Thermodynamic anomaly of the free damped quantum particle: the bath perspective

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Abstract. A possible definition of the specific heat of open quantum systems is based on the reduced partition function of the system. For a free damped quantum particle, it has been found that under certain conditions, this specific heat can become negative at low temperatures. In contrast to the conventional approaches focusing on the system degree of freedom, here we concentrate on the changes induced in the environment when the system is coupled to it. Our analysis is carried out for an Ohmic environment consisting of harmonic oscillators and allows to identify the mechanism by which the specific heat becomes negative. Furthermore, the formal condition for the occurrence of a negative specific heat is given a physical interpretation in terms of the total mass of bath oscillators and the system mass.

1 Introduction

The standard definition of the thermodynamic equilibrium quantities in a canonical ensemble relies on the assumption that the coupling between the system of interest and its thermal environment is arbitrarily weak. In the real world, this approximation never strictly holds and important deviations from the usual picture can be expected in particular for systems on the nanoscale. Beyond the study of effects of finite coupling to the environment on the thermodynamic properties of system, the more fundamental question arises of how to properly define quantities like an internal energy, a specific heat or an entropy in such a situation [1]. The last five years or so have seen considerable activities addressing this issue and related ones [2–19].

In the quantum regime, the thermodynamic equilibrium properties not only depend on the strength of the coupling to the environment. Even more importantly, it turns out that the very definition of these quantities is no longer unique [1]. As an example, we consider here the specific heat which for a damped quantum system can be defined in at least two different ways.

The first approach defines the internal energy of the system as expectation value of the system Hamiltonian taken with respect to the thermal ensemble of the coupled system. By the latter we mean here and in the following the coupled complex of system (S) and heat bath (B). Quantities related to the coupled system will be indicated by a subscript "S+B". Based on the definition of the internal energy just introduced, one obtains the associated specific heat by taking the derivative with respect to temperature. Obviously, in the absence of a coupling between system and bath, the specific heat defined in this way reduces to the standard specific heat of the system.

An alternative approach is based on the reduced partition function of the system defined as [20–22]

$$\mathcal{Z} = \frac{\mathcal{Z}_{\mathrm{S+B}}}{\mathcal{Z}_{\mathrm{B}}}. \tag{1}$$

In the absence of a coupling between the system and its environment, $\mathcal{Z}$ equals the partition function of the system. Even though we thus can consider $\mathcal{Z}$ to be a quantity associated with the system, we omit a subscript "S" in order to emphasize the fact that $\mathcal{Z}$ also takes into account the coupling between system and bath. Here, we will employ the ratio (1) only in the context of equilibrium thermodynamics, but recently it has also been used in the discussion of fluctuation theorems for open quantum systems in nonequilibrium situations [7,8,17].

The partition function (1) can be used to define thermodynamic equilibrium quantities by means of the standard relations valid in the absence of a coupling between the system and its environment. We thus obtain a second expression for the specific heat reading

$$C = k_{\mathrm{B}}\beta^2 \frac{\partial^2 \ln(\mathcal{Z})}{\partial \beta^2}, \tag{2}$$

where $\beta = 1/k_{\mathrm{B}}T$. In the absence of a coupling between system and bath, this definition of a specific heat also reduces to the usual definition and thus agrees with our first definition in the limit of vanishing coupling. Again we omit a subscript "S" to underline the dependence of the specific heat on the coupling, but we do so also in view of the interpretation (3) given below which emphasizes the role of the heat bath.

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It should be noted that, in general, the two specific heats just defined differ for finite coupling to the environment already in the leading high-temperature corrections to the classical specific heat. For a bilinear coupling between system and bath, the classical specific heats still agree [1,3] while this need no longer be the case for anharmonic couplings [9].

The difference between the two approaches is most spectacular in situations where the specific heat (2) becomes negative in contrast to the positive specific heat based on the expectation value of the system Hamiltonian [1,3]. In the following, we exclusively consider the specific heat obtained from the reduced partition function so that the symbol C will always refer to (2).

