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Thermodynamics of quantum Brownian motion with internal degrees of freedom: the role of entanglement in the strong-coupling quantum regime

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Abstract

We study the influence of entanglement on the relation between the statistical entropy of an open quantum system and the heat exchanged with a low temperature environment. A model of quantum Brownian motion of the Caldeira–Leggett type—for which a violation of the Clausius inequality has been stated by Th M Nieuwenhuizen and A E Allahverdyan (2002 *Phys. Rev. E* **66** 036102)—is re-examined and the results of the cited work are put into perspective. In order to address the problem from an information theoretical viewpoint a model of two coupled Brownian oscillators is formulated that can also be viewed as a continuum version of a two-qubit system. The influence of an additional internal coupling parameter on heat and entropy changes is described and the findings are compared to the case of a single Brownian particle.

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1. Introduction

Open systems are subject to dissipation of energy and fluctuations in their degrees of freedom. Within the theory of quantum dissipative systems [1, 2] the starting point in describing noise and damping is the Hamiltonian $H_{\text{tot}} = H_S + H_E + H_{SE}$ where the Hamiltonian of the total system H_{tot} is expressed as a sum of the Hamiltonian of the subsystem of interest H_S , a Hamiltonian H_E modelling the environmental degrees of freedom and an interaction term H_{SE} . For quantum objects this coupling to the environment in addition leads to the phenomena of decoherence and entanglement. These entanglement effects play an important role if the bath temperature is low or the system–bath interaction is strong. Under the unitary evolution of the density operator $\rho_{\text{tot}}(t) = U(t, 0)\rho_{\text{tot}}(0)U^\dagger(t, 0)$ with $U(t, 0) = \exp[-\frac{i}{\hbar}H_{\text{tot}}t]$ an initial product state of subsystem S and bath E evolves into a

correlated state with $\rho_{\text{tot}}(t) \neq \rho_S(t) \otimes \rho_E(t)$ for $t > 0$. For zero temperature the total closed system ρ_{tot} is in its ground state and therefore the von Neumann entropy $S(\rho_{\text{tot}}(t))$ stays zero for all times. But for $t > 0$ the pure state of the whole system is an entangled state of subsystem and bath with $S(\rho_{\text{tot}}(t)) \leq S(\rho_S(t)) + S(\rho_E(t))$. The subsystem therefore is in a mixed state with $S(\rho_S(t)) > 0$ even for zero bath temperature.

In most applications, especially in quantum optics [3, 4], the coupling between system and bath can be assumed to be weak which allows neglecting entanglement effects (Born–Markov approximation) and applying the formalism of Markovian quantum master equations. In this case the reduced density matrix of the open system is Gibbsian. If the total Hamiltonian is harmonic, a Gaussian initial state of the subsystem remains Gaussian for all times. In the strong-coupling quantum regime, the stationary state of the subsystem $\rho_S(t)$ is therefore still Gaussian but non-Gibbsian due to the entanglement with the bath. Its density matrix $\rho_S(t)$ is completely characterized by the first and second moments of the relevant operators. The Heisenberg equation of motion for these operators is the quantum Langevin equation [5, 6]. The characterizing moments are determined by the stationary values of the quantum Langevin equation and can be calculated alternatively by applying the quantum fluctuation-dissipation theorem. The statistical entropy associated with that stationary quantum state is the von Neumann entropy. The systems exchange of heat with the environment—which is defined as the change in energy due to redistributions in phase space—is related to the thermodynamic entropy by the Clausius inequality. This thermodynamic entropy can only be identified with the statistical entropy when ρ_S takes the form of the canonical density matrix. This is just the case for negligible interaction between subsystem and environment.

From an information-theoretical point of view, above considerations become important. The Landauer principle [7, 8] which is based on the Clausius inequality states that ‘many-to-one’ operations like erasure of information require the dissipation of energy. Deleting one bit of information is accompanied by a released amount of heat of at least $kT \ln 2$. This erasure is connected with a reduction of entropy, and thus cannot be realized in a closed system. Therefore the information-carrying system has to be coupled to its environment. To avoid a rapid destruction of the necessary quantum coherence the quantum subsystem should be placed in a low temperature environment. Thus the coupling might be relatively strong compared to thermal energy. Since the Landauer principle is dealing with information processing and erasure, the relevant entropy is the statistical entropy of the system. Statistical entropy and heat are defined separately. Thus, the relation between both the quantities can be examined.

The purpose of our paper is to study deviations from the Clausius inequality and Landauer bound respectively in the strong-coupling quantum regime. An analytic treatment of this issue is given within the framework of the Caldeira–Leggett model of quantum Brownian motion.

In the first part of this paper we want to discuss quite controversial recent work [9–12] and put some of those results into perspective. Therefore the quantum Langevin equation of a harmonically bound quantum particle based on the Caldeira–Leggett model is presented. The stationary moments that are obtained from this equation characterize the reduced density matrix completely. This density matrix is used to define thermodynamic quantities. Then, changes in heat and in statistical entropy for adiabatic parameter variations are compared and the applicability of the Clausius inequality in the strong coupling/low temperature quantum regime is discussed. In the second main part we will focus on a model of Brownian motion of two coupled oscillators, which can be understood as a continuum version of a two-qubit system [13]. With regard to recent work done on continuous variable computing [14, 15] the impact on quantum information theory is studied. It will become clear that additional internal

degrees of freedom can lead to different results as in the case of quantum motion of a single Brownian particle.

2. Caldeira–Leggett model of quantum Brownian motion

Brownian motion is a prominent example of an open quantum system [16]. The standard model of quantum Brownian motion, often referred to as the Caldeira–Leggett model [17, 18], is a system-plus-reservoir model. The whole system is governed by the Hamiltonian

$$H_{\text{tot}} = \frac{p^2}{2m} + V(q) + \sum_{i=1}^N \left[\frac{p_i^2}{2m_i} + \frac{m_i \omega_i^2}{2} x_i^2 \right] + \sum_{i=1}^N \left[-c_i x_i q + \frac{c_i^2}{2m_i \omega_i^2} q^2 \right] \quad (1)$$

where q and p are the Heisenberg operators for coordinate and momentum of the Brownian particle moving in the harmonic potential $V(q) = \frac{1}{2}m\omega_0^2 q^2$. The particle is coupled to a bath of N harmonic oscillators with variables x_i and p_i and uniformly spaced modes $\omega_i = i\Delta$. The interaction is bilinear in coordinates of system q and bath x_i . For the coupling-parameters c_i the so-called Drude–Ullersma spectrum [19] with large cutoff-frequency Γ and coupling constant γ is chosen: $c_i = \sqrt{2\gamma m_i \omega_i^2 \Delta \Gamma^2 / \pi (\omega_i^2 + \Gamma^2)}$. The bath is characterized by its spectral density $J(\omega)$, which takes the form of the Drude spectrum $J(\omega) = \gamma \omega \Gamma^2 / (\omega^2 + \Gamma^2)$ in the thermodynamic limit (sending $\Delta \rightarrow 0$, $N \rightarrow \infty$ and keeping $\Gamma = N\Delta = \text{const}$). The potential renormalization term $\sum c_i^2 / (2m_i \omega_i^2) q^2$ ensures that $V(q)$ remains the bare potential. Neglecting this self-interaction term, the positive definiteness of the total Hamiltonian H_{tot} would just be guaranteed for $\gamma \leq m\omega_0^2/\Gamma$ and—since Γ is large—would restrict the applicability of the model to weak-coupling approximations ($\gamma \ll m\omega_0$).

