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Statistical thermodynamics of quantum Brownian motion: Construction of perpetuum mobile of the second kind

Th. M. Nieuwenhuizen[1] and A. E. Allahverdyan[2,1,3]

[1]*Institute for Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands*

[2]*Service de Physique Théorique, CEA Saclay, 91191 Gif-sur-Yvette Cedex, France*

[3]*Yerevan Physics Institute, Alikhanian Brothers Street 2, Yerevan 375036, Armenia*

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The Brownian motion of a quantum particle in a harmonic confining potential and coupled to harmonic quantum thermal bath is exactly solvable. Though this system presents at high temperatures a pedagogic example to explain the laws of thermodynamics, it is shown that at low enough temperatures the stationary state is non-Gibbsian due to an entanglement with the bath. In physical terms, this happens when the cloud of bath modes around the particle starts to play a nontrivial role, namely, when the bath temperature T is smaller than the coupling energy. Indeed, equilibrium thermodynamics of the total system, particle plus bath, does not imply standard equilibrium thermodynamics for the particle itself at low T. Various formulations of the second law are found to be invalid at low T. First, the Clausius inequality can be violated, because heat can be extracted from the zero point energy of the cloud of bath modes. Second, when the width of the confining potential is suddenly changed, there occurs a relaxation to equilibrium during which the entropy production is partly negative. In this process the energy put on the particle does not relax monotonically, but oscillates between particle and bath, even in the limit of strong damping. Third, for nonadiabatic changes of system parameters the rate of energy dissipation can be negative, and, out of equilibrium, cyclic processes are possible which extract work from the bath. Conditions are put forward under which perpetuum mobility of the second kind, having one or several work extraction cycles, enter the realm of condensed matter physics. Fourth, it follows that the equivalence between different formulations of the second law (e.g., those by Clausius and Thomson) can be violated at low temperatures. These effects are the consequence of quantum entanglement in the presence of the slightly off-equilibrium nature of the thermal bath, and become important when the characteristic quantum time scale $\hbar/k_BT$ is larger than or comparable to other time scales of the system. They show that there is no general consensus between standard thermodynamics and quantum mechanics. The known agreements occur only due to the weak coupling limit, which does not pertain to low temperatures. Experimental setups for testing the effects are discussed.

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I. INTRODUCTION

Faith in the laws of thermodynamics has been strengthened time and again because numerous counterarguments and perpetuum mobile setups failed. It was summarized in the classical statement of Eddington in 1948 [1]: ‘‘The law that entropy always increases—the second law of thermodynamics—holds, I think, the supreme position among the laws of Nature. If someone points out to you that your pet theory of the universe is in disagreement with Maxwell's equations—then so much the worse for Maxwell's equations. If it is found to be contradicted by observation, well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but collapse in deepest humiliation.'' Nevertheless, we intend to show in this paper that there are *several formulations of the second law that may not apply to systems coupled to a bath in the quantum regime*. This paves the way for a different, modest definition of the most despised objects of modern physics, *perpetuum mobile of the second kind*. We shall propose realizations wherein they can make a few or even many cycles, though not infinitely many. A short version of the material appeared already [2], which was discussed in the scientific literature [3,4].

The laws of equilibrium thermodynamics apply both to (quasi)closed quantum and classical systems, and to open classical subsystems [5]. This can all be traced back to the general character of the Gibbs distribution that describes the equilibrium state. The same laws are *believed* to apply as well to open quantum subsystems. Our aim will be to show that, though this belief is proper for weak coupling, it is not justified for nonweak coupling between system and bath. Nonweak coupling means, physically, that a cloud of bath modes has been formed around the particle, which we shall still consider as a part of the bath. Although one could defend the opinion that—as an example—for Kondo-type problems there is no need or no sense to describe the impurity spin (‘‘the subsystem'') separately from the Kondo cloud of conduction electrons (‘‘the bath''), such a viewpoint is not obvious for an array of mesoscopic Josephson junctions, where the ‘‘bath'' is the electromagnetic field, to which they may be strongly coupled. Since that regime shows up in many systems at low enough temperature even for a small but fixed coupling, there is an important case to make.

When deriving the Gibbs distribution for a (quasi)closed system [5,6], the underlying statistical assumptions do not depend much on the quantum or classical nature. An open subsystem is usually considered as being in contact with an initially equilibrium bath. Under some general statistical

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conditions concerning the bath [6–10], which are again the same for the quantum and classical cases, one derives a Langevin equation. The general behavior of the classical Langevin equation is well known [6]. The stationary distribution is Gibbsian, and, at least for the white noise case, the equivalent Fokker-Planck equation is the main tool to describe the nonequilibrium statistical theory [11].

Much less is known about the quantum Langevin equation [6,7,9,10,12–14], first proposed by Senitzky [15] in the weakly damped (weakly coupled) case, and in a more general form by Ford, Kac, and Mazur [8], see also Ref. [16]. Its stationary distribution has been obtained for the harmonic potential, in which case it depends explicitly on the coupling constant, becoming Gibbsian only in the limit of weak coupling [10,14,17].

Let us recall that the situation where a particle is interacting with an equilibrium bath is known as Brownian motion, and the particle as well is referred to as a Brownian particle. As one of the paradigms of nonequilibrium statistical mechanics, the theory of Brownian motion has numerous applications in condensed matter physics [6,9,11,13,18,19], atomic physics [6,20], quantum optics, and chemistry [10,21]. It is believed that some of those practical realizations can be considered as being weakly coupled with their thermal baths, and then standard methods of statistical physics can be applied [10,22]. However, there are nowadays well-known experimental situations, which are essentially far from the weak-coupling regime. The main example of this is the case of weak links between superconductive regions, the so-called Josephson junctions, in their overdamped regime [18,19], where the relevant ranges of parameters were achieved already 20 years ago. Even in quantum optics, which has often been satisfactorily described by weak-coupling theories [10], there are recent experiments showing the necessity for moderate and strong coupling approaches (see, e.g., Ref. [23]). In nuclear magnetic resonance experiments, on the other hand, very weak coupling occurs, but it leads to a T_2 relaxation time of transverse (nonclassical) correlations, which can reach up to minutes. During that time, related nonthermodynamic effects can occur.

The cause of the crucial differences between quantum and classical Brownian motion lies in quantum entanglement. A complete description in terms of a wave function is possible only for a closed system; subsystems are necessarily in a mixed state. Since the quantum Gibbs distribution tends to the pure vacuum state for $T\to 0$, it is in that limit not an adequate candidate for the description of the quantum subsystem nonweakly interacting with its thermal bath. Where, typically, researchers have just guessed that thermodynamics would apply anyhow, we shall provide the opposite answer by analyzing exactly solvable models.

Another important property is embodied in the structure of the quantum Langevin equation [17]. As predicted by the quantum fluctuation-dissipation theorem, but in contrast to the classical case, the time-scales of fluctuations and dissipation are different, and even in the limit of instantaneous friction, the noise does not become white, but has the characteristic quantum time scale $\hbar/k_B T$. During this period the noise has a memory and thus has the possibility to cause nonstatistical but "mechanical" or "quenched," in any case nonthermodynamic, behavior of the system on which it acts [5,7]. The physical meaning of the classical fluctuation-dissipation theorem thus is stronger, since it insists on equal time scales of friction and noise, which induces the standard thermodynamic behavior.

The new properties become noneffective if the interaction with the thermal bath is weak or if temperature is high, in which case the subsystem relaxes to its own quantum or classical Gibbs distribution. Both these cases will be referred to as the Gibbsian limit. We recall that its existence is typically not connected with very low temperatures, since even for a small but generic coupling between the system and the thermal bath, one always goes out of the weak coupling limit by taking the temperature low enough.

It is a crucial fact that a non-Gibbsian stationary state implies the inadequacy of equilibrium thermodynamics. In the present paper we propose a generalized thermodynamical description of a quantum Brownian particle in a harmonic confining potential. This description is self-consistent, and does not use *a priori* the concepts of the equilibrium (Gibbsian) statistical thermodynamics. Instead we employ the methods of nonequilibrium statistical thermodynamics developed recently for glasses and applied to black holes, where a separation of time scales allows for a two-temperature approach [24–27].

The universal character of equilibrium thermodynamics led to the general expectation that in one way or the other, thermodynamics will be applicable to the full quantum domain. A somewhat stronger point was expressed by Landau and Lifshitz [5], namely, that the proper formulation of equilibrium thermodynamics must be based on quantum mechanics. For the strongly coupling quantum situation one might, however, not be convinced. Let us give three principal arguments that question common wisdom.

(1) The bath modes are correlated during the quantum time scale $\hbar/T$, even when damping is instantaneous. When this time scale is larger than the (largest) relaxation time of the system, the bath acts more like a quenched disorder than as a white noise. Thus the standard condition for going from a Langevin equation to a Gibbs distribution is not fulfilled and new behavior should be expected.

(2) Assume that the overall system (the Brownian particle plus the bath) is in equilibrium at a low temperature. One of the many formulations of the second law states that no heat can be extracted from the bath. This just follows from the Clausius inequality: $đ\mathcal{Q}\leqslant TdS$ (here $đ\mathcal{Q}$ is the heat flowing from the bath to the subsystem, the Brownian particle, while S is the entropy of the subsystem) for $T\to 0$. A naive argument in support of this statement will be that the bath is close to its ground state, and therefore its energy cannot be lowered. However, this argument is invalidated by quantum entanglement: Since the bath is not an isolated system itself, it cannot be in a definite energy eigenstate. In particular, it cannot be in the ground state, and its energy fluctuates even for $T\to 0$.

(3) If a closed quantum system is its ground state, the only change can be to do work on it. Now suppose that this system consists of a subsystem coupled to a bath, and that

the external coupling connects to the subsystem, and not to the bath. Then typically the action of doing work will reshuffle also the separate energies of the subsystem and the bath. As the direction of the exchange depends on the question whether externally work was added or subtracted, in one of the cases the subsystem receives energy from the bath. Since this comes from the unobserved bath modes, it cannot be identified as work, and must be identified as heat extracted from the bath, even at $T=0$.

Because these arguments question common wisdom, the only way to investigate the practical situation is to start from first principles, namely, from standard quantum mechanics. This is the general strategy of the present paper.

Statements on violations of certain formulations of the second law in the quantum microworld already appeared in literature. Capek and his co-workers [28] noticed such effects in certain biophysically inspired models; Novotny recently pointed out that in a related model the violations cannot pertain to the long time limit [29]. Nikulov [30] reported on violations of the second law in mesoscopic superconductivity; the latter author bases his view on results for permanent currents in inhomogeneous superconducting rings [31]. Older works on violations in plasmas are due to Sheehan [32].

Since the subject of violating the second law and introducing perpetuum mobile has such a notorious history, new works in this field should be as convincing as possible. Therefore we present now a somewhat extensive, but self-contained exact analysis that leads to our conclusions, partly already presented in Ref. [2]. Our methods are exact since the case of a quantum particle in a harmonic confining potential and coupled to a bath of harmonic oscillators with bilinear couplings is exactly solvable. Notice that in a previous work [2] we also entered the discussion of the approximate solution for a weakly anharmonic force; this will not be touched here.

Our paper is organized as follows. In Sec. II we recall the derivation of the quantum Langevin equation. In Sec. III we solve the statics of the total system (subsystem plus bath) by elementary techniques. In Sec. IV we show that the thermodynamics of adiabatic changes can be described through two effective temperatures, and that analogies with the usual two-temperature thermodynamics can be stated much further: The generalized relations will have the effective form of the first and second law. Next we first present details on the violation of the Clausius inequality. In Sec. V we consider the dynamics of the system for the case where the initial state is Gibbsian, and for which the spring constant is slightly modified at time zero. In Sec. VI we use those results to derive the energy relaxation and the entropy production. In Sec. VII we consider work done on the system for that situation of an instantaneously changed spring constant, and we also consider work for smooth, cyclic changes. In Sec. VIII we mention a number of experiments where our results have applications. In Sec. IX we view those results from the foundations of thermodynamics and the definition of perpetuum mobile. Finally in Sec. X we close the paper with a discussion.

II. THE QUANTUM LANGEVIN EQUATION

It is common wisdom that the analysis of Brownian motion of noninteracting particles may be restricted to a single Brownian particle. This insight goes back to Szilard in his somewhat related work on Maxwell's demon [33], for a translation see Ref. [34]. In our analysis we shall also make this simplification, but insist that the bath has many degrees of freedom. Therefore it is equally equipped to couple to a gas of N noninteracting Brownian particles, and our results for energy, work, heat, entropy, etc., must just be multiplied by N. Because of this, our results yield, without any change, the intrinsic variables of a large Brownian system in its thermodynamic limit.

A. The Hamiltonian

The quantum Langevin equation is derived from the exact Hamiltonian description of a subsystem (Brownian particle) and a thermal bath, by tracing out the degrees of freedom of the bath. The influence of the particle on the bath is assumed to be sufficiently small. Thus, only the linear modes of the bath are excited, and the interaction of the particle with the bath is assumed to be linear. To be as pedagogic as possible, we first take a definite model for the bath, namely, a collection of harmonic oscillators; later we will relax this assumption. For the total Hamiltonian we thus assume [9]

$$\mathcal{H}_{\rm tot}=\mathcal{H}+\mathcal{H}_B+\mathcal{H}_I,$$

$$\mathcal{H}=\mathcal{K}(p)+\mathcal{V}(x),\quad \mathcal{K}(p)=\frac{p^2}{2m},\quad \mathcal{V}(x)=\frac{1}{2}ax^2, \tag{2.1}$$

$$\mathcal{H}_B=\sum_i\left[\frac{p_i^2}{2m_i}+\frac{m_i\omega_i^2}{2}x_i^2\right],$$

$$\mathcal{H}_I=\sum_i\left[-c_ix_ix+\frac{c_i^2}{2m_i\omega_i^2}x^2\right],$$

where $\mathcal{H}$ is the Hamiltonian of the particle, consisting of the kinetic and potential energies $\mathcal{K}$ and $\mathcal{V}$, $\mathcal{H}_B$ is the Hamiltonian of the bath, and $\mathcal{H}_I$ is the interaction Hamiltonian, p,p_i,x,x_i are the momenta and coordinate operators of the particle and the linear modes of the bath, $\mathcal{V}(x)$ is the confining potential of the particle and m and m_i are the corresponding masses.

Notice that our total system is closed and its energy is conserved, except for the periods when work is done on it by externally changing a system parameter such as m or a. When we later on take as initial density matrix the Gibbs distribution $\exp(-\beta\mathcal{H}_{\rm tot})/Z$, this still refers to our closed system; in particular, it is not part of a larger thermodynamic system, with which heat exchange would be possible [35,36].

The x_i terms of $\mathcal{H}_B+\mathcal{H}_I$ form a complete square, since $\mathcal{H}_I$ includes a self-interaction term proportional to x^2. This guarantees that the total Hamiltonian $\mathcal{H}_{\rm tot}$ will be positive definite. In certain physical situations (e.g., electromagnetic interaction), such a term is generated automatically by the coupling [13]. Indeed, under a canonical transformation.

$$x_i \to \frac{p_i}{m_i\omega_i}, \quad p_i \to -x_i m_i \omega_i, \tag{2.2}$$

$\mathcal{H}_{\rm tot}$ becomes

$$\mathcal{H}'_{\rm tot} = \frac{p^2}{2m} + \frac{1}{2}ax^2 + \sum_i \left[\frac{1}{2m_i}\left(p_i - \frac{c_i}{\omega_i}x \right)^2 + \frac{m_i\omega_i^2}{2}x_i^2 \right], \tag{2.3}$$

which corresponds to the minimal coupling (or subtraction) scheme.

In other situations (such as certain cases in nuclear and atomic physics, see Ref. [13] for more details) the self-interaction term is absent, and one has [12]

$$\tilde{\mathcal{H}} = \frac{p^2}{2m} + \tilde{\mathcal{V}}(x), \quad \tilde{\mathcal{H}}_I = -x\sum_i c_i x_i, \tag{2.4}$$

while $\mathcal{H}_B$ is unchanged. For a harmonic system one will have $\tilde{\mathcal{V}}(x) = \frac{1}{2}bx^2$. In general, the potential energy will have a minimum only if $b \equiv \tilde{\mathcal{V}}''(0)$ is large enough. This happens when the combination

$$a = b - \sum_i \frac{c_i^2}{m_i\omega_i^2} \tag{2.5}$$

is positive. In the case we shall consider below, with the c_i given by Eq. (2.23), this sum can be evaluated, leading to $a = b - \gamma\Gamma$, where γ is the coupling strength (damping constant) and Γ is a large cutoff frequency. So this system can be mapped on the previous one provided we define $\tilde{\mathcal{V}}(x) = \mathcal{V}(x) + \frac{1}{2}\gamma\Gamma x^2$. In doing so we identify with Hamiltonian of the subsystem the expression $\mathcal{H} = \mathcal{K} + \mathcal{V}$ of Eq. (2.1), rather than $\mathcal{K} + \tilde{\mathcal{V}}$, and with $\mathcal{H}_I$ the combination $\tilde{\mathcal{H}}_I + \frac{1}{2}\gamma\Gamma x^2$. To give some motivation for this, let us notice that we shall take Γ large and γ finite. In that case the expectation value $\langle \tilde{\mathcal{V}} \rangle$ is large, proportional to $\gamma\Gamma$, but this is almost fully compensated by an opposite term arising from $\langle \tilde{\mathcal{H}}_I \rangle$. These cancellations have been accounted for by the mapping to $\mathcal{H}$ and $\mathcal{H}_I$, leaving at most a $\ln\Gamma$ divergence for large Γ, which actually arises at small temperatures from $\langle K \rangle$. We shall come back to the pros and cons of this identification in Sec. IV B 5, where we notice that it is already needed to obtain the standard thermodynamics at very large T.

Some word of nomenclature is called for. The case of a harmonic potential $\mathcal{V}(x) = \frac{1}{2}ax^2$ is often called "the linear case" in literature, of course referring to its linear force. The expressions "linear potential" and "nonlinear potential," that are sometimes found in the literature, are misnomers, and will be avoided by us.

B. Derivation of general quantum Langevin equation

The operator equations of motion for the bath modes read

$$\dot{x}_i = \frac{1}{m_i}p_i, \tag{2.6}$$

$$\dot{p}_i = -x_i m_i \omega_i^2 + c_i x. \tag{2.7}$$

After introducing the creation and annihilation operators by

$$x_i = \sqrt{\frac{\hbar}{2m_i\omega_i}}(a_i + a_i^\dagger), \quad p_i = i\sqrt{\frac{\hbar m_i\omega_i}{2}}(a_i^\dagger - a_i) \tag{2.8}$$

we can write Eqs. (2.6), and (2.7) in the form

$$\dot{a}_i(t) = -i\omega_i a_i(t) + i\sqrt{\frac{c_i^2}{2\hbar m_i\omega_i}}x(t). \tag{2.9}$$

This equation is solved readily,

$$a_i(t) = e^{-i\omega_i t}a_i(0) + i\sqrt{\frac{c_i^2}{2\hbar m_i\omega_i}}\int_0^t {\rm d}s\, e^{-i\omega_i(t-s)}x(s), \tag{2.10}$$

yielding

$$x_i(t) = x_i(0)\cos\omega_i t + \frac{p_i(0)}{m_i\omega_i}\sin\omega_i t + \frac{c_i}{m_i\omega_i}\int_0^t ds\,\sin\omega_i(t-s)x(s), \tag{2.11}$$

$$p_i(t) = -m_i\omega_i x_i(0)\sin\omega_i t + p_i(0)\cos\omega_i t + c_i\int_0^t ds\,\cos\omega_i(t-s)x(s). \tag{2.12}$$

The Heisenberg equations of motion for the Brownian particle read

$$\dot{x} = \frac{1}{m}p, \tag{2.13}$$

$$\dot{p} = -ax + \sum_i c_i x_i - x\sum_i \frac{c_i^2}{m_i\omega_i^2}. \tag{2.14}$$

Combined with Eq. (2.11) the last equation becomes

$$m\ddot{x}(t) = -ax(t) + \eta(t) - \int_0^t dt'\,\dot{\gamma}(t-t')x(t') - \gamma(0)x(t), \tag{2.15}$$

where

$$\eta(t)=\sum_i c_i\left[x_i(0)\cos\omega_i t+\frac{p_i(0)}{m_i\omega_i}\sin\omega_i t\right]$$
$$=\sum_i \sqrt{\frac{\hbar c_i^2}{2m_i\omega_i}}[a_i^\dagger(0)e^{i\omega_i t}+a_i(0)e^{-i\omega_i t}], \tag{2.16}$$

$$\gamma(t)=\sum_i \frac{c_i^2}{m_i\omega_i^2}\cos(\omega_i t), \tag{2.17}$$

are the noise related to the *unperturbed* bath, and the friction kernel, respectively. A partial integration brings

$$m\ddot{x}(t)=-ax(t)-x(0)\gamma(t)-\int_0^t ds\,\gamma(t-s)\dot{x}(s)+\eta(t), \tag{2.18}$$

Notice that in this derivation the back reaction of the bath on the particle has been taken into account in an exact manner. It is described by the integrals in Eqs. (2.11) and (2.12), and brings the damping terms $x(t)\gamma(0)-x(0)\gamma(t)-\int_0^t ds\,\gamma(t-s)\dot{x}(s)$ in going from Eq. (2.14) to Eq. (2.18).

C. Interaction energy and energy of the bath

The interaction Hamiltonian and the bath Hamiltonian can be expressed in $\eta(t)$ and $x(t)$. Using Eqs. (2.11) and (2.12) and the definition (2.16) of $\eta(t)$ and definition (2.17) of $\gamma(t)$, one gets, using trigeometric relations,

$$\mathcal{H}_I(t)=-\eta(t)x(t)+\int_0^t ds\,\dot{\gamma}(s)x(t-s)x(t)+\frac{1}{2}\gamma(0)x^2(t) \tag{2.19}$$

$$=-\eta(t)x(t)+\gamma(t)x(0)x(t)-\frac{1}{2}\gamma(0)x^2(t)+\int_0^t ds\,\gamma(s)\dot{x}(t-s)x(t).$$

Since the $x_i(t)$ commute with $x(t)$, there is an equivalent expression by putting $x(t)$ to the left in all terms. Furthermore,

$$\mathcal{H}_B(t)=\mathcal{H}_B(0)+\frac{1}{2}\int_0^t ds\,\gamma(s)\{\dot{\eta}(s),x(s)\}-\frac{1}{2}\int_0^t ds_1\int_0^t ds_2\,\ddot{\gamma}(s_1-s_2)x(s_1)x(s_2) \tag{2.20}$$
$$=\mathcal{H}_B(0)+\frac{1}{2}\int_0^t ds\,\gamma(s)\{\dot{\eta}(s),x(s)\}-\frac{1}{2}\int_0^t ds\,\dot{\gamma}(s)\{x(s),x(0)\}-\frac{1}{2}\int_0^t ds_1\int_0^{s_1} ds_2\,\dot{\gamma}(s_2)\{x(s_1),\dot{x}(s_1-s_2)\},$$

where $\mathcal{H}_B(0)$ is the unperturbed bath and $\{A,B\}=AB+BA$ is an anticommutator. An equivalent expression is

$$\mathcal{H}_B(t)=\mathcal{H}_B(0)+\frac{1}{2}\int_0^t ds\,\gamma(s)\{\dot{\eta}(s),x(s)\}-\frac{1}{2}\gamma(t)\{x(t),x(0)\}+\frac{1}{2}\gamma(0)[x^2(t)+x^2(0)]+\frac{1}{2}\int_0^t ds\,\gamma(s)[\{\dot{x}(s),x(0)\}$$
$$-\{\dot{x}(t-s),x(t)\}]+\frac{1}{2}\int_0^t ds_1\int_0^t ds_2\,\gamma(s_1-s_2)\dot{x}(s_1)\dot{x}(s_2). \tag{2.21}$$

The last equalities of $\mathcal{H}_I$ and $\mathcal{H}_B$ can be used in the limit where $\gamma(t)\approx\gamma\delta_+(t)+\gamma\delta_-(t)$.

D. Drude-Ullersma spectrum

For some, but not all, of our applications it is beneficial to consider a fully explicit case for the bath. The bath is assumed to have uniformly spaced modes,

$$\omega_i=i\Delta,\quad i=1,2,3,\ldots, \tag{2.22}$$

and for the couplings we choose the Drude-Ullersma spectrum [9,12]

$$c_i=\sqrt{\frac{2\gamma m_i\omega_i^2\Delta}{\pi}\frac{\Gamma^2}{\omega_i^2+\Gamma^2}}. \tag{2.23}$$

Here Γ is the characteristic Debye cutoff frequency of the bath, and γ stands for the coupling constant; it has the dimension of kg/s. Our parameter γ, related to another one ($\gamma'=\gamma/m$) that is sometimes employed, see, e.g., Ref. [9], allows us to consider changes in the effective mass m at fixed coupling to the bath.

The thermodynamic limit for the bath is taken by sending $\Delta\to 0$, which induces relaxational behavior. As usual, the ‘‘Heisenberg’’ time scale $1/\Delta$ will be extremely large, implying that in the remaining approach the limit of ‘‘large times’’ always means the quasistationary nonequilibrium state where time is still much less than $1/\Delta$. In the limit $\Delta\to 0$ each coupling $c_i\sim\sqrt{\Delta}$ is very weak. The fact that the bath has many modes nevertheless induces its nontrivial influence. At finite but small Δ the system would have an initial relaxational behavior, which at times of order $1/\Delta$ is changed in a recurrent behavior.

It is customary to define the spectral density

$$J(\omega)=\frac{\pi}{2}\sum_i \frac{c_i^2}{m_i\omega_i}\,\delta(\omega-\omega_i)=\frac{\gamma\omega\Gamma^2}{\omega^2+\Gamma^2}. \tag{2.24}$$

It has the Ohmic behavior $J\approx\gamma\omega$ for $\omega\ll\Gamma$, and γ is called the interaction strength or damping constant. As $J(\omega)$ is cut off at the ''Debye'' frequency Γ, it is called a quasi-Ohmic spectrum.

For many applications only the spectral density needs to be defined. However, for our further calculations it is advantageous to stick to the fully specified linear bath, with its frequencies (2.22) and couplings (2.23). It can then be shown that the friction kernel (2.17) becomes

$$\gamma(t)=\frac{2\gamma}{\pi}\int_0^\infty d\omega\,\frac{\Gamma^2}{\omega^2+\Gamma^2}\cos\omega t=\gamma\Gamma\, e^{-\Gamma|t|}. \tag{2.25}$$

It is nonlocal in time, but on time scales much larger than $1/\Gamma$ it may be replaced by $\gamma\delta_+(t)+\gamma\delta_-(t)$.

Finally, we wish to mention that there are alternative ways to derive the quantum Langevin equation [9], since many of its properties are rigidly determined by general statements such as the quantum fluctuation-dissipation theorem [5]. Nevertheless, we choose to focus on concrete models, because they show in detail how the quantum Langevin equation arises from first principles, and thus are better suited for pedagogical purposes.

III. GIBBSIAN STATE FOR A HARMONIC CONFINING POTENTIAL

The case of an oscillator subject to a parabolic confining potential is a celebrated exactly solvable problem in quantum mechanics,

$$\mathcal{H}(p,x)=\mathcal{K}(p)+\mathcal{V}(x)=\frac{p^2}{2m}+\frac{1}{2}ax^2. \tag{3.1}$$

The eigenfrequency is already known from the classical treatment,

$$\omega_0=\sqrt{\frac{a}{m}}. \tag{3.2}$$

When this oscillator is coupled to an oscillator bath with bilinear coupling, as was done in Eq. (2.1), the problem remains exactly solvable. It is in the true sense ''the harmonic oscillator model'' for quantum Brownian motion.

It is well known that, besides its direct physical meaning, the harmonic oscillator can be interpreted as an LC circuit [17]. Then x may correspond to the charge Q on a capacitor, $1/a$ to its capacitance C,m to an inductance L,p to a flux $L\dot{Q}$, γ to a resistance R, and $\eta(t)$ to a random electromotoric force. Although we will not use this language explicitly, it is useful to keep it in mind, especially when considering variations of parameters. Indeed, in this setup there should be nothing very difficult in varying L or C, in our notation m and a.

The theory of the dissipative harmonic oscillator is considered in many works (see Ref. [9] and references therein, as well as a recent work for the driven case [37]). We will now be primarily interested in thermodynamical aspects of this problem.

A. Shift of the bath frequencies due to coupling with the central particle

In Fourier space the equation of motion of the particle may be written as

$$\left(a-m\omega^2+\sum_i \frac{c_i^2}{m_i\omega_i^2}\right)x=\sum_i c_i x_i, \tag{3.3}$$

and for the bath

$$(-m_i\omega^2+m_i\omega_i^2)x_i=c_i x. \tag{3.4}$$

From these relations one derives a condition for the eigenfrequencies ν_k,

$$\begin{aligned}\frac{a}{m}-\nu^2&=\nu^2\sum_{i\geqslant 1}\frac{c_i^2}{m\, m_i\omega_i^2(\omega_i^2-\nu^2)}\\&=\frac{2\gamma\Gamma^2\nu^2}{\pi}\sum_{i\geqslant 1}\frac{\Delta}{(\omega_i^2+\Gamma^2)(\omega_i^2-\nu^2)} \qquad (3.5)\\&=-\frac{2\gamma\Gamma^2\nu^2}{\pi(\nu^2+\Gamma^2)}\sum_{i\geqslant 1}\frac{\Delta}{\omega_i^2+\Gamma^2}+\frac{\gamma\Gamma^2\nu}{\pi(\nu^2+\Gamma^2)}\\&\quad\times\sum_{i\geqslant 1}\left[\frac{\Delta}{\omega_i-\nu}-\frac{\Delta}{\omega_i+\nu}\right], \qquad (3.6)\end{aligned}$$

where we inserted the definition (2.23) of the c_i. The first sum may be replaced by an integral, while the second can be carried out exactly,

$$\begin{aligned}\sum_{i=1}^{\infty}\left[\frac{\Delta}{\omega_i-\nu}-\frac{\Delta}{\omega_i+\nu}\right]&=\lim_{N\to\infty}\left[\psi\left(N-\frac{\nu}{\Delta}\right)-\psi\left(1-\frac{\nu}{\Delta}\right)\right.\\&\quad\left.-\psi\left(N+\frac{\nu}{\Delta}\right)+\psi\left(1+\frac{\nu}{\Delta}\right)\right]\\&=\frac{\Delta}{\nu}-\pi\cot\frac{\pi\nu}{\Delta}, \qquad (3.7)\end{aligned}$$

where $\psi(z)=d\ln\Gamma(z)/dz$ is the di-Γ function and we used

$$\psi(z+1)=\psi(z)+\frac{1}{z},\qquad \psi(1-z)=\psi(z)+\pi\cot\pi z. \tag{3.8}$$

The eigenfrequencies ν_k of the coupled system thus follow as the roots of

$$\cot\frac{\pi\nu}{\Delta}-\frac{\Delta}{\pi\nu}=-\frac{(a/m-\nu^2)(\nu^2+\Gamma^2)+\gamma\Gamma\nu^2}{\gamma\Gamma^2\nu}. \tag{3.9}$$

The transcendental equation has no solution for $0\leqslant\nu\leqslant\Delta$. For $\nu>\Delta$ there is one solution in each period of the cotangent, except for the period that contains the point $\nu=\omega_0\equiv\sqrt{a/m}$, where there occur either three solutions or one. One can then check that in the limit of vanishing coupling $\gamma\to 0$, there occur the modes $\omega_i=i\Delta$ $(i=1,2,\ldots)$, and ω_0. Notice, however, that this behavior only pertains to the regime of infinitesimal coupling $\gamma<\gamma_c$ with $\gamma_c\sim m\Delta$. For $\gamma\geqslant\gamma_c$, however, the interval containing ω_0 has only one solution, so ω_0 is lost as a separate mode, its influence being taken by a shift of neighboring modes.

For finite γ the solution of Eq. (3.9) shows that the bath modes $\omega_k\geqslant\Delta$ now get shifted to

$$\nu_k=k\Delta-\frac{1}{\pi}\phi(k\Delta)\Delta=\omega_k-\frac{1}{\pi}\phi(\omega_k)\Delta, \tag{3.10}$$

where

$$\phi(\nu)=\arctan\frac{\gamma\Gamma^2\nu}{(a-m\nu^2)(\nu^2+\Gamma^2)+\gamma\Gamma\nu^2}. \tag{3.11}$$

Here the definition of the arctan is such that ϕ goes monotonously from $\phi(0)=0$ to $\phi(\infty)=\pi$. We shall need

$$\begin{aligned}\sin\phi(\nu)&=\frac{\gamma\Gamma^2\nu}{\{[(a-m\nu^2)(\nu^2+\Gamma^2)+\gamma\Gamma\nu^2]^2+(\gamma\Gamma^2\nu)^2\}^{1/2}}\\&\approx\frac{\gamma\nu}{\{(a-m\nu^2)^2+\gamma^2\nu^2\}^{1/2}},\end{aligned} \tag{3.12}$$

where the approximation holds for large Γ.

B. The Gibbsian state of the particle and its bath

The steps of the preceding subsection allow to calculate the Gibbs free energy of the total system,

$$\beta F_{\mathrm{tot}}(T,\gamma)=\sum_k \ln 2\sinh\frac{1}{2}\beta\hbar\nu_k. \tag{3.13}$$

For small Δ one may use the identity

$$\begin{aligned}\sum_{k=1}^{\infty}A(\nu_k)&=\frac{1}{\Delta}\int_0^\infty d\omega_k A(\nu_k)\\&=\frac{1}{\Delta}\int_0^\infty d\nu_k\frac{d\omega_k}{d\nu_k}A(\nu_k)\\&=\int_0^\infty d\nu\left[\frac{1}{\Delta}+\frac{1}{\pi}\frac{d\phi(\nu)}{d\nu}\right]A(\nu)+\mathcal{O}(\Delta)\end{aligned} \tag{3.14}$$

and one gets

$$F_{\mathrm{tot}}(T,\gamma)=F_B(T,\gamma=0)+F_p(a,\gamma,\Gamma,m,T), \tag{3.15}$$

where the first term is the free energy of the bath in absence of the particle. Neglecting its divergent zero point energy one gets

$$F_B(T,\gamma=0)=\frac{T}{\Delta}\int_0^\infty d\omega\,\ln(1-e^{-\beta\hbar\omega})=-\frac{\pi^2T^2}{6\hbar\Delta}. \tag{3.16}$$

It is of order $1/\Delta$, showing the extensivity of the bath, and implies the energy

$$U_B(T,\gamma=0)=\frac{\pi^2}{6\hbar\Delta}T^2 \tag{3.17}$$

and the linear specific heat and entropy

$$C_B(T,\gamma=0)=S_B(T,\gamma=0)=\frac{\pi^2 T}{3\hbar\Delta}. \tag{3.18}$$

The free energy shift due to the central particle, its coupling to the bath, and the resulting disturbance of the bath, follows from Eq. (3.14) as [16]

$$\beta F_p=\frac{1}{\pi}\int_0^\infty d\nu\,\ln\left[2\sinh\frac{1}{2}\beta\hbar\nu\right]\frac{d\phi}{d\nu} \tag{3.19}$$

$$\begin{aligned}&=\frac{\gamma\Gamma^2}{\pi}\int_0^\infty d\nu\,\ln\left[2\sinh\frac{1}{2}\beta\hbar\nu\right]\\&\quad\times\frac{a\Gamma^2+(m\Gamma^2+\gamma\Gamma-a)\nu^2+3m\nu^4}{[(a-m\nu^2)(\nu^2+\Gamma^2)+\gamma\Gamma\nu^2]^2+\gamma^2\Gamma^4\nu^2}.\end{aligned} \tag{3.20}$$

A useful identity is

$$\begin{aligned}\beta F_p=\ln 2\sinh\left(\frac{1}{2}\beta\hbar\nu_1\right)+\frac{1}{2}\beta\hbar\int_0^\infty d\nu\,\Bigg[\theta(\nu-\nu_1)\\-\frac{1}{\pi}\phi(\nu)\Bigg]\coth\left(\frac{1}{2}\beta\hbar\nu\right),\end{aligned} \tag{3.21}$$

where ν_1 is arbitrary and θ is the Heaviside step function.