Although the reduced partition function (1) appears to be a rather formal starting point, the quantities derived from it have a clear physical meaning. Due to the fact that thermodynamic equilibrium properties depend on the logarithm of the partition function, these quantities in the presence of a finite coupling to a heat bath possess a natural interpretation in terms of the difference between the quantity evaluated for the coupled system and the quantity evaluated for the bath alone [6,23]. For the specific heat (2), we thus have

$$C = C_{\mathrm{S+B}} - C_{\mathrm{B}}. \tag{3}$$

The two quantities involved in this difference, $C_{\mathrm{S+B}}$ and C_{B}, constitute measurable quantities. Even though one may invoke a superbath imposing the temperature on the bath and on the coupled system, the coupling to the superbath may be assumed to be negligible. Therefore, we are certainly allowed to employ the standard thermodynamic definition for the quantities on the right-hand side of (3). C thus is not a specific heat in the proper sense but it is the natural replacement for a specific heat in a situation where the system of interest is coupled with non-negligible strength to an environment. The approach discussed here was recently employed in the analysis of thermal data obtained for a metal phosphate compound [24]. For the sake of simplicity, we will occasionally refer to C as specific heat of the system. In doing so, we should however keep in mind the preceding discussion.

With the above interpretation of the specific heat (2), negative values should not give rise to concerns with respect to thermodynamic instabilities. In fact, there is no reason why the difference of two positive quantities should be positive. The situation considered here should therefore be distinguished from the negative specific heat appearing e.g. in self-gravitating systems within a microcanonical description [25–27].

Apart from the free damped quantum particle which we focus on in this paper, negative entropies and/or specific heats have been discussed e.g. in the context of the Casimir effect [28–35], Kondo systems [36,37], XY spin chains [12], two-level fluctuators [8] and energy transport in proteins [38]. While for a single harmonic oscillator coupled to an Ohmic bath [1,3] or to a single bath oscillator [6] the specific heat was found to be positive, this is not necessarily the case if a system consisting of several harmonic oscillators is coupled to a finite environment [19].

In the treatment of dissipative systems, the system degree of freedom usually is in the focus of interest. On the other hand, the difference (3) of specific heats, even though conceptually associated with the system degree of freedom, provides the motivation to take a different point of view, namely the one of the environment. The question answered by the specific heat (3) really is: How does the specific heat of the environment change when a system degree of freedom is coupled to it?

In the following we shall address this question by studying the change in the spectral density of the environment when a system degree of freedom is coupled to it. In Section 2 we briefly introduce the model for the damped free quantum particle which will allow us to obtain the change in the spectral density of the environment in Section 3. From these results, we derive in Section 4 the thermodynamic properties of the system in the sense explained above. We will show that these results can indeed be expressed in terms of properties of the system degree of freedom. In Section 5 we will give a physical interpretation of the condition under which the specific heat (3) of the free damped quantum particle becomes negative. Finally, we present our conclusions in Section 6.

2 Free particle coupled to harmonic oscillators

As our model for the study of the appearance of a negative specific heat we consider a particle of mass M which is bilinearly coupled to a set of harmonic oscillators constituting the environment. The corresponding Hamiltonian is given by

$$H = \frac{P^2}{2M} + \sum_{n=1}^{\infty} \left[\frac{p_n^2}{2m_n} + \frac{m_n \omega_n^2}{2} \left(Q - x_n\right)^2 \right]. \tag{4}$$

The sum describes the environmental oscillators of mass m_n and frequency ω_n, the bilinear coupling and a potential renormalization. The latter ensures that the effective equation of motion of the system position Q corresponds indeed to the Langevin equation of a free damped particle taking the form

$$M\ddot{Q} + M \int^t ds \gamma(t-s) \dot{Q}(s) = \xi(t). \tag{5}$$

Below, we will relate the damping kernel $\gamma(t)$ to the properties of the environment. The properties of the noise term $\xi(t)$ are irrelevant for our discussion so that we refer the reader to the literature for details [20–22,39]. The coupling constant of the bilinear term in x_n and Q in (4) has been expressed in terms of the masses and frequencies of the environmental oscillators which is possible without loss of generality [40,41]. The Hamiltonian is manifestly invariant under spatial translations of all degrees of freedom, confirming once more that we are treating a free damped particle.

In our discussion, two spectral densities play a key role and it is important to carefully distinguish them. We refer to the first quantity as spectral density of eigenmodes ρ.

This quantity is defined in terms of the eigenfrequencies of the quadratic Hamiltonian (4). For the bath alone, we have the spectral density of eigenmodes

$$\rho_{\mathrm{B}}(\omega) = \sum_{n=1}^{\infty} \delta\left(\omega - \omega_n\right). \tag{6}$$

Correspondingly, we define a spectral density of eigenmodes $\rho_{\mathrm{S+B}}(\omega)$ in which the frequencies ω_n appearing in (6) are replaced by the eigenfrequencies of the coupled system described by (4). The difference $\rho_{\mathrm{S+B}} - \rho_B$ will form the basis for the derivation of various thermodynamic quantities in Section 4.