2.1. Quantum Langevin equation

From the Hamiltonian (1) the Heisenberg equations of motion for the operators q and p and the bath variables x_i , p_i are received. By eliminating the bath degrees of freedom the quantum Langevin equation [5, 6] of a particle moving in the potential $V(q)$ can be derived:

$$m\ddot{q}(t) + \frac{dV(q)}{dq} + \int_0^t dt' \gamma(t-t') \dot{q}(t') = \eta(t) - q(0)\gamma(t). \quad (2)$$

The stochastic character of this integro-differential equation with the friction kernel $\gamma(t) = \gamma\Gamma e^{-\Gamma|t|}$ comes into play by considering the initial distribution of the bath variables which determines the noise term $\eta(t)$:

$$\eta(t) = \sum_{i=1}^N c_i \left(x_i(0) \cos \omega_i t + \frac{p_i(0)}{m_i \omega_i} \sin \omega_i t \right). \quad (3)$$

Assuming an uncorrelated initial state with the reservoir being in canonical equilibrium at temperature $T = \beta^{-1}$, $\rho_E \sim \exp(-\beta H_E)$, $\eta(t)$ is a stationary Gaussian operator noise with $\langle \eta(t) \rangle_{\rho_E} = 0$ and the correlation function [3]:

$$\begin{aligned} K(t-t') &= \frac{1}{2} \langle \eta(t)\eta(t') + \eta(t')\eta(t) \rangle_{\rho_E} \\ &= \frac{\hbar}{\pi} \int_0^\infty d\omega \frac{\gamma \Gamma^2 \omega}{\Gamma^2 + \omega^2} \coth \left(\frac{1}{2} \beta \hbar \omega \right) \cos \omega(t-t'). \end{aligned} \quad (4)$$

In the case of initial correlations of particle and bath the correlation function contains additional terms which affect the dynamics on the timescale $t \leq 1/\Gamma$. To fully characterize the reduced dynamics it is thus important to specify the initial preparation.

2.2. Stationary state

The relaxation dynamics of the moments $\langle q^2(t) \rangle$ and $\langle p^2(t) \rangle$ described by equation (2), end up in a stationary state for $t \rightarrow \infty$. The stationary correlations can be calculated alternatively by applying the quantum fluctuation-dissipation theorem [20], which establishes a connection between the quantum mechanical dynamical susceptibility $\tilde{\chi}(\omega) = \int_{-\infty}^{\infty} \chi(t-t') e^{i\omega t} = [m\omega_0^2 - m\omega^2 - i\omega\tilde{\gamma}(\omega)]^{-1}$ and the equilibrium fluctuations $\langle q^2 \rangle$ and $\langle p^2 \rangle$:

$$\langle q^2 \rangle = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \coth\left(\frac{1}{2}\beta\hbar\omega\right) \tilde{\chi}''(\omega), \quad (5)$$

$$\langle p^2 \rangle = \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega m^2 \omega^2 \coth\left(\frac{1}{2}\beta\hbar\omega\right) \tilde{\chi}''(\omega). \quad (6)$$

If the dissipative part of the susceptibility $\tilde{\chi}''(\omega)$ of the non-Markovian damped oscillator with three characteristic frequencies λ_1, λ_2 and λ_3 (poles in the complex plane) is inserted, an analytic expression for equations (5) and (6) is derived [1]:

$$\langle q^2 \rangle = \frac{\hbar}{m\pi} \sum_{i=1}^3 \frac{(\lambda_i - \Gamma)\psi\left(\frac{\beta\hbar\lambda_i}{2\pi}\right)}{(\lambda_{i+1} - \lambda_i)(\lambda_{i-1} - \lambda_i)} - T, \quad (7)$$

$$\langle p^2 \rangle = m^2 \omega_0^2 \langle q^2 \rangle + \frac{\hbar\gamma\Gamma}{\pi} \sum_{i=1}^3 \frac{\lambda_i \psi\left(\frac{\beta\hbar\lambda_i}{2\pi}\right)}{(\lambda_{i+1} - \lambda_i)(\lambda_{i-1} - \lambda_i)}, \quad (8)$$

where $\psi(x)$ is the Digamma function and $\lambda_0 = \lambda_3, \lambda_4 = \lambda_1$. The stationary state of the Brownian particle is fully characterized by the variances (7) and (8) which determine the stationary density matrix ρ_S of the subsystem [1, 21]:

$$\rho_S(q, q') = \frac{1}{\sqrt{2\pi\langle q^2 \rangle}} \exp\left[-\frac{(q+q')^2}{8\langle q^2 \rangle} - \frac{(q-q')^2}{2\hbar^2/\langle p^2 \rangle}\right]. \quad (9)$$

This reduced density matrix is different from the canonical equilibrium density matrix $\rho_{\text{th}} \sim \exp(-\beta H_S)$ for any finite coupling γ . The statistical entropy of the quantum state ρ_S —the von Neumann entropy $S(\rho_S)$ —is [9, 22]

$$\begin{aligned} S(\rho_S) &= -\text{Tr}[\rho_S \ln \rho_S] = -\sum_n p_n \ln p_n \\ &= \left(v + \frac{1}{2}\right) \ln\left(v + \frac{1}{2}\right) - \left(v - \frac{1}{2}\right) \ln\left(v - \frac{1}{2}\right), \end{aligned} \quad (10)$$

with Boltzmann constant set to $k_B = 1$ and the subsystems phase space volume v defined by

$$v = \frac{1}{\hbar} \sqrt{\langle q^2 \rangle \langle p^2 \rangle}, \quad (11)$$

as well as the eigenvalues of $\rho_S(q, q')$,

$$p_n = 1/(v + 1/2)[(v - 1/2)/(v + 1/2)]^n, \quad (12)$$

which are obtained as solution of the problem $\int dx' \rho_S(q, q') f_n(q') = p_n f_n(q)$, where the eigenfunctions f_n are given by $f_n \sim \sqrt{c} H_n(cq) e^{-c^2 q^2/2}$ with Hermite polynomials H_n and $c = [\langle p^2 \rangle / (\hbar^2 \langle q^2 \rangle)]^{1/4}$.

