpha}}}{\pi\left(y^2\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) + \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right)^2 + \left(-iy\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) - \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right) + 2\left(y^2 - y_0^2\right)e^{\frac{iy}{\alpha}}\right)^2\right)} \tag{5.87}$$

$$\tilde{\mathbb{P}}_k^A(y) = \frac{4y^2\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) + \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right)e^{\frac{iy}{\alpha}}}{\pi\left(y^2\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) + \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right)^2 + \left(-iy\left(e^{\frac{2i}{\alpha}y}\,\mathrm{E}_1\left(\frac{iy}{\alpha}\right) - \mathrm{E}_1\left(-\frac{iy}{\alpha}\right)\right) + 2\left(y^2 - y_0^2\right)e^{\frac{iy}{\alpha}}\right)^2\right)} \tag{5.88}$$

Their graphical representation is shown in Figs. 21 and 22.

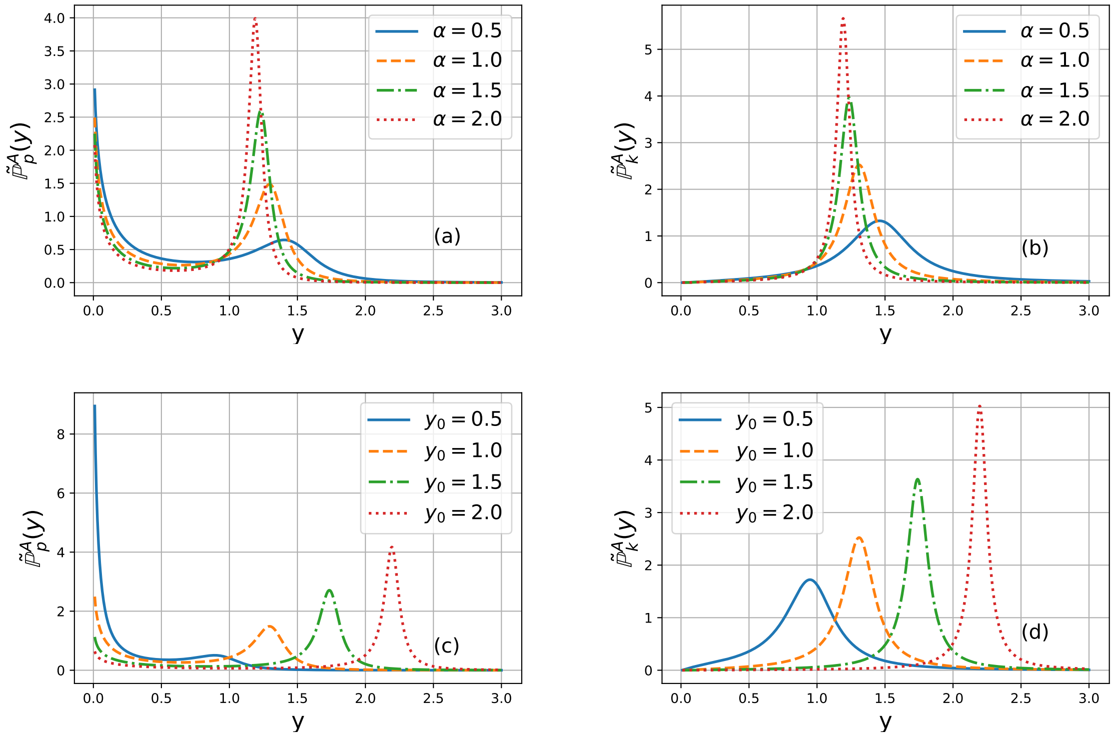

Figure 21: Probability density functions for the algebraically decaying memory function $\gamma(t) = \gamma_0/(t + \tau_c)$. Panels (a) and (c) depict probability density functions for potential energy. Panels (b) and (d) are for kinetic energy. Panels (a) and (b) are for fixed $y_0 = 1$ and selected values of $\alpha = \tau_v/\tau_c$. Panels (c) and (b) are for $\alpha = 1$ with selected values of the dimensionless parameter $y_0 = \omega_0\tau_v$ ($\tau_v = M/\gamma_0$ is fixed).

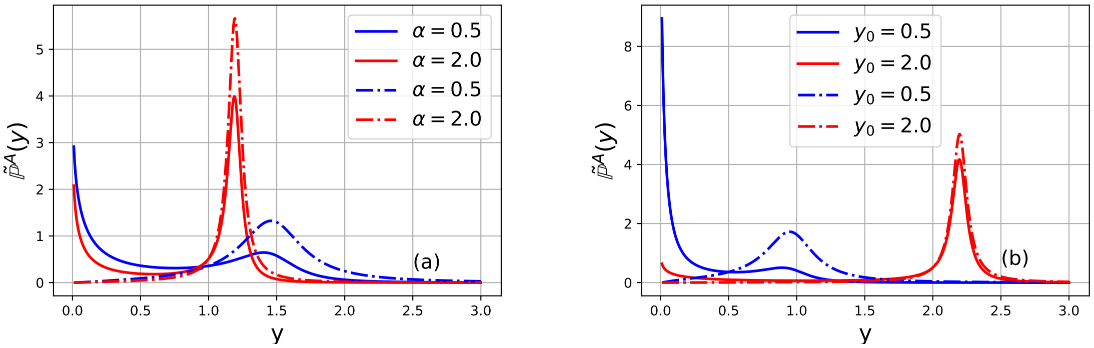

Figure 22: A comparison of probability density functions for potential energy (with solid line) and kinetic energy (dash-dot line) in the case of the algebraically decaying memory kernel defined as $\gamma(t) = \gamma_0/(t + \tau_c)$. Panel (a) is fixed $y_0 = 1.0$ and different values of $\alpha = \tau_v/\tau_c$. Panel (b) is for fixed $\alpha = 1.0$ and selected values of $y_0 = \omega_0\tau_v$ ($\tau_v = M/\gamma_0$ is fixed).

## 5.8 Gaussian memory kernel

The last model of dissipation which we want to present is defined by the Gaussian decay of the memory kernel:

$$\gamma(t) = \frac{\gamma_0 e^{-\frac{t^2}{\tau_c^2}}}{\sqrt{\pi}\tau_c} \tag{5.89}$$

The Laplace transform:

$$\hat{\gamma}_L(t) = \frac{\gamma_0}{2}\left(-\operatorname{erf}\left(\frac{\omega\tau_c}{2}\right) + 1\right) e^{\frac{\omega^2\tau_c^2}{4}} \tag{5.90}$$

where erf is the error function defined as:

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt \tag{5.91}$$

$$A(\omega) = \frac{\gamma_0}{2} e^{-\frac{\omega^2\tau_c^2}{4}} \tag{5.92}$$

$$B(\omega) = -\frac{i\gamma_0}{2} e^{-\frac{\omega^2\tau_c^2}{4}} \operatorname{erf}\left(\frac{i\tau_c}{2}\omega\right) \tag{5.93}$$

Probability density functions:

$$\mathbb{P}_p(\omega) = \frac{M\gamma_0\omega_0^2 e^{-\frac{\omega^2\tau_c^2}{4}}}{\pi\left(\frac{\gamma_0^2\omega^2}{4} e^{-\frac{\omega^2\tau_c^2}{2}} + \left(M\left(-\omega^2 + \omega_0^2\right) - \frac{i\omega}{2}\gamma_0 e^{-\frac{\omega^2\tau_c^2}{4}} \operatorname{erf}\left(\frac{i\tau_c}{2}\omega\right)\right)^2\right)} \tag{5.94}$$

$$\mathbb{P}_k(\omega) = \frac{M\gamma_0\omega^2 e^{-\frac{\omega^2\tau_c^2}{4}}}{\pi\left(\frac{\gamma_0^2\omega^2}{4}e^{-\frac{\omega^2\tau_c^2}{2}} + \left(M\left(-\omega^2+\omega_0^2\right) - \frac{i\omega}{2}\gamma_0 e^{-\frac{\omega^2\tau_c^2}{4}}\,\mathrm{erf}\left(\frac{i\tau_c}{2}\omega\right)\right)^2\right)} \tag{5.95}$$

Furthermore if we introduce scaling:

$$x = \omega\tau_c \tag{5.96}$$

$$x_0 = \omega_0\tau_c \tag{5.97}$$

the rescalled probability density functions are:

$$\mathbb{P}_p^G(x) = \frac{4\alpha x_0^2 e^{\frac{x^2}{4}}}{\pi\left(x^2 + \left(2\alpha\left(x^2 - x_0^2\right)e^{\frac{x^2}{4}} + ix\,\mathrm{erf}\left(\frac{ix}{2}\right)\right)^2\right)} \tag{5.98}$$

$$\mathbb{P}_k^G(x) = \frac{4\alpha x^2 e^{\frac{x^2}{4}}}{\pi\left(x^2 + \left(2\alpha\left(x^2 - x_0^2\right)e^{\frac{x^2}{4}} + ix\,\mathrm{erf}\left(\frac{ix}{2}\right)\right)^2\right)} \tag{5.99}$$

where:

$$\alpha = \frac{M}{\gamma_0\tau_c} = \frac{1}{\mu_0\tau_c} \tag{5.100}$$

These distributions are depicted in Figs. 23 and 24.