In addition, in order to characterize the properties of the heat bath and its coupling to the system, a quantity commonly referred to as spectral density of bath oscillators [42]

$$J(\omega) = \frac{\pi}{2} \sum_{n=1}^{\infty} m_n \omega_n^3 \delta\left(\omega - \omega_n\right) \tag{7}$$

is introduced. In contrast to the spectral density of eigenmodes (6) in the absence of coupling, the spectral density of bath oscillators (7) not only depends on the frequencies of the bath oscillators but also on their masses. For our choice of coupling constants (cf. discussion below (5)) this is tantamount to saying that (7) depends also on the coupling constants between system degree of freedom and bath oscillators. $J(\omega)$ contains all information about the heat bath required to describe the properties of the damped quantum system.

Although it is not obvious, it will turn out that even within our bath-centered approach all quantities of interest will eventually be expressible in terms of the spectral density of bath oscillators (7). This already indicates that even though we take the point of view of the environment, we will learn something about the properties of the system.

In our results, it will be natural to express the dependence on $J(\omega)$ in terms of the Laplace transform of the damping kernel $\gamma(t)$ appearing in (5). The two quantities are related by means of [20–22]

$$\hat{\gamma}(z) = \frac{2}{\pi M} \int_0^{\infty} d\omega \frac{J(\omega)}{\omega} \frac{z}{\omega^2 + z^2}. \tag{8}$$

For the purpose of our discussion, we will restrict ourselves to so-called Ohmic damping which implies that the spectral density of bath oscillators is continuous and linear in the frequency at least for small frequencies. At high frequencies, the spectral density of bath oscillators will typically be suppressed with respect to this linear behavior. To be specific, in cases where such a cutoff is of relevance, we will employ the so-called Drude model with

$$J_{\mathrm{D}}(\omega) = M\gamma\omega \frac{\omega_{\mathrm{D}}^2}{\omega^2 + \omega_{\mathrm{D}}^2}. \tag{9}$$

Here, the low-frequency behavior is characterized by the damping constant γ and ω_{D} is the cutoff frequency. The corresponding Laplace transform of the damping kernel reads

$$\hat{\gamma}_{\mathrm{D}}(z) = \frac{\gamma\omega_{\mathrm{D}}}{z + \omega_{\mathrm{D}}}. \tag{10}$$

Because the damping constant γ combines with the inverse temperature β to form a dimensionless quantity $\hbar\beta\gamma$ and thus merely sets the temperature scale, the cutoff frequency ω_{D} will be an important parameter determining the properties of the damped free particle.

3 Change in the spectral density of bath oscillators

In our environment-centered approach, we start out with a set of uncoupled environmental oscillators with frequencies ω_n. In addition, we have one system degree of freedom corresponding to an undamped free particle. We now couple the environmental oscillators to the free particle as prescribed by the Hamiltonian (4). As discussed in the previous section, the system and environment together are translationally invariant.

In the spirit of Ullersma's analysis of the damped harmonic oscillator [43] we determine the eigenmode spectrum of the free particle coupled to its environment. Diagonalizing the Hamiltonian, we recover a zero-mode which replaces the zero-mode corresponding to the uncoupled free particle. We thus concentrate on the non-zero frequencies which due to the coupling are shifted with respect to the original environmental oscillator frequencies. The new frequencies are obtained as solutions Ω of the equation

$$\sum_{n=1}^{\infty} \frac{m_n \omega_n^2}{\Omega^2 - \omega_n^2} = M. \tag{11}$$

For the following intermediate steps it is convenient to explicitly consider an equidistant set of discrete frequencies $\omega_n = n\Delta$ with $n = 1, 2, \ldots$ for the environmental oscillators. Later, we will take the limit of vanishing frequency spacing Δ to recover a continuous spectral density of environmental oscillators. In view of (7), we have the relation

$$\int_0^{\infty} d\omega\, J(\omega) f(\omega) = \frac{\pi}{2} \sum_{n=1}^{\infty} m_n \omega_n^3 f(n\Delta) \tag{12}$$

which holds for any function f for which the integral and the sum exist. If, on the other hand, we replace the integral on the left-hand side by a Riemann sum with step width Δ, we can express the masses m_n of the environmental oscillators in terms of the continuous spectral density of bath oscillators $J(\omega)$ according to

$$m_n = \frac{2}{\pi} \frac{J(n\Delta)}{(n\Delta)^3} \Delta. \tag{13}$$

The eigenfrequency condition (11) thus becomes

$$\sum_{n=1}^{\infty} \frac{J(n\Delta)}{n\left[\Omega^2 - (n\Delta)^2\right]} = \frac{\pi}{2} M. \tag{14}$$