1. Intermezzo: the characteristic frequencies of the damped oscillator

The present model for a damped harmonic oscillator has three characteristic frequencies that do not depend on temperature. They just follow from the linear equations of motion, and thus have the same value at high and low temperatures.

The denominator in Eq. (3.20) is a fourth-order polynomial in ν^2. It decomposes as

$$m^2(\nu^2+\Gamma^2)P_3(i\nu)P_3(-i\nu), \tag{3.22}$$

where

$$\begin{aligned} P_3(\omega) &= \omega^3 - \Gamma\omega^2 + \frac{a+\gamma\Gamma}{m}\omega - \frac{a\Gamma}{m} \\ &= (\omega-\Gamma)\left(\omega^2+\frac{a}{m}\right) + \frac{\gamma\Gamma}{m}\omega. \end{aligned} \tag{3.23}$$

The roots $\omega_{1,2,3}$ of P_3 satisfy the relations

$$\omega_1+\omega_2+\omega_3=\Gamma, \tag{3.24}$$

$$\omega_1\omega_2+\omega_2\omega_3+\omega_3\omega_1=\frac{a+\gamma\Gamma}{m}, \tag{3.25}$$

$$\omega_1\omega_2\omega_3=\frac{a\Gamma}{m}. \tag{3.26}$$

Two different situations can arise. Either all three roots are real (this is the case in the overdamped regime), or, in the underdamped regime, two of them are complex conjugate: $\omega_1^*=\omega_2$, whereas ω_3 is real. In both cases one has Re $\omega_{1,2,3}>0$, which indicates that with time the particle relaxes toward a stationary state.

For small γ these roots read

$$\omega_{1,2}=\pm i\omega_0+\frac{\gamma}{m}\,\frac{\Gamma}{2(\Gamma\mp i\omega_0)}+\left(\frac{\gamma}{m}\right)^2\frac{\Gamma^2(\Gamma\pm i\omega_0)}{8\omega_0(\Gamma\mp i\omega_0)^3}, \tag{3.27}$$

$$\omega_3=\Gamma-\frac{\gamma\Gamma^2}{m(\Gamma^2+\omega_0^2)}-\left(\frac{\gamma}{m}\right)^2\frac{\Gamma^3(\Gamma^2-\omega_0^2)}{(\Gamma^2+\omega_0^2)^3}. \tag{3.28}$$

On the other hand, for a large Γ one gets

$$\begin{aligned} \omega_{1,2} &= \frac{\gamma}{2m}\left(1\pm\sqrt{1-\frac{4am}{\gamma^2}}\right)+\frac{1}{2\Gamma}\left(\frac{\gamma}{m}\right)^2 \\ &\quad\times\left[1\pm\frac{1-2am/\gamma^2}{\sqrt{1-4am/\gamma^2}}\right], \end{aligned} \tag{3.29}$$

$$\omega_3=\Gamma-\frac{\gamma}{m}-\frac{1}{\Gamma}\left(\frac{\gamma}{m}\right)^2. \tag{3.30}$$

We shall only need them to leading order in $1/\Gamma$,

$$\omega_1=\frac{\gamma(1-w)}{2m}=\frac{2a}{\gamma(1+w)},\quad \omega_2=\frac{\gamma(1+w)}{2m},$$

$$\omega_3=\Gamma-\frac{\gamma}{m}, \tag{3.31}$$

where we denoted

$$\varepsilon=\frac{am}{\gamma^2},\quad w=\sqrt{1-4\varepsilon}. \tag{3.32}$$

Later on we shall need

$$a\frac{dw}{da}=m\frac{dw}{dm}=-\frac{1-w^2}{2w},\quad a\frac{d\omega_{1,2}}{da}=\mp\frac{\gamma(1-w^2)}{4mw},$$

$$m\frac{d\omega_{1,2}}{dm}=\pm\frac{\gamma}{4mw}(1\mp w)^2. \tag{3.33}$$

For overdamping ($\varepsilon<\frac{1}{4}$) w is real positive. Our interest is, in particular, the strong damping regime $\gamma^2\gg am$, where

$$\omega_1=\frac{a}{\gamma},\quad \omega_2=\frac{\gamma}{m}\left(1-\frac{am}{\gamma^2}\right),\quad \omega_3=\Gamma-\frac{\gamma}{m} \tag{3.34}$$

and the approximations hold to leading order in ε.

Already in the classical regime, our system has three characteristic relaxation times: for the coordinate, for the momentum, and for the noise. For large Γ and γ they are well separated,

$$\tau_x=\frac{1}{\omega_1}\approx\frac{\gamma}{a}\gg\tau_p=\frac{1}{\omega_2}\approx\frac{m}{\gamma}\gg\tau_\eta=\frac{1}{\Gamma}. \tag{3.35}$$

In the quantum regime the quantum time scale

$$\tau_\hbar=\frac{\hbar}{T} \tag{3.36}$$

can be comparable to or larger than τ_x, inducing quantum coherence effects of the noise and thus new physics.

In case of underdamping, ($\varepsilon>\frac{1}{4}$) one has $w=i\bar{w}$, with

$$\bar{w}=\sqrt{4\varepsilon-1},\quad \omega_{1,2}=\frac{\gamma(1\mp i\bar{w})}{2m}. \tag{3.37}$$

This leads to the renormalized oscillation time τ_0 and the damping time τ_d,

$$\tau_0=\frac{1}{\sqrt{\omega_0^2-\gamma^2/4m^2}},\quad \tau_d=\frac{2m}{\gamma}. \tag{3.38}$$

Since τ_d differs from τ_p by a factor of order unity, we may skip the latter and use τ_p and τ_0 as the relevant time scales in the underdamped regime.

It is worth mentioning that the weak-coupling limit commutes with the quasi-Ohmic limit, in the sense that taking large Γ in Eqs. (3.27) and (3.28) we get the same main term and at least the first correction as having taken small γ limit in Eqs. (3.31) and (3.30).

2. Continuing the main argument for the Gibbsian state

In order to calculate the free energy (3.20), we shall first determine the following integral:

$$I(a,A,B)=\int_0^\infty\frac{d\nu\quad\nu\coth\left(\frac{1}{2}a\nu\right)}{(A^2+\nu^2)(B^2+\nu^2)}. \tag{3.39}$$

We can write

$$
\begin{aligned}
I(a,A,B) &= \int_0^\infty \frac{d\nu\,\nu}{(A^2+\nu^2)(B^2+\nu^2)} + 2\int_0^\infty \frac{d\nu\,\nu}{(e^{a\nu}-1)(A^2+\nu^2)(B^2+\nu^2)} \\
&= \frac{1}{B^2-A^2}\ln\frac{B}{A} + \frac{2}{B^2-A^2}\left[\int_0^\infty \frac{d\nu\,\nu}{(e^{a\nu}-1)(A^2+\nu^2)} - \int_0^\infty \frac{d\nu\,\nu}{(e^{a\nu}-1)(B^2+\nu^2)}\right] \\
&= \frac{1}{B^2-A^2}\left[\psi\left(\frac{aB}{2\pi}\right) - \psi\left(\frac{aA}{2\pi}\right)\right] - \frac{\pi}{a}\,\frac{1}{AB(A+B)},
\end{aligned}
\tag{3.40}
$$

where we used the known formula

$$
2\int_0^\infty \frac{t\,dt}{[\exp(2\pi t)-1](t^2+z^2)} = \ln z - \psi(z) - \frac{1}{2z}.
\tag{3.41}
$$

By integration we obtain

$$
\begin{aligned}
J(a,A,B) &= \int_0^\infty \frac{d\nu}{\pi}\ \ln\left(2\sinh\frac{1}{2}a\nu\right)\left(\frac{1}{A^2+\nu^2} - \frac{1}{B^2+\nu^2}\right) \\
&= -\frac{1}{A}\ln\Gamma\left(\frac{aA}{2\pi}\right) - \frac{1}{2A}\ln\frac{aA}{4\pi^2} + \frac{1}{B}\ln\Gamma\left(\frac{aB}{2\pi}\right) \\
&\quad + \frac{1}{2B}\ln\frac{aB}{4\pi^2}.
\end{aligned}
\tag{3.42}
$$

In terms of the roots ω_i, we may write Eq. (3.11) as

$$
\phi(\nu) = \arctan\frac{\nu}{\omega_1} + \arctan\frac{\nu}{\omega_2} + \arctan\frac{\nu}{\omega_3} - \arctan\frac{\nu}{\Gamma}.
\tag{3.43}
$$

The derivation follows immediately after using Eq. (3.22) with $P_3(s)=(s-\omega_1)(s-\omega_2)(s-\omega_3)$ and expressing the arctan in logarithms. The integral in Eq. (3.20) can now be done by adding to $\phi(\nu)$ a term $[(\Gamma-\omega_1-\omega_2-\omega_3)/\omega_4]\arctan(\nu/\omega_4)$, which vanishes for any ω_4 on account of Eq. (3.24), and then using Eq. (3.42) with $a=\hbar\beta$.

This finally brings the shift of the free energy due to the presence of the Brownian particle

$$
\begin{aligned}
\beta F_p &= \ln\Gamma\left(\frac{\beta\hbar\Gamma}{2\pi}\right) - \ln\Gamma\left(\frac{\beta\hbar\omega_1}{2\pi}\right) - \ln\Gamma\left(\frac{\beta\hbar\omega_2}{2\pi}\right) \\
&\quad - \ln\Gamma\left(\frac{\beta\hbar\omega_3}{2\pi}\right) - \ln\frac{\beta\hbar\omega_0}{(2\pi)^2}.
\end{aligned}
\tag{3.44}
$$

This is just equal to $-\ln Z'$ with Z' calculated in Eq. (4.20) of Grabert *et al.* [38]. These authors did not point at the physical role of their Z'. Here we see that it is the part of the partition sum of the total system related to the central particle and its coupling to the bath with its linear unperturbed spectrum $\omega_k=k\,\Delta$. We nevertheless expect that the statics and the dynamics hold for more general bath spectra, as long as the interaction is bilinear, and the spectra ensure relaxation.

The internal energy of the total system reads

$$
\begin{aligned}
U_p &= \frac{\hbar\Gamma}{2\pi}\psi\left(\frac{\beta\hbar\Gamma}{2\pi}\right) - \frac{\hbar\omega_1}{2\pi}\psi\left(\frac{\beta\hbar\omega_1}{2\pi}\right) - \frac{\hbar\omega_2}{2\pi}\psi\left(\frac{\beta\hbar\omega_2}{2\pi}\right) \\
&\quad - \frac{\hbar\omega_3}{2\pi}\psi\left(\frac{\beta\hbar\omega_3}{2\pi}\right) - T.
\end{aligned}
\tag{3.45}
$$

C. The effective temperatures

We shall now study two objects, $T_x=a\langle x^2\rangle$ and $T_p=\langle p^2\rangle/m$, that would in classical equilibrium be equal to T and which we shall interpret below as effective temperatures. As in the classical situation, it holds that [38]

$$
T_x = a\langle x^2\rangle = 2a\,\frac{\partial F_p}{\partial a}.
\tag{3.46}
$$

We find

$$
T_x = -T + \frac{\hbar a}{\pi m}\left\{\frac{(\omega_1-\Gamma)\,\psi\left(\frac{\beta\hbar\omega_1}{2\pi}\right)}{(\omega_2-\omega_1)(\omega_3-\omega_1)} + \frac{(\omega_2-\Gamma)\,\psi\left(\frac{\beta\hbar\omega_2}{2\pi}\right)}{(\omega_1-\omega_2)(\omega_3-\omega_2)} + \frac{(\omega_3-\Gamma)\,\psi\left(\frac{\beta\hbar\omega_3}{2\pi}\right)}{(\omega_1-\omega_3)(\omega_2-\omega_3)}\right\}.
\tag{3.47}
$$

Likewise,

$$
T_p = \frac{\langle p^2\rangle}{m} = -2m\,\frac{\partial F_p}{\partial m} = T_x + \frac{\hbar\gamma\Gamma}{\pi m}\left\{\frac{\omega_1\,\psi\left(\frac{\beta\hbar\omega_1}{2\pi}\right)}{(\omega_2-\omega_1)(\omega_3-\omega_1)} + \frac{\omega_2\,\psi\left(\frac{\beta\hbar\omega_2}{2\pi}\right)}{(\omega_1-\omega_2)(\omega_3-\omega_2)} + \frac{\omega_3\,\psi\left(\frac{\beta\hbar\omega_3}{2\pi}\right)}{(\omega_1-\omega_3)(\omega_2-\omega_3)}\right\}.
\tag{3.48}
$$

To find the Gibbsian values for $\gamma \to 0$ one has to notice that

$$\psi\left(\frac{i\omega_0}{2\pi T}\right)-\psi\left(-\frac{i\omega_0}{2\pi T}\right)=\frac{2\pi i}{\hbar\omega_0}\ T+i\pi\coth\ \frac{\hbar\omega_0}{2T} \tag{3.49}$$

and this yields the standard weak-coupling result known from all the books,

$$U=\frac{1}{2}T_x+\frac{1}{2}T_p=T_x=T_p=\frac{\hbar\omega_0}{2}\coth\frac{\beta\hbar\omega_0}{2}=\frac{1}{2}\hbar\omega_0+\frac{\hbar\omega_0}{e^{\beta\hbar\omega_0}-1}\quad(\gamma\to 0). \tag{3.50}$$

1. Thermodynamics and effective temperatures at high T

Using that for small z

$$\ln\Gamma(z)=-\ln z-\gamma_E z+\frac{\pi^2}{12}z^2, \tag{3.51}$$

where $\gamma_E=0.577\,215\,6$ is Euler's constant, one gets the free energy

$$F_p=T\ln\beta\hbar\omega_0+\frac{\beta\hbar^2}{48}[\Gamma^2-\omega_1^2-\omega_2^2-\omega_3^2]$$

$$\approx T\ln\beta\hbar\omega_0+\frac{\beta\hbar^2(a+\gamma\Gamma)}{24m}, \tag{3.52}$$

where $\omega_0=\sqrt{a/m}$ and Γ has been taken large in the second identity. The internal energy and entropy become

$$U_p=T+\frac{\beta\hbar^2(a+\gamma\Gamma)}{12m},\quad S_p=\ln\frac{T}{\hbar\omega_0}+1+\frac{\beta\hbar^2(a+\gamma\Gamma)}{6m}. \tag{3.53}$$

From Eqs. (3.47) and (3.48) we obtain at large T

$$T_x=T+\frac{\beta\hbar^2 a}{12m}-\frac{\beta^3\hbar^4 a(a+\gamma\Gamma)}{720m^2} \tag{3.54}$$

and

$$T_p=T+\frac{\beta\hbar^2(a+\gamma\Gamma)}{12m}-\frac{\beta^2\hbar^3\gamma\Gamma^2}{4\pi^3 m}\zeta(3)$$

$$+\frac{\beta^3\hbar^4[\gamma\Gamma^3 m-(a+\gamma\Gamma)^2]}{720m^2}. \tag{3.55}$$

2. Thermodynamics and effective temperatures at low T

Further results can be obtained with the improved Stirling formula,

$$\ln\Gamma(z)=\left(z-\frac{1}{2}\right)\ln z-z+\frac{1}{2}\ln(2\pi)+\frac{1}{12z}-\frac{1}{360z^3}. \tag{3.56}$$

One gets for arbitrary and for large Γ,

$$F_p=\frac{\hbar}{2\pi}\left[\Gamma\ln\Gamma-\sum_{k=1}^{3}\omega_k\ln\omega_k\right]-\frac{\pi\gamma}{6\hbar a}T^2$$

$$=\frac{\hbar\gamma}{2\pi m}\left[\ln\frac{2m\Gamma}{\gamma}+1\right]-\frac{\hbar\gamma}{4\pi m}[(1+w)\ln(1+w)$$

$$+(1-w)\ln(1-w)]-\frac{\pi\gamma}{6\hbar a}T^2, \tag{3.57}$$

$$U_p=\frac{\hbar}{2\pi}\left[\Gamma\ln\Gamma-\sum_{k=1}^{3}\omega_k\ln\omega_k\right]+\frac{\pi\gamma}{6\hbar a}T^2$$

$$=\frac{\hbar\gamma}{2\pi m}\left[\ln\frac{2m\Gamma}{\gamma}+1\right]-\frac{\hbar\gamma}{4\pi m}[(1+w)\ln(1+w)$$

$$+(1-w)\ln(1-w)]+\frac{\pi\gamma}{6\hbar a}T^2, \tag{3.58}$$

$$S_p=\beta(U_p-F_p)=\frac{\pi\gamma}{3\hbar a}T. \tag{3.59}$$

Notice that S_p, the shift in total von Neumann entropy due to the presence of the Brownian particle, differs strongly from the von Neumann entropy of the particle itself, which remains finite at $T=0$, as we shall show in Eqs. (4.35) and (4.36). The non-additivity of entropies encountered here is a deep aspect of quantum physics, where a subsystem can have a larger von Neumann entropy than the full system.

Using Eq. (3.33) one finds at low temperatures and arbitrary am/γ^2, $w=\sqrt{1-4am/\gamma^2}$ [48],

$$T_p=\frac{\hbar\gamma}{\pi m}\ln\frac{2\Gamma m}{\gamma}+\frac{\hbar\gamma}{4\pi m\,w}[(1-w)^2\ln(1-w)$$

$$-(1+w)^2\ln(1+w)]+\mathcal{O}(T^4), \tag{3.60}$$

$$T_x=\frac{\hbar a}{\pi\gamma}\frac{1}{w}\ln\frac{1+w}{1-w}+\frac{\pi\gamma}{3\hbar a}T^2+\mathcal{O}(T^4). \tag{3.61}$$

The above expressions simplify in the limit of strong damping, see Eq. (3.31),

$$F_p(T)=\frac{\hbar\gamma}{2\pi m}\left(\ln\frac{\Gamma m}{\gamma}+1\right)+\frac{\hbar a}{2\pi\gamma}\ln\frac{\gamma^2}{am}-\frac{\pi\gamma}{6\hbar a}T^2,$$

$$U_p(T)=\frac{\hbar\gamma}{2\pi m}\left(\ln\frac{\Gamma m}{\gamma}+1\right)+\frac{\hbar a}{2\pi\gamma}\ln\frac{\gamma^2}{am}+\frac{\pi\gamma}{6\hbar a}T^2 \tag{3.62}$$

and [48]

$$T_p=\frac{\hbar\gamma}{\pi m}\ln\frac{\Gamma m}{\gamma}+\frac{\hbar a}{\pi\gamma}+\mathcal{O}(T^4), \tag{3.63}$$

$$T_x=\frac{\hbar a}{\pi\gamma}\ln\frac{\gamma^2}{am}+\frac{\pi\gamma}{3\hbar a}T^2+\mathcal{O}(T^4). \tag{3.64}$$

D. Interaction energy and bath energy

Some results can be obtained by studying the dependence of $\mathcal{H}_{\text{tot}}$ and $F_{\text{tot}}=F_{\text{tot}}(\gamma=0)+F_p$ on γ, Γ, and Δ. Let us first write Eq. (2.1) as

$$\mathcal{H}_{\text{tot}}=\mathcal{H}+\mathcal{H}_B+\mathcal{H}_I, \tag{3.65}$$

$$\mathcal{H}_B=\sum_i \hbar\Delta_i\left(a_i^\dagger a_i+\frac{1}{2}\right),\quad \mathcal{H}_I=-\eta(0)x+\frac{1}{2}\gamma\Gamma\,x^2.$$

where $\eta(0)=\Sigma_i c_i x_i$. Now due to the expression Eq. (2.23) for c_i it holds that $\eta(0)\sim\sqrt{\gamma}$. This implies

$$\gamma\frac{\partial\mathcal{H}_{\text{tot}}}{\partial\gamma}=-\frac{1}{2}\eta(0)x+\frac{1}{2}\gamma\Gamma\,x^2. \tag{3.66}$$

The relation $\langle\partial\mathcal{H}_{\text{tot}}/\partial\gamma\rangle=\partial F_{\text{tot}}/\partial\gamma$ yields the result

$$\langle\eta(0)x\rangle=\gamma\Gamma\langle x^2\rangle-2\gamma\frac{\partial F_p}{\partial\gamma}=\frac{\gamma\Gamma}{a}T_x-2\gamma\frac{\partial F_p}{\partial\gamma}. \tag{3.67}$$

Putting things together we get

$$U_I=\langle\mathcal{H}_I\rangle=-\frac{\gamma\Gamma}{2a}T_x+2\gamma\frac{\partial F_p}{\partial\gamma}. \tag{3.68}$$

In a similar manner we look at the Δ dependence. Using $\omega_i=i\,\Delta$ and the decomposition in creation and annihilation operators (2.8), we get from Eq. (2.16) at $t=0$,

$$\Delta\partial_\Delta\eta(0)=\tilde{\eta}(0)\equiv\sum_i\frac{\Gamma^2}{\omega_i^2+\Gamma^2}c_i x_i, \tag{3.69}$$

implying $\Delta\partial_\Delta\mathcal{H}_{\text{tot}}=\mathcal{H}_B-\tilde{\eta}(0)x$. Taking averages and using Eqs. (3.15), (3.16), and (3.17) brings

$$U_B-\langle\tilde{\eta}(0)x\rangle=\langle\Delta\partial_\Delta\mathcal{H}_{\text{tot}}\rangle=\Delta\partial_\Delta F_{\text{tot}}=U_B(\gamma=0). \tag{3.70}$$

Finally we can change the Debye cutoff Γ. One has

$$\Gamma\partial_\Gamma\mathcal{H}_{\text{tot}}=-\eta(0)x+\tilde{\eta}(0)x+\frac{1}{2}\gamma\Gamma x^2. \tag{3.71}$$

This implies

$$\langle\tilde{\eta}(0)x\rangle=\langle\eta(0)x\rangle-\frac{\gamma\Gamma}{2a}T_x+\Gamma\partial_\Gamma F_p, \tag{3.72}$$

and thus

$$U_B=U_B(\gamma=0)+\frac{\gamma\Gamma}{2a}T_x+\Gamma\partial_\Gamma F_p-2\gamma\partial_\gamma F_p. \tag{3.73}$$

These results yield for the total energy

$$U_{\text{tot}}=U+U_I+U_B=\frac{1}{2}T_x+\frac{1}{2}T_p+U_B(\gamma=0)+\Gamma\partial_\Gamma F_p. \tag{3.74}$$

On the other hand, we have from Eqs. (3.15), (3.16), and (3.17) $U_{\text{tot}}=U_B(\gamma=0)+U_p$. Employing definition (3.46), $T_x=2a\partial_a F_p$ and definition (3.48), $T_p=-2m\partial_m F_p$ and $U_p=\partial_\beta(\beta F_p)$, one reaches the consistency relation

$$(a\partial_a-m\partial_m+\Gamma\partial_\Gamma)\beta F_p=\beta\partial_\beta(\beta F_p). \tag{3.75}$$

It holds because Eq. (3.23) taken at a root ω_i implies

$$(a\partial_a-m\partial_m+\Gamma\partial_\Gamma)\omega_i=\omega_i\quad(i=1,2,3). \tag{3.76}$$

Typically the Debye frequency Γ will be large. Therefore, when γ is not very small, the dimensionless parameter $\gamma\Gamma/a$ has no reason to be small; it can even be large when γ is moderately small. This means that the term $-\langle\eta x\rangle$, usually taken as definition of the interaction energy, is not small; rather, it is large negative. But it is compensated by the self-interaction energy $\frac{1}{2}\gamma\Gamma\langle x^2\rangle=\gamma\Gamma T_x/(2a)$ and by a similar term that is present in the bath energy (3.73).

Recalling that F_p diverges most logarithmically in Γ, we have thus seen that the interaction energy U_I diverges linearly. It is thus rather large, but nevertheless compensated by a similar term from the bath. This behavior is not at all restricted to the quantum regime; it occurs in the same manner at arbitrary large T where $T_x\approx T$.

IV. THERMODYNAMIC ASPECTS OF ADIABATIC CHANGES

A. Generalized thermodynamic formulation

We now make it clear that the relation with standard thermodynamics can be continued much further by introducing the two *effective temperatures*

$$T_p=\frac{\langle p^2\rangle}{m},\quad T_x=a\langle x^2\rangle. \tag{4.1}$$

One reason to do this is that the stationary state for the harmonic potential has a quasi-Gibbsian expression for the Wigner function

$$W(p,x)=W_p(p)W_x(x)=\frac{e^{-\mathcal{K}(p)/T_p}}{\sqrt{2\pi m T_p}}\,\frac{e^{-\mathcal{V}(x)/T_x}}{\sqrt{2\pi T_x/a}} \qquad (4.2)$$

with $\mathcal{K}(p)=p^2/2m$ the kinetic energy and $\mathcal{V}(x)=\frac{1}{2}ax^2$ the potential energy. This expression is quasi-Gibbsian, since there occur two different temperaturelike variables. (Notice that the normalization is $\int dx dp W=1$). There occur the Boltzmann entropies of momenta and coordinate,

$$S_p=-\int dp W(p)\ln[W(p)\sqrt{\hbar}\,]=\frac{1}{2}\ln\frac{mT_p}{\hbar}+\frac{1}{2}, \qquad (4.3)$$

$$S_x=-\int dx W(x)\ln[W(x)\sqrt{\hbar}\,]=\frac{1}{2}\ln\frac{T_x}{\hbar a}+\frac{1}{2} \qquad (4.4)$$

(in S_p and S_x we skipped terms $\ln 2\pi$). The complete ''Boltzmann'' entropy is

$$S_B=S_p+S_x=-\int dp dx W(p,x)\ln[W(p,x)\hbar]$$
$$=\frac{1}{2}\ln\frac{mT_pT_x}{\hbar^2 a}+1. \qquad (4.5)$$

1. Internal energy and interaction energy

The energy of the central particle reads

$$U=\frac{\langle p^2\rangle}{2m}+\frac{1}{2}a\langle x^2\rangle=\frac{1}{2}T_p+\frac{1}{2}T_x. \qquad (4.6)$$

For a discussion of this identification in systems without a self-interaction term, see Sec. II A.

The interaction energy, i.e., the energy of the cloud of bath modes that surround the particle, is defined as

$$U_{\rm int}=U_{\rm tot}-U_B(\gamma=0)-U=U_p-U=U_p-\frac{1}{2}T_p-\frac{1}{2}T_x. \qquad (4.7)$$

Comparing with Eq. (3.74) one gets the shorter result

$$U_{\rm int}=\Gamma\frac{\partial F_p}{\partial\Gamma}. \qquad (4.8)$$

At high temperatures one gets from Eqs. (3.53) and (3.54)

$$U=T+\frac{\beta\hbar^2}{24m}(2a+\gamma\Gamma),\qquad U_{\rm int}=\frac{\beta\hbar^2}{24m}(6a+7\gamma\Gamma). \qquad (4.9)$$

Since the energy of the cloud involves $\hbar$, the nontriviality of the cloud is a quantum effect.

At low temperatures one gets the internal energy

$$U=\frac{\hbar\gamma}{2\pi m}\ln\frac{2m\Gamma}{\gamma}-\frac{\hbar\gamma}{2\pi m}[(1+w)\ln(1+w)+(1-w)$$
$$\times\ln(1-w)]+\frac{\pi\gamma}{6\hbar a}T^2. \qquad (4.10)$$

For large damping this reduces to

$$U=\frac{\hbar\gamma}{2\pi m}\ln\frac{m\Gamma}{\gamma}+\frac{\hbar a}{2\pi\gamma}\left[\ln\frac{\gamma^2}{am}+1\right]+\frac{\pi\gamma}{6\hbar a}T^2. \qquad (4.11)$$

The interaction energy of the cloud is now independent of w,

$$U_{\rm int}=\frac{\hbar\gamma}{2\pi m}+\mathcal{O}(T^4), \qquad (4.12)$$

provided that Γ is large.

2. Generalized free energy and the first and second law

The definition of the effective temperatures admits a clear thermodynamical interpretation. For studying the role of an adiabatically slow variation of an arbitrary parameter, such as a or m, that we shortly denote by α, the free energy F is defined as

$$F=-T_p\ln Z_p-T_x\ln Z_x. \qquad (4.13)$$

The definitions $Z_p=\int dp\,\exp[-\mathcal{K}(p)/T_p]$, $Z_x=\int dx\,\exp[-\mathcal{V}(x)/T_x]$ bring

$$F=-\frac{1}{2}T_p\ln mT_p-\frac{1}{2}T_x\ln\frac{T_x}{a}. \qquad (4.14)$$

For considering changes in system parameters one needs

$$d[-T_p\ln Z_p]=-\ln Z_p dT_p-\frac{T_p}{Z_p}dZ_p$$
$$=\frac{1}{Z_p}\int dp e^{-\beta_p\mathcal{K}(p)}d\mathcal{K}(p)-S_p dT_p,$$

$$d[-T_x\ln Z_x]=-\ln Z_x dT_x-\frac{T_x}{Z_x}dZ_x$$
$$=\frac{1}{Z_x}\int dx e^{-\beta_x\mathcal{V}(x)}d\mathcal{V}(x)-S_x dT_x. \qquad (4.15)$$

Equation (4.13) then yields

$$dF=-S_x dT_x-S_p dT_p+\text{đ}\mathcal{W}_{\rm rev} \qquad (4.16)$$

with, in agreement with the derivations (4.22) and (4.25) below, the work added to the system

$$\text{đ}\mathcal{W}_{\rm rev}=-T_p\frac{dm}{2m}+T_x\frac{da}{2a}. \qquad (4.17)$$

These relations are valid in spite of the fact that T_x and T_p are functions of a and m.

Because of Eqs. (4.6), (4.3), and (4.4), the definition (4.13) is compatible with the standard identification [24,25]

$$F=U-T_pS_p-T_xS_x \tag{4.18}$$

that one would write immediately for a two-temperature system. From this relation one will indeed reproduce the standard formulation for the first law for situations with two temperatures,

$$dU=\text{đ}\mathcal{Q}_{\rm rev}+\text{đ}\mathcal{W}_{\rm rev}, \tag{4.19}$$

$$\text{đ}\mathcal{Q}_{\rm rev}=T_p dS_p+T_x dS_x, \tag{4.20}$$

where $\text{đ}\mathcal{Q}_{\rm rev}$ is the heat reversible added to the particle. A detailed discussion concerning the general definitions of the work and heat is given below, in Sec. VII A.

The generalized thermodynamical relations (4.16)–(4.20) are in close analogy with those proposed recently for nonequilibrium glassy systems [24–26]. Analogously to that situation, F pertains to the particle alone and, except at high T, it differs from the F_p of Eq. (3.44) in the preceding section, which relates to the whole system—to be more precise, to the particle and the cloud of bath modes around it.

Let us recall that F_p satisfies Gibbsian thermodynamics, while F does not. There are many physical systems, such as a Josephson junction strongly coupled to the electromagnetic field, where the natural object to study is nevertheless F, since it relates for that case to properties of the junction only.

It is common wisdom that energy is dispersed if the variations are nonadiabatic changes. This is confirmed by Eq. (7.43), which holds provided the whole time domain where m and a vary is accounted for. This leads to the general result

$$\text{đ}\mathcal{Q}\leqslant T_p dS_p+T_x dS_x \tag{4.21}$$

that is also known from the study of glasses and, more generally, from two-temperature systems.

B. Violation of the Clausius inequality

1. The Clausius inequality at small T

Let us now consider two concrete examples, and study the Clausius inequality $\text{đ}\mathcal{Q}\leqslant T dS_{vN}$, which is one of the possible formulations of the second law.

For a very slow variation of the spring constant a one gets

$$\text{đ}\mathcal{W}_{\rm rev}=\int dx\,dp\,W(p,x)\frac{\partial H}{\partial a}da=\int dx\,W(x)\frac{1}{2}x^2 da$$
$$=T_x\frac{da}{2a}, \tag{4.22}$$

in agreement with Eq. (4.17). The first law implies for the heat added adiabatically to the particle at low T,

$$\text{đ}\mathcal{Q}_{\rm rev}=dU-\text{đ}\mathcal{W}_{\rm rev}=\left(\frac{\partial T_p}{\partial a}+\frac{\partial T_x}{\partial a}-\frac{T_x}{a}\right)\frac{da}{2}$$
$$=-\frac{\pi\gamma}{3\hbar a^2}T^2\,da\;+\mathcal{O}(T^4\,da). \tag{4.23}$$

It is seen that $\text{đ}\mathcal{Q}_{\rm rev}=0$ at $T=0$ for all γ. Using Eqs. (4.1) and (4.5) we derive for large γ and very large Γ

$$dS_B=-\frac{da}{2a}\Bigg[\frac{1}{\ln(\gamma^2/am)}-\frac{ma}{\gamma^2\ln(\Gamma m/\gamma)}$$
$$+\frac{\pi^2\gamma^2T^2}{3\hbar^2a^2\ln(\gamma^2/am)}\left(2-\frac{1}{\ln(\gamma^2/am)}\right)+\mathcal{O}(T^4)\Bigg]. \tag{4.24}$$

At $T=0$ the Clausius inequality says that no heat can be taken from the bath; at best, heat can go from the central system (here, the Brownian particle) to the bath. In our situation $\text{đ}\mathcal{Q}$ is of order T^2, while TdS_{vN} is of order T. Since we only do powercounting in T and both expressions are nontrivial, we may replace here S_{vN} by S_B. Thus for the case $da>0$, where an amount of work $\text{đ}\mathcal{W}_{\rm rev}>0$ is done on the system, the Clausius relation is violated at low but nonzero T.