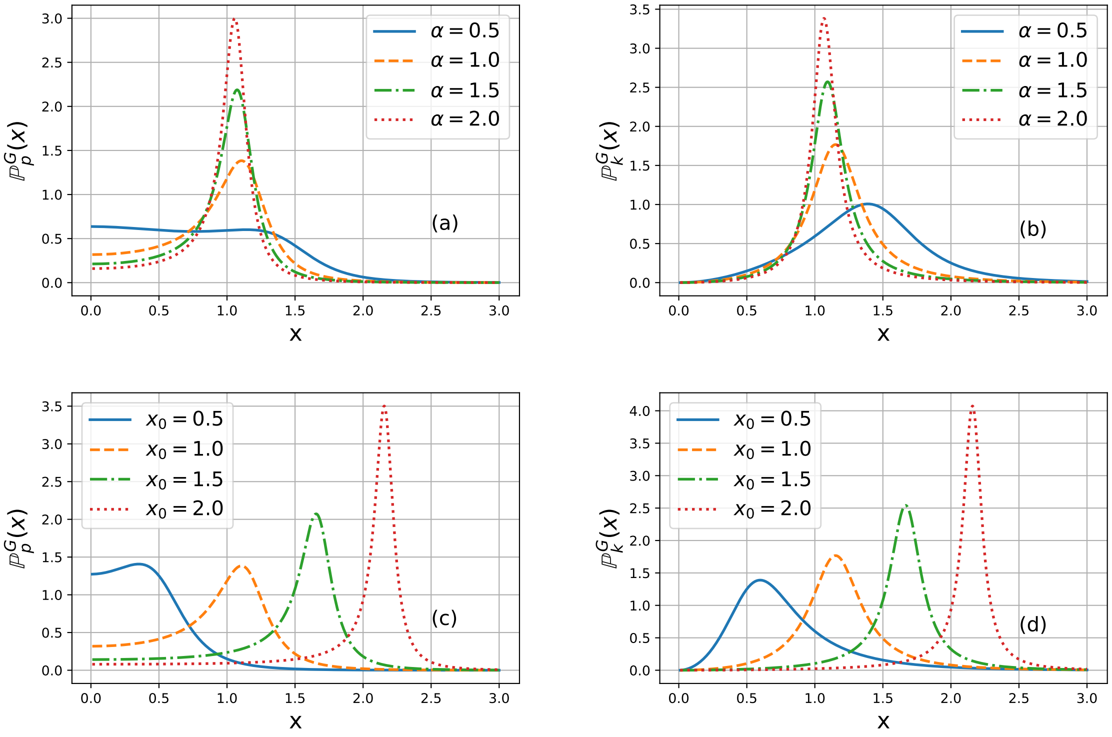

Figure 23: Probability density functions for the Gaussian model of dissipation. Memory kernel in this model is $\gamma(t) = \gamma_0 \exp\left(-t^2/\tau_c^2\right) / \left(\sqrt{\pi}\tau_c\right)$. Panel (a) is for potential energy with fixed $x_0 = 1.0$ and for different $\alpha$. Panel (b) corresponds to kinetic energy. In panel (c) $\alpha = 1.0$ and $x_0$ is changed. Panel (d) is for kinetic energy with fixed $\alpha = 1$.

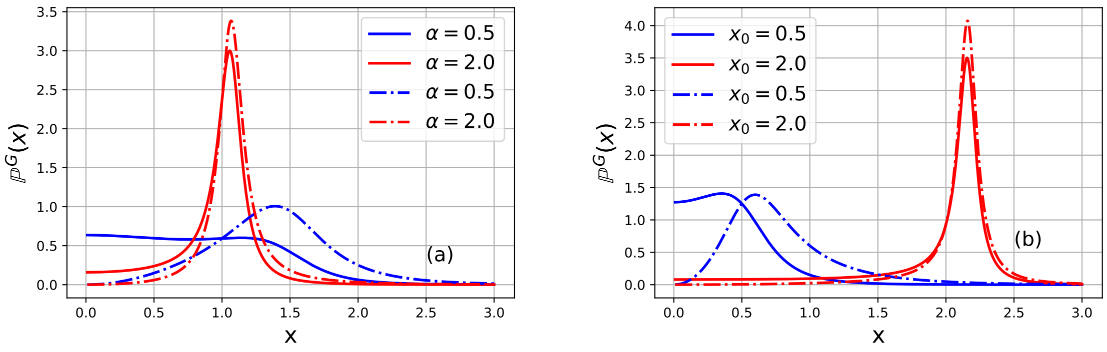

Figure 24: A comparison of probability density functions for the Gaussian model of dissipation: The probability density for potential energy is depicted by solid line and dash-doted line corresponds to kinetic energy. In panel (a) $x_0 = 1.0$ and impact of $\alpha$ is shown. Panel (b) is for fixed $\alpha = 1$ with different $x_0$.

For this rescaling parameter $\tau_c$ is fixed. If we are interested on the impact of the memory time $\tau_c$ upon behavior of probability density function we ought to use different rescaling with fixed parameter $\mu_0$. For the this type of rescaling:

$$y = \frac{\omega}{\mu_0} \tag{5.101}$$

$$y_0 = \frac{\omega_0}{\mu_0} \tag{5.102}$$

the dimensionless probability density functions are:

$$\tilde{\mathbb{P}}_p^G(y) = \frac{4y_0^2 e^{\frac{y^2}{4\alpha^2}}}{\pi\left(y^2 + \left(iy\,\mathrm{erf}\left(\frac{iy}{2\alpha}\right) + 2\left(y^2 - y_0^2\right)e^{\frac{y^2}{4\alpha^2}}\right)^2\right)} \tag{5.103}$$

$$\tilde{\mathbb{P}}_k^G(y) = \frac{4y^2 e^{\frac{y^2}{4\alpha^2}}}{\pi\left(y^2 + \left(iy\,\mathrm{erf}\left(\frac{iy}{2\alpha}\right) + 2\left(y^2 - y_0^2\right)e^{\frac{y^2}{4\alpha^2}}\right)^2\right)} \tag{5.104}$$

They are shown in Figs. 25 and 26.

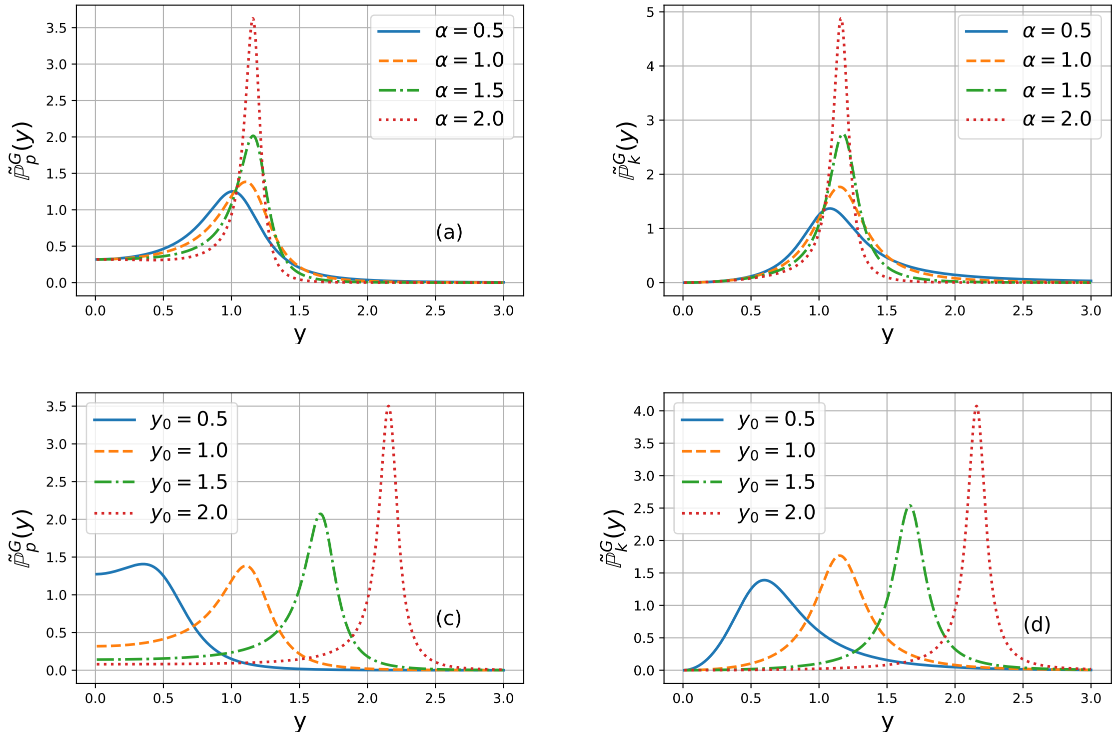

Figure 25: Probability density functions for the Gaussian model of dissipation with the frequency scaling $y = \tau_v \omega$.