In order to treat frequencies Ω close to an unperturbed environmental frequency $n\Delta$ correctly, we rewrite this condition as

$$\Delta\frac{J(\Omega)}{\Omega}\sum_{n=1}^{\infty}\frac{1}{\Omega^2-(n\Delta)^2}+\Delta\sum_{n=1}^{\infty}\frac{1}{\Omega^2-(n\Delta)^2}\times\left(\frac{J(n\Delta)}{n\Delta}-\frac{J(\Omega)}{\Omega}\right)=\frac{\pi}{2}M. \quad (15)$$

Performing the first sum exactly and replacing the second sum by an integral, we finally obtain

$$\cot\left(\frac{\pi\Omega}{\Delta}\right)-\frac{\Delta}{\pi\Omega}=g(\Omega) \quad (16)$$

with

$$g(\Omega)=\frac{M\Omega}{J(\Omega)}\left(\Omega+\mathrm{Im}\hat{\gamma}(\mathrm{i}\Omega)\right). \quad (17)$$

The coupling of the environment to the system degree of freedom modifies the original spacing Δ between adjacent environmental eigenfrequencies yielding a new spacing $\Delta+\epsilon$. The correction ϵ depends on the spectral bath density via the function g defined in (17) and can be shown to be of order Δ^2. Exploiting the latter fact and making use of the addition theorem of the cotangent, one determines ϵ from (16). For the change in the spectral density of eigenmodes, one thus finds as a central result

$$\rho_{\mathrm{S+B}}(\Omega)-\rho_{\mathrm{B}}(\Omega)=\frac{1}{\Delta+\epsilon(\Omega)}-\frac{1}{\Delta}=\frac{1}{\pi}\frac{g'(\Omega)}{1+g(\Omega)^2}. \quad (18)$$

Here, the prime denotes a derivative with respect to the argument.

Further insight into the change of the spectral density of eigenmodes can be obtained by specifying the properties of the bath. We choose a Drude model with the spectral density of environmental oscillators given by (9) and a Laplace transform of the damping kernel as specified in (10). From (18) one obtains

$$\rho_{\mathrm{S+B}}-\rho_{\mathrm{B}}=\frac{1}{\pi}\left[\frac{\omega_1}{\Omega^2+\omega_1^2}+\frac{\omega_2}{\Omega^2+\omega_2^2}-\frac{\omega_{\mathrm{D}}}{\Omega^2+\omega_{\mathrm{D}}^2}\right] \quad (19)$$

where

$$\omega_{1,2}=\frac{\omega_{\mathrm{D}}}{2}\left(1\pm\sqrt{1-\frac{4\gamma}{\omega_{\mathrm{D}}}}\right) \quad (20)$$

and ω_{D} is the Drude frequency providing the high-frequency cutoff. These three frequencies are the eigenfrequencies associated with the deterministic version of the Langevin equation (5) for a Drude damping kernel [3].

The change in the spectral density of eigenmodes is shown as thick solid line in Figure 1 for various values of $\omega_{\mathrm{D}}/\gamma$. The dotted lines represent the Lorentzian contributions according to (19). For the sake of clarity, they are depicted also in the grey regions of negative frequencies which are irrelevant for the spectral density of eigenmodes. As long as the cutoff frequency is sufficiently high,