In the same way one can consider the variation of the (effective) mass m. Here one has

$$\text{đ}\mathcal{W}_{\rm rev}=\int dx\,dp\,W(p,x)\frac{\partial H}{\partial m}dm=-\int dp\,W(p)\frac{p^2}{2m^2}dm$$
$$=-T_p\frac{dm}{2m}, \tag{4.25}$$

again in concordance with Eq. (4.17). This implies

$$\text{đ}\mathcal{Q}_{\rm rev}=\left(T_p\frac{\partial S_p}{\partial m}+T_x\frac{\partial S_x}{\partial m}\right)dm=\left(\frac{\partial T_p}{\partial m}+\frac{\partial T_x}{\partial m}+\frac{T_p}{m}\right)\frac{dm}{2}$$
$$=\frac{\hbar\gamma}{2\pi m^2}dm+\mathcal{O}(T^2). \tag{4.26}$$

In contrast to the previous case there is a transfer of heat even if the bath temperature is zero. Thus, violation of the Clausius inequality is even stronger in this case, since for $dm>0$ one has $\text{đ}\mathcal{Q}>0$, even though $TdS_{vN}=0$ (for $T\rightarrow 0$). This situation with $\text{đ}\mathcal{W}_{\rm rev}<0$ corresponds to the work performed by the system on the environment. To emphasize that the heat comes from the cloud of bath modes, we note that the general relations

$$\text{đ}\mathcal{W}_{\rm rev}=dF_p,\qquad dU=dU_p-dU_{\rm int}=\text{đ}\mathcal{Q}_{\rm rev}+\text{đ}\mathcal{W}_{\rm rev} \tag{4.27}$$

imply

$$\text{đ}\mathcal{Q}_{\rm rev}=TdS_p-dU_{\rm int}. \tag{4.28}$$

For changing m in the $T=0$ situation it indeed holds that

$$đ\mathcal{Q}_{\text{rev}}=-dU_{\text{int}} \tag{4.29}$$

for all values of w, even when Γ is not very large. For a change in a it holds that $dU_{\text{int}}=\mathcal{O}(T^4)$, but Eq. (4.28) nevertheless reproduces Eq. (4.23), because of relation (3.59).

Let us briefly discuss consequences drawn from the violation of the Clausius inequality in the quantum regime. First of all, it appears that it occurs in the overall Gibbsian state, so that globally (i.e., when applied to the overall closed system) thermodynamics is valid by definition. In particular, since the overall system does not absorb heat during any variation of a parameter, and $đ\mathcal{Q}=0$ is consistent with the $T\to 0$ case of the Clausius inequality (later we will see that this is also the case at finite temperatures, where $đ\mathcal{Q}$ is still zero). Nevertheless, the local state of the particle is not Gibbsian and does allow violations as we have seen. We stress that this violation arises due to quantum entanglement, which leads to non-Gibbsian effective temperatures for the stationary state of the Brownian particle. If the effective temperatures for $T\to 0$ would equal their Gibbsian values $\hbar\omega_0/2$, the state of the particle would be pure, which is impossible since it does interact with the bath.

When later discussing the Thomson's formulation of the second law, we will see that it is perfectly valid for the overall Gibbsian state, so that the above violation of the Clausius inequality provides us with an explicit example showing that at low temperatures the very equivalence between different formulations of the second law is lost.

A further aspect of this matter is the squeezing of phase space and entropy, relevant for computing in the quantum regime. In a separate paper we have shown that the so-called Landauer bound for the erasure of one bit of information, that arises from the Clausius inequality, is violated in a similar manner [39].

Notice again that the effective temperatures remain finite in the limit $T\to 0$ [see Eqs. (3.63), (3.64) and Fig. 1], and both are larger than the bath temperature T. The fact that they are nonequal is due to a mixed state of the particle. Indeed, a quantum system nonweakly interacting with its environment, will be in a mixed state even if the whole closed system (the particle and environment together) is in a pure state (e.g., the vacuum state).

The existence of different temperatures T_x, T_p, and T for the subsystem and bath should be compared with the zeroth law, which states that systems interacting for a long time are in equilibrium, and share common temperature. Notice especially that the above difference between temperatures is not a consequence of any metastability and/or incomplete equilibration, so that our effective temperatures do not depend on the dynamics of the particle and have somewhat more definite status compared with those defined, e.g., for glassy systems [24,25,27]. Typical derivations of the zeroth law (see, e.g., Ref. [5] for one of the most clear examples) essentially use the assumptions that the interaction with the bath is very weak, and that the total entropy can be considered as the sum of entropies of the subsystem and the bath. Evidently, this last condition is not satisfied in our case, except for the limit $\gamma\to 0$, where T_x and T_p tend to their Gibbsian value [see Eq. (3.50)] of the harmonic oscillator coupled very weakly to its bath, the situation treated in all textbooks.

Let us notice that in literature some other ways were proposed to establish effective characteristics for nonunderdamped Brownian oscillator. In Ref. [9] it is shown that there is a mapping to the Gibbsian (underdamped) oscillator through the definition of an effective mass and frequency. For the description of He$_3$, Prokof'ev studies a related model with a gap in $J(\omega)$ at small ω [40]. In this approach he makes a different identification for the effective temperature. Surely, choosing a quantity as "effective temperature" is to some extent a matter of taste, that can only be justified by the induced simplification of the physical results. For our thermodynamic approach other definitions of effective temperatures will not be very helpful. Our T_p and T_x, however, allow us to formulate the generalized Clausius inequality and they also occur in the Maxwell-Boltzmann-like form (4.2) of the Wigner function. Last but not the least, these effective temperatures enter in the same way as in glasses and other two-temperature systems, such as black holes.

2. Von Neumann entropy

In the next section we shall discuss the von Neumann entropy of the central particle. To investigate it one needs the density matrix corresponding to the Wigner function (4.2). For the harmonic oscillator this can be worked out explicitly. One approach is to introduce an effective mass and an effective frequency [9], and insert these results in the expression for the entropy of the effective harmonic oscillator. We found it more insightful to redo the derivation. The standard relation

$$\left\langle x+\frac{u}{2}\middle|\rho\middle|x-\frac{u}{2}\right\rangle=\int dp\, e^{-ipu/\hbar}W(p,x) \tag{4.30}$$

connects the density matrix in coordinate representation with the Wigner function. From this relation one gets the following formula [38]:

$$\langle x|\rho|x'\rangle=\frac{1}{\sqrt{2\pi\langle x^2\rangle}}\exp\left[-\frac{(x+x')^2}{8\langle x^2\rangle}-\frac{(x-x')^2}{2\hbar^2/\langle p^2\rangle}\right]. \tag{4.31}$$

The physical meaning of Eq. (4.31) is clear The diagonal elements ($x=x'$) are distributed at the scale $\sqrt{\langle x^2\rangle}$, while the maximally off-diagonal elements ($x=-x'$), which characterize coherence, are distributed with the characteristic scale $\hbar/\sqrt{\langle p^2\rangle}$.

We have to find eigenfunctions and eigenvectors of this density matrix,

$$\int dx'\langle x|\rho|x'\rangle f_n(x')=p_n f_n(x). \tag{4.32}$$

The solution of this problem uses some tabulated formulas for Hermite polynomials, and results in

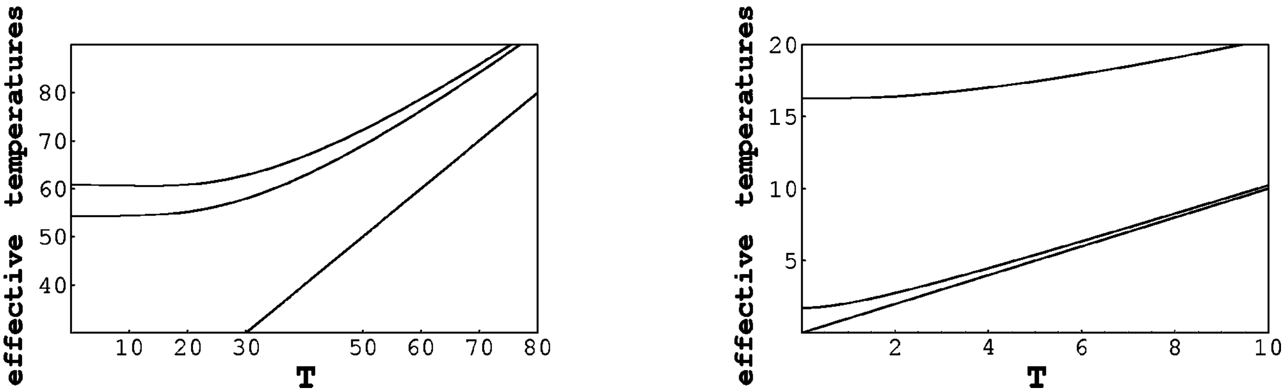

FIG. 1. The effective temperatures T_p, T_x vs the bath temperature T for two values of the dimensionless damping. For the parameters involved we take the following values: $\hbar\gamma/(4\pi m)=1$, $\hbar\Gamma/(2\pi)=100$. Left part, $am/\gamma^2=80$ (underdamping), from top to bottom, T_p, T_x, T. Right part, the same but with $am/\gamma^2=0.2$ (moderate overdamping).

$$p_n=\frac{1}{v+\frac{1}{2}}\left[\frac{v-\frac{1}{2}}{v+\frac{1}{2}}\right]^n, \tag{4.33}$$

$$f_n(x)=c\,H_n(c\,x)e^{-c^2x^2/2}, \tag{4.34}$$

$$c=\left(\frac{\langle p^2\rangle}{\hbar^2\langle x^2\rangle}\right)^{1/4}, \quad v=\frac{\Delta p\,\Delta x}{\hbar}=\sqrt{\frac{\langle p^2\rangle\langle x^2\rangle}{\hbar^2}}=\sqrt{\frac{mT_pT_x}{\hbar^2 a}}, \tag{4.35}$$

where H_n are Hermite polynomials, and it holds that $v\geqslant\frac{1}{2}$ due to the Heisenberg uncertainty relation. The result for the von Neumann entropy now reads [9]

$$\begin{aligned}S_{vN}&=-\sum_n p_n\ln p_n\\&=\left(v+\frac{1}{2}\right)\ln\left(v+\frac{1}{2}\right)-\left(v-\frac{1}{2}\right)\ln\left(v-\frac{1}{2}\right).\end{aligned} \tag{4.36}$$

The first terms in its large v expansion are

$$S_{vN}=\ln v+1-\frac{1}{24v^2}-\frac{1}{320v^4}-\frac{1}{2688v^6}. \tag{4.37}$$

From Eqs. (4.3), (4.4), and (4.5) we notice that the same quantity v governs behavior of the Boltzmann entropy,

$$S_B=\frac{1}{2}\ln\frac{\langle x^2\rangle\langle p^2\rangle}{\hbar^2}+1=\ln v+1. \tag{4.38}$$

This appears to coincide with the leading terms of Eq. (4.37). It is known to be larger than the von Neumann entropy, and this is obvious from the sign of the correction terms.

If some parameter (a or m) is varied, then the derivative of S_{vN} with respect to it reads

$$dS_{vN}=\ln\frac{v+\frac{1}{2}}{v-\frac{1}{2}}\,dv. \tag{4.39}$$

In other words, the sign of the change in S_{vN} is determined by the sign of the change in v. This holds as well for the change in S_B, so qualitatively they carry the same information, and this already was used above to simplify one point of the discussion, namely, the Clausius inequality at low T.

Let us stress that von Neumann entropy S_{vN} is the unique quantum measure of localization, whereas the entropies S_p and S_x characterize localizations of momentum and coordinate separately. The differences between S_B and S_{vN} are due to the fact that in quantum theory momentum and coordinate cannot be measured simultaneously; in this sense S_p and S_x characterize two different measurement setups. Nevertheless, for the harmonic particle if S_{vN} increases (decreases), then S_p+S_x increases (decreases) as well. Notice that the real importance of S_p and S_x becomes clear when they have to be used to generalize the Clausius inequality. The von Neumann entropy cannot be used for this purpose whenever $T_x\neq T_p$.

3. Clausius inequality at large T

At low T only power counting in T was needed for showing the violation of the Clausius inequality. The precise definition of entropy, and the quantitative difference between the Boltzmann entropy and the von Neumann entropy were not essential, since then $TdS\to 0$ anyhow. Here we wish to show that the same violation already happens at arbitrarily large temperature. To do this we have to use the von Neumann entropy of the subsystem.

In this section we consider very large temperatures, $T\gg\hbar\Gamma$. Using Eq. (3.54) we find from Eq. (4.26) for a change in m that

$$\text{đ}\mathcal{Q}=\left[1-\frac{\beta^2\hbar^2 a}{12m}\right]\frac{T}{2m}dm,$$

$$dS_{vN}=\left[1-\frac{\beta^2\hbar^2(a+\gamma\Gamma)}{12m}\right]\frac{1}{2m}dm. \tag{4.40}$$

So, for a change $dm>0$ it is seen that at arbitrarily large temperature the Clausius inequality is violated. The relative violation $(đ\mathcal{Q}-TdS_{vN})/đ\mathcal{Q}$ is of order $\hbar^2\gamma\Gamma/(mT^2)$.

For a change in a we find

$$đ\mathcal{Q}=\left\{-\frac{1}{2a}+\frac{\hbar^2\beta^2}{24m}-\frac{\beta^4\hbar^4[a+(2/3)\gamma\Gamma]}{480m^2}\right\}T\,da, \tag{4.41}$$

$$TdS_{vN}=\left\{-\frac{1}{2a}+\frac{\hbar^2\beta^2}{24m}-\frac{\beta^4\hbar^4[a+\gamma\Gamma]}{480m^2}\right\}T\,da. \tag{4.42}$$

These expressions differ at relative order $\beta^4\hbar^4\gamma\Gamma/m^2$, and the Clausius inequality is violated for $da>0$.

The important conclusion of this Sec. is that the violation of the Clausius inequality already occurs at arbitrarily high temperatures. Later we point out that a similar conclusion can be drawn about the violation of the zeroth law at large temperatures.

We stress that the Clausius inequality is violated for any finite coupling, and the violating terms only disappear in the weak coupling limit $\gamma\to 0$, or in the classical limit $\hbar\to 0$, equivalent to the high-temperature limit.

4. Clausius inequality for comparing two systems

For nonequilibrium systems the question has not been settled as to whether the von Neumann entropy is the true physical entropy. As we are inclined to believe that it is, we have discussed that entropy above.

Let us, however, now consider cases where there is no doubt. For systems in true Gibbsian equilibrium the proper entropy of the subsystem is surely its von Neumann entropy. We can now compare two such equilibrium systems, having slightly different system parameters. In standard thermodynamics such a comparison does not yield a new insight, as the equilibrium state of the system is independent of its history. We should point out that in the thermodynamics of glasses it is customary to compare cooling experiments at different but fixed pressures. A related comparison was also made for black holes: it could be shown that comparing the situation of a single black hole before and after a small amount of matter was added, is analogous to comparing two different black holes with slightly different masses [41]. This universality pointed at a thermodynamic behavior of black holes, and the physical framework could indeed be provided by one of us, by drawing an analogy with the thermodynamics of glasses [27].

For our present case we can compare two equilibrium systems at slightly different temperatures. This has the benefit that the work term is absent, thus needing no interpretation, and it implies $đ\mathcal{Q}=dU$. Using the fully exact expressions for the energy and the von Neumann entropy, it is then straightforward to show that at large T,

$$đ\mathcal{Q}-TdS_{vN}=\frac{\beta^2\hbar^2\gamma\Gamma}{24m}dT. \tag{4.43}$$

The standard *expectation* that this should vanish is again seen to be invalid, and the Clausius inequality is violated for $dT>0$. As before, the terms in the right hand side vanish only in the weak coupling limit $\gamma\to 0$, the classical limit $\hbar\to 0$, or the infinite temperature limit $\beta\to 0$.

5. On our identification of the energy of the subsystem

In Sec. II A we have considered two physical situations. In the first case the Hamiltonian contains a self-interaction term $\sim x^2$. For that case the above results on the Clausius inequality apply unambiguously. In the second case there is no such self-interaction, but the potential energy $\frac{1}{2}bx^2$ is split as $\frac{1}{2}ax^2+\frac{1}{2}\gamma\Gamma x^2$, and the first part is counted in the energy of the subsystem, while the last part is counted with the interaction energy. Let us now shortly look at what happens when this is not done, and $\tilde{U}=\langle\tilde{H}\rangle$ is considered as energy of the subsystem. At large T one will have $\tilde{U}=U+\frac{1}{2}(\gamma\Gamma/a)T=T+\frac{1}{2}(\gamma\Gamma/a)T$. Since the work is not modified by this identification, one will have a shift in the change of heat, $d\tilde{Q}=dQ+\frac{1}{2}\gamma\Gamma[dT/a-Tda/a^2]$. From Eqs. (4.42) and (4.43) it is seen that then even at very large temperatures $d\tilde{Q}-TdS_{vN}$ will not vanish whenever γ is nonzero. Thus, when there is no self-interaction our identification of $\mathcal{H}$ as the Hamiltonian of the subsystem is already mandatory for having a proper classical limit. The underlying reason is that the Wigner function has the Maxwell-Boltzmann form

$$\exp\left(-\left[\frac{1}{2m}p^2+\tfrac{1}{2}ax^2\right]/T\right),$$

involving a and not $b=a+\gamma\Gamma$. This fixes the entropy, and by the Clausius inequality also the change in heat, thus leaving one consistent choice for the energy.

V. EXACT DYNAMICAL SOLUTION

We now consider the situation where our closed system starts at time $t=0^-$ from a Gibbsian initial distribution. It could arise if long before the total system was coupled to a "superbath," that allowed relaxation to equilibrium, after which the connection was cut [36]. A more realistic situation occurs when the bath has small nonlinearities, that drive the whole system to its global Gibbsian state.

A. The case when the initial state is a modified Gibbsian

We assume that for $t<0$ the system is in a Gibbsian state at temperature T with certain parameters $a=a_0$, $m=m_0$, $\gamma=\gamma_0$. At $t=0$ these parameters are instantaneously changed to a, m and γ, and the system will relax to a steady state. This setup generalizes previous studies in which for times $t\leqslant 0$ particle and bath are uncoupled, described by $\gamma_0=0$. An important benefit is that in the strong damping limit the present initial state can be close to the final state, which is, of course, impossible if $\gamma_0=0$ but γ is large. When making the change $\gamma_0 \to \gamma$ at $t=0$, an amount of work $\frac{1}{2}(\gamma - \gamma_0)\Gamma \langle x^2 \rangle_0$ has to be supplied to the system. This was truly large in our paper [2], where we took $\gamma_0 = 0$, but Γ and γ large. In the present setup we can choose $\gamma_0 = \gamma$, but $a_0 \neq a$, implying that the work need not be large, even when the Debye frequency Γ is large.

1. The eigenmodes of the initial state

In the most general case the Hamiltonian has for $t<0$ the parameters a_0, γ_0, and m_0. It reads

$$\mathcal{H} = \sum_{i \geqslant 0} \frac{p_i^2}{2m_i} + \frac{1}{2} \sum_{i,j \geqslant 0} \sqrt{m_i m_j}\, x_i A_{ij} x_j \tag{5.1}$$

with

$$A_{00} = \frac{a_0 + \gamma_0 \Gamma}{m_0}, \quad A_{0i} = A_{i\,0} = -\frac{c_i^{(0)}}{\sqrt{m_0 m_i}}, \quad A_{ij} = \omega_i^2 \delta_{ij}, \tag{5.2}$$

where $c_i^{(0)}$ is given by Eq. (2.23) with γ_0 replacing γ,

$$c_i^{(0)} = \sqrt{\frac{2\gamma_0 m_i \omega_i^2 \Delta}{\pi} \frac{\Gamma^2}{\omega_i^2 + \Gamma^2}}. \tag{5.3}$$

Let us denote the eigenvalues of A by ν_k^2. From a previous section, Eqs. (3.10) and (3.12), we infer that the eigenfrequencies are shifted,

$$\nu_k = \omega_k - \frac{1}{\pi} \phi_0(\omega_k)\, \Delta, \tag{5.4}$$

where ϕ_0, satisfying $0 \leqslant \phi_0 \leqslant \pi$, is given by

$$\phi_0(\nu) = \arctan \frac{\gamma_0 \Gamma^2 \nu}{(a_0 - m_0 \nu^2)(\nu^2 + \Gamma^2) + \gamma_0 \Gamma \nu^2}. \tag{5.5}$$

In later sections we only need that for large Γ,

$$\sin \phi_0(\nu) = \frac{\gamma_0 \nu}{\{(a_0 - m_0 \nu^2)^2 + \gamma_0^2 \nu^2\}^{1/2}}. \tag{5.6}$$

The eigenvectors are

$$e_0^k = \alpha_k, \quad e_i^k = \frac{c_i^{(0)} \alpha_k}{\sqrt{m_0 m_i}(\omega_i^2 - \nu_k^2)} \tag{5.7}$$

with normalization factor

$$\frac{1}{\alpha_k^2} = 1 + \sum_{i \geqslant 1} \frac{[c_i^{(0)}]^2}{m_0 m_i (\omega_i^2 - \nu_k^2)^2}. \tag{5.8}$$

The following normalization conditions hold:

$$\sum_k e_i^k e_j^k = \delta_{ij}, \quad \sum_{i \geqslant 0} e_i^k e_i^l = \delta_{kl}. \tag{5.9}$$

For small Δ one may use

$$\sum_{i=-\infty}^{\infty} \frac{1}{[(i-k)\pi + \phi_0(\omega_k)]^2} = \frac{1}{\sin^2 \phi_0(\omega_k)} \tag{5.10}$$

to find

$$\alpha_k = \sqrt{\frac{2\Delta m_0 (\Gamma^2 + \omega_k^2)}{\pi \gamma_0 \Gamma^2}} \sin \phi_0^k,$$

$$e_i^k = \sqrt{\frac{\Gamma^2 + \omega_k^2}{\Gamma^2 + \omega_i^2}} \frac{2\Delta \omega_i \sin \phi_0^k}{\pi(\omega_i^2 - \nu_k^2)}, \tag{5.11}$$

where $\phi_0^k = \phi_0(\omega_k)$. In the zero coupling limit $\gamma_0 \to 0$ one has $\phi_0^k \to 0$, so that $\nu_k \to \omega_k$ and indeed $e_i^k \to \delta_{ik}$. The latter setup occurs in the standard treatments where bath and subsystem are initially uncoupled.

2. The noise

We assume Gibbsian equilibrium for $t \leqslant 0$. Let us now introduce for the creation and annihilation operators $b_k^\dagger$, b_k, satisfying $[b_k, b_l^\dagger] = \delta_{kl}$ by

$$x_i = \sum_k \sqrt{\frac{\hbar}{2 m_i \nu_k}} e_i^k (b_k^\dagger e^{i\nu_k t} + b_k e^{-i\nu_k t}),$$

$$p_j = i \sum_k \sqrt{\frac{\hbar m_j \nu_k}{2}} e_j^k (b_k^\dagger e^{i\nu_k t} - b_l e^{-i\nu_k t}), \tag{5.12}$$

$$x = \sum_k \sqrt{\frac{\hbar \Delta (\Gamma^2 + \nu_k^2)}{\pi \gamma_0 \Gamma^2 \nu_k}} \sin \phi_0^k\, (b_k^\dagger e^{i\nu_k t} + b_k e^{-i\nu_k t}),$$

$$p = \sum_k \sqrt{\frac{\hbar \Delta (\Gamma^2 + \nu_k^2)}{\pi \gamma_0 \Gamma^2 \nu_k}} \sin \phi_0^k\, m_0 \nu_k (i\, b_l^\dagger e^{i\nu_k t} - i\, b_l e^{-i\nu_k t}). \tag{5.13}$$

They indeed satisfy $[x_i, p_j] = i\hbar \delta_{ij}$ due to the normalization condition, as well as $[x,p] = i\hbar$, $[x, p_i] = [x_i, p] = 0$. For $t<0$ the Hamiltonian then reads

$$\mathcal{H} = \frac{1}{2} \sum_k \hbar \nu_k (b_k^\dagger b_k + b_k b_k^\dagger) = \sum_k \hbar \nu_k \left(b_k^\dagger b_k + \frac{1}{2} \right). \tag{5.14}$$

In the Gibbsian state that describes our closed system for $t<0$, the density matrix is

$$\rho = \frac{1}{Z} e^{-\beta \mathcal{H}}. \tag{5.15}$$

It has the Bose occupation numbers

$$\langle b_k^\dagger b_k + b_k b_k^\dagger \rangle = 1 + \frac{2}{e^{\beta\hbar\nu_k}-1} = \coth\left(\frac{1}{2}\beta\hbar\nu_k\right). \tag{5.16}$$

Combining Eqs. (2.16) and (5.12) we now have for the noise

$$\eta(t) = \sum_{i\geqslant 1}\sum_k \sqrt{\frac{\hbar}{2m_i\nu_k}}\, c_i\, e_i^k\left[(b_k^\dagger + b_k)\cos\omega_i t + i\frac{\nu_k}{\omega_i}(b_k^\dagger - b_k)\sin\omega_i t\right]. \tag{5.17}$$

To carry our the i sum, we have to evaluate

$$\sum_{i\geqslant 1}\frac{c_i e_i^k \cos\omega_i t}{\sqrt{m_i}} = \sqrt{\frac{2\gamma\Gamma^2\Delta}{\pi(\Gamma^2+\nu_k^2)}}\,\frac{2\Delta\sin\phi_0^k}{\pi}\sum_{i\geqslant 1}\left(\frac{\nu_k^2}{\omega_i^2-\nu_k^2} + \frac{\Gamma^2}{\omega_i^2+\Gamma^2}\right)\cos\omega_i t. \tag{5.18}$$

Gradstein and Rhyzhik [42] present on p. 40, Eq. (1.445.2) the equality

$$\sum_{k=1}^{\infty}\frac{\cos kx}{k^2+\alpha^2} = -\frac{1}{2\alpha^2} + \frac{\pi}{2\alpha}\,\frac{\cosh(\pi\alpha - \alpha x)}{\sinh \pi\alpha}. \tag{5.19}$$

According to them it holds for $0\leqslant x\leqslant 2\pi$, but it actually only holds for $0\leqslant x\leqslant\pi$, while further it is symmetric and periodic. We have to apply this with $x = t\Delta$, which is surely between 0 and π, for the cases $\alpha = i\nu/\Delta$ and $\alpha = \Gamma/\Delta$,

$$\sum_{i\geqslant 1}\frac{c_i e_i^k\cos\omega_i t}{\sqrt{m_i}} = \sqrt{\frac{2\gamma\Gamma^2\Delta}{\pi(\Gamma^2+\nu_k^2)}}\sin\phi_0^k\left[\Gamma\frac{\cosh(\pi\Gamma/\Delta - \Gamma t)}{\sinh(\pi\Gamma/\Delta)} - \frac{\nu_k\cos(\pi\nu_k/\Delta - \nu_k t)}{\sin(\pi\nu_k/\Delta)}\right] \tag{5.20}$$

$$= \sqrt{\frac{2\gamma\Gamma^2\Delta}{\pi(\Gamma^2+\nu_k^2)}}[\Gamma\sin\phi_0^k\, e^{-\Gamma t} + \nu_k\cos(\phi_0^k + \nu_k t)]. \tag{5.21}$$

In the last step we have used Eq. (5.4) and neglected terms of order $\exp(-2\Gamma/\Delta)$, which are extremely small. The primitive of this relation yields

$$\sum_{i\geqslant 1}\frac{c_i e_i^k\sin\omega_i t}{\sqrt{m_i}\,\omega_i} = \sqrt{\frac{2\gamma\Gamma^2\Delta}{\pi(\Gamma^2+\nu_k^2)}}[-\sin\phi_0^k\, e^{-\Gamma t} + \sin(\phi_0^k + \nu_k t)]. \tag{5.22}$$

When we insert this in expression (5.18) for the noise we have the explicit result

$$\eta(t) = \sum_k\sqrt{\frac{\gamma\hbar\nu_k\Gamma^2\Delta}{\pi(\Gamma^2+\nu_k^2)}}\left[\left(\frac{\Gamma - i\nu_k}{\nu_k}b_k^\dagger + \frac{\Gamma + i\nu_k}{\nu_k}b_k\right)\times\sin\phi_0^k e^{-\Gamma t} + e^{i\phi_0^k + i\nu_k t}b_k^\dagger + e^{-i\phi_0^k - i\nu_k t}b_k\right]. \tag{5.23}$$

The memory of the initial state (i.e., the dependence on a_0, m_0, and γ_0, coded in ϕ_0^k) is washed out after a time $\tau_\eta = 1/\Gamma$, apart from a harmless phase factor. Notice that the time dependencies are $\exp(i\nu_k t)$, as one would have expected from Eq. (5.12). Also note that the $\exp(-\Gamma t)$ terms underline the special role of $t=0$, just as it does elsewhere in Eq. (2.18). We shall later verify that this passes a consistency check.

3. The noise correlator

The noise correlator now decomposes in two parts:

$$K(s,t) = \frac{1}{2}\langle\, \eta(t)\,\eta(s) + \eta(s)\,\eta(t)\,\rangle = K_0(s-t) + K_1(s,t). \tag{5.24}$$

The first term is the stationary noise known from the situation where system and bath were initially uncoupled:

$$K_0(s-t) = \frac{1}{\pi}\int_0^\infty d\omega\,\bar{K}_0(\omega)\cos\omega(t-s) \tag{5.25}$$

$$= \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\bar{K}(\omega)e^{i\omega(s-t)},$$

with spectrum

$$\bar{K}_0(\omega) = \frac{\gamma\hbar\omega}{\tanh\frac{1}{2}\beta\hbar\omega}\,\frac{\Gamma^2}{\Gamma^2+\omega^2}. \tag{5.26}$$

It indeed does not involve parameters of the initial state. The connection between properties of the noise and the friction kernel is the consequence of quantum fluctuation-dissipation theorem [5,9,17].

As shown in Ref. [43], the quantum noise has correlation $K_0(t)=-\ln(\Gamma t)>0$ at small times, $t\ll 1/\Gamma$. At $T=0$ there occurs for large times the celebrated power-law, anticorrelated decay

$$K_0(t)=-\frac{\hbar\gamma}{\pi t^2}. \tag{5.27}$$

This is cut off at times larger than the universal quantum coherence time $\tau_\hbar=\hbar/T$, where

$$K_0(t)=-\frac{\pi\gamma T^2}{\hbar}\left[\sinh\left(\frac{\pi t}{\beta\hbar}\right)\right]^{-2}. \tag{5.28}$$

The divergence of this expression at $t=0$ shows that a regulator like Γ is needed.

Let us briefly explain the qualitative reasons for the above structure of the quantum noise. As seen from Eq. (2.16), the quantum noise is just a weighted sum of the unperturbed coordinates of the baths oscillators. For $T\to 0$ the unperturbed bath appears in its lowest energy level, and since energy and coordinate do not commute (just because coordinate and momentum do not commute), the quantum noise fluctuates even for $T\to 0$, and brings a nontrivial structure to $K(t)$ in contrast to the classical case, where the noise is just absent for zero temperatures. On the other hand, the total intensity of the quantum noise is zero for $T\to 0$: as seen from Eq. (5.26), $\int dt K(t)=2\gamma T$. For the total integral to be zero, the correlator $K(t)$ should change its sign at some intermediate time t. For longer times the quantum noise is anticorrelated. The correlator displays a power-law behavior, since the correlation timescale $\hbar/T$ is now infinite. A colored noise generated by the low-temperature quantum thermal bath will be the main cause of our effects. The classical white noise situation $K_0(t)=2\gamma T\delta(t)$ is recovered by taking the high-temperature limit ($T\gg\hbar\Gamma$).

The second term of Eq. (5.24) is due to the initial correlation of particle and bath,

$$K_1(s,t)=K_{11}e^{-\Gamma(s+t)}+K_{12}(s)e^{-\Gamma t}+K_{12}(t)e^{-\Gamma s}, \tag{5.29}$$

$$K_{11}=\frac{1}{\pi}\int_0^\infty d\omega\,\bar{K}_0(\omega)\frac{\Gamma^2+\omega^2}{\omega^2}\sin^2\phi_0(\omega), \tag{5.30}$$

$$K_{12}(t)=\frac{1}{\pi}\int_0^\infty d\omega\,\bar{K}_0(\omega)\left[\frac{\Gamma}{\omega}\cos[\phi_0(\omega)+\omega t]\right. \\ \left.-\sin[\phi_0(\omega)+\omega t]\right]\sin\phi_0(\omega), \tag{5.31}$$

where ϕ_0 is defined by Eq. (5.5).

The standard case of initially uncoupled Brownian particle and bath is recovered for $\gamma_0\to 0$, where $\phi_0\to 0$. Then K_{12} and K_{11} vanish, making the noise correlator time-translation invariant. In the general case, the initial correlation only affects the very short time regime $t\leqslant\tau_\eta=1/\Gamma$ (remember that we assume that Γ is larger than other characteristic frequencies of the damped Brownian particle).

4. Variances and covariance arising from the initial state

The Gibbsian initial state leads to three coupled Gaussian random variables: the random initial conditions, $z_1=p_0$ and $z_2=x_0$, and the noise $z_3(t)=\eta(t)$ for $t\geqslant 0$. More precisely, when we discretize the time axis in points t_i, the function $z_3(t)$ becomes a set of variables $z_{3,i}$. Their correlations and cross correlations are

$$\langle p_0^2\rangle=m_0T_p(a_0,m_0,\gamma_0),\quad \langle x_0^2\rangle=\frac{T_x(a_0,m_0,\gamma_0)}{a_0},$$

$$K(s,t)=\frac{1}{2}\langle\eta(s)\eta(t)+\eta(t)\eta(s)\rangle, \tag{5.32}$$

$$\langle p_0x_0\rangle=0,\quad S_1(t)=\frac{1}{2}\langle\eta(t)p_0+p_0\eta(t)\rangle,$$

$$S_2(t)=\frac{1}{2}\langle\eta(t)x_0+x_0\eta(t)\rangle. \tag{5.33}$$

For $t'\leqslant 0$ we also define the more general quantities

$$S_1(t,t')=\frac{1}{2}\langle\eta(t)p(t')+p(t')\eta(t)\rangle,$$

$$S_2(t,t')=\frac{1}{2}\langle\eta(t)x(t')+x(t')\eta(t)\rangle. \tag{5.34}$$

It holds that

$$S_1(t,t')=m_0\frac{\partial}{\partial t'}S_2(t,t'). \tag{5.35}$$

The most interesting term reads

$$S_2(t,t')=\frac{\hbar\sqrt{\gamma}}{\pi\sqrt{\gamma_0}}\int_0^\infty d\nu\sin\phi_0(\nu)\ \coth\frac{1}{2}\beta\hbar\nu \\ \times\left[\left(\frac{\Gamma}{\nu}\cos\nu t'-\sin\nu t'\right)\sin\phi_0(\nu)\,e^{-\Gamma t}\right. \\ \left.+\cos[\phi_0(\nu)+\nu t-\nu t']\right]. \tag{5.36}$$

It yields

$$S_1(t)=\frac{\hbar m_0\sqrt{\gamma}}{\pi\sqrt{\gamma_0}}\int_0^\infty d\nu\,\nu\sin\phi_0(\nu)\coth\frac{1}{2}\beta\hbar\nu \\ \times\{-\sin\phi_0(\nu)\,e^{-\Gamma t}+\sin[\phi_0(\nu)+\nu t]\} \tag{5.37}$$

and $S_2(t)=S_2(t,0)$.