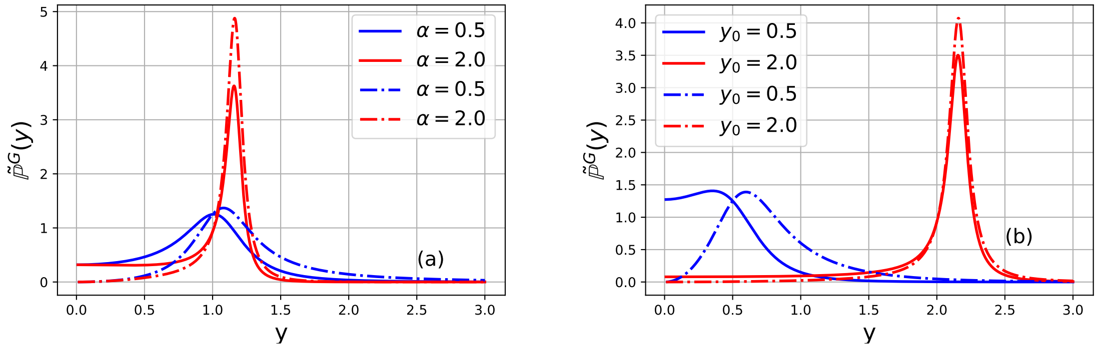

Figure 26: A comparison of probability density functions for the Gaussian model of dissipation. The remaining is the same as in the previous figures.

Fig. 26 illustrates comparison between the probability density function for potential energy with the probability density function for kinetic energy. In the panel (a) we can observe influence of the memory time $\tau_c$ via parameter $\alpha = \frac{\tau_v}{\tau_c}$ with fixed parameter

$y_0 = \tau_v \omega_0$. The functions $\tilde{\mathbb{P}}_p^G(y)$ and $\tilde{\mathbb{P}}_k^G(y)$ are defined in (5.103) and in (5.104). It is interesting to note that for this scalling the value of $\tilde{\mathbb{P}}_p^G(0)$ does not depend on the parameter $\alpha$ as it was in previously considered models, like in figure 17. The value of $\tilde{\mathbb{P}}_p^G(0)$ depends only on the value of parameter $y_0$ as can be seen in the panel (b).

## 5.9 Discussion and remarks

In literature, one can find various expressions for potential and kinetic energy of the dissipative quantum harmonic oscillator. Nonetheless, the formulas introduced in this chapter for potential energy:

$$E_p = \int_0^{+\infty} d\omega \, \mathcal{E}_p(\omega) \mathbb{P}_p(\omega) \tag{5.105}$$

and kinetic energy:

$$E_k = \int_0^{+\infty} d\omega \, \mathcal{E}_k(\omega) \mathbb{P}_k(\omega) \tag{5.106}$$

are similar as in the case of a free Brownian particle and their interpretation, *mutatis mutandis*, is also similar. Nevertheless, we summarize main results to make this chapter to be independent on Chapter 4. Let us list:

I. In the equilibrium state, the mean potential energy $E_p$ of the central oscillator equals averaged potential energy $\langle \mathcal{E}_p \rangle$ of the thermostat degree of freedom, i.e. $E_p = \langle \mathcal{E}_p \rangle$

II. The mean kinetic energy $E_k$ of the central oscillator equals the mean kinetic energy $\langle \mathcal{E}_k \rangle$ of the thermostat degree of freedom, i.e. $E_k = \langle \mathcal{E}_k \rangle$. The form of this statement is similar as for classical systems, see Eq. (2.9): The mean kinetic energy of a free classical particle equals the average kinetic energy of the thermostat degree of freedom.

III. The functions $\mathbb{P}_p(\omega)$ and $\mathbb{P}_k(\omega)$ are probability density functions, i.e. they are non-negative and normalized on the interval $[0; +\infty)$. From probability theory it follows that there exist random variables $\xi_1$ and $\xi_2$ for which $\mathbb{P}_p$ and $\mathbb{P}_k$ are their probability distributions. These random variables can be interpreted as frequencies of thermostat oscillators. In the thermodynamic limit for thermostat, there are infinitely many oscillators of various frequencies $\omega$ which contribute in a various way to $E_p$ and $E_k$ according to $\mathbb{P}_p(\omega)$ and $\mathbb{P}_k(\omega)$, respectively. It is worth to stress that in general, the same thermostat oscillators of frequencies in the interval $(\omega_1, \omega_2)$ contribute to $E_k$ in a different way than to $E_p$.

IV. The thermostat oscillators contribute to $E_p$ and $E_k$ in a non-uniform way according to the probability density functions $\mathbb{P}_p(\omega)$ and $\mathbb{P}_k(\omega)$. The form of these distributions do not depend on temperature $T$. However, they depend on coupling between the Brownian particle and thermostat. There is no restriction on the value of this coupling - it means that strong coupling is included as well. They also depend on the memory time - it means that non-Markovian regime is included as well. And finally, it depends on mass $M$ of the central oscillator and its frequency. Note that for classical systems, there is no mass and frequency dependence.

### 5.9.1 Remarks on mean energy

We show how energy of a quantum oscillator depends on some parameters of the model. The results presented here are published in our paper [21]. In Fig. 27, we illustrate the mean kinetic and potential energy for the Drude model, see Eqs. (5.47) and (5.48) with (5.105) and (5.106), as a function of temperature for selected values of the model parameters. In particular, in panel (a) we present the influence of the memory time $\tau_c$ via the parameter $\alpha = \tau_v/\tau_c$ with fixed $\tau_v = M/\gamma_0$ and the oscillator eigenfrequency $\tilde{\omega}_0 = 1$. We note that regardless of the value of the memory time for this set of parameters the potential energy is always smaller than the kinetic one. Moreover, when the memory time decreases (i.e. $\alpha$ increases) the kinetic energy increases whereas the potential one is decreasing. On the other hand if time $\tau_c$ increases (i.e. $\alpha$ decreases) then the difference between the kinetic and potential energy is getting smaller and smaller and in the limit of infinitely long memory time it tends to zero.

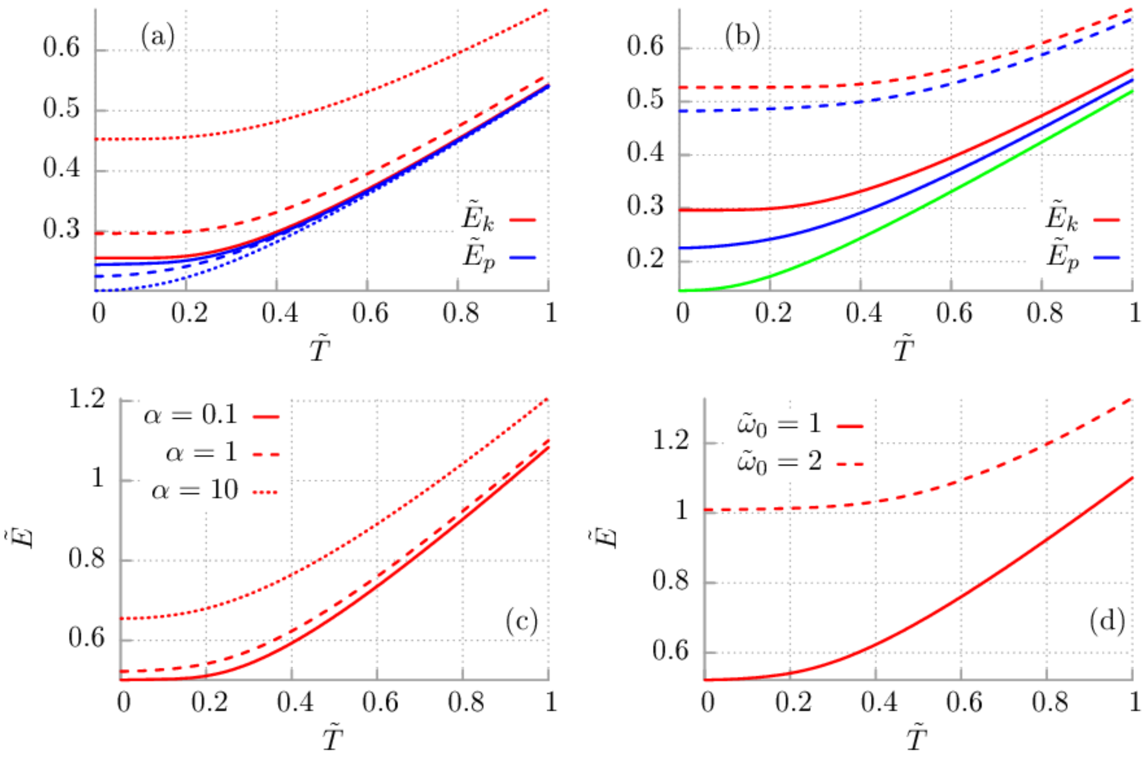

Figure 27: Harmonic oscillator with Drude dissipation. The dimensionless mean kinetic energy $\tilde{E}_k = \tau_v E_k/\hbar$ (red) and mean potential energy $\tilde{E}_p = \tau_v E_p/\hbar$ (blue) versus dimensionless temperature $\tilde{T} = \tau_v k_B T/\hbar$, where $\tau_v = M/\gamma_0$ is fixed. Panel (a): Solid line $\alpha = \tau_v/\tau_c = 0.1$, dashed line: $\alpha = 1$, dotted line $\alpha = 10$; all for the fixed eigenfrequency $\tilde{\omega}_0 = \omega_0\tau_v = 1$. Panel (b): Solid line $\tilde{\omega}_0 = 1$, dashed line $\tilde{\omega}_0 = 2$ and fixed $\alpha = 1$. The exception here is the green solid line which shows the mean kinetic energy $\tilde{E}_k$ for the free Brownian particle with $\tilde{\omega}_0 = 0$. Panel (c): The total energy $\tilde{E} = \tilde{E}_k + \tilde{E}_p$ corresponding to the regime of panel (a). Panel (d): The total energy corresponding to the regime of panel (b).