The von Neumann entropy of the subsystem is increased with raising the coupling γ at a given temperature (figure 1). Even at $T \rightarrow 0$ the subsystems entropy is larger than zero.

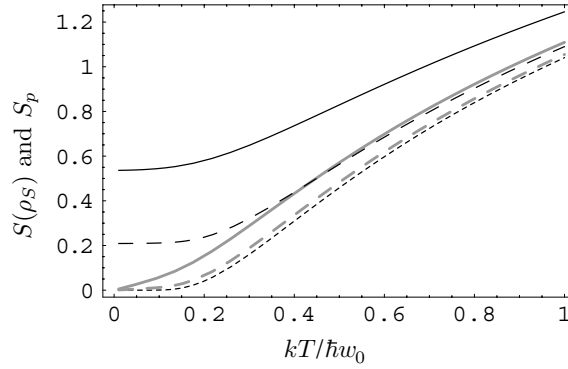


Figure 1. Temperature dependence of the entropy expressions $S(\rho_S)$ and S_p for different values of the system–bath couplings γ (in units of $m\omega_0^2/\Gamma$). Dark lines from bottom to top: $S(\rho_S)_{\gamma=0}$; $S(\rho_S)_{\gamma=1}$; $S(\rho_S)_{\gamma=5}$. Grey lines: $S_{p,\gamma=1}$ (dashed) and $S_{p,\gamma=5}$. Other parameters: $\omega_0 = 1$, $m = 1$, $\Gamma = 10$, $\hbar = 1$.

This effect is due to the correlations between subsystem and bath which prevent the subsystem from reaching a pure state for $T \rightarrow 0$. The probabilities to find the subsystem in an excited state depend on the coupling to the environment [23]. In the weak coupling limit, where $\rho_S = \rho_{th}$, expression (10) gives the entropy

$$S(\omega_0, T) = \frac{\beta\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1} - \ln(1 - e^{-\beta\hbar\omega_0}) \quad (13)$$

of an harmonic oscillator in canonical equilibrium.

It is important to remark here, that the entropy (10) deviates from the difference of the total entropy $S(\rho_{tot})$ and the entropy of the bath in the absence of the particle $S(\rho_E)_{\gamma=0}$ which is given by [24]

$$S_p = \frac{1}{\pi} \int_0^\infty S(\omega, T) \text{Im} \left\{ \frac{d \ln \tilde{\chi}(\omega)}{d\omega} \right\} d\omega. \quad (14)$$

In the same way the thermodynamic potentials F_p and U_p can be derived which are related by $S_p = \beta(U_p - F_p)$. One can see from figure 1 that S_p vanishes at $T \rightarrow 0$ whereas $S(\rho_S)$ does not. Proceeding in this way, the entropy S_p also contains the part of entropy that is associated with the quantum mechanical correlations of particle and bath. Since this conditional entropy is negative for entangled systems, the statistical entropy of the Brownian oscillator alone is underestimated by S_p . Thus, in our further treatment we will concentrate on the entropy $S(\rho_S)$.

2.3. Thermodynamics of adiabatic changes

Nieuwenhuizen and Allahverdyan [11] examined the validity of the Clausius inequality respectively the Landauer bound in the strong coupling quantum regime. They found a violation of these principles at very low temperatures due to the existing correlations between subsystem and bath. With respect to quantum information theory they concluded that quantum mechanical information carrier therefore could be more efficient than their classical counterparts. A controversial subject in this context is the appropriate choice of heat and entropy expressions. Our purpose in this section is to clarify this issue and to put the findings of Nieuwenhuizen and Allahverdyan into perspective.

The internal energy of the Brownian oscillator can be defined as the mean energy in the stationary state [9]:

$$U_S = \text{Tr}[H_S \rho_S] = \langle H_S \rangle = \frac{1}{2m} \langle p^2 \rangle + \frac{1}{2} m \omega_0^2 \langle q^2 \rangle. \quad (15)$$

This expression differs from the equivalent to (14) defined internal energy U_p . The difference $U_p - U_S$ can be interpreted as the interaction energy $U_{\text{int}} (\neq \langle H_{SE} \rangle!)$ which is related to the free energy F_p by

$$U_{\text{int}} = U_p - U_S = \Gamma \frac{\partial F_p}{\partial \Gamma}. \quad (16)$$

Choosing the parameter values m , ω_0 and Γ as in figure 1 the ratio $\tau = U_{\text{int}}/U_p$ at zero bath temperature is given by $\tau_{(\gamma=m\omega_0^2/\Gamma)} \approx 0.03$ and $\tau_{(\gamma=5m\omega_0^2/\Gamma)} \approx 0.10$. For $kT = \hbar\omega_0$ the ratios are $\tau_{(\gamma=m\omega_0^2/\Gamma)} \approx 0.01$ and $\tau_{(\gamma=5m\omega_0^2/\Gamma)} \approx 0.05$, respectively.

The total differential dU_S of the internal energy U_S ,

$$dU_S = \text{Tr}[\rho_S dH_S] + \text{Tr}[H_S d\rho_S] = \delta W + \delta Q \quad (17)$$

can be divided into two parts [25]. The first term results from the change of the parameters m and ω_0 in the Hamiltonian, so it is a mechanical, non-statistical object and will be referred to as work δW :

$$\delta W = m\omega_0 \langle q^2 \rangle d\omega_0 + \left(\frac{\omega_0^2 \langle q^2 \rangle}{2} - \frac{\langle p^2 \rangle}{2m^2} \right) dm. \quad (18)$$

The second term $\text{Tr}[H_S d\rho_S]$ represents the variation of U_S due to the statistical redistribution of the phase space, which will be associated with the change in heat δQ :

$$\delta Q = \delta_\omega Q + \delta_m Q$$

with

$$\delta_\omega Q = \left(\frac{1}{2} m \omega_0^2 \frac{\partial \langle q^2 \rangle}{\partial \omega_0} + \frac{1}{2m} \frac{\partial \langle p^2 \rangle}{\partial \omega_0} \right) d\omega_0, \quad (19)$$

$$\delta_m Q = \left(\frac{1}{2} m \omega_0^2 \frac{\partial \langle q^2 \rangle}{\partial m} + \frac{1}{2m} \frac{\partial \langle p^2 \rangle}{\partial m} \right) dm. \quad (20)$$