For the sake of completeness we also mention that for $t\leqslant 0,\ t'\leqslant 0$

$$\frac{1}{2}\langle x(t)x(t')+x(t')x(t)\rangle=\frac{\hbar}{\pi\gamma_0}\int_0^\infty d\nu\frac{\Gamma^2+\nu^2}{\nu\Gamma^2}\sin^2\phi_0(\nu)\times\coth\frac{1}{2}\beta\hbar\nu\cos\nu(t-t'), \tag{5.38}$$

which allows us to determine $\langle x(t)x(0)+x(0)x(t)\rangle$ and $\langle x^2(t)\rangle$. The results pertain for $t>0$, $t'\geqslant 0$ if the system is not modified at $t=0$, viz. $a_0=a$, $m_0=m$, $\gamma_0=\gamma$. Therefore they allow a consistency check on the average of $\mathcal{H}_I$ of Eq. (2.19) in the stationary state. For large Γ there occurs an apparent time dependence $\sim\Gamma\exp(-\Gamma t)$, arising from its first two terms $-\langle\eta(t)x(t)\rangle+\gamma\Gamma\exp(-\Gamma t)\langle x(0)x(t)\rangle$. It can now be verified that, in the stationary state, these large, fast terms cancel, and so do the other time dependencies.

The general case where the system is modified at $t=0$ will be considered now.

B. Exact solution of the Langevin equation

Now we consider the exact solution of the quantum Langevin equation,

$$\dot{x}=\frac{p}{m},\quad \dot{p}=-ax-\gamma(t)x(0)-\int_0^t dt'\,\gamma(t-t')\dot{x}(t')+\eta(t), \tag{5.39}$$

The general solution of Eq. (5.39) is obtained with the help of Laplace transformation. The reader may recall the following standard relations between functions $A(t)$, $B(t)$ and their Laplace-transforms $\mathcal{L}\{A\}=\hat{A}(s)=\int_0^\infty dt\,e^{-st}A(t)$:

$$\mathcal{L}\left\{\int_0^t dt' A(t-t')B(t')\right\}=\hat{A}(s)\hat{B}(s),$$
$$\mathcal{L}\{\dot{A}\}=-A(0)+s\hat{A}(s). \tag{5.40}$$

One gets

$$ms\hat{x}(s)-mx(0)=\hat{p}(s),$$
$$s\hat{p}(s)-p(0)=-a\hat{x}(s)-\hat{\gamma}(s)s\hat{x}(s)+\hat{\eta}(s). \tag{5.41}$$

Together this yields

$$\hat{x}(s)=\frac{1}{m}[mx(0)s+p(0)+\hat{\eta}(s)]\,\hat{f}(s), \tag{5.42}$$

where

$$\hat{f}(s)=\frac{m}{ms^2+a+s\hat{\gamma}(s)}. \tag{5.43}$$

Thus, the solution of Eq. (5.39) reads

$$x(t)=x(0)\dot{f}(t)+\frac{1}{m}p(0)f(t)+\frac{1}{m}\int_0^t dt' f(t-t')\,\eta(t'), \tag{5.44}$$

$$p(t)=p(0)\dot{f}(t)+mx(0)\ddot{f}(t)+\int_0^t dt'\,\dot{f}(t-t')\,\eta(t'), \tag{5.45}$$

where $\hat{f}(s)$ and $\hat{\gamma}(s)$ are the Laplace transforms of $f(t)$, $\gamma(t)$. Expanding $\hat{f}(s)$ for small s, one finds that $f(0)=\ddot{f}(0)=0$, $\dot{f}(0)=1$. Now we turn to our standard case of the Drude-Ullersma spectrum,

$$\gamma(t)=\gamma\Gamma e^{-\Gamma|t|},\quad \hat{\gamma}(s)=\frac{\gamma\Gamma}{\Gamma+s}. \tag{5.46}$$

For $\hat{f}(s)$ one has

$$\hat{f}(s)=\frac{m(\Gamma+s)}{(s+\Gamma)(ms^2+a)+s\gamma\Gamma}=\frac{\Gamma+s}{(s+\omega_1)(s+\omega_2)(s+\omega_3)}=\frac{\Gamma+s}{P_3(-s)}, \tag{5.47}$$

where $P_3(s)$ was defined in Eq. (3.23), where also its roots $\omega_{1,2,3}$ are discussed.

Likewise, one has for the initial Gibbsian states

$$\hat{f}_0(s)=\frac{m_0(\Gamma+s)}{(s+\Gamma)(m_0s^2+a_0)+s\gamma_0\Gamma}. \tag{5.48}$$

One may write

$$\hat{f}(s)=\sum_{i=1}^3\frac{f_i}{s+\omega_i},\quad f(t)=\sum_{i=1}^3 f_i e^{-\omega_i t},$$
$$f_i=\frac{\Gamma-\omega_i}{(\omega_{i+1}-\omega_i)(\omega_{i-1}-\omega_i)}, \tag{5.49}$$

where, in this connection, $\omega_0=\omega_3$, not to be confused with the definition $\omega_0=\sqrt{a/m}$ elsewhere in the work.

For large Γ one has

$$f_1=-f_2=\frac{m}{\gamma w},\quad f_3=\frac{1}{\Gamma} \tag{5.50}$$

with w defined in Eq. (3.32).

Let us now set, in analogy with Eq. (5.13),

$$x(t)=\sum_k\sqrt{\frac{\hbar\Delta(\Gamma^2+\nu_k^2)}{\pi\gamma\Gamma^2\nu_k}}\,[\beta_k(t)b_k^\dagger+\beta_k^*(t)b_k]. \tag{5.51}$$

This implies

$$p(t)=m\sum_k\sqrt{\frac{\hbar\Delta(\Gamma^2+\nu_k^2)}{\pi\gamma\Gamma^2\nu_k}}\,[\dot{\beta}_k(t)b_k^\dagger+\dot{\beta}_k^*(t)b_k]. \tag{5.52}$$

One has from Eqs. (5.44), (5.47), and (5.49) $\beta_k=\beta(\nu_k)$, with

$$\beta(\nu)=\sqrt{\frac{\gamma}{\gamma_0}}\sin\phi_0(\nu)\sum_{i=1}^{3} f_i(-\omega_i+i\nu)e^{-\omega_i t}+\frac{\gamma\Gamma^2\nu}{m(\Gamma^2+\nu^2)}\sum_{i=1}^{3} f_i\left[\sin\phi_0(\nu)\frac{\Gamma-i\nu}{\nu}\frac{e^{-\omega_i t}-e^{-\Gamma t}}{\Gamma-\omega_i}+e^{i\phi_0(\nu)}\frac{e^{i\nu t}-e^{-\omega_i t}}{\omega_i+i\nu}\right]. \tag{5.53}$$

The $e^{-\Gamma t}$ terms cancel since, due to Eq. (5.47),

$$\sum_i \frac{f_i}{\omega_i-\Gamma}=\hat{f}(-\Gamma)=0. \tag{5.54}$$

Next one can check that

$$e^{i\phi(\nu)}=\frac{m(\Gamma^2+\nu^2)\sin\phi(\nu)}{\gamma\Gamma^2\nu\hat{f}(i\nu)},$$

$$e^{i\phi_0(\nu)}=\frac{m_0(\Gamma^2+\nu^2)\sin\phi_0(\nu)}{\gamma_0\Gamma^2\nu\hat{f}_0(i\nu)}, \tag{5.55}$$

which brings

$$\frac{\gamma\Gamma^2\nu}{m(\Gamma^2+\nu^2)}e^{i\phi_0(\nu)}\sum_{i=1}^{3}\frac{f_i}{\omega_i+i\nu}=\frac{\gamma m_0\hat{f}(i\nu)}{\gamma_0 m\hat{f}_0(i\nu)}\sin\phi_0(\nu). \tag{5.56}$$

This leads to the exact result

$$\beta(\nu,t)=\beta_0 e^{i\nu t}+\sum_{i=1}^{3}\beta_i(\nu)e^{-\omega_i t},$$

$$\beta_0(\nu)=\sin\phi(\nu)\, e^{i\phi_0(\nu)-i\phi(\nu)},$$

$$\beta_i(\nu)=\sin\phi_0(\nu)\, f_i\left[\sqrt{\frac{\gamma}{\gamma_0}}(-\omega_i+i\nu)+\frac{\gamma\Gamma^2}{m(\Gamma+i\nu)(\Gamma-\omega_i)}-\frac{\gamma m_0}{\gamma_0 m\,\hat{f}_0(i\nu)(\omega_i+i\nu)}\right]. \tag{5.57}$$

For large times only the first term remains, and the initial condition only enters through its phase factor $\exp(i\phi_0-i\phi)$, which has no physical effect, thus showing that the central particle relaxes to its equilibrium state independent of its initial condition. In the case $\gamma_0=\gamma$, the expression for β_i can be simplified by writing it as the ratio of two polynomials, and using the fact that ω_i is a zero of $1/\hat{f}(-\omega)$, allowing to eliminate the ω_i^3 term of the numerator. This brings

$$\beta_i(\nu)=\sin\phi_0(\nu)\ \frac{a-a_0+(m_0-m)\nu^2}{m}\ \frac{f_i}{\omega_i+i\nu}, \tag{5.58}$$

which is still exact. Using Eq. (5.55) we can also express the result as

$$\beta(\nu,t)=\frac{\gamma\Gamma^2\nu\ e^{i\phi_0(\nu)}}{m(\Gamma^2+\nu^2)}\left\{\hat{f}(i\nu)e^{i\nu t}+[a-a_0-(m-m_0)\nu^2]\times\hat{f}_0(i\nu)\sum_{i=1}^{3}\frac{f_i}{\omega_i+i\nu}e^{-\omega_i t}\right\}. \tag{5.59}$$

It is trivial to check that, when no change is made at $t=0$ ($\gamma_0=\gamma$, $m_0=m$, and $a_0=a$), the result $\beta(\nu)=\sin\phi\exp(i\nu t)$ shows that Eq. (5.51) extends the negative time behavior (5.13) to all positive times, even though the noise and the damping had a special (but in that case unphysical) role in $t=0$.

In the rest of this work we shall be mainly interested in the situation $\gamma_0=\gamma$, $m_0=m$ while a_0 is different from but close to a. One gets in the regime of large Γ and $t\gg 1/\Gamma$ to linear order in $a-a_0$,

$$\beta(\nu)=\sin\phi(\nu)\ e^{i\phi_0(\nu)-i\phi(\nu)+i\nu t}\left[1+\frac{a-a_0}{\gamma w}\left(\frac{e^{-\omega_1 t-i\nu t}}{\omega_1+i\nu}-\frac{e^{-\omega_2 t-i\nu t}}{\omega_2+i\nu}\right)\right], \tag{5.60}$$

where w is defined in Eq. (3.32) and $\omega_{1,2}$ in Eqs. (3.24)–(3.38).

VI. ENERGY OSCILLATION AND NEGATIVE ENTROPY PRODUCTION

We consider the dynamical evolution of a system initially in equilibrium characterized by a spring constant a_0, which at $t=0$ is instantaneously changed to $a_1=a$. These parameters are connected as

$$a_0=(1-\alpha_0)a. \tag{6.1}$$

We shall assume that $|\alpha_0|\ll 1$. We also assume a large Debye frequency Γ, but this does not lead to principal changes.

A. Nonmonotonous relaxation of the energy at low *T*

Let us now consider how the system relaxes to its steady state. From Eqs. (5.51) and (5.16) one has

$$\langle x^2\rangle = \int_0^\infty \mathrm{d}\nu\, \frac{\hbar(\Gamma^2+\nu^2)}{\pi\gamma\Gamma^2\nu}\,\beta^*\beta\coth\frac{1}{2}\beta\hbar\nu,$$

$$\langle p^2\rangle = m^2\int_0^\infty \mathrm{d}\nu\, \frac{\hbar(\Gamma^2+\nu^2)}{\pi\gamma\Gamma^2\nu}\,\dot\beta^*\dot\beta\coth\frac{1}{2}\beta\hbar\nu. \qquad (6.2)$$

The infinite time values, discussed already in Eqs. (3.47) and (3.48), can be checked from these expressions. For the evolution from the initial state to these values, we shall consider times $t \gg 1/\Gamma$, and we can just take the limit $\Gamma\to\infty$ since no divergences occur, except for the $\ln\Gamma$ term of the static part $\langle p^2\rangle$ at $T=0$. Inserting Eq. (5.60) we get to linear order in α_0,

$$V(t)=\frac{1}{2}a\langle x^2\rangle = \frac{1}{2}T_x+\alpha_0\frac{\hbar a}{2\pi\gamma}C_x\left(\frac{\gamma t}{2m}\right), \qquad (6.3)$$

$$K(t)=\frac{\langle p^2\rangle}{2m}=\frac{1}{2}T_p+\alpha_0\frac{\hbar a}{2\pi\gamma}C_p\left(\frac{\gamma t}{2m}\right), \qquad (6.4)$$

$$U(t)=\frac{1}{2}T_p+\frac{1}{2}T_x+\alpha_0\frac{\hbar a}{2\pi\gamma}C_E\left(\frac{\gamma t}{2m}\right), \qquad (6.5)$$

with the relaxation functions of coordinate, momentum, and energy,

$$C_x(\tau)=\frac{2(1-w^2)}{w}\int_{-\infty}^{\infty}\frac{dy\, y\coth(\beta\hbar\gamma y/4m)}{[(1+w)^2+y^2][(1-w)^2+y^2]} \times\left[\frac{e^{-(1-w+iy)\tau}}{1-w+iy}-\frac{e^{-(1+w+iy)\tau}}{1+w+iy}\right], \qquad (6.6)$$

$$C_p(\tau)=\frac{2}{w}\int_{-\infty}^{\infty}\frac{dy\, y\coth(\beta\hbar\gamma y/4m)}{[(1+w)^2+y^2][(1-w)^2+y^2]} \times\left[\frac{iy(1-w)e^{-(1-w+iy)\tau}}{1-w+iy}-\frac{iy(1+w)e^{-(1+w+iy)\tau}}{1+w+iy}\right], \qquad (6.7)$$

$$C_E(\tau)=\frac{2}{w}\int_{-\infty}^{\infty}\frac{dy\, y\coth(\beta\hbar\gamma y/4m)}{[(1-iy)^2-w^2]} \times\left[\frac{(1-w)e^{-(1-w+iy)\tau}}{(1-w+iy)^2}-\frac{(1+w)e^{-(1+w+iy)\tau}}{(1+w+iy)^2}\right]. \qquad (6.8)$$

Of course, one just has $C_E=C_p+C_x$. The integration variable is $y=2m\nu/\gamma$. The appearance of the dimensionless time scale $\tau=\gamma t/2m$ is natural, since in the underdamped regime, where w is imaginary, the damping time is just $\tau_d=2m/\gamma$, see Eq. (3.38). In the overdamped regime the time scales τ_x and τ_p from Eq. (3.35) are coded in the terms $(1\mp w)\tau$ in the exponentials, respectively. In particular, for strong overdamping one has $t/\tau_x=(1-w)\gamma t/2m\to at/\gamma$.

1. Classical regime

At large T the tanh linearizes. One can do contour integration to find for overdamping, i.e., for $\varepsilon = am/\gamma^2<\frac{1}{4}$ and $w=\sqrt{1-4\varepsilon}>0$, the exact results

$$C_x(\tau)=\frac{\pi\gamma T}{\hbar a}e^{-2\tau}\left[\cosh(w\tau)+\frac{\sinh(w\tau)}{w}\right]^2, \qquad (6.9)$$

$$C_p(\tau)=\frac{\pi\gamma T}{\hbar a}e^{-2\tau}(1-w^2)\left[\frac{\sinh(w\tau)}{w}\right]^2, \qquad (6.10)$$

$$C_E(\tau)=\frac{\pi\gamma T}{\hbar a}e^{-2\tau}\left\{\left[\cosh(w\tau)+\frac{\sinh(w\tau)}{w}\right]^2+(1-w^2) \times\left[\frac{\sinh(w\tau)}{w}\right]^2\right\}. \qquad (6.11)$$

For overdamping $(0<w<1)$ these functions are strictly positive. For underdamping one has to replace $w\to i\bar{w}$, implying $\cosh w\tau\to\cos\bar{w}\tau$ and $\sinh(w\tau)/w\to\sin(\bar{w}\tau)/\bar{w}$. Then C_x and C_p get zeroes, but remain non-negative, while C_E remains strictly positive (Figs. 2 and 3).

For the relaxation of the energy this implies

$$U=T+\frac{1}{2}\alpha_0 T\left\{\left[\cosh(w\tau)+\frac{\sinh(w\tau)}{w}\right]^2 +(1-w^2)\left[\frac{\sinh(w\tau)}{w}\right]^2\right\}e^{-2\tau}. \qquad (6.12)$$

For strong overdamping $(\varepsilon\to 0,\ w\approx 1-2\varepsilon)$ this becomes a simple exponential decay,

$$U=T+\frac{1}{2}\alpha_0 T\, e^{-4\varepsilon\tau}. \qquad (6.13)$$

In case of underdamping, $\varepsilon>\frac{1}{4}$, one has $w=i\bar{w}$ with $\bar{w}=\sqrt{4\varepsilon-1}$. This yields by analytic continuation

$$U=T+\frac{1}{2}\alpha_0 T\left\{\left[\cos(\bar{w}\tau)+\frac{\sin(\bar{w}\tau)}{\bar{w}}\right]^2 +\frac{1+\bar{w}^2}{\bar{w}^2}\sin^2(\bar{w}\tau)\right\}e^{-2\tau}. \qquad (6.14)$$

The term multiplying α_0 is an oscillating function, and is strictly positive. Its derivative

$$\dot U=-\frac{\gamma\alpha_0 T}{m}\,\frac{1+\bar{w}^2}{\bar{w}^2}\sin^2(\bar{w}\tau)\,e^{-2\tau} \qquad (6.15)$$

has zeros but does not change sign. Physically this means: depending on the sign of α_0, both the kinetic and the potential energy oscillate either above or below their final value, and the total energy flow is unidirected; it goes towards the bath when $a>a_0$, i.e., $\alpha_0>0$ and from the bath to the particle in the opposite case.

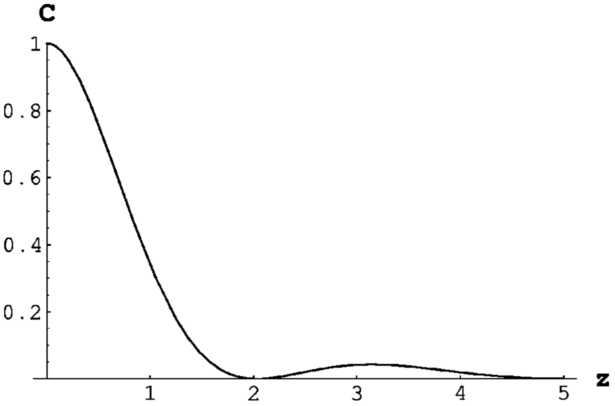

FIG. 2. The underdamped situation. C_x as a function of the rescaled dimensionless time $z=\tau\delta=\tau/|w|$, normalized to unity at $z=0$, for large T and $\delta=0.5$.

In the limit of weak damping ($\bar{w}\gg 1$) one gets

$$U=T+\frac{1}{2}\alpha_0 T\left\{1+\frac{\sin(2\omega_0 t)}{\bar{w}}\right\}e^{-\gamma t/m},$$

$$\dot{U}=-\frac{\gamma\alpha_0 T}{m}\sin^2(\omega_0 t)\,e^{-\gamma t/m}. \tag{6.16}$$

Notice that the small but oscillating term in U has become of leading order for $\dot{U}$.

2. Weak damping regime

In the weak damping limit it holds that

$$\bar{w}=-iw\approx\frac{2\sqrt{am}}{\gamma}\gg 1. \tag{6.17}$$

For performing the integrals, we write $C_x(\tau)$ first as an integral from 0 to infinity, and make the shift $y\to\bar{w}+u$, yielding up to order $1/\bar{w}^2$,

$$C_x(\tau)=e^{-\tau}\int_{-\bar{w}}^{\infty}du\,\frac{\coth(b+bu/\bar{w})}{u^2+1}\left(-\frac{u\cos u\tau+\sin u\tau}{1+u^2}+\frac{\cos(2\omega_0 t+u\tau)}{2\bar{w}}\right), \tag{6.18}$$

where a correction factor $1+u/\bar{w}$ in numerator and denominator have canceled, and we denoted

$$b=\frac{1}{2}\beta\hbar\omega_0. \tag{6.19}$$

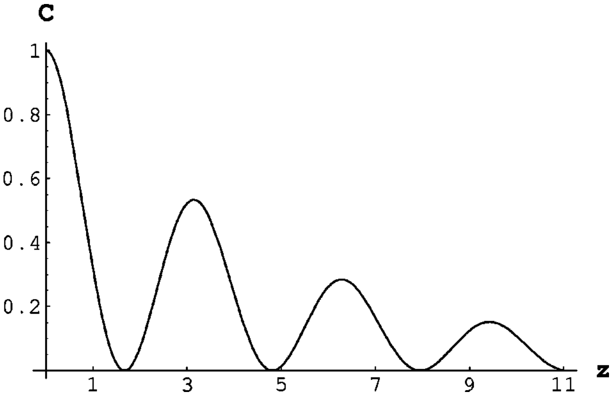

FIG. 3. The underdamped situation. C_x as a function of the rescaled dimensionless time $z=\tau\delta=\tau/|w|$, normalized to unity at $z=0$, for large T and $\delta=0.1$.

Evaluating this to leading order in $1/\bar{w}$ we get

$$C_x(\tau)=\frac{\pi\gamma}{4\sqrt{am}}\left(\frac{\frac{1}{2}\beta\hbar\omega_0}{\sinh^2\frac{1}{2}\beta\hbar\omega_0}+\coth\tfrac{1}{2}\beta\hbar\omega_0\cos 2\omega_0 t\right)e^{-2\tau}. \tag{6.20}$$

For large T this agrees with Eq. (6.9), of which the last factor now becomes $\cos^2\omega_0 t$. For $T=0$ and $\tau=0$ it agrees with Eq. (6.27) below. Likewise,

$$C_p(\tau)=\frac{\pi\gamma}{4\sqrt{am}}\left(\frac{\frac{1}{2}\beta\hbar\omega_0}{\sinh^2\frac{1}{2}\beta\hbar\omega_0}-\coth\tfrac{1}{2}\beta\hbar\omega_0\cos 2\omega_0 t\right)e^{-2\tau}. \tag{6.21}$$

As in the classical limit, $C_E'=C_x'+C_p'$ picks up a contribution of C_E that is subleading but oscillating; it is most easily obtained by evaluating C_E' in a manner similar to Eq. (6.18),

$$C_E'(\tau)=-\frac{\pi\gamma}{\sqrt{am}}\left(\frac{\frac{1}{2}\beta\hbar\omega_0}{\sinh^2\frac{1}{2}\beta\hbar\omega_0}-\coth\tfrac{1}{2}\beta\hbar\omega_0\cos 2\omega_0 t\right)e^{-2\tau}. \tag{6.22}$$

When inserting C_p+C_x in Eq. (6.5) we have for the leading decay of the energy

$$U=\frac{1}{2}\hbar\omega_0\coth\frac{1}{2}\beta\hbar\omega_0+\frac{1}{2}\alpha_0 T\frac{(\frac{1}{2}\beta\hbar\omega_0)^2}{\sinh^2\frac{1}{2}\beta\hbar\omega_0}e^{-\gamma t/m}, \tag{6.23}$$

showing that to leading order in γ in the weak damping limit the energy does not oscillate, but monotonically leaks into the bath (when $\alpha_0>0$) or is taken from the bath (when $\alpha_0<0$). At low temperature this happens with an exponentially small rate. But the rate of energy transfer, determined by Eq. (6.22),

$$\dot{U}=-\frac{\gamma\alpha_0 T}{2m}\left(\frac{(\frac{1}{2}\beta\hbar\omega_0)^2}{\sinh^2\frac{1}{2}\beta\hbar\omega_0}-\frac{\frac{1}{2}\beta\hbar\omega_0}{\tanh\frac{1}{2}\beta\hbar\omega_0}\cos 2\omega_0 t\right)e^{-\gamma t/m}, \qquad (6.24)$$

is an oscillating function that changes sign in each period whenever T is not infinite. Thus the rate of energy transfer is not unidirected except for the classical limit. When averaged over one period, the cosine is subleading and a unidirected flow emerges.

3. Quantum regime for nonweak damping

At $T=0$ one has $y\coth(\beta\hbar\gamma y/4m)=|y|$. For time $\tau=0$ one finds by direct integration

$$C_x(0)=\frac{1}{w^2}-\frac{1-w^2}{2w^3}\ln\frac{1+w}{1-w}, \qquad (6.25)$$

and we define the shorthand

$$\lambda(w)=\frac{1}{2w}\ln\frac{1+w}{1-w}. \qquad (6.26)$$

It further holds that

$$C_p(0)=-C_x(0), \quad C_E(0)=0. \qquad (6.27)$$

These results can be verified using the relations

$$a\langle x^2(t=0^+)\rangle-T_x(a)=\frac{a}{a_0}T_x(a_0)-T_x(a)$$
$$=-\alpha_0 a^2\frac{d(T_x/a)}{da}=\alpha_0\frac{\hbar a}{\pi\gamma}C_x(0),$$
$$\frac{1}{m}\langle p^2(t=0^+)\rangle-T_p(a)=-\alpha_0 a\frac{dT_p}{da}=\alpha_0\frac{\hbar a}{\pi\gamma}C_p(0). \qquad (6.28)$$

So after the instantaneous change of the spring constant ($t\gg 1/\Gamma$), the deviation of the potential energy from its final value is, to leading order in α_0, just opposite to the one of the kinetic energy. Consequently, the particle already has the proper energy, but this will not remain so; for $\alpha_0>0$ first a flow from the bath will occur and then a reversed flow, after which the equilibrium will be reached by a second energy flow from the bath to the particle.

At large times ($\tau\gg 1$) and still $T=0$ one gets in case of overdamping ($w>0$)

$$C_x(\tau)=-\frac{1}{2\varepsilon^2\tau^2}e^{-\tau}\left[\cosh w\tau+\frac{\sinh w\tau}{w}\right],$$
$$C_p(\tau)=-\frac{1}{\varepsilon^2\tau^3}e^{-\tau}\frac{\sinh w\tau}{w},$$
$$C_E(\tau)=-\frac{1}{2\varepsilon^2\tau^2}e^{-\tau}\left[\cosh w\tau+\frac{\sinh w\tau}{w}\right], \qquad (6.29)$$

and for underdamping ($\bar{w}>0$)

$$C_x(\tau)=-\frac{1}{2\varepsilon^2\tau^2}e^{-\tau}\left[\cos\bar{w}\tau+\frac{\sin\bar{w}\tau}{\bar{w}}\right],$$
$$C_p(\tau)=-\frac{1}{\varepsilon^2\tau^3}e^{-\tau}\frac{\sin\bar{w}\tau}{\bar{w}},$$
$$C_E(\tau)=-\frac{1}{2\varepsilon^2\tau^2}e^{-\tau}\left[\cos\bar{w}\tau+\frac{\sin\bar{w}\tau}{\bar{w}}\right]. \qquad (6.30)$$

The latter expressions all exhibit an infinity of oscillations around $C=0$. For overdamping one has $C_x(0)>0$, while it has a negative tail; consequently there remains one oscillation even in the limit of strong damping. In that limit (γ large), one may set $\sigma=(1-w)\tau=at/\gamma$. For large, but fixed σ one gets $C_x=C_E=-2\exp(-\sigma)/\sigma^2$, $C_p=-8\varepsilon\exp(-\sigma)/\sigma^3$.

4. Strong damping at low T

Let us now write $C_x(t)$ as

$$C_x(t)=f_x(\tau,w)+f_x(\tau,-w), \qquad (6.31)$$

$$f_x(\tau,w)=\frac{2(1-w^2)}{w}e^{-(1-w)\tau}\int_{-\infty}^{\infty}dy\,\frac{y\coth(by/\sqrt{1-w^2})[(1-w)\cos y\tau-y\sin y\tau]}{[(1+w)^2+y^2][(1-w)^2+y^2]^2}, \qquad (6.32)$$

where b was defined in Eq. (6.19).

We investigate in some greater detail two particular cases: $w \rightarrow 1$ (strong overdamping) and $w = 0$ (the border between overdamping and underdamping). For the first case one changes the integrating variable $y \rightarrow y/(1-w)$ and arrives at

$$f_x(\tau,w) = f_1(2\varepsilon\tau),$$

$$f_1(\sigma) = e^{-\sigma}\int_{-\infty}^{\infty} \mathrm{d}y \, \frac{y\coth(\,b\,y\sqrt{\varepsilon})[\cos y\sigma - y\sin y\sigma]}{[\,1+y^2\,]^2}, \tag{6.33}$$

$$f_x(\tau,-w) = -\varepsilon e^{-2\tau}\int_{-\infty}^{\infty} \mathrm{d}y \, \frac{y\coth(b\,y\sqrt{\varepsilon})\cos 2\varepsilon y\tau}{[1+y^2]^2}. \tag{6.34}$$

Recall that $w = \sqrt{1-4\varepsilon}$, and in the limit $\varepsilon \rightarrow 0$ one has $w = 1-2\varepsilon \rightarrow 1$. It is seen that in this limit $f_x(\tau,-w)$ is small compared to $f_x(\tau,w)$ due to an extra factor ε and, above all, a quickly decaying exponential $e^{-2\tau} = e^{-\sigma/\varepsilon}$. Thus, we will omit $f_x(\tau,-w)$. Then one has a scaling form

$$C_E(\tau,\varepsilon) = C_x(\tau,\varepsilon) = f_1(2\varepsilon\tau) = f_1\left(\frac{at}{\gamma}\right) = f_1\left(\frac{t}{\tau_x}\right). \tag{6.35}$$

Notice also that for this function small and large temperatures are determined by the dimensionless ratio: $b\sqrt{\varepsilon} = \frac{1}{2}\beta\hbar a/\gamma = \frac{1}{2}\hbar/(\tau_x T)$. If this parameter is small (which is always achieved for large temperature and also for fixed temperature and large damping), then we go back to the situation of Eq. (6.13) because

$$f_1(2\varepsilon\tau) = \frac{\pi T}{\hbar\omega_0\sqrt{\varepsilon}}e^{-4\varepsilon\tau} \tag{6.36}$$

combined with Eqs. (6.5) and (6.35) yield (6.13).

In the zero-temperature limit one takes $y\coth(b\,y\sqrt{\varepsilon}) = |y|$ and gets

$$f_1(\sigma) = 2e^{-\sigma}\int_0^{\infty} \mathrm{d}y \, \frac{y\,[\cos y\sigma - y\sin y\sigma\,]}{[1+y^2]^2}. \tag{6.37}$$

This function can be exactly expressed through Meijer functions, but we will not write this representation explicitly, since it is useful only for numerical computations. Notice that Eq. (6.47) can be once more checked with help of Eq. (6.37). The behavior of $f_1(\sigma)$ for different temperatures is presented in Fig. 4.

It starts with $f(0) = 1$, becomes negative at $\tau_0 = 0.407\,211\,889\,989$, goes through a minimum, and finally bends up to 0^- for $\tau \rightarrow \infty$. The minimum is characterized by

$$\sigma_{\mathrm{min}} = 0.879\,087\,308\,04,$$

$$f_1(\sigma_{\mathrm{min}}) = -0.091\,898\,049\,6, \quad c_2 \equiv f_1''(\sigma_{\mathrm{min}}) = 0.404\,842. \tag{6.38}$$

In this limit C_p has an interesting behavior. We discussed already that $C_p(0) = -C_x(0)$. For small σ, C_p quickly grows, goes through zero, and then becomes of order ε, starting as $\varepsilon\ln 1/\sigma$ for small, but not too small σ. For finite σ one thus has $C_E \approx C_x$, implying that now the total energy makes one oscillation, despite the strong damping.

For $\alpha_0 > 0$ it says that, after initially energy has been put on the particle by the change of $a_0 \rightarrow a > a_0$, this energy leaks away into the bath. However, at intermediate times more energy leaks away than in the final state, so a part has to come back at moderately late times. This nonmonotonic behavior (“bouncing”) is familiar of the noise correlator, which is anticorrelated at large times in the quantum regime.

Let us now turn to the behavior of C_x for $w = 0$,

$$C_x(\tau) = 8\tau e^{-\tau}\int_0^{\infty} dy \, \frac{y\coth(b\,y)\,[\cos y\tau - y\sin y\tau\,]}{[1+y^2]^3} + 8\,e^{-\tau}\int_0^{\infty} dy \, \frac{y\coth(b\,y)\,[\,(1-y^2)\cos y\tau - 2y\sin y\tau\,]}{[1+y^2]^4}. \tag{6.39}$$

The behavior of this function is depicted in Fig. 5. It is seen that the cases $w = 0$ and $w = 1$ are qualitatively similar. As expected, the negative tail of $C_x(t)$ is more pronounced for $w = 0$. For $C_p(t)$ one has

$$C_p(t) = f_p(\tau,w) + f_p(\tau,-w), \tag{6.40}$$

$$f_p(\tau,w) = \frac{2(1-w)}{w}e^{-(1-w)\tau}\int_{-\infty}^{\infty} dy \, \frac{y\coth(\,b\,y/\sqrt{1-w^2}\,)[\,y^2\cos y\tau + y(1-w)\sin y\tau]}{[(1+w)^2+y^2]\,[(1-w)^2+y^2]^2}. \tag{6.41}$$

The behavior of $C_p(t)$ in the overdamped situation can be studied along exactly the same lines as for $C_x(t)$,

$$C_p(t) = 2\epsilon\, e^{-2\epsilon\tau}\int_0^{\infty} dy \, \frac{y\coth(b\,y\sqrt{\varepsilon})[y^2\cos(2\,\epsilon\,\tau y) + y\sin(2\,\epsilon\,\tau y)\,]}{[1+y^2]^2\,(1+\epsilon^2 y^2)}$$

$$-2\,e^{-2\tau}\int_0^{\infty} dy \, \frac{\coth(\,b\,y/\sqrt{\varepsilon}\,)[y\cos(2\,\tau y) + \sin(2\,\tau y)]}{[1+y^2]^2}. \tag{6.42}$$

Due to the additional factor ϵ, this is smaller than $C_x(t)$ for $\tau > 1$, and this justifies Eq. (6.35). Nevertheless, on the qualitative level $C_p(t)$ displays nearly the same behavior as $C_x(t)$. This is demonstrated by Figs. 6 and 7.

Let us now investigate properties of $C_x(t)$ in the underdamped limit, where $w = i\overline{w} = i\sqrt{4\varepsilon - 1}$, and $\overline{w}$ is real. In the additional weak damping limit one has $\overline{w} \sim 1/\gamma \to \infty$. Using Eqs. (6.32) and (6.33) one gets

$$C_x(t) = \frac{8(\overline{w}^2+1)}{\overline{w}^4} e^{-\tau} \operatorname{Im}\left[e^{i\tau\overline{w}} \int_0^\infty dy \frac{y \coth\left(\frac{by\overline{w}}{\sqrt{\overline{w}^2+1}}\right) [(1/\overline{w}-i)\cos(y\tau\overline{w}) - y\sin(y\tau\overline{w})]}{[(1/\overline{w}+i)^2+y^2][(1/\overline{w}-i)^2+y^2]^2} \right], \tag{6.43}$$

$$C_p(t) = \frac{8}{\overline{w}^2} e^{-\tau} \operatorname{Im}\left[(1/\overline{w}-i)\, e^{i\tau\overline{w}} \int_0^\infty dy \frac{y \coth\left(\frac{by\overline{w}}{\sqrt{\overline{w}^2+1}}\right) [y^2\cos(y\tau\overline{w}) + (1/\overline{w}-i)y\sin(y\tau\overline{w})]}{[(1/\overline{w}+i)^2+y^2][(1/\overline{w}-i)^2+y^2]^2} \right]. \tag{6.44}$$

The behavior of these functions, as well as $C_E(t) = C_x(t) + C_p(t)$, is depicted in Figs. 8 and 9 for $T = 0$. It is seen that for the initial time of order $1/\overline{w}$, C_x and C_p oscillate with the amplitude higher for larger $\overline{w}$.