Alternatively, if the memory time $\tau_c$ is fixed and we change $\tau_v = M/\gamma_0$ in $\alpha = \tau_v/\tau_c$ we observe that the kinetic and potential energy approaches the same value in the limit of large values of $\alpha$ (not depicted). It implies that either:

(i) the mass $M$ of the particle is large or

(ii) the coupling $\gamma_0$ between the system and thermostat is weak.

In the latter situation one could say that the system may be approximated by a free harmonic oscillator, which especially in the low temperature limit approaches a coherent state, where the position and momentum variances (proportional to kinetic and potential energy) match. The problem of relation between the kinetic and potential energy is discussed also in Ref. [43]. In panel (b) of Fig. 27 we present the same characteristics but now depicted for the fixed memory time $\alpha = 1$ and different values of the oscillator eigenfrequency $\tilde{\omega}_0$. The observation is that for increasing values of the latter parameter both the kinetic and potential energy is growing. However, still the kinetic one is larger than the potential energy. The reader should note there also the interesting comparison with the case of a free quantum Brownian particle $\tilde{\omega}_0 = 0$ which is marked by the green colour. It turns out that the kinetic energy of a quantum harmonic oscillator is always greater than in the corresponding case of the free particle.

In panels (c) and (d) of Fig. 27 we analyse the dependence of the total averaged energy $E = E_k + E_p$ of the quantum oscillator versus the previously discussed parameters. It is instructive to observe in the panel (c) that when the memory time $\tau_c$ decreases (i.e. $\alpha$ increases) the total energy of the system increases to infinity. It means that the limiting case of vanishing memory is non-physical for quantum systems. Since the time scale $\tau_c$ can be viewed also as the leading correlation time of the quantum thermal fluctuations one would say in analogy to classical physics that there is no limit of white noise in the quantum realm. In other words it implies that quantum thermal fluctuations are always correlated. Qualitatively, the dependence of the kinetic, potential or total energy on temperature is robust with respect to changes of the model parameter values. For high enough temperature it always tends to the classical limit $k_B T/2$ while in the regime of low temperature it is higher than the corresponding classical value. Note that all curves are monotonically increasing functions of temperature which never intersect each other. Due to this fact for a qualitative analysis it is sufficient to study the oscillator energies corresponding to zero temperature limit $T = 0$.

Here, we mention two recent papers [10, 18] where similar problems are studied. There the variance of the position of the quantum Brownian particle is studied as a function of temperature and the system-thermostat coupling strength. One of the main results of analysis performed there is the particle position squeezing as temperature decreases and the interaction strength increases. For our system we observe a similar effect (not depicted). The potential energy $E_p$ (the particle position variance) decreases for fixed temperature $T$ and growing of the coupling constant $\gamma_0$. It then translates to the fact that the probability distribution $\mathbb{P}_p(\omega)$ corresponding to the mean potential energy rapidly decays meaning that relatively only the oscillators of low frequency bring the contribution to the average potential energy. Under this assumption they have small kinetic energy and therefore can transfer only little amount of it to the system. Consequently, the variance of the particle position is limited. In contrast, for weak system-thermostat coupling oscillators of high frequency dominate the probability distribution for the potential energy (position variance). Then they are allowed to have much larger kinetic energy and may transfer much bigger portion of it to the system resulting in increase of the particle position variance. Therefore the theorem of quantum partition of energy turns out to be quite helpful in qualitative interpretation of the mentioned particle position squeezing effect.

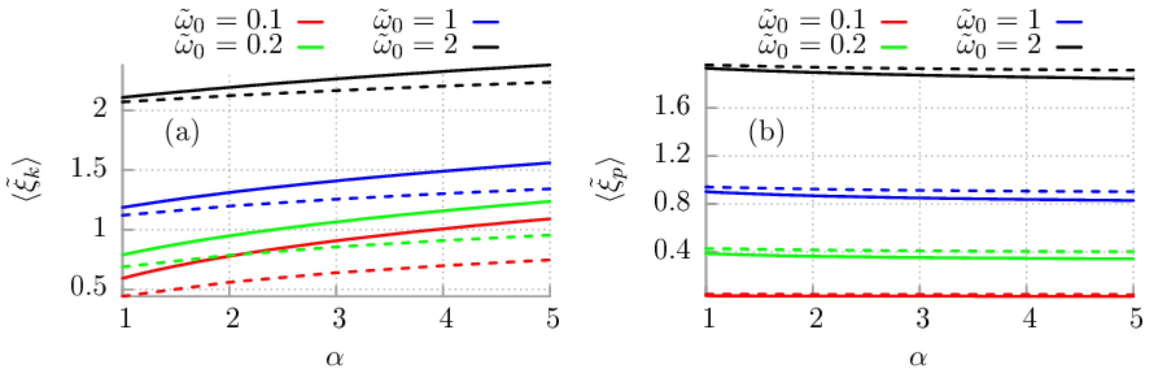

Figure 28: Panel (a): the mean value $\langle\tilde{\xi}_k\rangle = \tau_v\langle\xi_k\rangle$ of the random variable distributed according to the probability distribution $\tilde{\mathbb{P}}_k(x) = (1/\tau_v)\mathbb{P}_k(x/\tau_v)$ corresponding to the mean kinetic energy of the quantum harmonic oscillator is shown as the function of the parameter $\alpha = \tau_v/\tau_c$, where $\tau_v = M/\gamma_0$ is fixed, and different values of eigenfrequency $\tilde{\omega}_0 = \omega_0\tau_v$. Panel (b): the first statistical moment of the probability density $\tilde{\mathbb{P}}_p(x) = (1/\tau_v)\mathbb{P}_p(x/\tau_v)$ for the potential energy of the quantum harmonic oscillator. Solid lines correspond to the Drude (exponential) model and dashed lines to algebraic decay of $\gamma(t)$.

The case of zero temperature $T = 0$ is analysed in Fig. 28 where the impact of the memory time $\tau_c$ as well as the eigenfrequency $\tilde{\omega}_0$ is shown. Now additionally we compare the two mentioned mechanisms of dissipation. Panel (a) of this figure shows that when the memory time $\tau_c$ decreases (i.e. $\alpha$ increases) the kinetic energy monotonically increases. The opposite effect is for the potential energy: it slowly decreases as the memory time is shorter. One can note that kinetic energy for Drude model is greater than for the algebraic decay of $\gamma(t)$. For the potential energy it is opposite sequence: $E_p$ is greater for the algebraic decay of $\gamma$ than for the exponential one. Moreover, both the kinetic as well as potential energy grows as the eigenfrequency $\tilde{\omega}_0$ is increased. Finally, the influence of the coupling strength $\gamma_0$ should be pointed out (not shown in figures). It seems to be rather obvious that if the coupling is stronger then more channels are open to transmit energy from environment to the central system $S$ and therefore its energy is greater.

### 5.9.2 High temperature regime

As it was done in the previous chapter, one can investigate some special cases or interesting specific regimes. One of such a regime is the high temperature regime $T \to +\infty$ and the approximation

$$\coth\left(\frac{\hbar\omega}{2k_BT}\right) \approx \frac{2k_BT}{\hbar\omega} \tag{5.107}$$

can be utilized. Then

$$\begin{aligned} E_p = \langle \mathcal{E}_k \rangle &= \int_0^\infty d\omega \; \mathcal{E}_k(\omega)\mathbb{P}_p(\omega) = \int_0^\infty d\omega \; \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\mathbb{P}_p(\omega) \\ &\approx \frac{1}{2}k_BT\int_0^\infty d\omega \; \mathbb{P}_p(\omega) = \frac{1}{2}k_BT, \end{aligned} \tag{5.108}$$

$$\begin{aligned} E_k = \langle \mathcal{E}_k \rangle &= \int_0^\infty d\omega \; \mathcal{E}_k(\omega)\mathbb{P}_k(\omega) = \int_0^\infty d\omega \; \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_BT}\right)\mathbb{P}_k(\omega) \\ &\approx \frac{1}{2}k_BT\int_0^\infty d\omega \; \mathbb{P}_k(\omega) = \frac{1}{2}k_BT, \end{aligned} \tag{5.109}$$

This lead to classical relations for the harmonic oscillator.

### 5.9.3 Low temperature regime

For low temperature, $T \to 0$, the following approximation can be applied

$$\coth(x) = 1 + 2\,\frac{\mathrm{e}^{-2x}}{1-\mathrm{e}^{-2x}} \approx 1 + 2\mathrm{e}^{-2x}, \quad x = \frac{\hbar\omega}{2k_BT}. \tag{5.110}$$

We insert this expression into the formula for potential energy:

$$E_p = \int_0^{+\infty} d\omega \, \mathcal{E}_p(\omega)\mathbb{P}_p(\omega) \tag{5.111}$$

and kinetic energy:

$$E_k = \int_0^{+\infty} d\omega \, \mathcal{E}_k(\omega)\mathbb{P}_k(\omega) \tag{5.112}$$

We obtain:

$$E_p = E_p^{(0)} + E_p^{(1)}(T), \tag{5.113}$$

and:

$$E_k = E_k^{(0)} + E_k^{(1)}(T), \tag{5.114}$$

where

$$E_i^{(0)} = \frac{1}{4}\int_0^\infty d\omega\ \hbar\omega\,\mathbb{P}_i(\omega) \tag{5.115}$$

with $i = p$ for potential energy or $i = k$ for kinetic energy. It is average potential and kinetic energy for temperature $T = 0$, i.e. when the thermostat is in the vacuum state and

$$E_i^{(1)}(T) = \frac{1}{2}\int_0^\infty d\omega\ \hbar\omega\,\mathbb{P}_i(\omega)\exp\left[-\frac{\hbar\omega}{k_B T}\right] \tag{5.116}$$

is the first correction for small temperature $T > 0$.