Now the validity of the Clausius inequality

$$\delta Q \leq T dS \quad (21)$$

can be evaluated. The second law of thermodynamics in the formulation by Clausius states that in a quasi-static process, during which the system at all times passes through equilibrium states, one has $dS_{\text{th}} = \delta Q/T$. The thermodynamic entropy S_{th} defined by the Clausius equality can only be identified with the statistical entropy $S(\rho_S)$ at thermal equilibrium where $\rho_S = \rho_{\text{th}}$ with $\rho_{\text{th}} = Z^{-1} \exp(-\beta H_S)$ and $Z = \text{Tr} \exp(-\beta H_S)$, because

$$\begin{aligned} dS &= -\text{Tr}[d\rho_{\text{th}} \ln \rho_{\text{th}}] = \text{Tr}[d\rho_{\text{th}} \ln Z] + \beta \text{Tr}[d\rho_{\text{th}} H_S] \\ &= \beta \text{Tr}[\rho_{\text{th}} H_S] = \beta \delta Q = dS_{\text{th}}. \end{aligned} \quad (22)$$

Concerning the Landauer principle, which is based on the Clausius inequality, but deals with information processing and erasure, the relevant entropy is the statistical entropy $S(\rho_S)$. Therefore we want to compare changes in the statistical entropy dS to changes in heat δQ induced by adiabatic variation of the systems parameters. The total differential of the von Neumann entropy (10) is given by

$$dS = -\text{Tr}[d\rho_S \ln \rho_S] = \ln \left(\frac{v + \frac{1}{2}}{v - \frac{1}{2}} \right) dv. \quad (23)$$

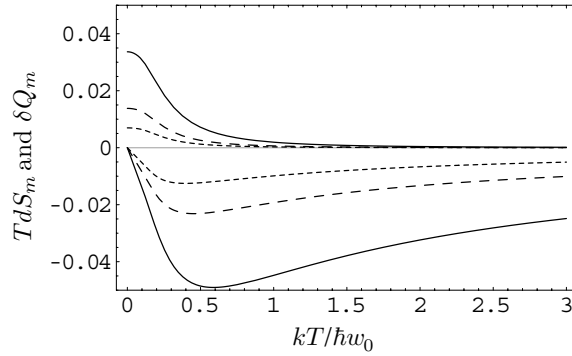


Figure 2. Changes in heat δQ_m (positive) and entropy-term $T dS_m$ (negative) versus bath temperature T for different values of the system–bath coupling γ (in units of $m\omega_0^2/\Gamma$): 0.5 (narrow dashed), 1 (dashed), 2.5 (solid line). The oscillator parameters are chosen to be $\omega_0 = 1$ and $m = 1$. The cutoff-frequency is set to $\Gamma = 10$ and $\hbar = 1$.

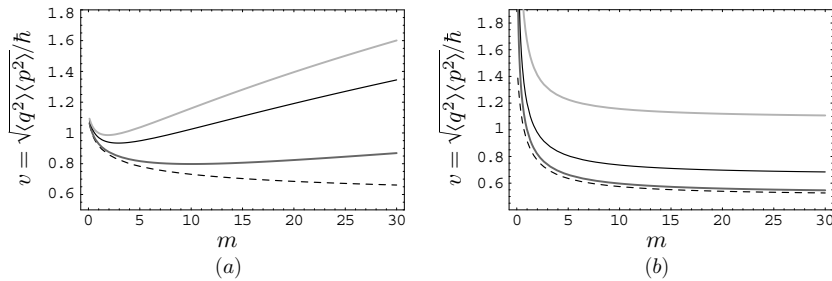


Figure 3. Phase space volume v versus mass m for different T -values. From bottom to top: $T = 0; 0.1; 0.2; 0.25$. Other parameters: $\gamma = 1, \Gamma = 500, \hbar = 1$. (a) Oscillator potential $V(q) = \frac{1}{2}aq^2$ with fixed spring constant $a = 1$ (see also [11]). (b) Oscillator potential $V(q) = \frac{1}{2}m\omega_0^2q^2$ with frequency $\omega_0 = 1$.

Thus, the sign of the change in $S(\rho_S)$ is determined by the sign of the change in v . Note here that the parameters m and ω_0 are chosen as independent quantities, so that we can examine $\delta Q_m \leq T dS_m$ and $\delta Q_\omega \leq T dS_\omega$ separately.

Figure 2 shows the temperature dependence of the changes in heat δQ_m and of the term $T dS_m$ for different coupling strength γ . While δQ_m is always positive, which means that the Brownian particle absorbs heat during an adiabatic increase of mass, the change of entropy and therefore the product $T dS_m$ remains negative. In the high-temperature limit one has $\delta Q_m \rightarrow 0$ as well as $T dS_m \rightarrow 0$ and therefore the behaviour of an uncoupled harmonic oscillator characterized by (13). The term $T dS_m$ converges relatively slowly towards zero because of the increasing factor T . The smaller the coupling γ , the faster is the convergence of the two terms δQ_m and $T dS_m$. If the temperature T goes to zero, then the product $T dS_m$ does as well. The amount of heat δQ_m exchanged with the bath stays positive even in this limit and equals $-d_m U_{\text{int}}$. Thus, the Brownian particle can extract heat from the bath even at $T = 0$, a fact that was already extensively discussed in [9, 11].

Figure 3(a) gives results of the cited work [11]. Nieuwenhuizen and Allahverdyan studied the influence of adiabatic changes in mass on the phase space volume v given by equation (11). At $T = 0$ one receives a monotonic decreasing function which should converge with increasing

mass to the minimal value $v_{\min} = 1/2$ which results from the uncertainty relation. They found, that at moderate temperatures the phase space volume first decreases for low masses, then reaches a minimum and finally increases nearly linearly with the mass. The increasing phase space volume means a positive sign for the entropy change dS . Therefore the authors conclude that the different signs of δQ and $T dS$ would only occur at very low temperatures due to quantum correlations between system and bath.

In contrast to that, figure 3(b) shows the mass dependence of the phase space volume using the moments defined by equations (7) and (8). One can clearly see that even for moderate temperatures the phase space volume does not increase, but reaches a temperature-dependent limit value. This value is given by the phase space volume of an uncoupled harmonic oscillator in canonical equilibrium: $v_{th} = \frac{1}{2} \coth \beta \hbar \omega_0 / 2$. Both, sending $m \rightarrow \infty$ or coupling $\gamma \rightarrow 0$, finally leads to the standard case of the quantum Gibbs distribution.