5. Moments of the relaxation functions at low temperature

We can also determine the integral

$$\int_0^\infty \mathrm{d}\tau C_x(\tau)$$

$$= 8(1-w^2)\int_{-\infty}^\infty \frac{dy\, y \coth(\beta\hbar\gamma y/4m)}{[(1+w)^2+y^2]^3[(1-w)^2+y^2]^3} \times [(1-w^2)^2 - 2y^2(1+w^2) - 3y^4]. \tag{6.45}$$

At $T = 0$ it can be simply checked that it vanishes at $w = 0$ and near $w = 1$,

$$\int_0^\infty d\tau C_x(\tau) = 8[B(1,5) - 2B(2,4) - 3B(3,3)] = 0,$$

$$\int_0^\infty d\tau C_x(\tau) = (1-w)\int_{-\infty}^\infty dy\, |y| \frac{(1-w)^2 - y^2}{[(1-w)^2+y^2]^3}$$

$$= \frac{1}{1-w}[B(1,2) - B(2,1)] = 0, \tag{6.46}$$

where $B(w,z) = \Gamma(w)\Gamma(z)/\Gamma(w+z)$ is the β function. It actually holds for all w that

$$C_x^{(0)}(T=0) \equiv \int_0^\infty d\tau C_x(\tau, T=0) = 0. \tag{6.47}$$

This surprising zero-temperature outcome will have important consequences when it comes to work extraction. It is

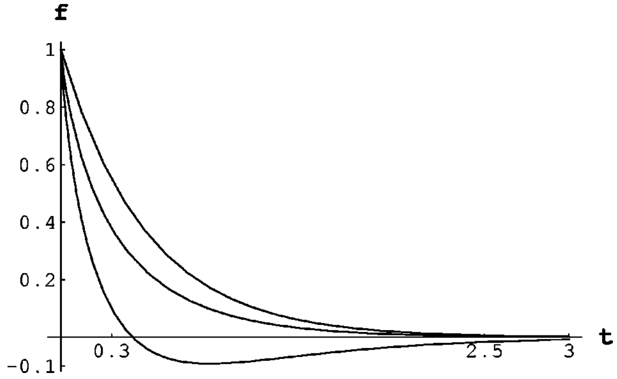

FIG. 4. The case of strong damping. $f_1(t)$ as a function of dimensionless time t, normalized to unity at $t = 0$, for different values of the dimensionless temperature $\theta = 1/(b\sqrt{\varepsilon}) = 2T\gamma/(\hbar a)$. Upper curve, $\theta \to \infty$ [taking into the normalization the expression given by Eq. (6.36)]. Middle curve, $\theta = 1$ [see Eq. (6.33)]. Lower curve, $T = \theta = 0$ [the expression given by (6.37)]. In the latter case there is still an oscillation, despite the strong damping.

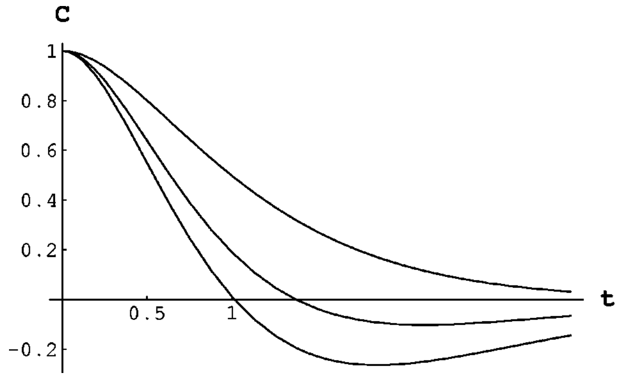

FIG. 5. The case with $w = 0$ (the border between overdamping and underdamping). $C_x(t)$ as a function of dimensionless time t, normalized to unity at $t = 0$, for different values of the dimensionless temperature $\theta = 1/b = T\sqrt{2m}/(\hbar\sqrt{a})$. Upper curve, $\theta = 1$, middle curve, $\theta = 0.2$, lower curve, $T = \theta = 0$. In the two latter cases there is an oscillation.

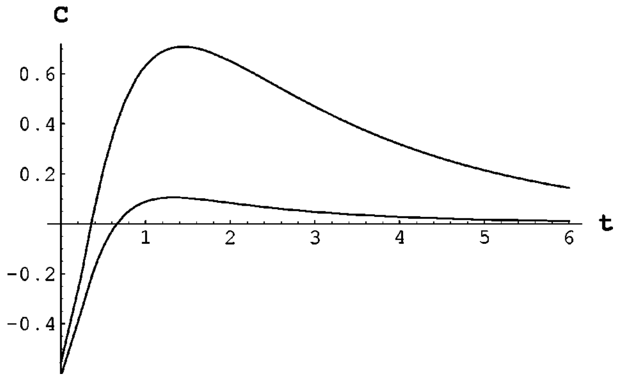

FIG. 6. The overdamped situation, $\epsilon=0.1$ ($w=0.7745$). $C_p(t)$ as a function of time, for different values of the dimensionless temperature $\theta=1/(b\sqrt{\varepsilon})=2T\gamma/(\hbar a)$. Upper curve, $\theta=33$; lower curve, $\theta=0$.

similar to $\int_{-\infty}^{\infty}dt\,K(t)=2\gamma T\to 0$ for $T\to 0$, where $K(t)$ is the autocorrelation function of the quantum noise. For small T one gets

$$C_x^{(0)}(T)=\int_0^\infty d\tau C_x(\tau)=\frac{64\pi^2}{3(1-w^2)}\left(\frac{mT}{\hbar\gamma(1-w^2)}\right)^2 =\frac{1}{12\varepsilon}\left(\frac{2\pi\gamma T}{\hbar a}\right)^2. \tag{6.48}$$

It can also be verified that at zero T and arbitrary ε,

$$C_x^{(1)}=-\int_0^\infty d\tau\,\tau C_x(\tau,T=0)=\frac{1}{24\varepsilon^2}\tilde{C}_x^{(1)},$$

$$\tilde{C}_x^{(1)}=\frac{(3+w^2)(3w^2-1)+3(1-w^2)^3\lambda(w)}{8w^4}, \tag{6.49}$$

where λ is defined in Eq. (6.26), and

$$C_x^{(2)}=-\int_0^\infty d\tau\,\tau^2 C_x(\tau,T=0)=\frac{8}{3(1-w^2)^3}=\frac{1}{24\varepsilon^3}. \tag{6.50}$$

These coefficients are exact and positive for all w. The minus signs in the integrals arise because the negative tail of $C_x(\tau,T=0)$ gets a larger weight than its positive center. These results follow from the Laplace transform

$$\begin{aligned}\hat{C}_x(2u,T=0)&=\int_0^\infty d\tau\,C_x(\tau,T=0)\,e^{-2u\tau}\\ &=\frac{1}{2uw^2}+\frac{1-w^2}{8u^2(1+u)}\Bigg[\frac{(1+2u-w)\ln(1+2u-w)}{(u-w)w(1+u-w)}-\frac{(1+2u+w)\ln(1+2u+w)}{(u+w)w(1+u+w)}\\ &\quad\times\frac{2u^2(1+u)^2+2u(1+u)w+w^2-w^3}{(u+w)w^3(1+u-w)}\ln(1-w)-\frac{2u^2(1+u)^2-2u(1+u)w+w^2+w^3}{(u-w)w^3(1+u+w)}\ln(1+w)\Bigg].\end{aligned} \tag{6.51}$$

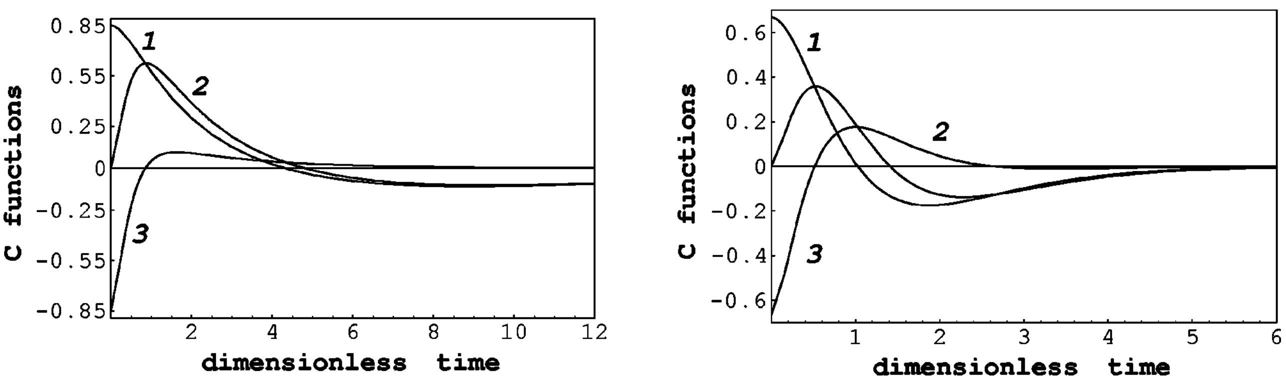

FIG. 7. The zero-temperature behavior of the C functions vs the dimensionless time. Left part, $w=0.9$ (strong overdamping), 1, C_x, 2, $C_E=C_p+C_x$, 3, C_p. Right part, the same but with $w=0.1$ (weak overdamping).

At $T=0$ all even moments of C_p vanish. This implies in particular that the integral of $C_E=C_p+C_x$ vanishes. The Laplace transform of C_E reads in that case

$$\hat{C}_E(2u,T=0)=\int_0^\infty d\tau\, C_E(\tau,T=0)\, e^{-2u\tau}$$
$$=\frac{(1+w)(1+2u+w)}{4u^2w(1+u)(1+u+w)}\ln\frac{1+2u+w}{1+w}-\frac{(1-w)(1+2u-w)}{4u^2w(1+u)(1+u-w)}\ln\frac{1+2u-w}{1-w}. \tag{6.52}$$

The Laplace transform $\hat{C}_p(2u,T=0)$ follows as $\hat{C}_E(2u,T=0)-\hat{C}_x(2u,T=0)$.

For later use we evaluate the related coefficients

$$C_E^{(0)}=\int_0^\infty d\tau C_E(\tau)=\frac{1}{12\varepsilon}\left(\frac{2\pi\gamma T}{\hbar a}\right)^2+\mathcal{O}(T^4),$$

$$C_E^{(1)}=-\int_0^\infty d\tau\tau C_E(\tau)=\frac{1}{24\varepsilon^2}+\mathcal{O}(T^2), \tag{6.53}$$

$$C_E^{(2)}=-\int_0^\infty d\tau^2\tau C_E(\tau)=\frac{1}{24\varepsilon^3}+\mathcal{O}(T^2).$$

They differ from the $C_x^{(0,1,2)}$ only by the factor $\tilde{C}_x^{(1)}$, which goes to unity for large damping.

B. Entropy production versus energy dispersion

To derive the rate of entropy production we first need the Wigner function and its temporal evolution.

1. Fokker-Planck equation for the Wigner function

To derive the evolution equation for the Wigner function, we shall write the Langevin Equation (2.18) in the form

$$\dot{p}=-ax-\frac{\gamma}{m}p+\eta+\delta\dot{p}, \tag{6.54}$$

where $\delta\dot{p}$ is small as $1/\Gamma$. Indeed, from this definition and the exact dynamical solution (5.44), (5.45) one may derive

$$\delta\dot{p}(t)=mx_0\dot{g}(t)+p_0g(t)+\int_0^t dt'\, g(t-t')\,\eta(t'), \tag{6.55}$$

where

$$g(t)=\frac{\gamma}{m}\sum_{i=1}^{3}\frac{\omega_i^2}{\Gamma-\omega_i}f_i\, e^{-\omega_i t} \tag{6.56}$$

is of order $1/\Gamma$ for large Γ. Now recall that for the harmonic situation the Wigner function is given as

$$W(p,x,t)=\int dp_0\ \ dx_0 W(p_0,x_0,0)\langle\delta(p(t)-p)\times\delta(x(t)-x)\rangle, \tag{6.57}$$

where the average is taken with respect to the noise, $W(p,x,t)$ and $W(p_0,x_0,0)$ are final and initial Wigner functions, while $p(t)$, $x(t)$ are the solutions of Eq. (2.18) for the corresponding initial conditions, and for a particular realization of the Gaussian noise. Equation (6.57) is not the most general definition of the Wigner function, but it is exact for harmonic systems.

We now seek a closed equation for the Wigner function (6.57). Differentiating $W(y_1,y_2,t)$ we get

$$\frac{\partial W(y_1,y_2,t)}{\partial t}=-\sum_{k=1}^{2}\frac{\partial(v_kW)}{\partial y_k}-\frac{\partial}{\partial y_1}\langle\delta(p(t)-y_1)\times\delta(x(t)-y_2)[\eta(t)+\delta\dot{p}(t)]\rangle, \tag{6.58}$$

where

$$v_1=-ax-\frac{\gamma}{m}p,\quad v_2=\frac{p}{m} \tag{6.59}$$

are the damped Newtonian acceleration and the velocity, respectively. The term $\delta\dot{p}$ is a linear combination of p_0, x_0, and $\eta(t')$. Due to the Gibbsian initial state, these are Gaussian random variables and their cross correlations were given

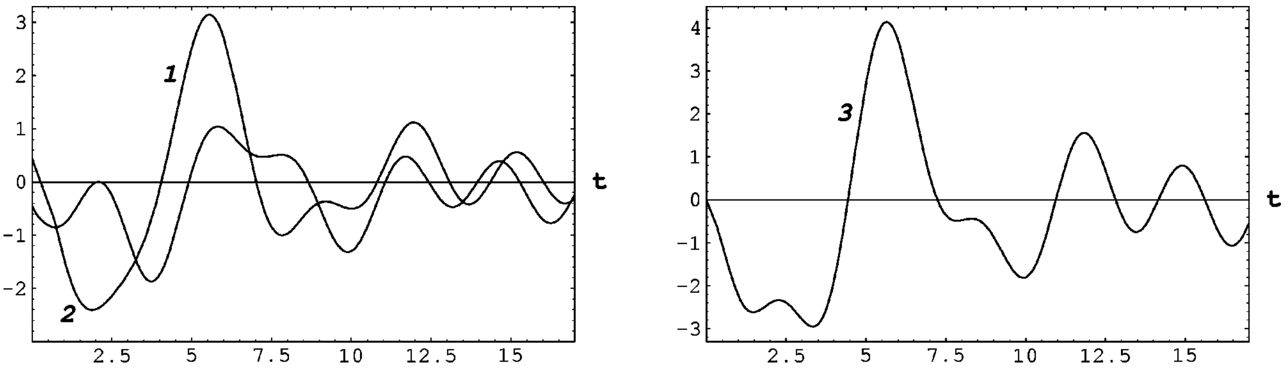

FIG. 8. The underdamped situation. 1, C_x as a function of the rescaled dimensionless time $t=\tau/|\overline{w}|$, for $T=0$ and $\overline{w}=2$, 2, C_p as a function of t, 3, C_E as a function of t both for the same values of the parameters.

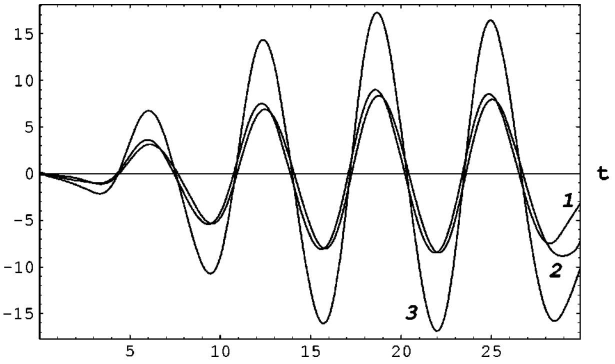

FIG. 9. The underdamped situation. 1, C_x, 2, C_p, 3, C_E, as functions of the rescaled dimensionless time $t=\tau/|\overline{w}|$, for $T=0$ and $\overline{w}=10$. As compared with Fig. (8), the amplitude of oscillations is much larger. It is seen also that C_x and C_p are quite close to each other.

in Eqs. (5.32)–(5.37). Let us denote these variables by the vector $z=\{p_0,x_0,\eta(t)\}$, and their correlations by the matrix $M_{ij}=\langle z_i z_j\rangle$. One then has for its joint distribution

$$P_0(z)=\frac{1}{\sqrt{\det(2\pi M)}}\exp\left(-\frac{1}{2}z_i M_{ij}^{-1}z_j\right). \tag{6.60}$$

Using the relation

$$z_i P_0(z)=-\sum_j M_{ij}\frac{\delta}{\delta z_j}P_0(z) \tag{6.61}$$

one can perform a partial integrations, which brings a closed equation for W. The final result is that we obtain a diffusion-type equation (Fokker-Planck-Kramers-Klein equation) for W itself,

$$\frac{\partial W(p,x,t)}{\partial t}=\mathcal{L}W=-\frac{p}{m}\frac{\partial W}{\partial x}+\frac{\partial}{\partial p}\left[\left(\frac{\gamma}{m}p+ax\right)W\right]+[D_x(t)-D_p(t)]\frac{\partial^2}{\partial p\,\partial x}W+\gamma D_p(t)\frac{\partial^2 W}{\partial p^2}, \tag{6.62}$$

where the diffusion coefficients D_x and D_p are instantaneous functions t. (Notice that in Ref. [2] we used the notation $D_{pp}=D_p$, $D=D_x$, $D_{xp}=D_x-D_p$.) The derivation along this road is somewhat lengthy. A quicker way to derive the result is to use the solution of the Fokker-Planck equation, determined by the moments

$$\langle p^2\rangle=2mK(t),\quad \langle px\rangle=\frac{m}{a}\dot{V}(t),\quad \langle x^2\rangle=\frac{2}{a}V(t), \tag{6.63}$$

where $K(t)=\langle\mathcal{K}(p)\rangle$ and $V(t)=\langle\mathcal{V}(x)\rangle$ are the expectation values of kinetic and potential energy, respectively. The time-dependent Wigner function thus reads

$$W(p,x,t)=\frac{a}{2\pi\sqrt{4amKV-m^2\dot{V}^2}}\times\exp\left(-\frac{aKx^2-\dot{V}px+Vp^2/m}{4KV-m\dot{V}^2/a}\right). \tag{6.64}$$

Inserting this in Eq. (6.62), one finally gets

$$D_p(t)=2K(t)+\frac{m}{\gamma}[\dot{K}(t)+\dot{V}(t)], \tag{6.65}$$

$$D_x(t)=2V(t)+\frac{m}{\gamma}[\dot{K}(t)+\dot{V}(t)]+\frac{\gamma}{a}\dot{V}(t)+\frac{m}{a}\ddot{V}(t). \tag{6.66}$$

Let us also define the time-dependent but currentless state

$$W_{st}(p,x,t)=\frac{\sqrt{a}}{2\pi\sqrt{mD_p(t)D_x(t)}}\exp\left(-\frac{p^2}{2mD_p(t)}-\frac{ax^2}{2D_x(t)}\right) \tag{6.67}$$

for which indeed the right hand side of the Fokker-Planck equation (6.62) vanishes, though the left hand side does not. This is the locally stationary distribution. For sufficiently long times, that is when $D_x(t)$ and $D_p(t)$ are changing with time slowly enough, W_{st} becomes a solution of the Fokker-Planck equation.

2. H function and entropy production

The $\mathcal{H}$ *function* is defined as the information theoretical distance between the actual Wigner function $W(x,p,t)$ and the locally stationary Wigner function $W_{st}(x,p,t)$,

$$\mathcal{H}=\int dx\,dp\,W(x,p,t)\ln\frac{W(x,p,t)}{W_{st}(x,p,t)}\geqslant 0. \tag{6.68}$$

The $\mathcal{H}$ function is non-negative due to the inequality

$$\frac{W}{W_{st}}\ln\frac{W}{W_{st}}\geqslant\frac{W}{W_{st}}-1, \tag{6.69}$$

$$\mathcal{H}\geqslant\int dxdp[W(x,p,t)-W_{st}(x,p,t)]=0. \tag{6.70}$$

Thus, $\mathcal{H}$ is equal to zero only for $W(x,p,t)=W_{st}(x,p,t)$, i.e., in the stationary state. Since values of $\mathcal{H}$ at intermediate times are higher than its final value, it is reasonable to look at its rate of change. In particular, $\mathcal{H}$ changes with time due to the time dependence of the reference Wigner distribution W_{st}, whereas the remaining part of $d\mathcal{H}/dt$ appears to be induced solely by the bath (see below). We define the *entropy production* d_iS/dt by

$$-\frac{d\mathcal{H}}{dt}=\int dx\,dp\,\dot{W}_{st}(x,p,t)\,\frac{W(x,p,t)}{W_{st}(x,p,t)}+\frac{d_iS}{dt}. \tag{6.71}$$

This leads to

$$\frac{d_iS}{dt}=-\int dx\,dp\,\dot{W}(x,p,t)\,\ln\frac{W(x,p,t)}{W_{st}(x,p,t)}. \tag{6.72}$$

This definition has the following properties.

(1) It is equal to zero in the stationary state.

(2) It is equal to zero if the Brownian particle does not couple with the bath.

(3) It is non-negative in the classical case, where $D_x=D_p=T$.

The last two properties are proved below.

Using Eq. (6.67) and denoting

$$R(x,p,t)=\frac{W(x,p,t)}{W_{st}(x,p,t)}, \tag{6.73}$$

one gets

$$\begin{aligned}\frac{d\mathcal{H}}{dt}&=\int dx\,dp\,[\,\mathcal{L}\,W(x,p,t)\,]\ln R(x,p,t)\\&\quad-\int dx\,dp\,R(x,p,t)\,\dot{W}_{st}(x,p,t)\\&=\int dx\,dp\,W(x,p,t)\,\mathcal{L}^{\dagger}\ln R(x,p,t)\\&\quad-\int dx\,dp\,R(x,p,t)\,\dot{W}_{st}(x,p,t).\end{aligned} \tag{6.74}$$

where $\mathcal{L}$ is the Fokker-Planck operator of the right hand side of Eq. (6.62). Noting that

$$\begin{aligned}\mathcal{L}^{\dagger}\ln R=\frac{1}{R}\mathcal{L}^{\dagger}R-\frac{1}{R^2}\bigg(\gamma D_p(t)\left[\frac{\partial R}{\partial p}\right]^2+[D_x(t)\\-D_p(t)]\frac{\partial R}{\partial x}\,\frac{\partial R}{\partial p}\bigg),\end{aligned} \tag{6.75}$$

and making once more integration by parts one ends up with

$$\begin{aligned}\frac{d_iS}{dt}=\int dx\,dp\,\frac{W(x,p,t)}{R^2(x,p,t)}\bigg(\gamma D_p(t)\left[\frac{\partial R(x,p,t)}{\partial p}\right]^2\\+[D_x(t)-D_p(t)]\frac{\partial R(x,p,t)}{\partial x}\,\frac{\partial R(x,p,t)}{\partial p}\bigg).\end{aligned} \tag{6.76}$$

Now it is clear that in the classical white-noise limit, where $D_x=D_p$, the entropy production is non-negative. The positivity of d_iS/dt just means that from the global viewpoint the approach to the stationary state is monotonous. In contrast, in the quantum case the positivity of the entropy production is endangered. It is also clear that for a free Brownian particle ($\gamma=0$) the entropy production is zero.

Finally, we mention that the difference between dS_B/dt and the entropy production is just the entropy flux,

$$\frac{d_eS}{dt}\equiv\frac{dS_B}{dt}-\frac{d_iS}{dt}=-\int dx\,dp\,\dot{W}(x,p,t)\ln W_{st}(x,p,t). \tag{6.77}$$

It takes the value

$$\frac{d_eS}{dt}=\frac{\dot{K}(t)}{D_p(t)}+\frac{\dot{V}(t)}{D_x(t)}. \tag{6.78}$$

Let us recall that in the relaxation process no work is performed, so a change in energy can only be due to a change of heat exchanged with the bath. Therefore, the last relation can be written as

$$\frac{d_eS}{dt}=\frac{\dot{\mathcal{Q}}_p}{D_p}+\frac{\dot{\mathcal{Q}}_x}{D_x}, \tag{6.79}$$

where $\dot{\mathcal{Q}}_p=\dot{K}$ and $\dot{\mathcal{Q}}_x=\dot{V}$ are the changes of heat in the momentum and coordinate sector, respectively, while $D_{p,x}$ are the corresponding diffusion coefficients in the Fokker-Planck operator $\mathcal{L}$ of Eq. (6.62). Notice that this entropy flow deviates from the standard expression $d_eS/dt=\dot{\mathcal{Q}}/T=\dot{\mathcal{Q}}_p/T+\dot{\mathcal{Q}}_x/T$, which does not make sense since $\dot{\mathcal{Q}}$ does not scale with T at low T.

The Boltzmann entropy reads

$$\begin{aligned}S_B&=-\int dp\,dx\,W(p,x,t)\ln\frac{1}{\hbar}W(p,x,t)\\&=1+\frac{1}{2}\ln\left[\frac{m}{\hbar^2a}\left(4KV-\frac{m}{a}\dot{V}^2\right)\right].\end{aligned} \tag{6.80}$$

Its rate of change is

$$\frac{dS_B}{dt}=\frac{2a\dot{K}V+2aK\dot{V}-m\dot{V}\ddot{V}}{4aKV-m\dot{V}^2}. \tag{6.81}$$

The entropy production is the difference between them and appears to be quadratic in the deviation from the equilibrium state. To second order in the small parameter α_0, defined in Eq. (6.1), it becomes

$$\begin{aligned}\frac{d_iS}{dt}=\frac{\hbar^2\gamma a\alpha_0^2}{16\pi^2m^2}\bigg\{\frac{C_x'^2}{T_x^2}+\varepsilon(C_x'+C_p')\left(\frac{C_p'}{T_p^2}+\frac{C_x'}{T_x^2}\right)\\+\frac{T_p-T_x}{2T_pT_x^2}C_x'C_x''\bigg\},\end{aligned} \tag{6.82}$$

where $C_{p,x}'$ denote the dimensionless derivatives $dC_{p,x}(\tau)/d\tau$.

3. Classical limit

In the classical limit, where $T_x = T_p = T$, the rate of entropy production thus becomes the sum of two squares, much like the energy relaxation function C_E of Eq. (6.11),

$$\frac{d_iS}{dt} = 4\frac{a\alpha_0^2}{\gamma} e^{-4at/\gamma} \frac{\sinh^2 w\tau}{w^2}\left\{\left(\cosh w\tau + \frac{\sinh w\tau}{w}\right)^2 + (1-w^2)\frac{\sinh^2 w\tau}{w^2}\right\}. \tag{6.83}$$

The total entropy production is thus

$$\Delta_i S = \int_0^\infty dt\, \frac{d_iS}{dt} = \frac{\alpha_0^2}{4}. \tag{6.84}$$

This result holds for all w.

In Eq. (7.42) we derive the general result for the energy dispersion. In the present setup we have $\alpha(t) = \alpha_0\theta(t)$, yielding

$$\Delta\Pi = \frac{\hbar a\alpha_0^2}{4\pi\gamma} C_x(0). \tag{6.85}$$

With the help of Eq. (6.9) we find

$$\frac{\Delta\Pi}{T} = \frac{\alpha_0^2}{4}. \tag{6.86}$$

This just coincides with $\Delta_i S$, explaining that both describe the same physics.

In the strong damping limit $w \to 1$ one has a simple exponential decay,

$$\frac{d_iS}{dt} = \frac{a\alpha_0^2}{\gamma} e^{-4at/\gamma}. \tag{6.87}$$

In the weak damping limit, but still at high temperatures, the result oscillates, but is non-negative,

$$\frac{d_iS}{dt} = \frac{\gamma\alpha_0^2}{m}\sin^2\omega_0 t\, e^{-2\gamma t/m}. \tag{6.88}$$

Notice the similarity with the rate of energy decay (6.16).

4. Weak damping limit at moderate temperature

In the weak-damping limit $\gamma \to 0$, where $T_p = T_x = \frac{1}{2}\hbar\omega_0 \coth(\frac{1}{2}\beta\hbar\omega_0)$, the entropy production follows from Eqs. (6.82), (6.20), and (6.22) to leading order as

$$\frac{d_iS}{dt} = \frac{\gamma\alpha_0^2}{4m}\left(\sin^2 2\omega_0 t + \left[\cos 2\omega_0 t - \frac{\beta\hbar\omega_0}{\sinh\beta\hbar\omega_0}\right]^2 + \frac{2}{\pi}\Delta\psi \tanh\frac{1}{2}\beta\hbar\omega_0 \sin 4\omega_0 t\right) e^{-2\gamma t/m}. \tag{6.89}$$

The term $\Delta\psi$ comes from the difference $T_p - T_x$, given in Eq. (3.48). It reads

$$\Delta\psi = \psi\left(\frac{\beta\hbar\Gamma}{2\pi}\right) - \mathrm{Re}\,\psi\left(i\frac{\beta\hbar\omega_0}{2\pi}\right). \tag{6.90}$$

At high T the last contribution of Eq. (6.89) vanishes (at least, it is of order $1/\Gamma$, which we discard everywhere in this work), so Eq. (6.88) is recovered.

The term with $\Delta\psi$ is responsible for the occurrence of both positive and negative values of the rate of entropy production. At low T one has $\Delta\psi \to \ln(\Gamma/\omega_0)$, which is moderately large. Therefore, below some specific temperature $T^* \sim \hbar\omega_0/\ln(\Gamma/\omega_0)$ the rate of entropy production can be negative, a surprising result. This finding goes against the formulation of the second law in the form of positivity of the entropy production. In our system the negative rates are not totally unexpected since oscillatory behavior is also exhibited already in the rate of energy decay Eq. (6.24).

The integrated entropy production is, to leading order in γ, insensitive to the oscillations. When averaged over one period, the cosine and sine are subleading and a positive rate emerges. The full integral reads

$$\Delta_i S = \frac{\alpha_0^2}{8}\left(1 + \frac{(\beta\hbar\omega_0)^2}{\sinh^2\beta\hbar\omega_0}\right) \tag{6.91}$$

while the energy dispersion is

$$\frac{\Delta\Pi}{T_x} = \frac{\alpha_0^2}{8}\left(1 + \frac{\beta\hbar\omega_0}{\sinh\beta\hbar\omega_0}\right). \tag{6.92}$$

Both expressions have the same order of magnitude, and coincide at large and small T.

Consequently, in the Gibbsian limit the rate of entropy production oscillates in the case of underdamping, as does the rate of internal energy. After averaging over one period the oscillations are washed out. This justifies our identifications of entropy flux and production.

5. Entropy production at zero temperature

Also at zero temperature the entropy production can be negative. Let us consider the case of strong damping, where $\varepsilon \ll 1$ and $T_x \sim \varepsilon T_p$, implying

$$\begin{aligned}\frac{d_iS_x}{dt} &\approx \frac{\hbar^2\gamma\alpha_0^2}{16\pi^2 m^2 T_x^2}\left\{(1+\varepsilon)C_x'^2 + \frac{1}{2}C_x'C_x''\right\}\\ &= \frac{a(1+\varepsilon)}{4\gamma\lambda^2} f'(\sigma)[f_1'(\sigma) + \varepsilon f_1''(\sigma)]\\ &\quad + \mathcal{O}(\varepsilon^2).\end{aligned} \tag{6.93}$$

Now we know that f_1 has a negative minimum at $\sigma_{\min}$. Let us expand, using the numerical constants from Eq. (6.38),

$$f_1(\sigma) = f_1(\sigma_{\min}) + \frac{1}{2}c_2(\sigma - \sigma_{\min})^2, \tag{6.94}$$

where $\sigma = at/\gamma$. Then we get

$$\frac{d_iS_x}{dt}=\frac{a(1+\varepsilon)\alpha_0^2}{4\gamma\lambda^2}c_2^2(\sigma-\sigma_{\min})(\sigma-\sigma_{\min}+\varepsilon). \tag{6.95}$$

This is negative for $\sigma_{\min}-\varepsilon<\sigma<\sigma_{\min}$. The minimum is of order $-\varepsilon^2$, and the area of the negative part is of order ε^3. Notice that negative value holds over a time window $\delta\sigma=\varepsilon$, corresponding to $\Delta t=\tau_p=m/\gamma$. This is much less than the free oscillation period $\tau_0=\sqrt{m/a}$, so after averaging over one period it disappears. However, in the (strongly) overdamped regime there are no oscillations, so there is no compelling reason to average over one period.

For a numerical investigation of the entropy production at $T=0$ we will first of all introduce a parametrization for the effective temperatures

$$T_p=\frac{\hbar\gamma}{\pi m}\theta_p,$$

$$\theta_p=\frac{1}{4w}\left[(1+w)^2\ln\left(\frac{\Lambda}{1+w}\right)-(1-w)^2\ln\left(\frac{\Lambda}{1-w}\right)\right]. \tag{6.96}$$

$$T_x=\frac{\hbar\gamma}{\pi m}\varepsilon\ \theta_x,\qquad \theta_x=\frac{1}{w}\ln\frac{1+w}{1-w}, \tag{6.97}$$

$$\theta=\frac{\theta_x}{\theta_p}, \tag{6.98}$$

where $\Lambda=2m\Gamma/\gamma$ is a large dimensionless parameter. Then Eq. (6.82) can be presented in a more convenient form,

$$\frac{d_iS}{dt}=\frac{a\alpha_0^2}{16\gamma}\frac{1}{\varepsilon^2\theta_x^2}\bigg((C_x')^2+\varepsilon(C_x'+C_p')(C_x'+\theta^2\varepsilon^2C_p') + \frac{1-\theta}{2}C_x'C_x''\bigg). \tag{6.99}$$

As for the functions involved in this expression, we recall that $C_{p,x}(\tau)=f_{p,x}(\tau,w)+f_{p,x}(\tau,-w)$ and notice that

$$\frac{df_x(\tau,w)}{d\tau}=-\frac{4(1-w^2)}{w}e^{-(1-w)\tau}\int_0^\infty dy\frac{y\coth\left(by\sqrt{\frac{1-w}{1+w}}\right)\cos[y(1-w)\tau]}{[(1+w)^2+(1-w)^2y^2][1+y^2]}, \tag{6.100}$$

$$\frac{d^2f_x(\tau,w)}{d\tau^2}=\frac{4(1-w^2)(1-w)}{w}e^{-(1-w)\tau}\int_0^\infty dy\frac{y\coth\left(by\sqrt{\frac{1-w}{1+w}}\right)\{\cos[y(1-w)\tau]+y\sin[y(1-w)\tau]\}}{[(1+w)^2+(1-w)^2y^2][1+y^2]}, \tag{6.101}$$

$$\frac{df_p(\tau,w)}{d\tau}=-\frac{4(1-w)^2}{w}e^{-(1-w)\tau}\int_0^\infty dy\frac{y^2\coth\left(by\sqrt{\frac{1-w}{1+w}}\right)\sin[y(1-w)\tau]}{[(1+w)^2+(1-w)^2y^2][1+y^2]}. \tag{6.102}$$

The behavior of the entropy production is depicted in Fig. 10. It is seen that there is a small region, where the curves are negative. For $w=0.1$ (weak overdamping) the negative region is yet noticeable, but already for $w=0.7$ (moderate overdamping) this region is almost indistinguishable. This is in agreement with the above analytical analysis in the limit $\varepsilon\to 0$.