# 6 Method via Callen-Wellton fluctuation-dissipation relations

Up to now, we have considered two physical systems: the free Brownian particle and oscillator. The natural question is whether the relation for energy partition is valid for arbitrary quantum systems. The answer is only partial. In this section, we show that a formal relation similar to that for two above mentioned examples can be obtained from the fluctuation-dissipation relation of the Callen-Welton type [44, 5, 6, 8]. We recall that in this theory the quantum system is characterized by the Hamiltonian $\tilde{H}$ and is in a thermal equilibrium state at temperature $T$ defined by the Gibbs canonical statistical operator $\rho \propto \exp[-\tilde{H}/k_BT]$. Next, the external force $F(t)$ is applied to the system which develops in time under the perturbed time-dependent Hamiltonian $H = \tilde{H} - F(t)Y$, where $Y$ is a hermitian operator. In the linear response approximation, one can calculate fluctuations of the operator $Y$. For a special choice of $Y$ one can get Eq. (4.19). One can exploit the results contained in the Zubarev book [7] [see Eq. (17.19g)] or the Landau-Lifshitz book [6] [see Eq. (124.10)]. We apply Eq. (17.19g), namely, the mean square deviation or variance of the operator $Y$ is given by the relation

$$\langle (Y - \langle Y \rangle)^2 \rangle = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \, \coth\left[\frac{\hbar\omega}{2k_BT}\right] \chi''(\omega) = \frac{\hbar}{\pi} \int_{0}^{\infty} d\omega \, \coth\left[\frac{\hbar\omega}{2k_BT}\right] \chi''(\omega), \quad (6.1)$$

where the odd function $\chi''(\omega)$ is the imaginary part of the generalized susceptibility,

$$\chi(\omega) = \chi'(\omega) + i\chi''(\omega). \quad (6.2)$$

The generalized susceptibility $\chi(\omega)$ is a Fourier transform

$$\chi(\omega) = \int_{-\infty}^{\infty} dt \, \mathrm{e}^{i\omega t} \, G_r(t) \quad (6.3)$$

of the response function $G_r(t)$ (sometimes unfortunately denoted as $\chi(t)$) which is in fact the retarded thermodynamic Green function [7]:

$$G_r(t-s) = \frac{i}{\hbar}\theta(t-s)\langle [Y(t), Y(s)] \rangle, \quad (6.4)$$

where $\theta(t)$ is the Heaviside step function and

$$Y(t) = \exp(i\tilde{H}t/\hbar) Y(0) \exp(-i\tilde{H}t/\hbar). \quad (6.5)$$

is the Heisenberg operator corresponding to $Y(0)$. The averaging is over the Gibbs canonical statistical operator $\rho \propto \exp[-\tilde{H}/k_B T]$.

Let $Y = p$ be a momentum operator of the Brownian particle and the Hamiltonian $\tilde{H}$ is given by Eq. (3.2). Then Eq. (6.1) takes the form

$$\langle p^2 \rangle = \frac{\hbar}{\pi} \int_0^\infty d\omega \, \coth\left[\frac{\hbar\omega}{2k_B T}\right] \chi''(\omega), \tag{6.6}$$

where now the response function reads

$$G_r(t) = \frac{i}{\hbar}\theta(t)\langle[p(t), p(0)]\rangle, \tag{6.7}$$

and the average momentum $\langle p \rangle = 0$ at the equilibrium state. If we compare Eqs. (6.6) and (4.19) then it follows that formally

$$\mathbb{P}(\omega) = \frac{2}{\pi M \omega}\, \chi''(\omega). \tag{6.8}$$

The question is whether this expression fulfils the property for the probability density. Its positivity follows from the spectral representation of $\chi''(\omega)$, see the equation just above Eq. (124.9) in the Landau-Lifshitz book [6]. The problem is to prove the normalization of (6.8):

$$\int_0^\infty \mathbb{P}(\omega) d\omega = \frac{1}{M}\, \frac{2}{\pi} \int_0^\infty \frac{\chi''(\omega)}{\omega} d\omega. \tag{6.9}$$

According to the Kramers-Kronig dispersion relation

$$\chi'(\omega) = \frac{2}{\pi}\, P \int_0^\infty \frac{u\chi''(u)}{u^2 - \omega^2} du, \tag{6.10}$$

the integral in (6.9) is related to the real part of the susceptibility, namely,

$$\chi'(0) = \frac{2}{\pi}\, P \int_0^\infty \frac{\chi''(u)}{u} du, \tag{6.11}$$

where $P$ denotes the principal value of the integral. Alternatively, we can apply Eq. (123.19) in the Landau-Lifshitz book [6] which reads

$$\chi(i\omega) = \frac{2}{\pi} \int_0^\infty \frac{u\chi''(u)}{\omega^2 + u^2} du. \tag{6.12}$$

For $\omega = 0$ it takes the form

$$\chi(0) = \frac{2}{\pi} \int_0^\infty \frac{\chi''(u)}{u} du. \tag{6.13}$$

On the other hand, from Eqs. (6.3) and (6.4) it follows that

$$\chi(0) = \int_{-\infty}^{\infty} G_r(t)dt = \frac{i}{\hbar} \int_0^{\infty} \langle [p(t), p(0)] \rangle dt. \tag{6.14}$$

We see that the problem of normalization of $\mathbb{P}(\omega)$ in Eq. (6.8) can be converted to the problem:

$$\chi(0) = M \quad ??? \tag{6.15}$$

For two cases considered in previous sections, it can be proved. Indeed, we know the form of the momentum operator at time $t$ [see Eqs. (4.9) or (5.15)], namely,

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

In literature, one can note confusion because $R(t)$ is also called the response function.

The commutator in (6.7) can be easily calculated yielding

$$G_r(t) = \theta(t) \int_0^t du\ R(t-u)\gamma(u) \tag{6.16}$$

The Fourier transform $\chi(\omega)$ in Eq. (6.3) is a Fourier transform of the convolution in Eq. (6.16) and as a result we obtain

$$\chi(\omega) = \hat{R}_L(-i\omega)\hat{\gamma}_L(-i\omega), \tag{6.17}$$

i.e., it is expressed by the Laplace transforms of the response function $R(t)$ and the dissipation function $\gamma(t)$. For the free Brownian particle it takes the form (see Eq. (4.11)),

$$\chi(\omega) = \frac{M\hat{\gamma}_L(-i\omega)}{-i\omega M + \hat{\gamma}_L(-i\omega)}$$

and it is seen that $\chi(0) = M$.

We can exploit representation (4.11) for $\hat{R}_L(z)$ and (4.28a) for $\hat{\gamma}_L(i\omega)$ to get another form of the generalized susceptibility,

$$\chi(\omega) = M\ \frac{A(\omega) + iB(\omega)}{-iM\omega + A(\omega) + iB(\omega)} \tag{6.18}$$

The imaginary part of it reads

$$\chi''(\omega) = \frac{M^2\omega A(\omega)}{A^2(\omega) + [B(\omega) - M\omega]^2} \tag{6.19}$$

and the relation (6.8) assumes the form

$$\mathbb{P}(\omega) = \frac{2M}{\pi} \, \frac{\omega A(\omega)}{A^2(\omega) + [B(\omega) - M\omega]^2} \tag{6.20}$$

which is the same as Eq. (4.29). It shows the equivalence of both approaches. We can quote the next example. In Ref. [3], the authors have obtained Eq. (4.14) therein:

$$E_k = \frac{\hbar}{2\pi} \int_0^\infty d\omega \, \coth\left[\frac{\hbar\omega}{2k_B T}\right] M\omega^2 \, \mathrm{Im}[\alpha(\omega + i0^+)]. \tag{6.21}$$

By comparing this equation with our formulas we see that $\mathbb{P}(\omega) = (2/\pi)M\omega \, \mathrm{Im}[\alpha(\omega + i0^+)]$, where $\alpha(\omega)$ is also called susceptibility.

Applying this fluctuation-dissipation relation (6.1) we see that Eq. (4.19) is valid for arbitrary systems in contact with bosonic thermostat. It means that Eq. (4.19) holds true for any potential $U(x)$ in the Hamiltonian (3.2). For this class of systems, the quantum partition of kinetic energy (4.19) is universal and the probability distribution is of the form (6.8), where the susceptibility $\chi(\omega)$ is the Fourier transform of the retarded thermodynamic Green functions.

**REMARKS**: If $\tilde{H} = H$ with the total Hamiltonian $H$ in Eq. (3.2) then all regimes, from weak to strong coupling with thermostat, can be analyzed. However, if $\tilde{H} = H_S = p^2/2M + U(x)$ (there is no interaction with thermostat) then it means that only the weak coupling limit can be considered because averaging is over the Gibbs canonical density operator $\rho \propto \exp(-H_S/k_B T)$ valid for the weak coupling limit.