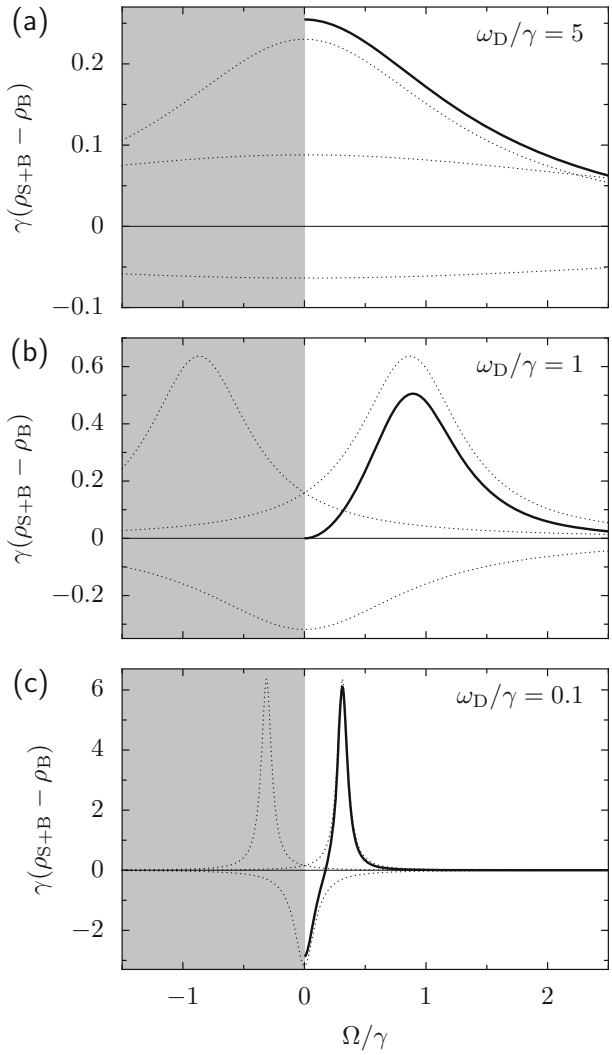

Fig. 1. The change in the spectral density of eigenmodes $\rho_{\mathrm{S+B}}-\rho_{\mathrm{B}}$ induced by the coupling to the system degree of freedom is depicted as thick solid line for Drude damping with (a) $\omega_{\mathrm{D}}/\gamma=5$, (b) $\omega_{\mathrm{D}}/\gamma=1$, and (c) $\omega_{\mathrm{D}}/\gamma=0.1$. The contributions of the three Lorentzians according to (19) are represented as dotted lines. Only the white regions of positive frequencies are of relevance for the spectral density of eigenmodes.

$\omega_{\mathrm{D}}>4\gamma$, (19) describes the sum of three Lorentzians centered at zero frequency. An example for this situation is given in Figure 1a. Coupling the system degree of freedom to the environment then leads to an increase of the spectral density at zero frequency by $(\omega_{\mathrm{D}}-\gamma)/\pi\gamma\omega_{\mathrm{D}}$. For smaller cutoff frequencies, if $\omega_{\mathrm{D}}<4\gamma$ like in the cases depicted in Figures 1b and 1c, the two frequencies (20) become complex and the first two Lorentzians in (19) are now centered at nonzero frequencies. As a consequence, the suppressing effect of the third Lorentzian on the spectral density of eigenmodes becomes relevant. For $\omega_{\mathrm{D}}<\gamma$ one finds in fact a suppression of the spectral density at zero frequency as is shown in Figure 1c for $\omega_{\mathrm{D}}/\gamma=0.1$. It is this suppression which leads to the negative specific heat as we will discuss in the following section.

Before doing so, we would like to emphasize that although the change in the spectral density of eigenmodes obtained in this section is mainly related to properties of the environment, the results are determined by properties of the damped system. In the general result (18) the environment appears only through the spectral density of bath oscillators (7) which is sufficient to provide a reduced description of the damped system. In the specific case of Drude damping, the three eigenfrequencies of the damped system turn out to be sufficient for the complete description of the change in the spectral density of eigenfrequencies.

Despite being closely related to the properties of the damped system, the change of the spectral density of eigenmodes discussed here should not be confused with the density of states which can be obtained from the reduced partition function (1) by its inverse Laplace transform [44]. Because the density of states defined in such a way is linearly related to the reduced partition function, it cannot be interpreted as a difference of a property of the coupled system on the one hand and the heat bath on the other hand [3].

4 Thermodynamic properties of the system

The change of the specific heat (2) due to the coupling of the system degree of freedom to the environment can be obtained from the change (18) of the spectral density of eigenfrequencies as

$$C = \int_0^\infty d\omega \left(\rho_{\mathrm{S+B}}(\omega) - \rho_{\mathrm{B}}(\omega)\right) C_{\mathrm{ho}}(\omega) \tag{21}$$

where

$$C_{\mathrm{ho}}(\omega) = k_{\mathrm{B}} \left(\frac{\hbar\beta\omega}{2\sinh\left(\hbar\beta\omega/2\right)}\right)^2 \tag{22}$$

is the specific heat of a harmonic oscillator with frequency ω. Equation (21) implies a negative specific heat C at low temperatures if the spectral density of eigenmodes is suppressed for small frequencies due to the coupling of the system degree of freedom to the bath.