The differences between our findings and the results in [11] which become obvious in figures 3(a) and (b) can be explained as follows: in the paper by Nieuwenhuizen and Allahverdyan [11] the harmonic potential $V(q) = \frac{1}{2} m \omega_0^2 q^2$ is expressed by $\frac{1}{2} a q^2$ with spring constant a . Varying m and keeping a fixed leads to the results of figure 3. But since the limit $m \rightarrow \infty$ and $\gamma \rightarrow 0$ should lead to the same result of $v = 1/2$ at $T = 0$, this choice of the potential is inconsistent. In figure 3 the phase space volume at $T = 0$ does not reach the value $v = 1/2$ even for high masses (instead $v \approx 0.6$ for the given parameter values). In order to receive the correct expressions for $\langle q^2 \rangle$, $\langle p^2 \rangle$ and U in the weak coupling or high temperature limit one has to set $a = m \omega_0^2$, which has also been done in the cited work [11] in different contexts.

Choosing the potential $V(q) = \frac{1}{2} m \omega_0^2 q^2$, which is then affected by the variation of the mass, shows that the anomaly of different signs is an even stronger effect than found in [11]. This indicates that not only quantum correlations at low temperatures might play a role but also classical correlations between the damped oscillator and its environment at moderate temperatures.

3. Quantum Brownian motion of two coupled harmonic oscillators

In order to study the influence of additional parameters on the results stated above we introduce a model of quantum Brownian motion of two coupled oscillators which can be viewed as a continuum version of a two-qubit system. In contrast to former work concerning the relaxation dynamics of two coupled oscillators [13, 26] we focus on the stationary state. The Hamiltonian $H_{S'}$ of the open quantum system S' now reads

$$H_{S'} = H_A + H_B + H_{AB}, \quad (24)$$

where H_A and H_B are the Hamiltonians of the two harmonic oscillators A and B with masses m_a, m_b and frequencies ω_a and ω_b . H_{AB} describes the interaction between them. Before deriving a quantum Langevin equation it is necessary to discuss different couplings between the oscillators as well as between the system $H_{S'}$ and the bath H_E and to choose an appropriate model.

3.1. Coupling between the two oscillators

In the framework of quantum optics the coupling between oscillators is often chosen to $H_{AB} = -D q_a q_b$ with coupling parameter D . In this case one problem is the constraint $D \leq \sqrt{m_a m_b} \omega_a \omega_b$ as a condition for real eigenfrequencies of the system which restricts the

range of allowed parameter variations. In our further treatment we will concentrate on the interaction Hamiltonian

$$H_{AB} = \frac{1}{2}D(q_a - q_b)^2. \quad (25)$$

This Hamiltonian is clearly inspired by its mechanical analogy—a restoring force proportional to the relative distance of the two oscillators—and leads to real eigenfrequencies of the system H_S for all values of the coupling parameter D .

3.2. Coupling between system and bath

In order to study the case of strong system–bath coupling γ , the positive definiteness of the Hamiltonian has to be guaranteed in the range of relevant γ -values. Therefore we will discuss different couplings between system and bath in the following section.

3.2.1. Oscillators separately coupled to the bath. If each oscillator is coupled separately to the bath according to the coupling in (1) then we receive the following interaction Hamiltonian $H_{S'E}$:

$$H_{S'E} = \sum_{i=1}^N \left[-c_i x_i (q_a + q_b) + \frac{c_i^2}{2m_i \omega_i^2} (q_a^2 + q_b^2) \right]. \quad (26)$$

The equation for the eigenvalues ν of the total system

$$H_{\text{tot}} = H_A + H_B + H_{AB} + H_E + H_{S'E} \quad (27)$$

reads

$$\nu^2 - \left(\omega_a^2 + \frac{D}{m_a} \right) = \sum_i \frac{c_i^2}{m_a m_i (\nu^2 - \omega_i^2)} \frac{\nu^2}{\omega_i^2} - \frac{\frac{1}{m_a m_b} (D - \sum_i \frac{c_i^2}{m_i (\nu^2 - \omega_i^2)})^2}{\omega_b^2 + \frac{D}{m_b} + \sum_i \frac{c_i^2}{m_b m_i (\nu^2 - \omega_i^2)} \frac{\nu^2}{\omega_i^2}}. \quad (28)$$

Figure 4(a) shows the influence of the system–bath coupling strength γ on the eigenfrequencies of a finite system consisting of the two oscillators coupled to an environment of eight oscillators. The lowest eigenvalue ν_1 decreases with increasing coupling strength and becomes imaginary at a critical value

$$\gamma_{\text{crit}} = \left(\frac{2\pi}{\Delta} \sum_{i=1}^N \frac{\Gamma^2}{\omega_i^2 + \Gamma^2} \right)^{-1} \left[\sqrt{(m_a \omega_a^2 + D)(m_b \omega_b^2 + D)} - D \right] \quad (29)$$

which means exponentially increasing amplitudes and therefore instability of the whole system. In the thermodynamic limit this critical value becomes very small, so that this model is only suitable in the weak coupling case.

3.2.2. Bath coupling to the centre of mass. A more adequate model is the bath-coupling attached to the centre of mass R of the system H_S , while the relative motion is an uncoupled internal degree of freedom. The system–bath interaction could then be described by the Hamiltonian

$$H_{S'E} = \sum_{i=1}^N \left[-c_i x_i R + \frac{c_i^2}{2m_i \omega_i^2} R^2 \right]. \quad (30)$$

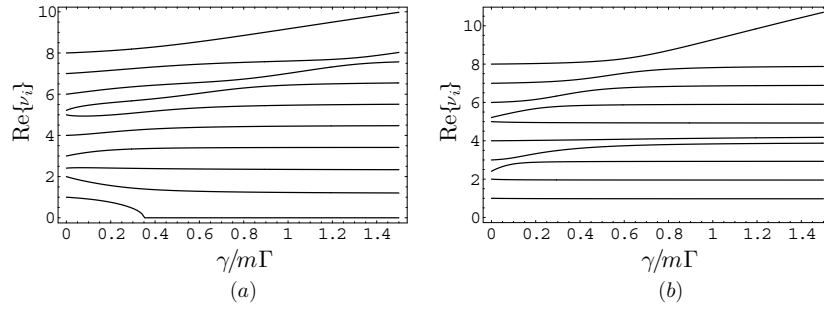


Figure 4. Eigenfrequencies of a finite model with $N + 2 = 10$ oscillators versus the system–bath coupling strength γ (in units of $m\Gamma$). Parameters: $\omega_a = 2$, $\omega_b = 5$, $m = m_{a,b} = 1$, $D = 2$ and $\Delta = 1$, $\Gamma = N\Delta = 8$. (a) Oscillators separately coupled to the bath with eigenfrequencies ν given by equation (28). The critical value γ_{crit} is given by equation (29). (b) Bath coupling to the centre of mass with eigenfrequencies ν given by equation (31).