VII. WORK AND HEAT

So far we have discussed the system's relaxation from a nonequilibrium initial state. Since the total system is isolated, in this process energy is transferred from the subsystem to the bath, or vice versa. This energy is related to the unobservable bath modes, so it is identified as heat. In particular, in no way work was added to or extracted from the system, except for the initial moment, where the strength of the central spring was modified.

We shall now consider the possibility of additional changes in the spring constant and its implications for work extracted from the system.

A. General definition of work and heat

The behavior of a statistical system under interaction with external macroscopic sources is the standard area of applications for any thermodynamical theory. As is well known, in this setup one neglects the influence of the statistical system

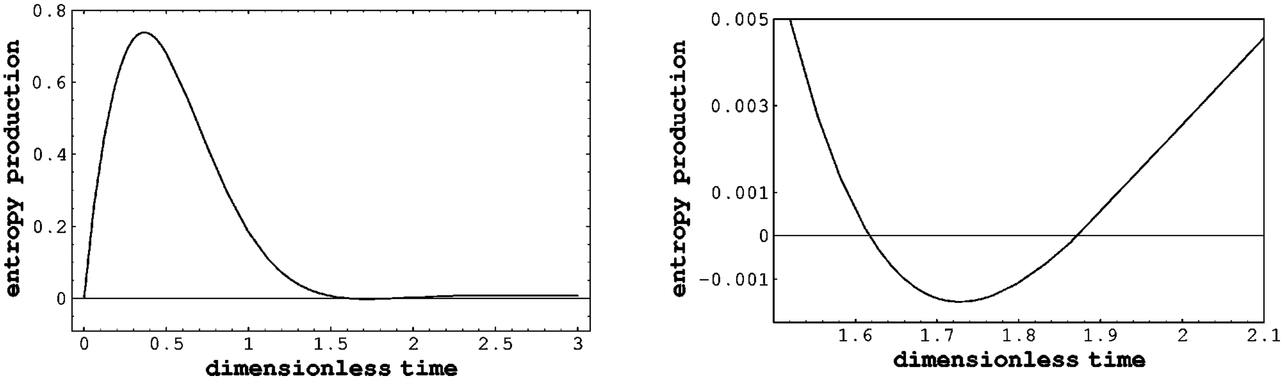

FIG. 10. Rate of entropy production [up to a factor $a\alpha_0^2/(16\gamma\varepsilon^2\theta_x^2)$] vs dimensionless time τ. Left part, $T=0$, $w=0.1$. Right part, magnification of the region around $\tau=1.75$.

to the dynamics of the source. Therefore, one can keep the parameters of the system as given functions of time, and solve the corresponding equations for the system's dynamics. We start with general remarks about the energy budget of any variation.

Let us consider the change of a system parameter α. It is assumed to be intrinsic, that is to say, to characterize the Brownian particle but not the bath or the interaction between the particle and bath. In the situation discussed in the body of this work, α can stand for the spring constant a of the harmonic potential, the effective width of the anharmonic potential, or the mass m (for electrical circuits and junctions mass is connected with inductivity and can be subjected to variations; this also makes sense in systems where m is an effective mass, that can be modified by changing other system parameters, such as pressure).

First one has to identify the Hamiltonian of the subsystem. In Eq. (2.1) we have chosen $\mathcal{H}=\frac{1}{2}p^2/m+\frac{1}{2}ax^2$, as in absence of the bath. It should be stressed that we did not include the self-coupling $\frac{1}{2}\gamma\Gamma x^2$ or (part of) the interaction energy in $\mathcal{H}$. Our choice is the natural one in the sense that the limits of large Debye frequency Γ and subsequent large damping γ lead to moderately large values of the energy of system and bath, and not to large terms of opposite sign that cancel in the total energy, as would occur, e.g., if $\frac{1}{2}\gamma\Gamma x^2$ were counted for the subsystem. See also the discussion in Sec. IV B 5.

A change with time of the mean energy is considered due to a variation of a parameter α according to the prescribed trajectory $\alpha(t)$

$$\begin{aligned} dU&=d\int dx dp\, W(p,x,t)\,\mathcal{H}(p,x)\\ &=\int dx dp\,\mathcal{H}(p,x)\,dW(p,x,t)\\ &\quad+\int dx dp\, W(p,x,t)\,d\mathcal{H}(p,x), \end{aligned}\tag{7.1}$$

where $W(p,x)$ is the Wigner function of the Brownian particle. The last term results from the change in the Hamiltonian, so it is a mechanical, nonstatistical object. Following other authors [5,6,44–46], we shall associate it with the work $\text{đ}W$ produced by external sources, in close relation with the definition of work in classical mechanics and standard thermodynamics. The first term in the right hand side represents the variation due to the statistical redistribution of the phase space. We shall identify it with the change in heat $\text{đ}\mathcal{Q}$. Equation (7.1) can then be written as the usual first law,

$$dU=\text{đ}\mathcal{Q}+\text{đ}\mathcal{W}\tag{7.2}$$

The work, as defined in Eq. (7.1) can be shown to be the change of the total closed system's (the particle plus bath) energy due to the variation of the parameter α. First one notices that for closed systems with a unitary evolution any change of energy is determined solely by work. This fact is due to the conservation of energy, and can be easily illustrated using the von Neumann equation of motion for the density matrix ρ_{tot} of the total system. Indeed, since

$$\frac{d\rho_{tot}}{dt}=-\frac{i}{\hbar}[\rho_{tot},\mathcal{H}_{tot}],$$

one has

$$\begin{aligned} dU_{tot}&=d\ \ \mathrm{tr}(\rho_{tot}\mathcal{H}_{tot})=\mathrm{tr}(\rho_{tot}\ \ d\mathcal{H}_{tot})+\mathrm{tr}(\mathcal{H}_{tot}\ \ d\rho_{tot})\\ &=\mathrm{tr}(\rho_{tot}\ \ d\mathcal{H}_{tot})-\frac{i}{\hbar}\ \ dt\ \ \mathrm{tr}(\mathcal{H}_{tot}\ \ [\rho_{tot},\mathcal{H}_{tot}])\\ &=\mathrm{tr}(\rho_{tot}\ \ d\mathcal{H}_{tot}) \end{aligned}\tag{7.3}$$

due to the cyclic character of the trace. If now $W_{tot}(p,x,p_1,x_1,\ldots)$ is the Wigner function of the whole system, then this implies the identity

$$\begin{aligned} dU_{tot}&=\int dp dx\prod_k\ dp_k dx_k\, W_{tot}(p,x,p_1,x_1,\ldots)\\ &\quad\times d\mathcal{H}_{tot}(p,x,p_1,x_1,\ldots)\\ &=\int dx\ \ dp\, W(p,x,t)\,d\mathcal{H}(p,x), \end{aligned}\tag{7.4}$$

since we only consider cases where forces are attached to the central particle, so $d\mathcal{H}_{tot}(p,x,p_1,x_1,\dots)=d\mathcal{H}(p,x)$, implying that the p_k, x_k integrals over the full Wigner function just bring the Wigner function of the subsystem. Taking into account that no heat was added to the total system, $đ\mathcal{Q}_{tot}=0$, we may conclude that the work $đ\mathcal{W}$ extracted from the subsystem equals the work subtracted from the total system, $đ\mathcal{W}_{tot}=dU_{tot}=đ\mathcal{W}$.

We again consider the situation where at $t=0$ the system was Gibbsian, with spring constant a_0, and it is instantaneously changed to a new value a. For achieving this an amount of work $\mathcal{W}_0$, given in Eq. (7.13) has to be added to the system. For $a>a_0$ this is just the work needed to make the spring attached to the particle stiffer. When $a_0<a$ this work is negative; energy is extracted, since the spring is weakened. For work extraction from the thus created nonequilibrium state we shall make additional changes in the spring constant.

B. Maximally extractable work

Now the total system consisting of central particle and bath is out of equilibrium, some work can be extracted from it. Before the interaction between the bath and the particle has been switched on, the total energy was

$$U_{\rm tot}(0^-)=U_B(T)+U_p(T,a_0), \tag{7.5}$$

where $U_B(T)=\pi^2T^2/(6\hbar\Delta)$ and $U_p(T)$ are the initial energies of the unperturbed bath and the perturbation due to the Brownian particle, defined in Eq. (3.17) and by $U_p=\partial[\beta F_p]/\partial\beta$ with F_p taken from Eq. (3.44), respectively. After the switching of the interaction has been completed, the energy has become

$$U_{\rm tot}(0^+)=\mathcal{W}_0+U_B(T)+U_p(T,a_0). \tag{7.6}$$

Let us now consider what the maximum amount of work is that can be extracted from the overall isolated system in the considered nonequilibrium state. First of all, we notice that we are interested in the work done due to the nonequilibrium character of this state, and not in the work which might be done due a change of the Hamiltonian. Therefore, during extraction processes the parameters of the Hamiltonian $\mathcal{H}_{\rm tot}$ will be either fixed or vary cyclically, such that after the process has been completed, the system has the same Hamiltonian as initially. To determine the maximum amount of extracted work we will employ the following formulations of the second law, which are undoubtedly valid for the considered thermally isolated system [5,44,45].

(i) No work can be extracted from a system in its equilibrium state. (Let us recall that thermal isolation means that no external supply of heat is given; the allowed transformations are variation of parameters by external sources).

(ii) The converse is true as well under certain general conditions [47]. If no work can be extracted by any means from a system in a given state, then this state is equilibrium.

As follows from (i) some work can be extracted from nonequilibrium states. In the same way (ii) implies that if work has been extracted in all possible ways, the system is left in an equilibrium state at some temperature $T_{\rm fin}$. Since the overall system is thermally isolated, the extracted work is in magnitude equal to the complete change of energy (this is the statement of the first law): $|\mathcal{W}_{\rm max}|=U_{\rm tot}(0^+)-U_{\rm fin}(T_{\rm fin})$, where $U_{\rm fin}(T_{\rm fin})=U_{\rm tot}(T_{\rm fin},a)$ is the energy of the final equilibrium state. Because the entropy is conserved during variations of parameters, the optimal final equilibrium state will have a density matrix

$$\rho_{\rm fin}=\frac{\exp[-\beta_{\rm fin}\mathcal{H}_{\rm tot}]}{Z}, \tag{7.7}$$

involving the temperature $T_{\rm fin}=1/\beta_{\rm fin}$, which is determined by constancy of the von Neumann entropy of the total system,

$$\begin{aligned}S_{\rm tot}(T)=S_B(T,\gamma=0)+S_p(T,a_0)=S_{\rm tot}(T_{\rm fin})=S_B(T_{\rm fin},\gamma=0)\\ +S_p(T_{\rm fin},a)\end{aligned} \tag{7.8}$$

with $S_B(T,\gamma=0)=\pi^2T/3\hbar\Delta$ from Eq. (3.18). Remembering that the level splitting Δ of the bath modes is very small, one can solve

$$T_{\rm fin}=T+\frac{3\hbar\Delta}{\pi^2}[S_p(T,a_0)-S_p(T,a)]. \tag{7.9}$$

This yields

$$\begin{aligned}|\mathcal{W}_{\rm max}|&=\mathcal{W}_0+U_{\rm tot}(T,a_0)-U_{\rm tot}(T,a)\\ &\quad-TS_p(T,a_0)+T_p(T,a)\\ &=\mathcal{W}_0+F_{\rm tot}(T,a_0)-F_{\rm tot}(T,a)\\ &=\mathcal{W}_0+F_p(T,a_0)-F_p(T,a).\end{aligned} \tag{7.10}$$

In the last step we canceled the contributions of the unperturbed bath. Not unexpectedly, the result just depends on the free energies of the total system.

Notice that for a cycle consisting of the changes $a_0\rightarrow a$ and (much) later $a\rightarrow a_0$, the maximally extractable work becomes the sum of the amounts of work, $\mathcal{W}_0(a_0\rightarrow a)+\mathcal{W}_0(a\rightarrow a_0)$, so for cycles in principle all work can be recovered.

1. Values at high and low T

In the classical limit the free energy is given by the first term in Eq. (3.52), just the value for a harmonic oscillator, whether or not it is coupled to other harmonic oscillators. The maximally extractable work is

$$|\mathcal{W}_{\rm max}|=\frac{1}{2}\left[\frac{\alpha_0}{1-\alpha_0}+\ln(1-\alpha_0)\right]T=\frac{1}{4}\alpha_0^2T+\mathcal{O}(\alpha_0^3). \tag{7.11}$$

At low T the difference in free energy of the total system between the equilibrium states at the initial and final value of the spring constant is

$$F_{\mathrm{tot}}(a)-F_{\mathrm{tot}}(a_0)=F_p(a)-F_p(a_0)=\frac{\hbar a}{2\pi\gamma}\left[\frac{\alpha_0}{w}\ln\frac{1+w}{1-w}+\frac{\alpha_0^2}{2w^2}\left(1-\frac{1-w^2}{2w}\ln\frac{1+w}{1-w}\right)\right]+(\alpha_0+\alpha_0^2)\frac{\pi\gamma T^2}{6\hbar a}. \tag{7.12}$$

The energy added at $t=0$ is

$$\mathcal{W}_0=\frac{1}{2}\left(\frac{a}{a_0}-1\right)T_x(a_0)=\frac{\hbar a}{2\pi\gamma}\left[\frac{\alpha_0}{w}\ln\frac{1+w}{1-w}+\frac{\alpha_0^2}{w^2}\left(1-\frac{1-w^2}{2w}\ln\frac{1+w}{1-w}\right)\right]+(\alpha_0+2\alpha_0^2)\frac{\pi\gamma T^2}{6\hbar a}. \tag{7.13}$$

So by making the instantaneous change in a the maximally extractable work (7.10) reads

$$|\mathcal{W}_{\max}|=\alpha_0^2\left[\frac{\hbar a}{4\pi\gamma}\frac{1}{w^2}\left(1-\frac{1-w^2}{2w}\ln\frac{1+w}{1-w}\right)+\frac{\pi\gamma T^2}{6\hbar a}\right]. \tag{7.14}$$

If we let the system relax, this will run away in the bath on a time scale τ_x. By making clever subtraction schemes, we may recover some of it, and in principle all of it.

For the case $T=T_{\mathrm{fin}}=0$ Eq. (7.10) merely says that that all energy exceeding the ground-state energy of the new system can, in principle, be extracted.

C. Work extraction by further sudden changes

Here we present the formalism of work extraction via sudden changes of a parameter. Besides presenting the general setup, we will display the validity of the Thomson's equilibrium formulation of the second law within the present situation.

Let there be a closed system with a Hamiltonian $\mathcal{H}$ in a state $\rho(t_1)$ at the moment t_1. Certain parameters of the Hamiltonian are varied in a very fast way such that for t_1^+ its Hamiltonian becomes $\mathcal{H}_1$, but the state remains $\rho(t_1)$ due to the sudden character of the variation. The work done by an external source reads

$$\mathcal{W}_1=\mathrm{tr}[\rho(t_1)(\mathcal{H}_1-\mathcal{H})]. \tag{7.15}$$

In the second step the system is allowed to evolve according to the new Hamiltonian $\mathcal{H}_1$. At moment t_2 when the system reaches the state

$$\rho(t_2)=e^{-i(t_2-t_1)\mathcal{H}_1/\hbar}\rho(t_1)e^{i(t_2-t_1)\mathcal{H}_1/\hbar}, \tag{7.16}$$

its parameters are suddenly returned to their original value. The work done in this step reads

$$\mathcal{W}_2=\mathrm{tr}[\rho(t_2)(\mathcal{H}-\mathcal{H}_1)]. \tag{7.17}$$

The total work done by the source for this cyclic variation of the parameter reads

$$\begin{aligned}\mathcal{W}&=\mathcal{W}_1+\mathcal{W}_2\\&=\mathrm{tr}[\rho(t_1)(e^{i(t_2-t_1)\mathcal{H}_1/\hbar}\,\mathcal{H}\,e^{-i(t_2-t_1)\mathcal{H}_1/\hbar}-\mathcal{H})],\end{aligned} \tag{7.18}$$

where we have used Eq. (7.16). Notice that we consider the closed overall system, and only due to this fact the evolution of the system for times between t_1 and t_2 is given by the Hamiltonian $\mathcal{H}_1$.

It is not difficult to see from Eq. (7.18) that the second law is satisfied for the present setup. Let us first assume that at the moment t the system was in the ground state of $\mathcal{H}$: $\rho(t_1)=|0\rangle\langle 0|$. Then one has

$$\mathcal{W}=\langle 0|\,e^{i(t_2-t_1)\mathcal{H}_1/\hbar}\,\mathcal{H}\,e^{-i(t_2-t_1)\mathcal{H}_1/\hbar}\,|0\rangle-\langle 0|\,\mathcal{H}\,|0\rangle\geqslant 0, \tag{7.19}$$

just by the definition of the ground state. The same statement, namely, $W\geqslant 0$, holds when $\rho(t)$ is the Gibbs distribution of the initial state at positive temperature $T=1/\beta$: $\rho(t_1)=\exp(-\beta\mathcal{H})/Z,\ Z=\mathrm{tr}\exp(-\beta\mathcal{H})$ [47,64].

Our work extraction mechanism involves a second change of the spring constant, which is cyclic: at time t_2 we impose a jump $a\to a_2=a(1-\alpha_2)$ and it keeps that value, until at t_3 it is put back to a. The work involved in this cyclic two-step process is

$$\begin{aligned}\Delta\mathcal{W}&=U_{\mathrm{tot}}(t_2^+)-U_{\mathrm{tot}}(t_2^-)+U_{\mathrm{tot}}(t_3^+)-U_{\mathrm{tot}}(t_3^-)\\&=\frac{1}{2}(a_2-a)[\langle x^2\rangle_{t_2}-\langle x^2\rangle_{t_3}].\end{aligned} \tag{7.20}$$

The change in particle energy between t_2^- and t_3^+ is

$$\Delta U=\frac{1}{2m}[\langle p^2\rangle_{t_3}-\langle p^2\rangle_{t_2}]+\frac{1}{2}a[\langle x^2\rangle_{t_3}-\langle x^2\rangle_{t_2}]. \tag{7.21}$$

Thus the change in heat during the work extraction process is

$$\Delta\mathcal{Q}=\frac{1}{2m}[\langle p^2\rangle_{t_3}-\langle p^2\rangle_{t_2}]+\frac{1}{2}a_2[\langle x^2\rangle_{t_3}-\langle x^2\rangle_{t_2}]. \tag{7.22}$$

The values of $\langle x^2\rangle$ and $\langle p^2\rangle$ at time t_2 are set by the spring constants a_0 and a solely, and can be taken from the preceding section. When we take t_3 large, we can take for that situation the limiting values for a system with spring constant a_2. We then find

$$\Delta\mathcal{W}=(a_2-a)\left[\frac{T_x(a)}{2a}+\frac{\alpha_0\hbar}{2\pi\gamma}C_x\left(\frac{\gamma t_2}{2m}\right)-\frac{T_x(a_2)}{2a_2}\right], \tag{7.23}$$

$$\Delta U=\frac{1}{2}T_p(a_2)-\frac{1}{2}T_p(a)+\frac{a}{2a_2}T_x(a_2)-\frac{1}{2}T_x(a)-\frac{\alpha_0\hbar a}{2\pi\gamma}C_E\left(\frac{\gamma t_2}{2m}\right), \tag{7.24}$$

$$\Delta\mathcal{Q}=\frac{1}{2}T_p(a_2)-\frac{1}{2}T_p(a)+\frac{1}{2}T_x(a_2)-\frac{a_2}{2a}T_x(a)-\frac{\alpha_0\hbar a}{2\pi\gamma}C_p\left(\frac{\gamma t_2}{2m}\right)-\frac{\alpha_0\hbar a_2}{2\pi\gamma}C_x\left(\frac{\gamma t_2}{2m}\right). \tag{7.25}$$

1. Classical regime

In the classical case with strong damping we use Eq. (6.13) and obtain

$$\Delta\mathcal{W}=\frac{1}{2}\alpha_2^2T-\frac{1}{2}\alpha_0\alpha_2Te^{-2at_2/\gamma}. \tag{7.26}$$

This has a minimum at

$$\alpha_2^*=\frac{1}{2}\alpha_0e^{-2at_2/\gamma},\quad \Delta\mathcal{W}_{\min}=-\frac{1}{8}\alpha_0^2T\ e^{-4at_2/\gamma}. \tag{7.27}$$

Work can only be extracted under proper conditions, that is to say, when α_2 is between 0 and $\alpha_0\exp(-2\omega_2t_2)$. Otherwise the cycle $a\rightarrow a_2\rightarrow a$ disperses energy.

The heat absorbed by the subsystem is at linear order in α_0 insensitive to the work extraction,

$$\Delta\mathcal{Q}=\Delta U=-\frac{1}{4}\alpha_0Te^{-4at_2/\gamma}. \tag{7.28}$$

There are two cases.

(1) $\alpha_0>0$. The central spring is stiffened, $a>a_0$, and energy is supplied at $t=0$. This energy leaks away, mostly as heat into the bath, $(\Delta\mathcal{Q}<0)$ and partly as work extracted from the total system $(\Delta W<0)$, more precisely, from the particle.

The ratio of extracted work to maximally extractable energy is, in the regime where α_0 is small but finite and $T\gg\hbar\omega_0$,

$$\eta=\frac{|\Delta\mathcal{W}|}{|\mathcal{W}_{\max}|}=\frac{1}{2}e^{-4\omega_2t_2}. \tag{7.29}$$

So our mechanism extracts maximally 50% of maximum; to do this it must start immediately $(t_2=0)$ and last as long as possible $(t_3=\infty)$.

(2) $\alpha_0<0$. The central spring is weakened at $t=0$. Energy is taken out from the system. The amount, $\frac{1}{2}T(|\alpha_0|-\alpha_0^2)$ is less than the amount that could have been extracted by an adiabatic change, $\frac{1}{2}T(|\alpha_0|+\frac{1}{2}\alpha_0^2)$. After that has been done, heat flows from the bath to the particle $(\Delta\mathcal{Q}>0)$, as if the particle were at a lower temperature. In the course of this process work can be extracted, maximally the absolute value of Eq. (7.27), as is usual for two-temperature systems. The basic issue to extract work is to have a mechanism that, given the initial change in a, is the closest to adiabaticity. These conclusions also hold for moderate and weak damping.

2. Low-temperature regime

At $T=0$ we get from Eq. (7.23)

$$\Delta\mathcal{W}=\frac{\hbar a}{2\pi\gamma}\left[\alpha_2^2C_x(0)-\alpha_0\alpha_2\,C_x\left(\frac{\gamma t_2}{2m}\right)\right], \tag{7.30}$$

where $C_x(0)$ is defined in Eq. (6.25) and $C_x(\tau)$ in Eq. (6.6). The minimum occurs for

$$\alpha_2^*=\frac{\alpha_0}{2C_x(0)}C_x\left(\frac{\gamma t_2}{2m}\right),\quad \Delta\mathcal{W}_{\min}=-\frac{\hbar\omega_2\alpha_0^2}{8\pi C_x(0)}C_x^2\left(\frac{\gamma t_2}{2m}\right). \tag{7.31}$$

The change in heat and internal energy is

$$\Delta\mathcal{Q}=\Delta U=-\alpha_0\frac{\hbar a}{2\pi\gamma}C_E\left(\frac{\gamma t_2}{2m}\right). \tag{7.32}$$

We consider again the following separate cases.

(1) $\alpha_0>0$. The spring is stiffened at $t=0$ and energy $\mathcal{W}_0$ is supplied. At $t=0^+$ the energy is, to linear order in α_0, equal to its final value, since $C_E(0)=0$. This changes since energy comes from the bath, on a time scale τ_p which is short for strong damping, where $\tau_p=m/\gamma$. In the initial time regime $\gamma t_2/2m<\tau_0$ this mainly leaks away to the bath, and a small part can be extracted as work. In the regime $\tau_0<\gamma t_2/2m<\sigma_{\min}$ this also happens, but the energy of the subsystem goes below its final value, so the particle becomes "too cold." In the final regime $\gamma t_2/2m>\sigma_{\min}$ energy flows back to the particle and again a small part can be extracted as work. This is then work extracted from the nonequilibrium bath, and the surprise is that this can be done although initially energy was put on the particle. This recovery of energy stored in the bath is a quantum effect.

$\Delta W<0$ means that work is extracted from the total system. Equation (7.31) is the maximally extractable amount of work with the present mechanism. As an efficiency factor we may normalize with respect to the maximally extractable energy from Eq. (7.11) the energy that would otherwise leak away into the bath,

$$\eta=\frac{-\Delta\mathcal{W}_{\min}}{|\mathcal{W}_{\max}|}=\frac{1}{2}C^2(\omega_2t_2). \tag{7.33}$$

When one starts the extraction quickly after the initial change $(\tau_1\approx0)$ one can still get half of the work back in this way, the same rate as in the classical regime. Even more is obtained when one still starts at $t_2=0$ but stops at the moment that the energy current goes no longer towards the particle, but away from it, i.e., at $\omega_2t_3=\sigma_{\min}$. One then has

$$\begin{aligned}\Delta\mathcal{W}&=-\frac{1}{2}\alpha_2 a[\langle x^2\rangle_{t=0;\,a_0}-\langle x^2\rangle_{t_3;\,a_2}]\\&=\frac{\hbar a}{2\pi\gamma}\{\alpha_2^2-\alpha_0\alpha_2[1-C_x(\omega_2 t_3)]\}\\&\geqslant-\frac{\hbar a}{8\pi\gamma}\alpha_0^2[1-C_x(\omega_2 t_3)]^2.\end{aligned}\tag{7.34}$$

The efficiency is

$$\eta=\frac{-\Delta\mathcal{W}}{|\mathcal{W}_{max}|}=\frac{1}{2}[1-C_x(\omega_2 t_3)]^2,\tag{7.35}$$

which indeed has the proper behavior for $t_3\rightarrow 0$ and $t_3\rightarrow\infty$. The maximum is, due to Eqs. (6.35) and (6.38),

$$\eta_{\max}=\frac{1}{2}[1-C_x(\sigma_{\min})]^2=0.5961;\tag{7.36}$$

it exceeds the classical efficiency $\eta=1/2$. So the quantum statistical excess energy flow from the particle into the bath indeed allows a more optimal recovery of energy initially put on the particle.

The most interesting feature is that with the present mechanism it is also possible to extract work solely from the bath a mechanism forbidden by the original Thomson formulation of the second law. Indeed, after $\omega_2 t=\sigma_{\min}$ energy will flow back from the bath to the particle. By starting the extraction mechanism at $\omega_2 t_2=\sigma_{\min}$ and exploiting all times after this for the work extraction, the maximal efficiency (7.33) is

$$\eta_{\max}=\tfrac{1}{2}C^2(\sigma_{\min})=0.004\,222\,625\,76.\tag{7.37}$$

In contrast to the classical case, it goes to a finite limit when $\alpha_0\rightarrow 0$. This occurs because in the quantum case the energy $\sim\alpha_0^2$, with respect to which the extracted work has been normalized, is one order of magnitude smaller than the initially supplied energy $\mathcal{W}_0\sim\alpha_0$.

(2) $\alpha_0<0$. The spring is weakened and energy $\mathcal{W}_0$ is extracted. Some energy can be extracted. For $\omega_2 t_2<\sigma_{\min}$ it comes from the bath, but in the regime $\omega_2 t_2>\sigma_{\min}$ the particle has excess energy, which then supplies the work.

D. Work extraction by smooth changes of the spring constant

Let us now consider the case where the spring constant $a(t)=[1-\alpha(t)]a$, is slightly changed ($|\alpha(t)|\ll 1$) in a smooth manner, starting from the equilibrium state $a(-\infty)=a$. In Appendix A we derive for the rate of work added to the system

$$\frac{d\mathcal{W}}{dt}=\frac{d\mathcal{W}_{\text{rev}}}{dt}+\frac{d\Pi}{dt},\tag{7.38}$$

where

$$\frac{d\mathcal{W}_{\text{rev}}}{dt}=-\frac{\gamma}{2m}\frac{d\alpha(\tau)}{d\tau}\left[\frac{1}{2}T_x+\frac{\hbar a}{2\pi\gamma}\alpha(\tau)C_x(0)\right],\tag{7.39}$$

with $\tau=\gamma t/(2m)$, is the adiabatic (“reversible” or “recoverable”) rate of work and

$$\frac{d\Pi}{dt}=\frac{\hbar a}{4\pi m}\frac{d\alpha(\tau)}{d\tau}\int_0^\infty d\sigma\,\alpha'\left(\frac{\gamma t}{2m}-\sigma\right)C_x(\sigma)\tag{7.40}$$

is the rate of energy dispersion.

1. *Completed changes*

Integrating over the full change one has

$$\mathcal{W}_{\text{rev}}=-\frac{1}{2}(\alpha_f-\alpha_i)T_x-\frac{\hbar a}{4\pi\gamma}C_x(0)[\alpha_f^2-\alpha_i^2],\tag{7.41}$$

where $\alpha_i=\alpha(-\infty)$ and $\alpha_f=\alpha(\infty)$, and

$$\Pi=\frac{\hbar a}{4\pi\gamma}\int_{-\infty}^{\infty}d\tau_1\,\alpha'(\tau_1)\int_{-\infty}^{\infty}d\tau_2\,\alpha'(\tau_2)C_x(|\tau_1-\tau_2|).\tag{7.42}$$

For a full process (covering the whole region where $\alpha'\neq 0$) Π is non-negative, since it is an integral over a non-negative function,

$$\Pi=\frac{\hbar a}{2\gamma}\int_{-\infty}^{\infty}d\zeta|A(\zeta)|^2\Re\,\hat{C}_x(i\zeta),\tag{7.43}$$

where the Laplace transform $\hat{C}_x$ was given in Eq. (6.51) for the case $T=0$; it can be verified that $\operatorname{Re}\hat{C}_x(i\zeta)$ is positive for all real ζ. Furthermore,

$$A(\zeta)=\int\frac{d\tau}{2\pi}\alpha'(\tau)\,e^{i\zeta\tau}.\tag{7.44}$$

The positive energy dispersion for a completed, nonadiabatic cyclic change of system parameters ($\alpha_i=\alpha_f$) is the Thomson formulation of the second law. We see that a positive dispersion also holds for noncyclic but completed changes $\alpha_i\neq\alpha_f$, as is known to occur on general grounds.

We can check previous case $\alpha(t)=\alpha_0\theta(-t)$, $\alpha'(\tau)=-\alpha_0\delta(\tau)$, for which Eq. (7.13) is, at $T=0$, equivalent to

$$\mathcal{W}_0=\mathcal{W}_{\text{rev}}+\Pi=\frac{1}{2}\alpha_0 T_x+\frac{\hbar a}{2\pi\gamma}\alpha_0^2 C_x^{(0)}.\tag{7.45}$$

2. *Incomplete changes*

Let us now consider the temporal build up of this result in the regime of strong damping. Let α have the form

$$\alpha(\tau)=\alpha_m h(\Omega t), \tag{7.46}$$

where α_m is a small amplitude and h is a bounded function ($|h|\leqslant 1$), with $h(-\infty)=0$, $h'(\infty)=0$. If $h(\infty)\neq 0$ it could be an error function; if $h(\infty)=0$ a Gaussian. $1/\Omega$ is the typical time duration of the change. Using Eqs. (6.48)–(6.50) we get from Eq. (A10)

$$\begin{aligned}\frac{d\Pi}{dt}&=\frac{\hbar a}{4\pi m}\,\alpha'\left[\alpha' C_x^{(0)}+\alpha'' C_x^{(1)}-\frac{1}{2}\alpha''' C_x^{(2)}\right]\\&=\frac{\hbar\Omega^2\alpha_{\rm m}^2}{12\pi}h'(\Omega t)\left[\left(\frac{2\pi\gamma T}{\hbar a}\right)^2 h'(\Omega t)+\frac{\gamma\Omega\tilde{C}_x^{(1)}}{a}h''(\Omega t)-\frac{\gamma^2\Omega^2}{a^2}h'''(\Omega t)\right],\end{aligned} \tag{7.47}$$

where $\tilde{C}_x^{(1)}$ was defined in Eq. (6.49); for weak damping it equals $3\pi\sqrt{am}/8\gamma$, while for large damping it becomes unity. The integrated effect is

$$\Pi(t)=\frac{\hbar\Omega\alpha_{\rm m}^2}{12\pi}\left\{\left(\frac{2\pi\gamma T}{\hbar a}\right)^2\int_{-\infty}^{\Omega t}d\xi[h'(\xi)]^2+\frac{\gamma\Omega\tilde{C}_x^{(1)}}{2a}[h'(\Omega t)]^2+\frac{\gamma^2\Omega^2}{a^2}\left[-h'(\Omega t)h''(\Omega t)+\int_{-\infty}^{\Omega t}d\xi[h''(\xi)]^2\right]\right\}. \tag{7.48}$$

For a completed change the second and third terms vanish, leading to a positive energy dispersion, in concordance with Eq. (7.43). It is seen that then the standard behavior $\Pi\sim\Omega$ applies when T is large enough or when Ω is small enough. However, in the quantum regime where the duration $1/\Omega$ is smaller than the quantum time scale $\tau_\hbar=\hbar/T$, the last term in Eq. (7.48) dominates, with a new behavior $\Pi\sim\Omega^3$.

Another quantum effect is that at low T and for typical times the second term in Eq. (7.47) is larger in magnitude than the other ones. This too occurs, since the integral of $C_x(\tau)$ vanishes at $T=0$, and leads to new possibilities, which we discuss now.