The above mentioned formula (6.8) establishes the relation between the probability distribution $\mathbb{P}(\omega)$ and the generalized susceptibility $\chi''(\omega)$. It means that properties of the quantum environment and its coupling to a given quantum system which are characterized by $\mathbb{P}(\omega)$ may be experimentally inferred from the measurement of the linear response of the system to an applied perturbation, for instance, electrical or magnetic. Consequently, the latter quantity may open a new pathway to study quantum open systems

# 7 Summary and discussion

In this dissertation analysis of some aspects of energetics of quantum Brownian motion is presented. This is by no means a new problem - quite the contrary - this is a well-known problem and as such has been investigated for many decades by scientists and there are hundreds of papers devoted to this very issue. Nevertheless, this old problem has proven to be worthy of investigation. We have proposed a new relation for kinetic energy of quantum systems named as the *theorem on quantum partition of energy*. The main result summarized in this form has been studied and described in a series of our papers [19, 20, 21, 22]. The relation for kinetic energy can be interpreted as long-awaited quantum counterpart of the classical *energy equipartition theorem* introduced by the founders of classical statistical physics - John James Waterston, James Clerk Maxwell and Ludwig Boltzmann in XIX century.

In Chapter 2, I have presented n two different methods of derivation of energy equipartition theorem: firstly I consider the standard Gibbs canonical distribution approach and next I have shown how this theorem can emerge by means of the Langevin equation methods.

In Chapter 3, I formulate a problem of dissipative quantum systems in terms of a generalized Langevin equation. In this chapter, the reader can find the step-by-step derivation of formulas and partial analysis of this problem. In the following two chapters I consider two exactly solvable models of dissipative quantum systems - that is a free Brownian particle coupled to the quantum thermostat (Chapter 4) and the harmonic oscillator interacting with its environment (Chapter 5). For these two cases, I have rigorously formulated the energy partition theorem.

In Chapter 6, I discuss a partially solved problem of such a theorem for arbitrary quantum systems. This topic is presented in the context of the Callen-Welton fluctuation-dissipation theorem. The challenge is to obtain the value of the momentum-momentum susceptibility at zero frequency, cf. Eq. (6.14). It is the inverse problem to the sum rules for thermodynamic Green functions which give the value of the integral of the susceptibility (a Fourier transform of the Green function) over all frequencies.

Another open problem is to derive similar results for the case of fermionic or spin thermostats.

For the sake of self-containment, this work includes a set of various appendices in which I present formulas and more detailed analysis for some specific topics which were dealt with in this dissertation.

**Remark on the white noise limit**: We have considered such a class of memory kernels $\gamma(t-s)$ that it tends to the Dirac delta $\delta(t-s)$. Then the integro-differential Langevin equation (4.1) becomes local in time (as for classical Markovian processes). It is similar to a classical Newton equation with noise $\eta(t)$ . However, we should also consider the correlation function $C(t)$ of noise $\eta(t)$. If $\gamma(t) = \delta(t)$ then the spectral function $J(\omega) = const.$. From the fluctuation-dissipation relation it follows that when $J(\omega)$ is constant then

$$C(t) \propto \int_0^{+\infty} d\omega \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2k_B T}\right) \cos(\omega t) \tag{7.1}$$

We see that it does not tend to white noise as in the classical case. It is even worse: the integral diverges! We refer the interested reader to Ref. [45] for a more detailed analysis and to Ref. [4] for discussion on the ohmic dissipation and Markovian limit. Another aspect of the short memory time limit has been discussed for dynamics of solitons in superfluids [46]. This formal limit and the corresponding Markovian approximation gives rise to the Abraham-Lorentz force (i.e., a term proportional to the derivative of the soliton's acceleration) which results in breaking of causality. The next issue is related to averaged kinetic energy. From Fig. 8 we infer that kinetic energy tends to infinity when $\tau_c \to 0$. It is also physically incorrect. The above non-physical effects lead to the conclusion that the limiting case of vanishing memory time is not allowable for quantum systems. In other words, quantum noise is always correlated.

**Interpretation revisited**: Finally, I have to explain and discuss in detail the interpretation of the basic relation for the partition of energy. Let us remind that we assume the factorized initial state of the composite system, i.e.,

$$\rho(0) = \rho_S \otimes \rho_E, \tag{7.2}$$

where $\rho_S$ is an arbitrary state of the Brownian particle and $\rho_E$ is the equilibrium canonical state of the thermostat of temperature $T$, namely,

$$\rho_E = \exp(-H_E/k_BT)/\mathrm{Tr}[\exp(-H_E/k_BT)], \tag{7.3}$$

where:

$$H_E = \sum_i \left[\frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_i^2 q_i^2\right] \tag{7.4}$$

is the Hamiltonian of the thermostat. The factorization means that there are no initial correlations between the particle and thermostat. In the gedankenexperiment we can assume the following situation: there is thermostat which is in the Gibbs state (7.3) for $(-\infty, 0)$. At some moment, say $t = 0$, we throw the Brownian particle into thermostat. Then we can realize the factorization state. At equilibrium determined by Eq. (7.3), the expression

$$\mathcal{E}_k(\omega) = \frac{\hbar\omega}{4}\coth\left(\frac{\hbar\omega}{2k_BT}\right) \tag{7.5}$$

is thermal kinetic energy per one degree of freedom of the thermostat consisting of free harmonic oscillators. It is true for time $t \le 0$. For time $t > 0$, the statistical operator $\rho(t)$ of the composite system S+E evolves according to the von Neumann equation, i.e.,

$$\rho(t) = \mathrm{e}^{-iHt/\hbar}\left[\rho_S \otimes \rho_E\right]\mathrm{e}^{iHt/\hbar} \tag{7.6}$$

The stationary state (which is a new thermodynamic equilibrium state) is determined as

$$\rho(\infty) = \lim_{t\to\infty} \mathrm{e}^{-iHt/\hbar}\left[\rho_S \otimes \rho_E\right]\mathrm{e}^{iHt/\hbar} \tag{7.7}$$

In the relation

$$E_k = \int_0^\infty d\omega\; \mathcal{E}_k(\omega)\mathbb{P}(\omega). \tag{7.8}$$

the term

$$\mathcal{E}_k(\omega_l) = \mathrm{Tr}\left\{\frac{p_l^2}{2m_l}\rho_E\right\} \tag{7.9}$$

is the value for $t \le 0$ while the term $\mathbb{P}(\omega)$ is an exact probability density for $t \to \infty$ (conventionally we write $t = \infty$). We could say that the system at $t = \infty$ remembers its initial state via $\mathcal{E}_k(\omega)$ valid for $t \in (-\infty, 0]$. So, the averaging in Eq. (7.8) is averaging of the random variable at $t = 0$ over the probability density at $t = \infty$. The averaged value of kinetic energy $\mathcal{E}_{st}(\omega)$ of the thermostat oscillator in the stationary state for $t = \infty$, i.e.,

$$\mathcal{E}_{st}(\omega_l) = \mathrm{Tr}\left\{ \frac{p_l^2}{2m_l}\, \rho(\infty) \right\} \tag{7.10}$$

is different from $\mathcal{E}_k(\omega)$ at $t = 0$, i.e., $\mathcal{E}_{st}(\omega_l) \neq \mathcal{E}_k(\omega_l)$. To the best of my knowledge, $\mathcal{E}_{st}(\omega)$ is not known (although in principle it could be calculated). We suppose and expect that the difference between $\mathcal{E}_k(\omega)$ and $\mathcal{E}_{st}(\omega)$ should be extremely small in the thermodynamic limit for thermostat but nevertheless, it is not zero. So, we treat it as an open and unsolved problem.

# Appendix A Mean values of boson operators

To investigate properties of quantum thermal noise it is convenient to work in the second quantization framework and rewrite operators $q_k$ and $p_k$ in terms of creation and annihilation operators. Thermostat consists of non-interacting quantum harmonic oscillators which can be described by creation and annihilation bosonic operators:

$$q_k = \sqrt{\frac{\hbar}{2m_k\omega_k}}\left(a_k + a_k^\dagger\right) \tag{A.1}$$

$$p_k = \frac{1}{\mathrm{i}}\sqrt{\frac{m_k\omega_k\hbar}{2}}\left(a_k + a_k^\dagger\right) \tag{A.2}$$

The Hamiltonian of thermostat in this notation reads:

$$H = \sum_k \hbar\omega_k\left(n_k + \frac{1}{2}\right) \tag{A.3}$$

where:

$$n_k = a_k^\dagger a_k \tag{A.4}$$

The commutation relations for creation and annihilation operators are :

$$\begin{aligned} [a_k; a_k] &= \left[a_k^\dagger; a_k^\dagger\right] = 0 \\ \left[a_k; a_j^\dagger\right] &= \delta_{kj} \end{aligned} \tag{A.5}$$