This interaction could also be understood as a model of two oscillators separately coupled to the bath including a self-interaction term proportional to the product $q_a q_b$. The coupling leads to the following eigenvalue equation of the total system H_{tot} :

$$\nu^2 - \frac{1}{M}(m_a \omega_a^2 + m_b \omega_b^2) = \sum_{i=1}^N \frac{c_i^2}{M m_i (\nu^2 - \omega_i^2)} \frac{\nu^2}{\omega_i^2} - \frac{\mu (\omega_a^2 - \omega_b^2)^2}{m_b \omega_a^2 + m_a \omega_b^2 + \frac{M}{\mu} D - M \nu^2}. \quad (31)$$

In figure 4(b) one can recognize that the lowest eigenvalue is only slightly reduced by increasing the coupling strength and remains real for all γ -values.

Since this interaction term assures the positive definiteness of the total Hamiltonian we will use this system–bath coupling in the further examination. Additionally this coupling allows us to transform the system easily to normal coordinates which simplifies the analysis in the case of identical oscillators. Physically speaking it can be interpreted as a model of a Brownian particle with an internal degree of freedom—in this case harmonic vibrations described by equation (25).

3.3. Langevin equation of two coupled Brownian oscillators

By transforming the Hamiltonian H_S onto coordinates for the centre of mass $R = 1/M(m_a q_a + m_b q_b)$ and the relative coordinate $x = (q_a - q_b)$ (with total mass M and reduced mass μ) and eliminating the bath variables, the following system of coupled equations for the Heisenberg operators x and R can be written down:

$$\ddot{x} = -\Omega_x^2 x(t) - (\omega_a^2 - \omega_b^2) R(t) \quad (32)$$

$$\ddot{R} = -\Omega_R^2 R(t) - \frac{1}{M} \int_0^t \gamma(t-t') \dot{R}(t') dt' - \gamma(t) R(0) - \frac{\mu}{M} (\omega_a^2 - \omega_b^2) x(t) + \eta(t) \quad (33)$$

with the frequencies

$$\Omega_x^2 = \frac{1}{M} \left(m_b \omega_a^2 + m_a \omega_b^2 + \frac{M}{\mu} D \right) \quad (34)$$

$$\Omega_R^2 = \frac{1}{M} (m_a \omega_a^2 + m_b \omega_b^2) \quad (35)$$

and damping term $\gamma(t)$ and noise term $\eta(t)$ as defined in section 2.1. Solving equation (32) as an inhomogeneous differential equation and inserting the solution into (33) gives a Langevin equation for the centre of mass R with new damping term $\tilde{\gamma}(t)$ and new noise term $\tilde{\eta}(t)$:

$$M\ddot{R} + \frac{d\tilde{V}(R)}{dR} + \int_0^t dt' \tilde{\gamma}(t-t')\dot{R}(t') = \tilde{\eta}(t) - R(0)\tilde{\gamma}(t) \quad (36)$$

which describes the motion of R in the effective potential $\tilde{V}(R) = 1/2M\tilde{\Omega}_R^2 R^2$ with frequency

$$\tilde{\Omega}_R^2 = \Omega_R^2 - \frac{\mu(\omega_a^2 - \omega_b^2)^2}{M\Omega_x^2} \quad (37)$$

influenced by the generalized damping and noise

$$\tilde{\gamma}(t-t') = \gamma\Gamma e^{-\Gamma|t-t'|} + \mu \frac{(\omega_a^2 - \omega_b^2)^2}{\Omega_x^2} \cos \Omega_x(t-t') \quad (38)$$

$$\begin{aligned} \tilde{\eta}(t) = \sum_{i=1}^N c_i \left[x_i(0) \cos(\omega_i t) + \frac{p_i(0)}{m_i \omega_i} \sin(\omega_i t) \right] \\ + \mu(\omega_b^2 - \omega_a^2) \left[x(0) \cos(\Omega_x t) + \frac{p_x(0)}{M\Omega_x} \sin(\Omega_x t) \right]. \end{aligned} \quad (39)$$

In the case of identical oscillators equations (32) and (33) are decoupled. The relative coordinate performs a harmonic oscillation and for R the Langevin equation of a Brownian particle with mass M and oscillator frequency Ω_R is received,

$$M\ddot{R} + M\Omega_R^2 R + \int_0^t dt' \gamma(t-t')\dot{R}(t') = \eta(t) - R(0)\gamma(t), \quad (40)$$

which is equivalent to quantum Langevin equation (2) in the first part of this paper.

3.4. Stationary state

In order to calculate the stationary correlations for the general case we again apply the quantum fluctuation-dissipation theorem.

From equation (36) one obtains the dynamical susceptibility $\tilde{\chi}_R''(\omega) = [M\tilde{\Omega}_R^2 - M\omega^2 - i\omega\tilde{\gamma}(\omega)]^{-1}$ and can express the variance of the centre of mass by

$$\begin{aligned} \langle R^2 \rangle &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{\chi}_R''(\omega) \coth\left(\frac{1}{2}\beta\hbar\omega\right) \\ &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{\gamma\Gamma^2\omega}{\xi^2\Gamma^2 + (\xi + \gamma\Gamma)^2\omega^2} \coth\left(\frac{1}{2}\beta\hbar\omega\right) \end{aligned} \quad (41)$$

where

$$\xi = M\Omega_R^2 - M\omega^2 - \mu \frac{(\omega_a^2 - \omega_b^2)^2}{\Omega_x^2 - \omega^2}. \quad (42)$$

Figure 5 shows the temperature dependence of the variance (41) in comparison to the limiting cases:

$$\langle R^2 \rangle_{\text{th}} = \frac{\hbar}{2M\tilde{\Omega}_R} \coth \frac{1}{2}\beta\hbar\tilde{\Omega}_R \quad \text{for } \gamma \rightarrow 0 \quad (43)$$

$$\langle R^2 \rangle_{\text{cl}} = \frac{kT}{M\tilde{\Omega}_R^2} \quad \text{for } T \gg m\tilde{\Omega}_R^2. \quad (44)$$

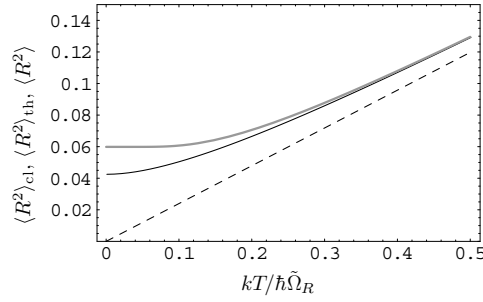


Figure 5. Temperature dependence of $\langle R^2 \rangle$ (41) for parameter values $\omega_a = 2$, $\omega_b = 3\omega_a$, $m_a = m_b = 1$, $D = M\Omega_R^2$, $\Gamma = 10$ and $\gamma = 5M\tilde{\Omega}_R^2/\Gamma$, (dark line). For increasing temperature $\langle R^2 \rangle$ converges to the limit cases $\langle R^2 \rangle_{th}$ (grey line) and $\langle R^2 \rangle_{cl}$ (dashed line) as given by equations (43) and (44).