3. Work extraction from a smooth cyclic change

One definition for a perpetuum mobile of the second kind is that there is a machine that performs a cycle in which it receives heat from a bath and converts it fully into work done on the surroundings. Additional requirements can occur; we shall discuss them in Sec. IX H. Here we analyze whether such a full energy conversion can be realized in our setup. The aim is thus to have a cyclic change of a system parameter with the properties

$$\Delta U=0,\quad \Delta\mathcal{Q}=-\Delta\mathcal{W}>0. \tag{7.49}$$

Including in Eq. (A6) also the contribution of the momentum, we have, to linear order in α,

$$\begin{aligned}U(t)=\frac{1}{2}T_p(a)+\frac{1}{2}T_x(a)+\frac{\hbar a}{2\pi\gamma}\Bigg[&\alpha\left(\frac{\gamma t}{2m}\right)C_E(0)\\&-\int_0^\infty d\tau\,\alpha'\left(\frac{\gamma t}{2m}-\tau\right)C_E(\tau)\Bigg].\end{aligned} \tag{7.50}$$

Let us choose for $\alpha(\tau)$ a curve in the shape of a double bell, and consider the system at some time t_1 after the first peak, and compare it to the situation at a later time t_2, after the second peak. We require that the spring constant has the same values at these instants, $\alpha(\tau_1)=\alpha(\tau_2)$, where $\tau_{1,2}=\gamma t_{1,2}/2m$. This implies for the internal energy

$$\begin{aligned}\Delta U&=U(t_2)-U(t_1)\\&=\frac{\hbar a}{2\pi\gamma}\int_0^\infty d\tau[\alpha'(\tau_1-\tau)-\alpha'(\tau_2-\tau)]C_E(\tau).\end{aligned} \tag{7.51}$$

At low T and for slow changes this can be expanded,

$$\begin{aligned}\Delta U=\frac{\hbar a}{2\pi\gamma}\Bigg\{&[\alpha'(\tau_1)-\alpha'(\tau_2)]C_E^{(0)}+[\alpha''(\tau_1)\\&-\alpha''(\tau_2)]C_E^{(1)}-\frac{1}{2}[\alpha'''(\tau_1)-\alpha'''(\tau_2)]C_E^{(2)}\Bigg\},\end{aligned} \tag{7.52}$$

where the coefficients are given in Eq. (6.53).

Let us assume that we have two consecutive changes, characterized by a common bell-shaped function $k(x)$ with $|k(x)|\leqslant 1$, but involving different rates of change $\Omega_{1,2}$,

$$h(\tau)=k(\Omega_1 t)+k(\Omega_2(t-t_2^c)), \tag{7.53}$$

where the parameters $\Omega_1>\Omega_2>0$ and $t_2^c>0$ are such that the profiles have negligible overlap. Choosing the times $t_{1,2}$ as

$$t_1=\frac{\bar{x}}{\Omega_1},\quad t_2=t_2^c+\frac{\bar{x}}{\Omega_2}, \tag{7.54}$$

we indeed satisfy the cyclic condition $\alpha(\tau_1)=\alpha(\tau_2)=\alpha_m k(\bar{x})$. The difference in energy is

$$\Delta U=\frac{\alpha_m\hbar(\Omega_1-\Omega_2)}{12\pi}\left\{\left(\frac{2\pi\gamma T}{\hbar a}\right)^2 k'(\overline{x})+\frac{\gamma(\Omega_1+\Omega_2)}{a}k''(\overline{x})-\frac{\gamma^2(\Omega_1^2+\Omega_1\Omega_2+\Omega_2^2)}{a^2}k'''(\overline{x})\right\}. \tag{7.55}$$

Let us assume that $\overline{x}$ is fixed but such that $k'<0$ while $k''>0$; this is possible because k has both convex and concave parts, implying that there is an interval with such behavior. In the example $k(x)=\exp(-x^2/2)$, there is an inflection point $x_{\rm if}=1$ and one needs $\overline{x}>1$. Let us also assume that $T\ll\hbar a/\gamma$. Then for

$$\Omega_1+\Omega_2=\frac{4\pi^2\gamma T^2}{\hbar^2 a}\frac{|k'(\overline{x})|}{k''(\overline{x})} \tag{7.56}$$

the first two terms can cancel, while the exposed correction term and the higher ones are small. Thus under these conditions it is possible to have a cyclic process with $\Delta U=0$ to order α_m; if $\alpha_{\rm m}^2$ corrections are taken into account, the condition for cancellation is shifted by an amount of order α_m and can again be met. Thus it is possible to start from the equilibrium state, make a first cyclic change of a and then a second, which process contains itself a cyclic change of a with $\Delta U=0$. The work during this cycle comes solely from the energy dispersion. Using Eq. (7.48) we obtain the leading terms

$$\begin{aligned}\Delta\mathcal{W}&=\frac{\alpha_{\rm m}^2\hbar}{12\pi}\left\{\left(\frac{2\pi\gamma T}{\hbar a}\right)^2\left(\Omega_1\int_{\overline{x}}^{\infty}d\xi[k'(\xi)]^2+\Omega_2\int_{-\infty}^{\overline{x}}d\xi[k'(\xi)]^2\right)+\frac{\gamma(\Omega_2^2-\Omega_1^2)\tilde{C}_x^{(1)}}{2a}[k'(\overline{x})]^2\right\}\\&=\frac{\hbar\alpha_{\rm m}^2}{12\pi}\left(\frac{2\pi\gamma T}{\hbar a}\right)^2\left\{\Omega_1\int_{\overline{x}}^{\infty}d\xi[k'(\xi)]^2+\Omega_2\int_{-\infty}^{\overline{x}}d\xi[k'(\xi)]^2+\frac{1}{2}(\Omega_2-\Omega_1)\tilde{C}_x^{(1)}\frac{|k'(\overline{x})|^3}{k''(\overline{x})}\right\}.\end{aligned} \tag{7.57}$$

The higher-order terms are small for the same reason as above. If $\Delta W<0$ this amounts to work exerted by the system on the environment. One can always have $k''(\overline{x})$ small enough (by choosing $\overline{x}$ close to the inflection point) to make the combination of the Ω_1 terms negative, and choose Ω_2 so small that the whole expression remains negative. So it is indeed possible to have a cycle where the extracted work $|\Delta\mathcal{W}|$ comes solely from the bath.

We should stress that these work cycles are realizable only because in the first part of the process, for $t<t_1$, energy was lost $[\mathcal{W}(t_1)-\mathcal{W}(-\infty)>0]$; a part of this is recovered. If, on the other hand, all the work is counted, then no work extraction is possible $[\mathcal{W}(\infty)-\mathcal{W}(-\infty)>0]$, cf. Eq. (7.42).

Alternatively, one may conclude that there are nonequilibrium initial conditions (for instance, the state of the total system at time t_1) which allow cycles that fully transform heat obtained from the bath into work done on the environment.

From the analysis it is clear that under less strict conditions it is even possible to make a cycle that extracts work that comes partly from the bath and partly from the system (“efficiency larger than 100%”).

4. Perpetuum mobile with many work extraction cycles

One can make several of these cycles. Even though the previous finding that complete cycles disperse energy should temper the hope to gain more work by doing more cycles, we consider the issue here, since work extraction from many cycles is one of the ways to express our unexpected results.

Let there be $\mathcal{N}$ cycles with $\alpha(\tau)=\alpha_m h(\tau)$ having $\mathcal{N}$ nonoverlapping bell-shaped parts, like in Eq. (7.53), where $k(x)$ could be the Gaussian $\exp(-\frac{1}{2}x^2)$. Each cycle is characterized by its typical inverse duration time $\Omega_n\ll a/\gamma$ and location t_n^c, and each new cycles is slower than the previous one, $\Omega_{n+1}<\Omega_n$. See Fig. 11 for a schematic plot. For having cyclic behavior in the energy one finds from Eq. (7.55) that for low T and small but almost equal Ω_n’s, one should choose $\overline{x}$ close to the inflection point $x_{\rm if}$ of k,

$$\overline{x}_n-x_{\rm if}=\frac{a}{2\gamma\Omega_n}\frac{|k'(x_{\rm if})|}{k'''(x_{\rm if})}\left(\frac{2\pi\gamma T}{\hbar a}\right)^2+\frac{3\gamma\Omega_n}{2a}+\mathcal{O}\left(\frac{\gamma^2\Omega_n^2}{a^2}\right). \tag{7.58}$$

In order that this be small for all n one needs that $\Omega_{\mathcal{N}}\gg\gamma T^2/\hbar^2 a$. Strictly speaking the $\alpha_n=\alpha_m h(\overline{x}_n)$ are now not exactly equal; this can be healed by slightly adjusting the profile in the nth cycle: $k(\Omega_n(t-t_n))\to k(\Omega_n(t-t_n^c))k(x_{\rm if})/k(\overline{x}_n)$, yielding $\alpha(\tau_n)=\alpha_m k(x_{\rm if})$ for all n. For small $\overline{x}_n-x_{\rm if}$ this correction factor is close to unity and can be omitted from the rest of the argument.

Let us define

$$\tilde{T}=\frac{2\pi\gamma T}{\hbar a}. \tag{7.59}$$

Taking Eq. (7.48) at $t=t_n$, where n cycles have been performed, and using that $\overline{x}-x_{\rm if}\ll 1$ and that $|\Omega_n-\Omega_{n+1}|\ll\Omega_n$, brings for the yield of the nth cycle

$$\Pi(t_n)-\Pi(t_{n-1})=\frac{\alpha_m^2}{12\pi}\hbar\left\{I_1\Omega_n\tilde{T}^2+I_2\frac{\gamma(\Omega_n^2-\Omega_{n-1}^2)}{2a}+I_3\frac{\gamma^2\Omega_n^3}{a^2}\right\}, \tag{7.60}$$

where

$$I_1=\int_{-\infty}^{\infty}d\xi[k'(\xi)]^2,\quad I_2=\tilde{C}_x^{(1)}[k'(x_{\rm if})]^2,$$
$$I_3=\int_{-\infty}^{\infty}d\xi[k''(\xi)]^2. \tag{7.61}$$

For having an equal yield per cycle, one demands

$$\Pi(t_n)-\Pi(t_{n-1})=\mathcal{W}_{\rm cycle}=-\frac{\alpha_m^2\hbar a}{12\pi\gamma}w=-\frac{\alpha_m^2\hbar a}{12\pi\gamma}\tilde{T}^3v, \tag{7.62}$$

where $v>0$ and $w=\tilde{T}^3v$ are dimensionless. It will turn out that there exists a consistent solution for v in some definite range. Assuming that $\Omega(n)=\Omega_n$ is a smooth function of n one obtains

$$I_1\Omega\tilde{T}^2+I_2\frac{\gamma}{a}\Omega\Omega'+I_3\frac{\gamma^2}{a^2}\Omega^3=-w. \tag{7.63}$$

Solving for $dn/d\Omega$ and going to a new variable $y=\beta\hbar\Omega/(2\pi)$ one gets the total number of cycles

$$\mathcal{N}=\frac{I_2}{\tilde{T}}\int_{\beta\hbar\Omega_{\mathcal{N}}/2\pi}^{\beta\hbar\Omega_1/2\pi}\frac{dy\,y}{v+I_1y+I_3y^3}. \tag{7.64}$$

The total yield is then

$$\mathcal{W}_{\rm tot}=\mathcal{N}\mathcal{W}_{\rm cycle}=-\frac{\alpha_m^2I_2}{12\pi}\frac{\hbar a}{\gamma}\tilde{T}^2\int_{\beta\hbar\Omega_{\mathcal{N}}/2\pi}^{\beta\hbar\Omega_1/2\pi}dy\frac{v\,y}{v+I_1y+I_3y^3}. \tag{7.65}$$

Here the minus sign indicates that work is performed by the system on the environment. This is possible because Eq. (7.48) expresses that, in order to make the work extraction cycles, one had to start from the equilibrium state and change α from $\alpha(-\infty)=0$ up to $\alpha(\tau_1)$. In this first part of the process energy was dispersed at an amount

$$\Pi(t_1)=+\frac{\alpha_m^2I_2}{24\pi}\frac{\hbar\gamma}{a}\Omega_1^2. \tag{7.66}$$

Notice that for $v\gg(\beta\hbar\Omega_1)^3$ the extracted work becomes, according to Eq. (7.65),

$$\mathcal{W}_{\rm tot}=-\frac{\alpha_m^2I_2}{24\pi}\frac{\hbar\gamma}{a}(\Omega_1^2-\Omega_{\mathcal{N}}^2), \tag{7.67}$$

so for $\Omega_{\mathcal{N}}\ll\Omega_1$ there is an almost perfect recovery, which is possible since the number of cycles is still large.

For moderate v more cycles are possible, but less work is recovered. For the lower integration variable Eq. (7.58) gives

$$y_{\mathcal{N}}\equiv\frac{\beta\hbar\Omega_{\mathcal{N}}}{2\pi}\gg\frac{\gamma T}{2\pi\hbar a}. \tag{7.68}$$

For strong damping the physical time scale is $\tau_x=\gamma/a$. One assumes that Ω_1 is a large but finite number of times $1/\tau_x$. Choosing $T\ll\hbar a/\gamma$ means that the upper integration limit $y_1=\beta\hbar\Omega_1/2\pi$ is much larger than unity. But it is still possible to choose $y_{\mathcal{N}}\ll1$, which is a useful condition for achieving many cycles. One then has for small v,

$$\mathcal{N}=\frac{I_2}{4\sqrt{I_1I_3}}\frac{\hbar a}{\gamma T}, \tag{7.69}$$

which is indeed large. In the overdamped regime the yield can thus be expressed as

$$\mathcal{W}_{\rm tot}=-\frac{\alpha_m^2I_2}{24\sqrt{I_1I_3}}\frac{\hbar a}{\gamma}v\tilde{T}^2=-\frac{\alpha_m^2\sqrt{I_1I_3}}{6\pi^2I_2}\frac{\hbar a}{\gamma}\frac{v}{\mathcal{N}^2}. \tag{7.70}$$

In the limit of weak damping we should notice that

$$I_2\equiv\tilde{I}_2\sqrt{\varepsilon}, \tag{7.71}$$

where $\varepsilon=am/\gamma^2\gg1$ and where $\tilde{I}_2$ is a numerical constant of order unity. Thus the work dispersed for achieving the nonequilibrium condition at t_1 is

$$\Pi(t_1)=+\frac{\alpha_m^2\tilde{I}_2}{24\pi}\frac{\hbar\Omega_1^2}{\omega_0}, \tag{7.72}$$

where $\omega_0=\sqrt{a/m}$ is the free oscillation frequency. Let us recall that $\tau_d=2m/\gamma$ is the damping time. For $T\ll\hbar\Omega_1$ it holds that

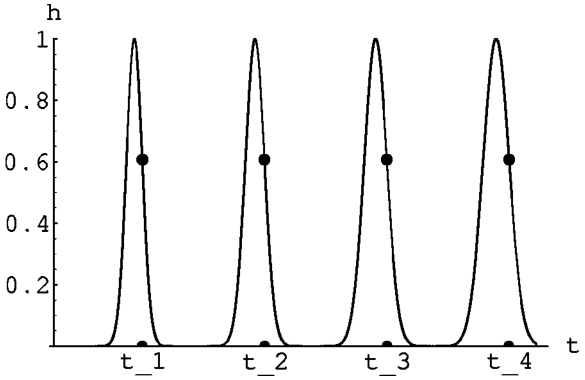

FIG. 11. Schematic plot of the cyclic changes in the spring constant, where successive cycles are slower and slower. h characterizes the size of the change and t denotes the dimensionless time. The interval $-\infty<t<t_1$ marks the process that establishes the nonequilibrium state at $t=t_1$. The picture shows three full cycles, in the intervals $t_i<t<t_{i+1}$ $(i=1,2,3)$. Their start and end points are indicated by bullets.

$$\mathcal{N}=\frac{\tilde{I}_2}{4\sqrt{I_1 I_3}}\varepsilon\frac{\hbar\omega_0}{T}. \tag{7.73}$$

At the typical temperature $T\lesssim\hbar\omega_0$ this carries an additional large factor ε. The yield per cycle carries a factor $1/\varepsilon$, so this total yield is independent of ε. For small v it reads

$$\mathcal{W}_{\mathrm{tot}}=-\frac{\alpha_m^2\pi^2\tilde{I}_2}{6\sqrt{I_1 I_3}}v\,\frac{T^2}{\hbar\omega_0}=-\frac{\alpha_m^2\pi^2\tilde{I}_2^3}{96(I_1 I_3)^{3/2}}\hbar\omega_0\frac{v\varepsilon^2}{\mathcal{N}^2}, \tag{7.74}$$

which can be comparable to the dispersed work, but it is always less.

Summarizing this section, we have investigated the presence of many work extraction cycles both in the strongly and weakly damped regimes. At low T their maximal number can be large but finite. The divergence $\mathcal{N}\sim 1/T$ is probably cut off at low enough T when the amplitude α_0 of our changes is small but finite. When more than $\mathcal{N}$ cycles are made, the possibility of work extraction is lost, because of the dispersion inherent to cycles. At moderate T the possibility of work extraction by cyclic changes is quickly lost; it is a strictly quantum effect.

VIII. EXPERIMENTS TO TEST THE BREAKDOWN OF THE SECOND LAW

In this section we will briefly comment on practical realizations of the low-temperature, nonweakly damped quantum Brownian motion. We do not intend to make detailed proposals for experimental setups, but we will mention certain fields which, according to commonly shared experimental views, display the above-mentioned strong-coupling and/or low-temperature regime.

A. Once more: the characteristic time scales

Let us first recall once more that there are several important time scales in the problem. τ_0 is the characteristic time brought about by the external potential, which the particle will have if there is no interaction with the thermal bath. For reasonably simple confining potentials there is only one such time. In particular, for the harmonic external potential $\mathcal{V}(x)=\frac{1}{2}ax^2$ it is read $\tau_0=1/\omega_0=\sqrt{m/a}$. Since no indications of damping are seen in this time, it can have a physical meaning only for very weak damping: $\gamma\rightarrow 0$.

If damping is large, then the characteristic dynamical times are $\tau_p=m/\gamma$, $\tau_x=\gamma/a$. The overdamped regime appears with $\tau_p\ll\tau_x$, and in this case τ_p and τ_x can be interpreted as the relaxation times of the momentum and coordinate, respectively.

In contrast, very weak damping means $\gamma\rightarrow 0$, and the damping time $\tau_d\sim\tau_p=m/\gamma$ is the longest characteristic time. For intermediate values of γ the characteristic dynamical times in the overdamped regime are $1/\omega_{1,2}$ defined in Eq. (3.31), and for the underdamped regime they are given in Eq. (3.38).

The aim of this work is to consider the regime where another time scale, the characteristic quantum time scale $\tau_\hbar=\hbar/T$, plays a dominant role. In particular, this time scale governs quantum correlations of the bath [35]. The high-temperature classical case naturally corresponds to $\tau_\hbar\ll\tau_0,\tau_p,\tau_x$ and there quantum correlation effects can be neglected.

Equilibrium quantum thermodynamics is recovered in the limit $\tau_\hbar,\tau_0\ll\tau_p$, which means that the momentary motion of the Brownian particle practically does not notice damping, though it does so at long times. Obviously, this condition cannot be satisfied at low temperatures. In the present paper we are interested in the regime where both damping and quantum correlation effects are important: $\tau_p\sim\tau_x\sim\tau_\hbar$, including possibilities of $\tau_p\ll\tau_x$ or $\tau_p,\tau_x\ll\tau_\hbar$, where our results are only strengthened. As noted at the end of Sec. VII, new possibilities for work extraction have been found to occur in this last domain, where the inequality $\tau_p\ll\tau_x\ll\tau_\hbar$ says that the noise is (anti)correlated throughout the systems relaxation. It thus looks more like a quenched random variable than an annealed one, thus not at all behaving like a white noise, the standard ingredient needed to derive from a Langevin equation a Gibbsian equilibrium state.

Before proceeding with concrete examples, let us just notice that there is nothing exotic in the quantum time scale itself: $\tau_\hbar=7.6$ ps at $T=1$ K, which is fully in range of the modern technologies.

B. Possible experimental realizations

1. Josephson junctions

The first example to be discussed is that of Josephson junctions [18,19,49,50]. This well-known phenomenon represents a standard example of quantum Brownian motion. The Josephson junction consists of two superconductors separated by a thin insulating barrier. Cooper pairs of electrons (or holes) are able to tunnel through this barrier, thereby maintaining phase coherence in the process, and leading to a possibility to have superconducting current. There is a direct map between properties of this junction, and the standard model of the quantum Brownian motion [18,19,49,50]. In particular, the coordinate x can correspond to the phase difference of the Cooper pair wave functions, the friction founds its place as resistance, mass is related to capacitance, and the current noise has the standard spectrum (5.25), (5.26), and can be related to $\eta(t)$. Under certain well-defined conditions one can neglect tunneling of the phase from one metastable state to another [18], and consider it in a confining, nearly harmonic potential. This system couples to the environment, which acts as the bath of our theory. In practice, one can notice the occurrence of strong coupling at low T since then a careful shielding of the sample is needed in order to prevent an influence of the environment to the measuring apparatus. It appears that the nonweakly damped and low-temperature limits are well known for Josephson junctions, and were a subject of rather long experimental activity [18,19,50]. For example, the following regime was explicitly realized as a condition of ‘‘really quantum effects’’ [19]: $\tau_p\sim 0.1$ ps which is smaller than $\tau_\hbar$ at 1 K. The ratio τ_p/τ_p need not be of order one, but can vary significantly (from 0.1 to 10) depending on the construction of the junction; for details see Ref. [19]. In experiments reported in Ref. [18] the authors achieved $\tau_\hbar/\tau_x \sim 10$ at $T=1$ K, and $\tau_p/\tau_x \sim 0.1$, which is a typical overdamped, low-temperature case. Notice that these experiments were among the first ones where the spectrum of the low-temperature quantum noise was measured and found to be in perfect agreement with the assumed standard form of the quantum Langevin equations.

C. Low-temperature electrical circuits

Experiments on mesoscopic, low-temperature electrical circuits [51,52] provide yet another example, where non-Gibbsian values of T_x were clearly observed, and found to be in good agreement with the theoretical predictions. We recall that the linear RLC can be mapped to the harmonic Brownian particle: the coordinate x and the momentum p of the particle correspond to the charge and the current of the circuit, and m and a are directly connected with the inductance L and the inverse capacitance $1/C$ of the circuit [see also our discussion after Eq. (3.1)]. Finally, the damping constant γ corresponds to the Ohmic resistance R. One notices that the (quasi-)Ohmic limit, where Γ is the largest characteristic frequency of the problem, is conveniently realized in the present context.

First of all we notice that for experiments described in Refs. [51,52] all the relevant characteristic time scales have basically similar values: $\tau_\hbar \sim \tau_p \sim \tau_x = 10^{-8}$ s, which makes the situation especially relevant for our purposes.

Here we will briefly discuss the possibilities of experimental detection the Clausius inequality violation at low temperatures, since this seems to be the simplest possible issue. Moreover, the most evident situation is realized upon a slow variation of the inductivity (mass) L, where for $T\to 0$—according to Eq. (4.26) and in clear contrast with the Clausius inequality $đQ \leqslant 0$—one gets a finite positive heat provided that $dm = dL > 0$. One needs to observe $\langle x^2 \rangle$ and $\langle p^2 \rangle$ for several different values of the inductivity (mass) L. This is sufficient to recover the corresponding changes of the average energy, as well as to recover the work according to Eq. (4.25). The heat is then obtained by subtracting the work from the energy. In the second step one can check the consistency of the results by observing directly the work done by the external source. Altogether, the challenge of the main experimental observation is in observation of the variances.

In Ref. [51] the authors considered mesoscopic electrical circuits in the context of single charge tunneling. The used circuits had thickness of the order 10 nm and width of the order 1 μm. The observations allowed indirect determination of $\langle x^2 \rangle$. With the subsequent improvement made in [52] the correspondence with the theoretical expression (3.47) is perfect. The observations were done with $C = 1/a = 4.5$ fF, $L = 4.5$ nH, and for $R = \gamma$ in the range 10^1–10^3 kΩ. For damped circuits the relative importance of damping is quantified by the quality factor τ_p/τ_0, which in the above range of parameters varies from 10^{-1} to 10^{-3}. To avoid thermal noises the circuits were cooled up to 20 mK. At such a low temperature quantum effects are dominating, since the quantum time scale $\tau_\hbar = \hbar/T \sim 10^{-8}$ s is larger than the other ones, $\tau_0 \sim 10^{-9} - 10^{-10}$, $\tau_p \sim 10^{-8}$, and $\tau_x \sim 10^{-9}$ s. To get an idea of the magnitude of the expected effect, let us estimate the outcome for $\Delta Q \simeq L \ dQ/dL$. With the above parameters and $R = \gamma = 10^3$ kΩ one gets from Eq. (4.26) $\Delta Q \sim 10^{-19}$ J$=1$ eV.

Since for mesoscopic circuits the formula for T_x was already verified, it is now a matter to perform three measurements (the equivalents of T_p, T_x and the work production) on a single sample, to verify unambiguously the breakdown of the Clausius inequality.

1. Trapped ions

As another more elementary example one can mention a trapped ion immersed in a photon bath. Taking as an estimate the mass of the proton ($m = 10^{-26}$ kg), and $\gamma = 10^{-15}$ kg s^{-1} [10], one gets $\tau_d \sim \tau_\hbar$ at 1 K, so the quantum coherence effects are still active. The ideal example of a harmonic Brownian particle will be an ion trapped in a so-called Paul trap [53], or an electron or ion in a Penning trap [54]. These electromagnetic traps are nowadays well realizable and suited for variation of parameters. In particular, high quantum number Rydberg states may have a long lifetime and a strong coupling to the radiation field.

IX. ON THE FOUNDATIONS OF THERMODYNAMICS AND PERPETUUM MOBILE

This section summarizes to what extent the standard relations and laws of thermodynamics can be applied to a quantum Brownian particle. There are many formulations of the second law, and some of them have been found to be invalid in previous discussion. One may go to the extreme limit by saying that there is no motivation to discuss thermodynamics in the way we did. To show that it is justified to do so, we summarize our results in the light of common thermodynamic wisdom, and point at the agreements and contradictions.

For a general, pedagogic text on the history and present status of thermodynamics and the second law, we refer the reader to the recent work by Uffink [55]. For a collection and discussion of the original papers, see the book by Kestin [56]. A very recent discussion on the basis of the axiomatic thermodynamics was presented by Lieb and Yngvason [57]. For a discussion of what can be meant by ‘‘the’’ entropy of a system, see Ref. [58].

A. Has the standard thermodynamics been violated or did it never apply?

The conclusion of our analysis is that thermodynamics does not work when, in the quantum regime, ones considers the Brownian particle in its reduced Hilbert space, thus summing out the bath variables of the total system. This makes sense when the characteristics of the particle are directly observable, as is indeed the case with the standard examples of the Brownian motion. There are, however, situations, where only some composite (system plus bath) quantities are measured, and the need for a separation between particle and bath is questionable (there still can be a possibility that such a separation can be given on a different, more coarse-grained description of the overall system, but we will not enter into that discussion). This is the case with a Kondo system, where the measured quantity is, for instance, the magnetization, which is set by the magnetic impurity and the bath together (i.e., it lives in the common space of the particle and the bath). Also for the dressing of a ''bare'' electron by photons, it is a standard practice of the quantum field theory to consider the dressed mass and charge as directly observable quantities. However, when the subsystem is a Josephson junction or a mesoscopic circuit, its own characteristics are perfectly measurable, so there is an important case to make. When looking at the budget of the junction alone, one has to keep in mind that it may exchange energy with its environment and, in particular, modify the cloud. At low enough temperature this mechanism displays unexpected behavior and is responsible for nonthermodynamic characteristics.

If one considers the subsystem as a Brownian particle immersed in a heat bath, then first it should be noticed that the particle acquires a cloud of bath modes around it. This dressing is a manifestation of the (strong) damping of the particle by the bath. One can then ask the question: ''if the *standard* thermodynamics does not apply, where was it lost?'' If no technical errors have been made in our derivations, then the answer must be: ''It never applied.'' Let us consider arguments for that point of view.

1. The full energy versus equilibrium energies of the bath and the particle

A well known sufficient condition for the derivation of the standard equilibrium thermodynamics is that the interaction energy between the bath and the particle is negligibly small. There are at least two things that can be meant by the term ''interaction energy.'' The standard approach, see, e.g., Ref. [59], connects this energy with the average value $U_I = \langle \mathcal{H}_I \rangle$ of the interaction Hamiltonian. According a different viewpoint the interaction energy can be associated with the full effect of the interaction $U_{\rm int} = \langle \mathcal{H} - \mathcal{H}(\gamma=0) \rangle$. Obviously, this last definition is only meaningful in the equilibrium state, since during the dynamical evolution from a nonequilibrium state it is just conserved and equal to its (arbitrarily chosen) initial value. In order to avoid any loophole, we will analyze below both definitions.

One notices that in the stationary state the full average energy of the system is not reduced to those of free equilibrium particle and bath, i.e., $U_{\rm int} \neq 0$. It reads in the stationary state

$$U_{\rm int} = U_p - \frac{1}{2} T_p - \frac{1}{2} T_x = \Gamma \frac{\partial F_p}{\partial \Gamma}. \tag{9.1}$$

The result is given explicitly by Eqs. (3.44), (3.45), (3.47), and (3.48). In a strict formulation of thermodynamics one may want to require that the equilibrium value of $U_{\rm int}$ be negligible. This may be viewed as a sufficient condition for separating of what is meant by the system from what is meant by the bath. In any case, the above examples stress that it is by no means necessary. In our case $U_{\rm int} \to 0$ would imply $\gamma \to 0$ or $T \to \infty$, and indeed in both limits the standard thermodynamics is recovered. However, for fixed γ the same system has at noninfinite T a nonzero $U_{\rm int}$. Whereas the limit of large T can be naturally achieved in practice, the weak-coupling limit $\gamma \to 0$ is much more difficult to realize, since coupling constants are generally fixed numbers whose magnitude cannot be manipulated at will. If one favors a viewpoint that thermodynamic quantities, such as heat, work, and temperature, should only be discussed for vanishing $U_{\rm int}$, then actually almost all realistic systems should not be considered as thermodynamic. This would apply to many systems at low enough temperature, leaving an uncomfortable situation with respect to the well behaved high-temperature properties of the same systems.

We recall that it is not meaningful to consider this quantity out of equilibrium. If one wishes to do something akin to it, one has to define a local region around the subsystem and consider how the system inside that region approaches its local equilibrium, while the surplus energy runs far away. We shall not entertain that scenario.

2. Classical thermodynamics does not need a vanishing interaction energy

Let us now analyze what are the consequences of the most standard understanding of the vanishing interaction energy

$$U_I \equiv \langle \mathcal{H}_I \rangle \to 0. \tag{9.2}$$

This condition can be applied also in the nonequilibrium situation. Here we notice that the classical thermodynamics itself provides a definite argument against the viewpoint that the use of thermodynamic quantities and the existence of thermodynamic laws must always be connected with condition (9.2). The simplest thing to notice is that the very existence of the classical (high-temperature) Gibbs distribution for the Brownian particle interacting with its thermal bath is *not* at all connected with a vanishing interaction energy [see Eq. (9.5) below]. A similar argument can be stated in the dynamical situation. Let us consider the H theorem [6,11,60–62] which is one of the most well known formulations of the second law in the nonequilibrium thermodynamics, and represents a particular case of the Clausius inequality. We already discussed this relation in Sec. VI B 2, where it was shown [see, e.g., Eq. (6.76)] that for our model this relation holds if temperature of the bath is high enough. In fact, this is a much more general relation, and for classical Brownian motion it can be stated as a rigorous theorem [6,11,60,61]. It was also generalized to the coarse-grained quantum Markovian dynamics, which is valid in the weak-coupling situation for not very low bath temperature; see Ref. [62] and references therein. The analogous inequality in the master-equation framework was derived in Ref. [60,61].

Our present purpose is to show that in the classical situation (high-temperature thermal bath) the H theorem, or the Clausius inequality, is *not* connected with any restriction on the average interaction energy $\langle \mathcal{H}_I \rangle$. In particular, the latter quantity can be as large as one wishes.

The motion of a classical Brownian particle interacting with an Ohmic thermal bath at temperature T is described by the classical Fokker-Planck-Kramers-Klein equation [6,11]. (Note that this equation is typically written for the case of separated initial conditions between the particle and the bath; this, however, will not influence the subsequent argument.) As can be deduced from this equation [6,11], the $\mathcal{H}$ function between the actual solution of the equation at some fixed time t and its stationary Gibbsian solution monotonously decays with time: $d\mathcal{H}/dt \leqslant 0$. This then implies the Clausius inequality $dU \equiv d\mathcal{Q} \leqslant T dS_B$, where U is the average energy of the particle, and $S_B = -\int f \ln f$ is its Boltzmann entropy; it is defined as in Eq. (6.80), where the Wigner function $W(x,p)$ should be substituted by the true probability distribution $f(x,p)$ of the coordinate and momentum. Since there is no external source, the whole change of energy is attributed to heat: $dU \equiv d\mathcal{Q}$, viz., $\dot{U} = \dot{\mathcal{Q}}$. For our particular situation this inequality can be derived from Eq. (6.76) upon noting that for the classical case W_{st} can be substituted by the Gibbs distribution, and that $D_x = D_p$. Now we are going to show that at the same time the average interaction energy can be *arbitrary* large. One uses Eq. (2.19), combines it with the solutions (2.11), (5.44), and (5.45) of the Langevin equations, and recalls that in the classical situation the noise is white: $\langle \eta(t)\eta(t')\rangle = 2\gamma T \delta(t-t')$. This leads to a result that could also have been taken from Eq. (2.19) in the limit of large Γ,

$$U_I(t) = -\langle x(t)\eta(t)\rangle + \gamma(t)\langle x(t)x(0)\rangle - \frac{\gamma(0)}{2}\langle x^2(t)\rangle + \gamma\langle x(t)\dot{x}(t)\rangle, \tag{9.3}$$

where $\gamma(t) = \gamma\Gamma\, e^{-\Gamma t}$ as given by Eq. (2.25). Recall that for large Γ one has $\gamma(t) = \gamma\delta_+(t) + \gamma\delta_-(t)$. Thus, the second term in the right hand side of Eq. (9.3) is zero. Also using Eq. (5.44) and assuming for simplicity $\langle \eta(t)x(0)\rangle = \langle \eta(t)p(0)\rangle = \langle p(0)x(0)\rangle = 0$ (separated initial condition), one finds

$$\langle x(t)\eta(t)\rangle = \frac{2\gamma T}{m}\int_0^t ds\, f(s)\delta(s) = \frac{\gamma T}{m} f(0) = 0, \tag{9.4}$$

where f is defined by Eqs. (5.49) and (5.50). Further transformations with help of Eqs. (5.44) and (5.45) lead to

$$U_I(t) = -\frac{\gamma\Gamma}{2}\langle x^2(t)\rangle + \gamma\left(\langle x^2(0)\rangle \dot{f}(t)\ddot{f}(t) + \langle \dot{x}^2(0)\rangle f(t)\dot{f}(t) + \frac{\gamma T}{m^2} f^2(t)\right). \tag{9.5}$$

It is seen that the interaction is not zero for both finite times, where the above Clausius inequality applies, and the infinite-time limit, where $\langle \mathcal{H}_I(t\to\infty)\rangle = -\gamma\Gamma T/(2a)$. Moreover, in the second case it is large by its absolute value due to the factor Γ. By means of this simple and well-known example we conclude that finite interaction energy by itself does not preclude the application of the second law.

Finally, it is interesting to mention that a discussion somewhat similar to that presented here appeared in the book by Terletskii [59]. This author carefully discusses the role of vanishing interaction energy in the standard equilibrium thermodynamics, and points out severe limitations of that assumption in the context of long-range interacting macroscopic systems, e.g., gravitationally interacting particles. He then conjectures that the standard thermodynamics could be a particular case of more general theories, where the assumption on the vanishing interaction energy is not valid anymore.