We need mean values of operators:

$$\langle q_k\rangle = \sqrt{\frac{\hbar}{2m_k\omega_k}}\left(\langle a_k\rangle + \left\langle a_k^\dagger\right\rangle\right) = 0 \tag{A.6}$$

$$\langle p_k\rangle = \frac{1}{\mathrm{i}}\sqrt{\frac{m_k\omega_k\hbar}{2}}\left(\langle a_k\rangle + \left\langle a_k^\dagger\right\rangle\right) = 0 \tag{A.7}$$

$$\langle q_k q_j\rangle = \frac{\hbar}{2\sqrt{m_k\omega_k m_j\omega_j}}\left(\langle a_k a_j\rangle + \left\langle a_k^\dagger a_j\right\rangle + \left\langle a_k a_j^\dagger\right\rangle + \left\langle a_k^\dagger a_j^\dagger\right\rangle\right) \tag{A.8}$$

$$\langle p_k p_j\rangle = -\frac{\hbar\sqrt{m_k\omega_k m_j\omega_j}}{2}\left(\langle a_k a_j\rangle - \left\langle a_k^\dagger a_j\right\rangle - \left\langle a_k a_j^\dagger\right\rangle + \left\langle a_k^\dagger a_j^\dagger\right\rangle\right) \tag{A.9}$$

$$\langle q_k p_j\rangle = \frac{\hbar}{2\mathrm{i}}\sqrt{\frac{m_k\omega_k}{m_j\omega_j}}\left(\langle a_k a_j\rangle + \left\langle a_k^\dagger a_j\right\rangle - \left\langle a_k a_j^\dagger\right\rangle - \left\langle a_k^\dagger a_j^\dagger\right\rangle\right) \tag{A.10}$$

$$\langle p_k q_j\rangle = \frac{\hbar}{2\mathrm{i}}\sqrt{\frac{m_j\omega_j}{m_k\omega_k}}\left(\langle a_k a_j\rangle - \left\langle a_k^\dagger a_j\right\rangle + \left\langle a_k a_j^\dagger\right\rangle - \left\langle a_k^\dagger a_j^\dagger\right\rangle\right) \tag{A.11}$$

Using commutation relations (A.5) we get:

$$\langle a_k a_j \rangle = \left\langle a_k^\dagger a_j^\dagger \right\rangle = 0 \tag{A.12}$$

$$\left\langle a_k a_j^\dagger \right\rangle = n_k \delta_{jk} \tag{A.13}$$

where

$$\bar{n_i} = \langle n_i \rangle = \left\langle a_i^\dagger a_i \right\rangle = \frac{1}{e^{\frac{\hbar\omega_k}{kT}} - 1} \tag{A.14}$$

and

$$\langle q_k q_j \rangle = \frac{\hbar}{\sqrt{m_k \omega_k m_j \omega_j}} \delta_{kj} \coth\left(\frac{\hbar\omega_k}{2kT}\right) \tag{A.15}$$

$$\langle p_k p_j \rangle = \hbar \sqrt{m_k \omega_k m_j \omega_j} \delta_{kj} \coth\left(\frac{\hbar\omega_k}{2kT}\right) \tag{A.16}$$

$$\langle q_k p_j \rangle = -\frac{\hbar}{2\mathrm{i}} \sqrt{\frac{m_k \omega_k}{m_j \omega_j}} \delta_{kj} \tag{A.17}$$

$$\langle p_k q_j \rangle = \frac{\hbar}{2\mathrm{i}} \sqrt{\frac{m_j \omega_j}{m_k \omega_k}} \delta_{kj} \tag{A.18}$$

# Appendix B Properties of response functions

Response functions are defined by theirs Laplace transforms:

$$\mathcal{L}\left\{Q(t)\right\}(z) = \hat{Q}_L(z) = \frac{1}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} \tag{B.1}$$

$$\mathcal{L}\left\{R(t)\right\}(z) = \hat{R}_L(z) = \frac{zM}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2}, \tag{B.2}$$

where to obtain proper definitions for the case of free Brownian particle it is sufficient to substitute $\omega_0$ with 0.

I would seem that for this kind of general and implicit definition for the response functions, there is not much information that can be learned for properties of the functions themselves. Nonetheless using the theorems from the integral transforms theory we can gain some understanding concerning the initial and final behavior.

For the sake of later reasoning it is useful to recall the Tauberian theorems[36]:

**Theorem 3** (Initial value theorem)**.**
*If* $\mathcal{L}\left\{f(t)\right\}(z) = \hat{f}_L(z)$ *exists, then:*

$$\lim_{z\to+\infty} \hat{f}_L(z) = 0 \tag{B.3}$$

*Moreover if* $f(t)$ *and its derivatives exist as* $t \to 0$*, we obtain* The Initial Value Theorem*:*

1. $$\lim_{z\to+\infty} z\hat{f}_L(z) = \lim_{t\to 0} f(t) = f(0) \tag{B.4}$$

2. $$\lim_{z\to+\infty} \left[z^2\hat{f}_L(z) - zf(0)\right] = \lim_{t\to 0} f'(t) = f'(0) \tag{B.5}$$

3. $$\lim_{z\to+\infty} \left[z^{n+1}\hat{f}_L(z) - z^n\hat{f}_L(z) - \ldots - zf(0)\right] = f^{(n)}(0) \tag{B.6}$$

**Theorem 4** (The Final Value Theorem)**.**
*If* $\hat{f}_L(z) = \frac{\hat{p}_L(z)}{\hat{q}_L(z)}$*, where* $\hat{p}_L(z)$ *and* $\hat{q}_L(z)$ *are polynomials in* $z$*, and the degree of* $\hat{p}_L(z)$ *is less than that of* $\hat{q}_L(z)$*, and all roots of* $\hat{q}_L(z)$ *have negative real parts with the possible of one root at* $z = 0$*, then:*

*1.*

$$\lim_{z\to 0}\hat{f}_L(z) = \int_0^{+\infty} f(t)dt, \tag{B.7}$$

*2.*

$$\lim_{z\to 0} z\hat{f}_L(z) = \lim_{t\to +\infty} f(t) \tag{B.8}$$

Using theorem 3 we can deduce the initial value of responses functions.

$$Q(0) = \lim_{z\to +\infty} z\hat{Q}_L(z) = \lim_{z\to +\infty} \frac{z}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} = 0 \tag{B.9}$$

$$R(0) = \lim_{z\to +\infty} z\hat{R}_L(z) = \lim_{z\to +\infty} \frac{Mz^2}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} = 1 \tag{B.10}$$

using the theorem 4 we can deduce value of integrals of response functions as well as their behavior at the infinity:

$$\int_0^{+\infty} Q(t)dt = \lim_{z\to 0} \frac{1}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} = \frac{1}{M\omega_0^2} \tag{B.11}$$

$$\lim_{t\to +\infty} Q(t) = \lim_{z\to 0} \frac{z}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} = 0 \tag{B.12}$$

$$\lim_{t\to +\infty} R(t) = \lim_{z\to 0} \frac{Mz^2}{Mz^2 + z\hat{\gamma}_L(z) + M\omega_0^2} = 0 \tag{B.13}$$

# Appendix C Putzer algorithm

In the relation (4.101), the exponential of the matrix $\mathbf{A}t$ is needed. We calculate it applying the Putzer method [42]. The exponential can be presented in the form

$$\mathrm{e}^{\mathbf{A}t} = \mathbf{R}(t) = r_1(t)I + r_2(t)P_1 + r_3(t)P_2, \tag{C.1}$$

where $I$ is the identity matrix, the matrices $P_1$ and $P_2$ are determined by the relations

$$P_1 = \mathbf{A} - \lambda_1 I, \quad P_2 = (\mathbf{A} - \lambda_2 I)\, P_1 \tag{C.2}$$

and $\lambda_j$ $(j = 1, 2, 3)$ are the eigenvalues (in any order and not necessarily distinct) of the matrix $\mathbf{A}$. The functions $r_j(t)$ takes the form

$$r_1(t) = \mathrm{e}^{\lambda_1 t}, \tag{C.3}$$

$$r_2(t) = \mathrm{e}^{\lambda_2 t} \int_0^t \mathrm{e}^{-\lambda_2 u}\, r_1(u)\, du = \frac{e^{\lambda_1 t} - e^{\lambda_2 t}}{\lambda_1 - \lambda_2}, \tag{C.4}$$

$$r_3(t) = \mathrm{e}^{\lambda_3 t} \int_0^t \mathrm{e}^{-\lambda_3 u}\, r_2(u)\, du = \frac{1}{\lambda_1 - \lambda_2} \left[ \frac{e^{\lambda_1 t} - e^{\lambda_3 t}}{\lambda_1 - \lambda_3} - \frac{e^{\lambda_2 t} - e^{\lambda_3 t}}{\lambda_2 - \lambda_3} \right]. \tag{C.5}$$

The eigenvalues $\lambda_j$ are the roots of the characteristic polynomial $|\mathbf{A} - \lambda I| = 0$ which explicitly reads

$$\lambda^3 + 2\varepsilon\lambda^2 + (\mu + \varepsilon^2 + \Omega^2)\lambda + \varepsilon\mu = 0. \tag{C.6}$$

All eigenvalues have negative real parts, i.e., $\mathrm{Re}\,\lambda_j < 0$. The necessary and sufficient conditions for this to hold are the Routh-Hurwitz conditions which for the cubic equation

$$\lambda^3 + a_2\lambda^2 + a_1\lambda + a_0 = 0 \tag{C.7}$$

take the form

$$a_2 = 2\varepsilon > 0, \quad a_0 = \varepsilon\mu > 0, \quad a_2 a_1 - a_0 = 2\varepsilon(\varepsilon^2 + \Omega^2) + \varepsilon\mu > 0. \tag{C.8}$$

In consequence, all functions $r_j(t)$ are decreasing functions of time.