In the same way we can specify the variance of the centre of mass momentum P_R :

$$\begin{aligned} \langle P_R^2 \rangle &= \frac{\hbar}{2\pi} M^2 \int_{-\infty}^{\infty} d\omega \tilde{\chi}_R''(\omega) \omega^2 \coth\left(\frac{1}{2}\beta\hbar\omega\right) \\ &= \frac{\hbar}{2\pi} M^2 \int_{-\infty}^{\infty} d\omega \frac{\gamma\Gamma^2\omega^3}{\xi^2\Gamma^2 + (\xi + \gamma\Gamma)^2\omega^2} \coth\left(\frac{1}{2}\beta\hbar\omega\right) \end{aligned} \quad (45)$$

as well as the variance of the relative coordinate x

$$\begin{aligned} \langle x^2 \rangle &= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hbar \coth\left(\frac{1}{2}\beta\hbar\omega\right) \tilde{\chi}_x''(\omega) \\ &= \frac{\hbar}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{(\omega_a^2 - \omega_b^2)^2}{(\Omega_x^2 - \omega^2)^2} \frac{\gamma\Gamma^2\omega \coth\left(\frac{1}{2}\beta\hbar\omega\right)}{\xi^2\Gamma^2 + (\xi + \gamma\Gamma)^2\omega^2} \end{aligned} \quad (46)$$

and the corresponding momentum p_x

$$\langle p_x^2 \rangle = \frac{\hbar}{2\pi} \mu^2 \int_{-\infty}^{\infty} d\omega \frac{(\omega_a^2 - \omega_b^2)^2}{(\Omega_x^2 - \omega^2)^2} \frac{\gamma\Gamma^2\omega^3 \coth\left(\frac{1}{2}\beta\hbar\omega\right)}{\xi^2\Gamma^2 + (\xi + \gamma\Gamma)^2\omega^2}. \quad (47)$$

The stationary correlation $\langle xR \rangle$ is obtained by transforming on normal coordinates $y = \zeta x + R$, $z = x + \vartheta R$. Because of $\langle yz \rangle = 0$ in the stationary state one receives

$$\langle xR \rangle = \frac{\zeta \langle x^2 \rangle + \vartheta \langle R^2 \rangle}{1 + \zeta\vartheta} \quad (48)$$

where

$$\begin{aligned} \zeta &= -\frac{\mu(\omega_a^2 - \omega_b^2)}{M\Omega_-^2 - (m_b\omega_a^2 + m_a\omega_b^2 + M/\mu D)} \\ \vartheta &= -\frac{M(\omega_a^2 - \omega_b^2)}{M\Omega_+^2 - (m_a\omega_a^2 + m_b\omega_b^2)} \end{aligned} \quad (49)$$

and Ω_{\pm} are the normal frequency of system (24) with H_{AB} given by (25)

$$\Omega_{\pm}^2 = \frac{1}{2} \left(\omega_a^2 + \omega_b^2 + \frac{D}{\mu} \right) \pm \frac{1}{2} \sqrt{\left(\omega_a^2 + \omega_b^2 + \frac{D}{\mu} \right)^2 - 4D \left(\frac{\omega_a^2}{m_b} + \frac{\omega_b^2}{m_a} \right) - 4\omega_a^2\omega_b^2}. \quad (50)$$

Further correlations, such as $\langle RP_R \rangle$, $\langle xp_x \rangle$, $\langle Rp_x \rangle$, ... are zero in the stationary state.

3.5. Thermodynamic of adiabatic changes

The stationary Gaussian state of the subsystem is completely characterized by the correlations (41), (45)–(48). The internal energy again is defined as the stationary mean value of the systems Hamiltonian (24):

$$U_{S'} = \frac{1}{2M} \langle P_R^2 \rangle + \frac{1}{2\mu} \langle p_x^2 \rangle + \frac{1}{2} \mu \Omega_x^2 \langle x^2 \rangle + \frac{1}{2} M \Omega_R^2 \langle R^2 \rangle + \mu (\omega_a^2 - \omega_b^2) \langle xR \rangle. \quad (51)$$

In the case of identical oscillators ($m_{a,b} = M/2$, $\omega_{a,b} = \omega$) the internal energy $U_{S'}$ turns into

$$U_{S'} = \frac{1}{2M} \langle P_R^2 \rangle + \frac{1}{2} M \omega^2 \langle R^2 \rangle + \frac{1}{2} \hbar \Omega_\mu \coth \left(\frac{1}{2} \beta \hbar \Omega_\mu \right), \quad (52)$$

where $\langle P_R^2 \rangle$ and $\langle R^2 \rangle$ are given by the moments defined in equations (7) and (8) with oscillator parameters M and ω . We can apply the weak coupling limit to the (free) oscillation of the relative coordinate so that the values $\langle x^2 \rangle$ and $\langle p_x^2 \rangle$ are determined by the quantum Gibbs distribution of an uncoupled oscillator with mass μ and frequency $\Omega_\mu = \sqrt{\omega^2 + D/\mu}$. The motion of R is described by equation (40) and leads to the stationary variances given by (7) and (8).

In this case of identical oscillators the von Neumann entropy $S(\rho_{S'})$ of the system $H_{S'}$ can be expressed as sum of the entropy of the centre of mass coordinate S_R and the entropy of the relative coordinate S_x :

$$S(\rho_{S'}) = S_x + S_R, \quad (53)$$

where S_R and S_x are defined similar to equation (10) with the phase space volumes $v_x = \sqrt{\langle x^2 \rangle \langle p_x^2 \rangle} / \hbar$ and $v_R = \sqrt{\langle R^2 \rangle \langle P_R^2 \rangle} / \hbar$. The exchange of heat δQ and the change in entropy $dS(\rho_{S'})$ are defined equivalent to equations (17) and (23) by $Q = \text{Tr}[H_{S'} d\rho_{S'}]$ and $dS = -\text{Tr}[d\rho_{S'} \ln \rho_{S'}]$.

We now want to study deviations from the Clausius inequality in the case of identical oscillators. Regarding variation of the mass M the Clausius inequality reads

$$\delta Q_M \leq T dS_M. \quad (54)$$

With regard to an information theoretical viewpoint, we use again the statistical entropy instead of the thermodynamic entropy S_{th} for which the Clausius equality—by definition—is fulfilled for quasi-static processes.