Let us mention a related model studied by us, where the central oscillator is replaced by a spin-$\frac{1}{2}$ particle (spin-boson model). This model has an exactly solvable limit, where the transverse field vanishes and the z component of the spin is conserved. Upon relaxation from a nonequilibrium initial state, the von Neumann entropy increases (H theorem). By applying fast pulses to this system, again situations occur where work is extracted from a quantum system in a nonequilibrium initial state [63]. In this system the interaction energy is a fixed constant, which can be absorbed in the spin energy.

Putting all arguments together, we reach the unavoidable conclusion: there are principle problems to get the standard thermodynamics at not very large temperatures and not very small couplings, more specifically, in the regime of quantum entanglement. There is no resolution to this, and in systems with standard thermodynamics at high temperatures, unexpected energy flows appear to be possible.

B. The nonthermodynamic regime of quantum entanglement between system and bath

Let us inspect in some detail the weak damping limit $\gamma \ll \sqrt{am}$. Here it can be shown that, even at $T=0$, one has $U_{\rm int} \ll U$, since, due to Eq. (3.48), $U_{\rm int} \sim \gamma$ but $U \to \frac{1}{2}\hbar\omega_0$, implying that the condition for the application of thermodynamics is almost fulfilled. Nevertheless, the Clausius inequality is typically violated, by an amount of, again, order γ.

In many subsystems coupled to a bath, the following three regimes will occur.

(1) At large T there is the classical regime, and equilibrium is described by the classical Gibbs distribution.

(2) There is a "standard" quantum regime where the bath only enters through its temperature, and equilibrium is now described by the quantum Gibbs distribution.

(3) At very low temperatures there occurs a quantum entanglement between subsystem and bath. Here the Gibbs distribution and standard thermodynamics are lost.

Regimes 1 and 3 always occur, while regime 2 may not occur if the coupling is strong. In regime 3 thermodynamics is endangered and typically not applicable.

C. Zeroth law

The zeroth law is often said to state that in an equilibrium situation there will be a unique temperature. A standard formulation is that if two bodies are each in equilibrium with a third body, then they are also in equilibrium with each other, and the three bodies have a common temperature. Let us look, however, at a careful formulation out of equilibrium: *If two parts of the system have an infinitesimally small tem-*

perature difference, then they will spontaneously equilibrate and reach a common temperature.

For the (nearly) harmonic situation two different *effective* temperatures T_p and T_x can be related to the momentum and the coordinate. Recall that these temperatures arise from the generalized form (4.15)–(4.19) of the Clausius inequality. The legitimation of such a definition of effective temperatures is confirmed by their successful use in glassy thermodynamics [24,26].

In our case, Eq. (3.54) shows that T_p deviates at large T from T_x by a term $\beta A\Gamma$, with $A=\hbar^2\gamma/12m$. So for any infinitesimal ϵ, the regime $T>A\Gamma/\epsilon$ indeed has temperatures T_p and T_x that differ less than ϵ. However, since they are parameters of the steady state, they will not equalize spontaneously, in conflict with the above formulation of the zeroth law. Instead, they become more and more different from each other at lower temperatures, and at zero bath temperature T_p and T_x are both finite but different from each other. The fact that they remain finite just indicates that the corresponding quantum state does not have sharp values for p and x; so this is a consequence of quantum complementarity. The fact that these effective temperatures take non-Gibbsian values is a consequence of the quantum entanglement. In the Gibbsian limit of weak coupling (i.e., $\gamma\to 0$) for the harmonic oscillator, both temperatures T_x, T_p tend to their common value $\frac{1}{2}\hbar\omega_0\coth(\frac{1}{2}\hbar\beta\omega_0)$ of the harmonic oscillator weakly coupled to its bath.

We should mention that the existence of the zeroth law is frequently viewed just as an axiom, but under certain conditions it can be derived from the second law (the entropy of a closed system never decreases) [5]. As we mentioned already, this derivation is based on the use of a weak interaction between the particle and its thermal bath. It confirms that if this weak-coupling condition is valid, then the two effective temperatures are indeed approximately equal.

D. First law

The first law relates the change of the system's energy into the heat added to it and the work done on it. It cannot be broken, since it is a direct consequence of energy conservation, a central concept in quantum mechanics. Nevertheless, the formulation of this law is not merely a tautology, because it allows to separate clearly those ingredients of the energy change, which arise from nonobservable degrees of freedom (heat obtained by the Brownian particle from the thermal bath) and external sources (work done by them on the whole system). Our identification of the energy of the subsystem as the expectation value of the Hamiltonian $\mathcal{H}$ was supported in Sec. IV B 5 by requiring application of standard thermodynamics at high T, and is imposed by the form of the Wigner function. We stress that, given this identification of energy, our identification of the heat $đ\mathcal{Q}$ added to the subsystem and the work $đ\mathcal{W}$ done on it are well accepted and widely discussed in literature; see, e.g., the books by Keizer [46], Balian [44], and Klimontovich [6].

E. Second law

Let us stress that there are many formulations of the second law. There are several formulations of the second law that are, at least apparently, violated by the solution of our problem.

1. Thomson's formulation, Kelvin's principle

The formulation by William Thomson, later Lord Kelvin of Largs, is: *It is impossible to perform a cyclic process with no other result than that heat is absorbed from a reservoir, and work is performed*. We call this the ''Thomson formulation,'' whereas Uffink [55] uses the name ''Kelvin's principle.'' An earlier and more particular version of this statement appeared due to Carnot: *Given an engine that is reversible and that operates between two fixed temperature baths. Then no other engine operating between these same temperatures can exceed this engine in efficiency.* Closely related is the Kelvin formulation: *It is impossible, by means of inanimate material agency, to derive mechanical effect from any portion of matter by cooling it below the temperature of the coldest of the surrounding objects* [56].

For general quantum systems starting from the equilibrium state, this can be proven mathematically [47]; a simplified proof will be presented elsewhere [64]. In our setups it can always be verified, see, for example, the fact that the energy dispersion (7.43) is non-negative. After finishing the cycle the bath is not exactly in its Gibbsian state, but it is still very close to it, because the bath is extensive. Basically the dispersed energy has run away to infinity, leaving the system locally again in a Gibbsian state. This implies also that successive cycles will further disperse energy.

However, out of equilibrium Thomson's formulation appears to be endangered. The first point to notice is that this can already occur at the classical level. The reason is simple. Consider, as we did in Sec. VII C, a sudden weakening of the central spring. In doing so, energy is extracted from the system, but, due to the sudden nature, it is not the optimal amount. One can improve on this by making the following cycle: quickly put the spring back at its original value, and then make the change slower. This cycle that started in a nonequilibrium state will yield work, and this work comes from the bath. We conclude that the Thomson's formulation can only refer to system changes on long enough time scales, such that the initial state is practically in equilibrium.

A more exciting violation of the nonequilibrium Thomson's formulation was observed for smooth changes of the spring constant at low enough temperature. In Sec. VII D 4 we discussed the case of $\mathcal{N}\gg 1$ bell-shaped cycles in the spring constant; each cycle has two inflection points, prepeak and postpeak. Starting in the Gibbsian state, the first cycle up to the postpeak inflection point is considered as a mechanism that produces for us a proper ''initial'' nonequilibrium state. If the typical duration of the successive cycles increases, parameters can be chosen such that after each return of the spring constant to its postpeak inflection point value, the system has the same energy, while a prescribed, fixed amount of work is extracted. There can be $\mathcal{N}\sim 1/T$ of these cycles, which can be large at low enough T. They extract heat from the bath and convert it fully into work, forbidden by the general (i.e., nonequilibrium) Thomson's formulation. It could be checked that the total amount of extracted work is less than the energy dispersed in the first part of the first cycle, so for the full process Thomson's formulation is not endangered. The interesting fact is nevertheless that there can be $\mathcal{N} \sim 1/T$ of these cycles, which can be large at low enough T. Actually, making more cycles implies a smaller total extracted work $\sim 1/\mathcal{N}^2$, since these cycles themselves lead to additional dispersion.

In contrast to the violation of the Clausius inequality, to be discussed below, the violation of Thomson's formulation is a consequence of both quantum regime (low temperatures) and the nonequilibrium character of the whole system (particle and bath). Indeed, any amount of work extracted by means of the particle is in fact extracted from the whole system. If this global system is in equilibrium (namely, it is exactly described by the Gibbs distribution), there will be no possibility to extract work by making a cyclic change of a system parameter, since this formulation of the second law applies as well to any closed equilibrium system [47,64]. On the other hand, the full account of quantum effects is necessary to show our work extraction, since it disappears in the Gibbsian limit, namely, both at moderate temperatures and/or for weak coupling to the thermal bath [69].

2. Clausius' principle

Clausius states: *It is impossible to perform a cyclic process which has no other result than that heat is absorbed from a reservoir with a low temperature and emitted into a reservoir with a higher temperature. It is impossible for a self-acting machine, unaided by any external agency, to convey heat from one body to another body at a higher temperature* [56].

The work gained could be used to drive some frictional process at a higher temperature, which would turn it into heat, in conflict with this principle. Nevertheless, this principle is obeyed at high temperatures, and only violated in the quantum regime at low T.

3. Clausius inequality

This formulation claims that in any thermodynamical process (in particular, for variation of a system parameter) the amount of heat received from the thermal bath by the particle is limited from above by the bath temperature times the change of the von Neumann entropy of the particle,

$$đQ \leqslant T dS_{vN}. \tag{9.6}$$

A particular formulation of this law is that no heat can be extracted from a zero-temperature thermal bath—it can only be dumped in it (i.e., then it is impossible to have $đQ \geqslant 0$). This situation is particularly interesting, since it does not employ in any way the concept of entropy, and therefore can be applied to situations, where entropy is not known, or not well defined. Physically it is also easy to understand. The energy of the cloud of bath modes around the subsystem will change if a system parameter is changed, even at $T=0$. This change in energy of nonobservable modes is heat, and it can be positive or negative, depending on the sign of the change. In one of the cases energy from the cloud will increase the subsystem's energy, violating the Clausius inequality. For a closed system $đQ$ goes to zero, and one recovers from the above inequality the more standard formulation $dS_{vN} \geqslant 0$, which appears to be a particular case of the Clausius inequality.

We have shown that both the general (all T) and particular ($T=0$) formulations are violated in the quantum case. Although at high temperatures these violations are small, they nevertheless do exist. For researchers who are reluctant to follow our identification of the effective temperatures, it will perhaps be hard to agree on the violation of the zeroth law, discussed above. However, the violation of the second law, which also sets in at arbitrarily large temperatures, should be easier to accept, since the Clausius inequality does not employ the notion of effective temperatures. Moreover, in Sec. IV B 4 we have discussed a formulation that compares only equilibrium systems.

For our harmonic system we succeeded in generalizing the Clausius inequality, involving two temperatures and two entropies, in the very same way it was done for glassy systems and which applies to black holes.

In hindsight, the derivation of the Clausius inequality is nontrivial in the case under consideration. In standard thermodynamics one formulation of the second law is that the total entropy of a closed system cannot decrease. When applied to a subsystem coupled to its equilibrium bath, this immediately leads to the Clausius inequality. Here one makes two assumptions: equilibration of the bath and additivity of the entropy. Let us follow the subsequent steps. Because of its equilibrium nature, the heat received by the bath is associated with an entropy change, $đ\mathcal{Q}_{bath} = T dS_{bath}$. Energy conservation says that $đ\mathcal{Q}_{bath} + đ\mathcal{Q} = 0$, where the latter is the heat received by the subsystem. This implies

$$dS - \frac{đ\mathcal{Q}}{T} = dS + dS_{bath} = dS_{\mathrm{tot}} \geqslant 0. \tag{9.7}$$

In the world of quantum entanglement, however, both assumptions are less obvious. First, it does not hold that $S_{\mathrm{tot}} = S + S_B$. We have shown this explicitly, since at $T=0$ one has $S_{\mathrm{tot}} = S_B = 0$, but $S = S_{vN} > 0$. Both the fact that energy is not quickly redistributed in the bath and the nonadditivity of the entropy imply that there is no *a priori* reason to expect that the Clausius inequality is satisfied. In concordance with that, we have shown that it is indeed not valid.

4. The rate of energy dispersion is non-negative

Positivity of the rate of energy dispersion underlies the classical no-perpetuum-mobile formulations of the second law, including those of Thomson and Clausius. In Sec. VII D 2 we have pointed out that at low enough temperatures the rate of energy dispersion can easily be negative. This holds even when one starts in equilibrium. Thus non-negativity of energy dispersion cannot serve as a universal formulation of the second law.

5. The total entropy of a closed system cannot decrease

The most standard formulation of the second law is that the (coarse grained) entropy of a closed system cannot decrease. In classical physics for a subsystem in contact with a heat bath the equivalent is that the rate of entropy production of the subsystem is non-negative. For situations close to equilibrium it can often be expressed as a bilinear expression in generalized currents, and the matrix elements are called Onsager coefficients; this matrix is positive definite in all examples known to us.

The rate of production of Boltzmann entropy was also considered by us. In the case of weak damping there occur oscillations in the production rate around zero in each period; this sets in at moderate temperatures, and is akin to the oscillations in energy that already occur at any noninfinite temperature. In Sec. VI B 4 and VI B 5 we have pointed out that even at low temperatures and in the limit of strong damping the rate of Boltzmann entropy production can be negative. So this criterion also does not qualify as a solid definition of the second law.

We should stress that we did not find sensible production rates for other entropies. Perhaps not accidentally, the Boltzmann entropies of the coordinate and momentum sectors are the ones that enter into our generalized, two-temperature version of the Clausius inequality.

In our setup the von Neumann entropy for the full closed system (fine-grained entropy) should not be confused with the von Neumann or Boltzmann entropies of the subsystem, which pertain to the Brownian particle only. The von Neumann entropy of the full system is not altered by changing the strength of the spring constant. This entropy remains constant during the overall unitary evolution of the whole system, and also remains constant during variations of a parameter, since also there the overall evolution is still unitary. The formulation of the second law in terms of nondecrease of entropy definitely refers to the coarse-grained entropy. In the classical situation the fine-grained entropy is conserved as well, by the Liouville dynamics. For more definitions of entropy, see Ref. [58].

In passing we note that if one starts from a Gibbsian state of the total system (central particle coupled to the bath), and changes a system parameter, then the conservation of entropy prevents the system from relaxing to a new Gibbsian state of the total system, since our total system is isolated. Nevertheless, the subsystem (the central particle) does relax to a state characterized by the parameters, which can be coded in the effective temperatures, of that would-be global Gibbsian state. It is the finite amount of energy dumped in the extensive bath that does not relax, since our bath lacks anharmonic interactions, or coupling to an external superbath. In contrast to a superbath, anharmonic interactions do not change the essence of the argument on the overall unitary evolution, conservation of both the von Neumann entropy and the energy. However, they can widen the set of observables having would-be Gibbsian values.

F. Third law

This law claims that if the ground state of the Brownian particle is nondegenerate, then its von Neumann entropy is equal to zero. This is a direct consequence of the quantum Gibbs distribution, which predicts the pure vacuum state at low temperatures. In our case neither the von Neumann entropy nor the Boltzmann entropy vanishes when the bath temperature is zero. This occurs because the quantum Brownian particle is in an entangled mixed state, and therefore cannot have vanishing von Neumann entropy.

The third law is recovered when taking the weak-coupling limit. In that case $T_p = T_x = \frac{1}{2}\hbar\omega_0 \mathrm{cotanh}(\frac{1}{2}\beta\hbar\omega_0)$, implying that the parameter v of Eq. (4.35) takes the value $v = \frac{1}{2}\,\mathrm{cotanh}\,\frac{1}{2}\beta\hbar\omega_0$, which causes the von Neumann entropy of the particle (4.36) to vanish at $T=0$. In a certain sense the violation of the third law reported here for nonweak coupling is the most straightforward consequence of quantum entanglement.

G. Perpetuum mobile of the first kind

Taken literally, a perpetuum mobile performs perpetual, i.e., everlasting, motion. Nevertheless, rotational currents in ordinary superconductors, which may exist for several days, are rarely connected to perpetual motion. We shall therefore employ the word ‘‘perpetuum mobile’’ for any principle that yields work.

One speaks of a perpetuum mobile of the first kind when the first law is violated, leading to an everlasting performance of work without any cost. Such a setup is impossible in quantum mechanics, since it satisfies the first law by principle. So there is no issue in the question what ‘‘perpetuum’’ means precisely.

H. Perpetuum mobile of the second kind

Another formulation of the second law is: *It is impossible to construct an engine which will work in a complete cycle, and convert all heat it absorbs from a reservoir, into mechanical work* [65]. A machine which would do so is called a *perpetuum mobile of the second kind*, and the second law states that such a machine is impossible.

1. ‘‘Perpetuum’’ mobile or perpetuum mobile?

When the first law is respected but the second is violated, one speaks of a ‘‘perpetuum mobile of the second kind.’’ However, we wish to make some remarks on the word ‘‘perpetuum.’’ Surely, in the eighteenth century such a perpetuum mobile was imagined, for instance, to cross the Atlantic by boat using only the energy stored in the ocean water. As such, there would be a basically infinite bath, and the mobile, if realized, could function perpetually, i.e., ‘‘forever.’’ In general, when the bath is finite, it obviously has a finite energy at its disposal. In many setups, such as those with a finite rate of energy extraction, this implies also finite duration of the process. Thus even in the classical situation, the term ‘‘perpetuum’’ need not be a precise adjective for this type of mobile, and the point of view could be taken that a perpetuum mobile of the second kind need not function arbitrarily long, but must only involve many cycles. In view of the failure to find so far any practical realization, this stretch of the definition seems allowable to us.

In quantum physics the situation is even more clear. In a closed system the energy can never go below the ground-state energy, so the amount of extracted work is always finite. As a result, there can never be an infinite amount of cycles for which a definite amount of work is extracted per cycle. One of the formulations of the second law is: ''Perpetuum mobiles of the second kind do not exist.'' Such a strong physical statement must, of course, be richer than the general statement on the existence of a ground state. The crux is that already one such cycle, which extracts work from a thermal bath, is forbidden. So, already in general, perpetual motion of the second kind does not have its literal meaning of everlasting motion; rather, it is a notion for a work extraction principle, and one cycle is therefore good enough for the construction of a ''perpetuum mobile.''

2. The present situation

For our purposes the allowance of noneternal duration of perpetuum mobile is relevant, since our effects only hold as long as both the particle does not relax, which happens on the time scale τ_x, and is quantum coherent, which involves the quantum time scale $\hbar/T$.

We have discussed a work extraction mechanism that cyclicly changes the spring constant in a certain time interval. Each of these cycles is slower than the relaxation time of the system. When the quantum time scale $\tau_\hbar=\hbar/T$ is also slower than the relaxation time, there occurs unexpected behavior: the contribution to the rate of dispersion inversely proportional to the duration of the cycle, normally the leading term, has a small prefactor quadratic in temperature. Therefore, quadratic and cubic terms in the inverse duration also play a role. Out of equilibrium cycles have been designed where a constant amount of heat extracted from the bath is fully converted into work, while the energy of the subsystem at the end of each cycle returns to its initial value. *In this sense, systems described by our models, with parameters in the appropriate regime, present at low temperatures true realizations of perpetuum mobile of the second kind*. Probably, it is also possible to extract work both from the bath and from the subsystem (''efficiency larger than 100%'').

In a more stringent definition of perpetuum mobile one requires that the cycle's work be extracted ''without any further change.'' For our system this can be expressed as the requirement that the Wigner function of the subsystem be back at its original value. This would imply the requirements that $\Delta K=0$, $\Delta V=0$, and $\Delta\dot{V}=0$ over each cycle, rather than only having $\Delta K+\Delta V=0$, where K is the expectation of the kinetic energy and V of the potential energy. The question whether this extended constraint can be satisfied by changing the spring constant and possibly also the mass, is left for the future.

We should stress the conceptual difference between the present situation and a well-known case, where work can be extracted due to a temperature difference between two thermal baths [5]. The latter is the standard setup for the thermodynamic heat engine: two baths are explicitly separated from each other, and therefore the whole system is in a nonequilibrium state, and can be used to perform work. If those baths are kept in a direct contact for a sufficiently long time, then they will go to equilibrium and after that no work can be extracted [66]. In contrast, here we have presented a case with *a single* thermal bath. After a sudden increase of the strength of the central spring, the central particle will go to equilibrium after one relaxation time τ_x or τ_d. But in doing so, more than the initial surplus energy is transfered to the bath, and in particular to the cloud of bath modes in its immediate surrounding. After a certain moment, this heat flow towards the bath stops, and then a smaller backflow occurs from the bath to the particle, before the whole comes into equilibrium. This backflow of heat is the mechanism that makes it possible to extract work from the bath by manipulating the particle, in a situation where this would be impossible classically. In particular, for smooth changes at zero temperatures the integral of this relaxation function is needed, but it appears to vanish, leading to a variety of effects at low temperatures.

On a thermodynamic level, the analogy with the classical case was strengthened because we could identify effective temperatures, though we also stressed that by themselves they do not tend to become equal to each other. All these intriguing aspects arise due to quantum effects, since we showed in detail that *the same system coupled to the same bath* displays at high temperatures the fully expected thermodynamical behavior.

I. Perpetuum mobile of the third kind

One can define a perpetuum mobile of the third kind when work is performed at the cost of a diminishing, but still nonvanishing, zero-temperature entropy. This can, in principle occur in systems such as glasses, which are able to relax to equilibrium, but are temporarily stuck in certain metastable states. Then the zero-temperature entropy can be used as a measure of this metastability [67].

One could wonder whether our extraction of work is due to the present nonvanishing zero-point entropy. However, this is not the case, since for the purely Gibbsian case of particle and bath, the particle would have the same zero-point entropy, but no work could be extracted. Moreover, in our case the zero point entropy is an indication of quantum entanglement and not of metastability.

X. CONCLUSION

This paper is devoted to the statistical thermodynamics of the quantum Brownian motion. The high-temperature case of this model can serve as a convenient pedagogic example, where almost all main statements of statistical thermodynamics are derived exclusively from first principles. Among other advantages, such an approach makes it possible to reveal the conceptual restrictions and limitations of the common thermodynamic wisdom. With this aim in mind we focussed in the paper on the low-temperature (quantum) situation of the Brownian motion model.

The stationary state of a quantum Brownian particle nonweakly interacting with its thermal bath is non-Gibbsian. It is this property which makes the quantum Brownian motion a challenging problem, and classical thermodynamic wisdom appears to be inadequate even if the total state of the system and the bath is Gibbsian. Both the classical and the quantum Gibbsian thermodynamic theories emerge as particular limits in this more general setup. The classical Gibbs distribution with all its thermodynamic consequences is recovered for high temperatures, and the quantum Gibbs distribution is obtained for very weak damping.

In Sec. II we start from the quantum Langevin equation. At low temperatures this equation contains a colored Gaussian noise; because of quantum coherence, the bath cannot generate white noise even in the limit where the friction has no memory. To achieve this interesting situation, no more is needed than the observation that quantum mechanics applies [see detailed explanations after Eq. (5.28)]. Moreover, the quantum fluctuation-dissipation theorem predicts different time-scales of noise and dissipation at low enough temperatures [5,6,9,17]. This is how quantum coherence enters into the considerations. Its characteristic time scale is $\hbar/T$, where we had set the Boltzmann constant k_B equal to unity so far. Restoring it, we have $t_\hbar=\hbar/(k_BT)=(6.23/T)$ K ps. At $T=1$ K one has $t_\hbar=6.23$ ps, in the range of typical microscopic processes in condensed matter.

Since the stationary distribution is non-Gibbsian there are conceptual differences compared with the equilibrium case. For the harmonic potential one can define effective temperatures (4.1) for momentum and coordinate. Both temperatures are different from the bath temperature T. Generalized thermodynamic relations can be introduced, which take a quasi-Gibbsian form, Eqs. (4.18) and (4.20), and are closely related to the ones in the thermodynamics of glasses [24–26].

The inapplicability of standard thermodynamics is most clearly illustrated by the violation of the Clausius relation, $đQ\leqslant TdS$, heat received by the particle from the bath is restricted by temperature of the bath times the change of the particle's entropy. In Sec. IV B we construct an explicit example which at low temperatures realizes $đQ>0$. This violation is significant at low temperatures, where quantum effects are relevant, and is small for high temperatures. It is important to notice that this violation exists already for the totally equilibrium (Gibbsian) state of the overall (particle plus bath) system [see our discussion after Eq. (4.28)]. Since Thomson's formulation of the second law is valid for such a state [47], we have the explicit counterexample showing that the very equivalence between different formulations of the second law is broken at low temperatures [69].

For the dynamical consideration we start from a nonequilibrium initial state obtained from the total Gibbsian by changing the width of the confining potential. This change involves a small, controllable energy input, and can be more realistic than the hitherto studied case where particle and bath are initially uncorrelated. After the nonequilibrium state has been prepared, the ensuing relaxation of the particle presents a number of thermodynamical anomalies at low temperatures of the bath. First, energy put into the bath does not completely dissipates there (in contrast to the classical situation), and thus work extraction from a single thermal bath is possible. This violates the second law in Thomson's formulation as applied to nonequilibrium. As a consequence of this, adiabatic changes of parameters are not the most optimal ones anymore. It is interesting to notice that at low temperatures a large (but finite) number of work-extracting cycles is possible. In our opinion, this explicitly realizes the basic nontrivial content of the perpetuum mobile of the second kind, because any possibility for infinite number of such cycles is ruled out merely by the existence of the ground state for the overall system.

The second aspect of the low-temperature relaxation is that no H theorem exists at low temperatures, i.e., the properly defined entropy production appears to be negative for some times. This holds even in the moderately overdamped regime, when the Brownian particle relaxes monotonically. (Recall that without any bath those frequencies are purely imaginary, which leads to the known oscillatory behavior.) Within the underdamped (weakly coupled) situation negative entropy production persists up to high temperatures, and disappears only in the explicitly classical limit.

Let us recall that Thomson's formulation of the second law in its most general and universally applicable form [5]: *In cyclic processes no work can be extracted from a closed equilibrium system*, remains satisfied. This statement was derived in Ref. [47], and we have presented a very simple proof elsewhere [64]. It obviously applies to the analysis of this paper, since we start from a Gibbsian with modified spring constant, and the work extraction disappears when the change in the spring constant vanishes [69]. Also for cyclic smooth changes that start from equilibrium we could verify the non-negativity of the energy dispersion.

We now make some remarks concerning the definition of the thermal bath in our problem. The harmonic oscillator bath model, which was used by us, is technically convenient, but at the same time it possesses all relevant properties of a thermal bath, which are typically postulated in the statistical thermodynamics. The most important of them is that the bath should have infinite amount of degrees of freedom, a necessary condition to ensure relaxation of the Brownian particle. On the other hand, the quantum Langevin equation, which is the starting point of our analysis, can be derived from rather different schemes (see, e.g., Ref. [9]), since in a sense they are more universal than the detailed properties of the considered thermal bath.

Finally, let us relax the conditions under which our results have been derived. We have already mentioned that they hold as well for $N\gg1$ Brownian particles in an external potential. Though mutual interactions would complicate the analysis, it would not modify our basic statements. This can already be seen from the case of noninteracting harmonically bound Brownian particles: under a change of variables they become interacting ones, while the characteristics of the bath remains basically unaffected because it has many degrees of freedom.

Our findings on the nonthermodynamical character of the low-temperature Brownian motion may have a wide scope of applications such as cooling, energy storage, and thermodynamical limits of low-temperature computing. Indeed, in the domain of information theory there is a large literature based on the fact that only the erasure of information must necessarily involve a dissipation of heat (see extensive reviews in Ref. [34]), and the claim that the erasure of one bit of information costs at least an amount of energy $k_BT\ln 2$, the so-called Landauer bound. It is well known that this bound is based on a straightforward application of the Clausius inequality. From our observations it is clear that the Landauer bound can also be broken, and strong effects may occur at low temperatures. This may have implications for computing in the quantum regime [39].

For spins coupled to a bath the quantum nature expresses itself in off-diagonal elements of the density matrix. These decay after the time $\mathcal{T}_2$, which can range up to seconds. In this regime related work extraction setups are possible [63].

Our results can be expressed in the statement that Maxwell's demon exists: it is the property of quantum entanglement in quantum mechanics [68]. They may further have implications for thermodynamics in high-energy physics and the early universe.

The aim of this paper has been to show that violations of the second law have a natural place in the physics of quantum particles that are nonweakly coupled to quantum baths. In this domain we have given conditions for the realization of the most notorious objects in the history of physics: perpetuum mobile of the second kind.

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APPENDIX A: SMOOTH CHANGES OF THE SPRING CONSTANT

In this appendix we derive the work for continuous changes of the spring constant. Here we first notice that perturbative expression (5.60) of the exact result (5.57), (5.58) can be derived directly by perturbation theory. Let us first denote a by a_1 and expand also ϕ to first order in a_1-a_0. We may use

$$\begin{aligned}\sin\phi\, e^{i\phi_0-i\phi} &= \sin\phi_0+(a_1-a_0)e^{-i\phi_0}\frac{d\phi}{da}\\ &= \sin\phi_0-(a_1-a_0)\sin^2\phi_0\, e^{-i\phi_0}\frac{\Gamma^2+\nu^2}{\gamma\Gamma^2\nu}.\end{aligned} \tag{A1}$$

Now inserting Eq. (5.55) and taking the large Γ limit of $\hat{f}(i\nu)$ from Eq. (5.47), we get from Eq. (5.60)

$$\begin{aligned}\beta(\nu)=\sin\phi_0(\nu)\, e^{i\nu t}\Bigg[1+\frac{a_0-a_1}{\gamma w}\Bigg(&\frac{1-e^{-\omega_1 t-i\nu t}}{\omega_1+i\nu}\\ &-\frac{1-e^{-\omega_2 t-i\nu t}}{\omega_2+i\nu}\Bigg)\Bigg].\end{aligned} \tag{A2}$$

Now let us remember that for $t<0$ the spring constant was a_0, while for $t>0$ it is a_1. Thus one could write in (5.39): $a\to a(t)=a_0+(a_1-a_0)\,\theta(t)$. By treating the term $(a_0-a_1)\,\theta(t)x(t)$ together with $\eta(t)$, one can read off the formal solution from the analog of Eq. (5.44), and solve it perturbatively to first order in (a_1-a_0). It can be verified that the result coincides with (A2).

This first order perturbation theory can immediately be generalized for many steps,

$$a(t)=a_k=(1-\alpha_k)a,\quad (t_k<t<t_{k+1}), \tag{A3}$$

where $t_0=-\infty$ and t_1 was taken equal to zero so far, but can be arbitrary. One writes $a(t)=a_0+\Sigma_{k\geqslant 1}(a_k-a_{k-1})\,\theta(t-t_k)$ and gets

$$\begin{aligned}\beta(\nu)=\sin\phi_0(\nu)\, e^{i\nu t}\Bigg[1-\sum_{k\geqslant 1}\frac{a_k-a_{k-1}}{\gamma w}\,\theta(t-t_k)&\\ \times\Bigg(\frac{1-e^{-(\omega_1+i\nu)(t-t_k)}}{\omega_1+i\nu}-\frac{1-e^{-(\omega_2+i\nu)(t-t_k)}}{\omega_2+i\nu}\Bigg)\Bigg].&\end{aligned} \tag{A4}$$

At a given instant of time the sum has a finite number of terms because of the θ functions.

In Eq. (A4) we considered that effect of many small changes in the spring constant. When we make many changes with small $\alpha(t)=\alpha_k$ in the domain $t_k<t<t_{k+1}$, we get

$$\begin{aligned}\langle x^2\rangle=\frac{T_x(a)}{a}+\frac{\hbar}{\pi\gamma}\Bigg[\alpha_k C_x(0)-\sum_{j=1}^{k}\,(\alpha_j-\alpha_{j-1})&\\ \times C_x\!\left(\frac{\gamma(t-t_j)}{2m}\right)\Bigg],&\end{aligned} \tag{A5}$$

where $t_1=t_i$ is the moment of the first change, taken equal to zero so far. Let us write $\alpha_k=\alpha(\tau_k)$ and assume that the changes are small. Then the sum can be replaced by an integral,

$$\begin{aligned}2V(t)=a\langle x^2(t)\rangle=T_x(a)+\frac{\hbar a}{\pi\gamma}\Bigg[\alpha\!\left(\frac{\gamma t}{2m}\right)C_x(0)&\\ -\int_0^\infty d\tau\,\alpha'\!\left(\frac{\gamma t}{2m}-\tau\right)C_x(\tau)\Bigg],&\end{aligned} \tag{A6}$$

where the upper integration border could be put equal to ∞, since α' vanishes for times less than t_i.

The work needed to make the change $a_{k-1}\rightarrow a_k$ at time t_k is equal to $\frac{1}{2}(a_k-a_{k-1})\langle x^2(t_k)\rangle$, so it equals

$$d\mathcal{W}_k=(\alpha_{k-1}-\alpha_k)\left\{\frac{1}{2}T_x(a)+\frac{\hbar a}{2\pi\gamma}\left[\alpha_k C_x(0)-\sum_{j=1}^{k}(\alpha_j-\alpha_{j-1})C_x\left(\frac{\gamma(t_k-t_j)}{2m}\right)\right]\right\}. \tag{A7}$$

If there are many steps with small increments, we can go to a continuum limit. Replacing the sum by an integral, we obtain the rate of work added to the system

$$\frac{d\mathcal{W}}{dt}=\frac{d\mathcal{W}_{\rm rev}}{dt}+\frac{d\Pi}{dt}, \tag{A8}$$

where, with $\tau\equiv\gamma t/(2m)$,

$$\frac{d\mathcal{W}_{\rm rev}}{dt}=-\frac{\gamma}{2m}\frac{d\alpha(\tau)}{d\tau}\left[\frac{1}{2}T_x+\frac{\hbar a}{2\pi\gamma}\alpha(\tau)C_x(0)\right] \tag{A9}$$

is the adiabatic (recoverable) rate of work and

$$\frac{d\Pi}{dt}=\frac{\hbar a}{4\pi m}\frac{d\alpha(\tau)}{d\tau}\int_0^\infty d\sigma\,\alpha'(\tau-\sigma)C_x(\sigma) \tag{A10}$$

is the rate of energy dispersion.

APPENDIX B: MODERATE CUTOFF FREQUENCY AND FINITE CHANGE OF SPRING CONSTANT

In this appendix we address the vanishing of work dispersion at $T=0$, without making the approximation of large Debye frequency Γ. Then the full equation (5.59) has to be employed, rather than the approximation (5.60). With the help of an algebraic manipulation program we have checked that at $T=0$ the important findings $C_x^{(0)}=0$, see Eq. (6.47), and $C_p^{(0)}=C_E^{(0)}=0$ (c.f. Eq. (6.53)) remain valid. So a negative rate of energy dispersion occurs also for a finite cutoff.

Let us mention, however, that the effect is weakened when α_0, the amplitude of the change of the spring constant, is not very small. This probably affects the maximal number of work extraction cycles.

If one changes the mass and not the spring constant, the system does not exhibit this interesting behavior, since the analog $C_x^{(0)}$ does not vanish then, implying that the leading term in the energy dispersion does not vanish at low T.

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