The explicit forms of the matrices in (C.1) read

$$P_1 = -\begin{bmatrix} \lambda_1 & 1 & 0 \\ -\mu & \lambda_1+\varepsilon & \Omega \\ 0 & -\Omega & \lambda_1+\varepsilon \end{bmatrix}, \tag{C.9}$$

$$P_2 = \begin{bmatrix} \lambda_1\lambda_2-\mu & \lambda_1+\lambda_2+\varepsilon & \Omega \\ -\mu\left(\lambda_1+\lambda_2+\varepsilon\right) & \left(\lambda_1+\varepsilon\right)\left(\lambda_2+\varepsilon\right)-\mu-\Omega^2 & \Omega\left(\lambda_1+\lambda_2+2\varepsilon\right) \\ \mu\Omega & -\Omega\left(\lambda_1+\lambda_2+2\varepsilon\right) & \left(\lambda_1+\varepsilon\right)\left(\lambda_2+\varepsilon\right)-\Omega^2 \end{bmatrix}. \tag{C.10}$$

What we need in Eq. (4.17) is the first element $R_{11}(t)$ of the matrix $R(t)$. We exploit the above formula (C.1)-(C.10) and get

$$R_{11}(t) = \left(\lambda_2\lambda_3-\mu\right) b_1 e^{\lambda_1 t} - \left(\lambda_1\lambda_3-\mu\right) b_2 e^{\lambda_2 t} + \left(\lambda_1\lambda_2-\mu\right)\, b_3 e^{\lambda_3 t}, \tag{C.11}$$

where

$$b_1 = \frac{1}{{\lambda_1}^2-\lambda_1\lambda_2-(\lambda_1-\lambda_2)\lambda_3}, \tag{C.12}$$

$$b_2 = -\frac{1}{\lambda_1\lambda_2-{\lambda_2}^2-(\lambda_1-\lambda_2)\lambda_3}, \tag{C.13}$$

$$b_3 = \frac{1}{\lambda_1\lambda_2-(\lambda_1+\lambda_2)\lambda_3+{\lambda_3}^2}. \tag{C.14}$$

# Appendix D Calculation of $I^1(\omega)$

In this Appendix, we calculate the function $I^1(\omega)$ defined by Equation (4.106). The integrand $R_{11}(t)$ is the sum of exponential functions (C.11) and the double integral in (4.106) can easily be calculated. The result reads:

$$\begin{aligned}
I^1(\omega) = {} & \frac{(\lambda_2\lambda_3-\mu)^2 b_1^2}{{\lambda_1}^2+\omega^2} + \frac{(\lambda_1\lambda_3-\mu)^2 b_2^2}{{\lambda_2}^2+\omega^2} + \frac{(\lambda_1\lambda_2-\mu)^2 b_3^2}{{\lambda_3}^2+\omega^2} \\
& - \frac{2\,(\lambda_1\lambda_2+\omega^2)(\lambda_1\lambda_3-\mu)(\lambda_2\lambda_3-\mu)b_1b_2}{{\lambda_1}^2{\lambda_2}^2+\omega^4+\left({\lambda_1}^2+{\lambda_2}^2\right)\omega^2} \\
& + \frac{2\,(\lambda_1\lambda_2-\mu)(\lambda_1\lambda_3+\omega^2)(\lambda_2\lambda_3-\mu)b_1b_3}{{\lambda_1}^2{\lambda_3}^2+\omega^4+\left({\lambda_1}^2+{\lambda_3}^2\right)\omega^2} \\
& - \frac{2\,(\lambda_1\lambda_2-\mu)(\lambda_1\lambda_3-\mu)(\lambda_2\lambda_3+\omega^2)b_2b_3}{{\lambda_2}^2{\lambda_3}^2+\omega^4+\left({\lambda_2}^2+{\lambda_3}^2\right)\omega^2}
\end{aligned} \tag{D.1}$$

Inserting the coefficients $b_j\,(j=1,2,3)$ from Equations (C.12) - (C.14) and using the Vieta's formulas for the roots of the polynomial (C.6), we obtain the final expression

$$I^1(\omega) = \frac{\left[(\omega+\Omega)^2+\varepsilon^2\right]\left[(\omega-\Omega)^2+\varepsilon^2\right]}{\omega^6+2\omega^4\left(\varepsilon^2-\Omega^2-\mu\right)+\omega^2\left(\mu^2+2\mu\Omega^2-2\mu\varepsilon^2+\Omega^4+2\Omega^2\varepsilon^2+\varepsilon^4\right)+\mu^2\varepsilon^2} \tag{D.2}$$

This function occurs in Equation (4.105) for average kinetic energy.

# Appendix E Series expansion for kinetic energy

We will present Eq. (4.19) in the form of a series. To this aim, we introduce the dimensionless integration variable $\theta$ and dimensionless parameters,

$$\theta = \tau_T \omega, \quad \tau_T = \frac{\hbar}{k_B T} \tag{E.1}$$

$$\hat{\mu}_0 = \tau_T \mu_0, \quad \hat{\varepsilon} = \tau_T \varepsilon, \quad \hat{\Omega} = \tau_T \Omega \tag{E.2}$$

Next, we exploit the series expansion [36]

$$\theta \coth\left(\frac{\theta}{2}\right) = 2 + 4 \sum_{n=1}^{\infty} \frac{\theta^2}{\theta^2 + 4\pi^2 n^2} \tag{E.3}$$

Using the above expansion we obtain the integrand of (4.19) in the form of uniformly convergent series. Therefore we can utilise the Weierstrass theorem [47] and integrate term by term as follows

$$\frac{2E_k}{kT} = I_0 + \sum_{n=1}^{\infty} I_n \tag{E.4}$$

$$I_0 = \frac{2}{\pi} \int_0^{\infty} \frac{\hat{\mu}_0 \hat{\varepsilon}^2 \left(\theta^2 + \hat{\Omega}^2 + \hat{\varepsilon}^2\right)}{\theta^6 - 2\theta^4 \left(\hat{\Omega}^2 + \hat{\mu}_0 \hat{\varepsilon} - \hat{\varepsilon}^2\right) + \theta^2 \left(\hat{\Omega}^4 + 2\hat{\Omega}^2 \hat{\mu}_0 \hat{\varepsilon} + 2\hat{\Omega}^2 \hat{\varepsilon}^2 + \hat{\mu}_0^2 \hat{\varepsilon}^2 - 2\hat{\mu}_0 \hat{\varepsilon}^3 + \hat{\varepsilon}^4\right) + \hat{\mu}_0^2 \hat{\varepsilon}^4} d\theta \tag{E.5}$$

$$I_n = \frac{1}{\pi} \int_0^{\infty} \frac{\hat{\mu}_0 \hat{\varepsilon}^2 \left(\theta^2 + \hat{\Omega}^2 + \hat{\varepsilon}^2\right)}{\theta^6 - 2\theta^4 \left(\hat{\Omega}^2 + \hat{\mu}_0 \hat{\varepsilon} - \hat{\varepsilon}^2\right) + \theta^2 \left(\hat{\Omega}^4 + 2\hat{\Omega}^2 \hat{\mu}_0 \hat{\varepsilon} + 2\hat{\Omega}^2 \hat{\varepsilon}^2 + \hat{\mu}_0^2 \hat{\varepsilon}^2 - 2\hat{\mu}_0 \hat{\varepsilon}^3 + \hat{\varepsilon}^4\right) + \hat{\mu}_0^2 \hat{\varepsilon}^4} \frac{4\theta^2}{4\pi^2 k^2 + \theta^2} d\theta \tag{E.6}$$

For all cases the integrands are rational functions. The polynomial degrees of denominators are higher by 4 than a degree of polynomials in numerators and therefore all integrals exist. We can use an elegant method of the residue theorem to calculate the integrals [48]. Manual calculations are long and tedious, but nowadays this problem can be overcome by using any computer algebra system. We used SymPy (the Python library) for symbolic mathematics.

The zero-th term is the same as (4.21) and therefore $I_0 = 1$. For remaining terms we obtain the expression for $I_n$ in the following form

$$I_n = \frac{2\hat{\mu}_0 \hat{\varepsilon} \left(\hat{\varepsilon} + 2\pi n\right)}{\hat{\mu}_0 \hat{\varepsilon} \left(\hat{\varepsilon} + 2\pi n\right) + 2\pi n \left(\hat{\varepsilon} + 2\pi n\right)^2 + 2\pi \hat{\Omega}^2 n}. \tag{E.7}$$

Finally,

$$\frac{2E_k}{k_B T} = 1 + \sum_{n=1}^{\infty} \frac{2\hat{\mu}_0 \hat{\varepsilon} \left(\hat{\varepsilon} + 2\pi n\right)}{\hat{\mu}_0 \hat{\varepsilon} \left(\hat{\varepsilon} + 2\pi n\right) + 2\pi n \left(\hat{\varepsilon} + 2\pi n\right)^2 + 2\pi \hat{\Omega}^2 n}. \tag{E.8}$$

Using this method we obtain a form which is more convenient for discussion on general properties of kinetic energy with respect to system parameters.

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