In the weak-coupling case of a single harmonic oscillator with mass M , entropy and heat are not affected by adiabatic variations of the mass: $\delta Q_M = T dS_M = 0$. This is different in the case of two coupled oscillators weakly interacting with the bath, where the additional coupling parameter D leads to an increase of δQ_M and $T dS_M$ with rising temperature. Nevertheless for $\gamma \rightarrow 0$ the equality $\delta Q_M = T dS_M$ holds for all values of T and D . Furthermore, in this weak coupling approximation one has $\delta Q_M \geq 0$ and $dS_M \geq 0$ for all T and D .

The impact of a non-zero system–bath coupling γ can be studied from figure 6(a): the exchanged amount of heat δQ_M is increased at a given bath temperature T , whereas the term $T dS_M$ is reduced. Since the product $T dS_M$ becomes negative at low temperature, changes in heat and entropy have opposite signs. This effect is more pronounced if the coupling γ rises. For $kT \gg \hbar\omega$ the two terms become equal.

If the coupling D between the oscillators is reduced ($D \rightarrow 0$), the system behaves like a single Brownian particle as could be supposed by comparing the dashed curves in figure 6(a) to figure 2. For $D \rightarrow \infty$ the behaviour is the same. This is shown by figure 6(b) which gives the D -dependence of δQ_M and $T dS_M$ at a certain temperature T and coupling γ . One can recognize that the values of δQ_M for $D \rightarrow \infty$ and $D \rightarrow 0$ are equal (as well as the

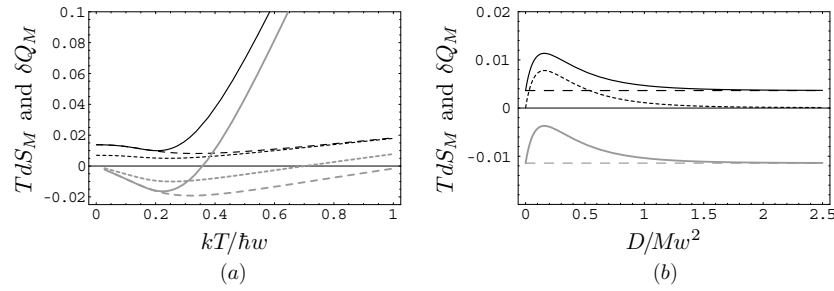


Figure 6. Changes in heat δQ_M and entropy-term $T dS_M$ due to variations of the bath temperature T (a) and the oscillator coupling D (b). The oscillator parameters are $\omega = \omega_{a,b} = 1$ and $M = 2m_{a,b} = 1$. The cutoff-frequency is set to $\Gamma = 10$ and $\hbar = 1$. (Compare to figure 2.) (a) δQ_M (dark lines) and $T dS_M$ (grey lines) versus T for various combinations of parameters ($D; \gamma$). Solid lines: (0.5; 1), Dashed lines: (0.01; 1). Dotted lines: (0.01; 0.5). (b) δQ_M (dark line) and $T dS_M$ (grey line) versus coupling D at bath temperature $T = 0.25\hbar\omega/k$. System–bath coupling $\gamma = 0.5M\omega^2/\Gamma$ compared to weak coupling limit (narrow dashed line).

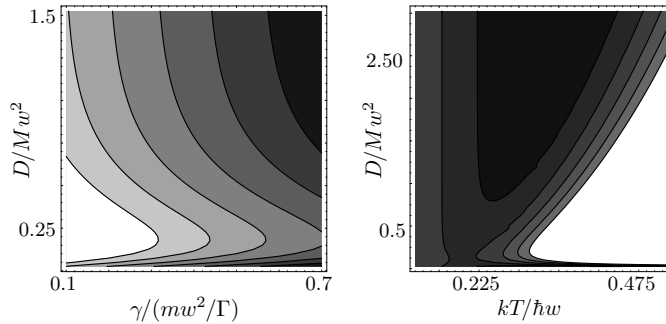


Figure 7. Contour plots in steps of $T dS_M = 0.0025$. White regions give those combinations of parameters where $T dS_M \geq 0$. On the left: bath temperature $T = 0.25\hbar\omega/k$. On the right: coupling $\gamma = 0.5M\omega^2/\Gamma$. Further parameters are chosen as in figure 6.

values for $T dS_M$) and correspond with the results for a single Brownian oscillator. For higher temperature, depending on the chosen parameter values of oscillators (M, ω) and bath (γ, Γ), there may exist a range of D -values where the terms $T dS_M$ and δQ_M have equal signs. This is shown by figures 7(a) and (b).

4. Summary and conclusions

We have discussed the statistical thermodynamics of quantum Brownian motion of two coupled oscillators where only the centre of mass is coupled to a bath. This model can be interpreted as a Brownian particle with an internal degree of freedom. We investigated especially the strong coupling quantum regime. As in the case of single Brownian motion the quantum correlations between subsystem and bath lead to deviations from the canonical equilibrium thermodynamics.

With regard to continuous variable quantum computing we examined the relation between changes in the subsystems statistical entropy and the exchange of heat with the environment. We found that this relation deviates from the Clausius (in)equality at low temperatures due to the existing correlations between system and bath. Related results of former work [9–11]

were put into perspective. Concerning quantum information processing, the validity of the Landauer principle which is based on the Clausius inequality but deals with the statistical entropy seems indeed questionable—at least for open quantum systems which are non-weakly interacting with a low temperature environment.

Our open quantum system with an internal degree of freedom shows additional effects. The quantum Langevin equation which has been derived for a system of two coupled Brownian oscillators describes the evolution of the Heisenberg operators. The stationary moments of these operators characterize the reduced density matrix completely. This density matrix contains all the accessible information about the quantum state. The statistical entropy of this state is measured by the von Neumann entropy. Reducing this entropy by quasi-static parameter variations is equivalent to a decrease in the information which is gained by a measurement. In our model the direction of heat and entropy flow due to mass variations depends on the coupling strength between both the oscillators. Already at moderate temperatures the flow of heat and entropy occurs in the same direction, whereas in the model of single Brownian motion this is reached only in the high temperature and weak coupling limit, respectively. Therefore varying the coupling parameter offers the possibility of adjusting the ratio of heat exchange and change in the subsystems entropy.

Of course, the resulting changes in heat and entropy depend on the chosen interaction between the oscillators. As pointed out at the beginning of the third section, this coupling has to be selected carefully to ensure the positive definiteness of the total Hamiltonian. We have chosen a system–bath coupling to the centre of mass which fulfills this condition and which allows us to derive an analytical results. The relative motion is then an uncoupled internal degree of freedom. This interaction could also be understood as a model of two oscillators separately coupled to the bath including a modified self-interaction Hamiltonian. Therefore this model provides an adequate example for studying the influence of an additional degree of freedom.

Furthermore, in view of future applications in continuous variable computing it will also be of interest to study the dynamical properties of decoherence and correlations of the two-mode state as well as the interplay between the external and internal coupling.

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