Assuming Ohmic damping, i.e. $J(\omega) \sim \omega$ at low frequencies, we can obtain the specific heat at low temperatures by inserting the change in the spectral density of eigenmodes (18) into (21). Together with (17) one finds

$$\frac{C}{k_{\mathrm{B}}} = \frac{\pi}{3}\frac{1+\hat{\gamma}'(0)}{\hat{\gamma}(0)}\frac{k_{\mathrm{B}}T}{\hbar} + \mathcal{O}\left(T^3\right) \tag{23}$$

in agreement with the findings of reference [3]. For

$$\hat{\gamma}'(0) < -1, \tag{24}$$

we thus obtain a negative specific heat at low temperatures. A physical interpretation of this result will be given in Section 5 below.

More explicit results can be derived for the case of Drude damping. There, the integral in (21) can be evaluated analytically and one finds

$$\frac{C}{k_{\mathrm{B}}} = \left(\frac{\hbar\beta\omega_1}{2\pi}\right)^2 \psi'\left(\frac{\hbar\beta\omega_1}{2\pi}\right) + \left(\frac{\hbar\beta\omega_2}{2\pi}\right)^2 \psi'\left(\frac{\hbar\beta\omega_2}{2\pi}\right) - \left(\frac{\hbar\beta\omega_{\mathrm{D}}}{2\pi}\right)^2 \psi'\left(\frac{\hbar\beta\omega_{\mathrm{D}}}{2\pi}\right) - \frac{1}{2}, \tag{25}$$

where $\psi'(z)$ denotes the digamma function. This result is in agreement with the expression obtained by proceeding according to the point of view of the system [3] and starting with the reduced partition function (1). The two approaches therefore are equivalent, but the approach presented here gives additional insight through the change in the spectral density of eigenvalues (18).

Instead of obtaining the internal energy and the specific heat from the reduced partition function, we can use our result (25) for the specific heat to obtain the other two quantities. In the limit of vanishing coupling to the heat bath, the internal energy U is related to the specific heat C by means of

$$C = -\beta^2 \frac{\partial U}{\partial \beta}. \tag{26}$$

In view of (3) we thus obtain from (25) by means of an integration the difference of internal energies induced by the system-bath coupling

$$\begin{aligned} U &= U_{\mathrm{S+B}} - U_{\mathrm{B}} \\ &= -\frac{\hbar\omega_1}{2\pi}\psi\left(\frac{\hbar\beta\omega_1}{2\pi}\right) - \frac{\hbar\omega_2}{2\pi}\psi\left(\frac{\hbar\beta\omega_2}{2\pi}\right) \\ &\quad + \frac{\hbar\omega_{\mathrm{D}}}{2\pi}\psi\left(\frac{\hbar\beta\omega_{\mathrm{D}}}{2\pi}\right) - \frac{1}{2\beta}. \end{aligned} \tag{27}$$

This result is only determined up to a constant of integration which, by comparison with the known result [3], turns out to vanish. In particular, at zero temperature, we thus find

$$U_0 = \frac{\hbar\omega_1}{2\pi}\ln\left(\frac{\omega_{\mathrm{D}}}{\omega_1}\right) + \frac{\hbar\omega_2}{2\pi}\ln\left(\frac{\omega_{\mathrm{D}}}{\omega_2}\right). \tag{28}$$

Furthermore, by means of the relation between the internal energy U and the partition function $\mathcal{Z}$

$$U = -\frac{d}{d\beta}\ln(\mathcal{Z}) \tag{29}$$

one reproduces the correct temperature dependence of the ratio of the partition functions of system and bath on the one hand and bath alone on the other hand [3]

$$\mathcal{Z} \sim \frac{1}{\beta^{1/2}} \frac{\Gamma\left(1+\frac{\hbar\beta\omega_1}{2\pi}\right)\Gamma\left(1+\frac{\hbar\beta\omega_2}{2\pi}\right)}{\Gamma\left(1+\frac{\hbar\beta\omega_{\mathrm{D}}}{2\pi}\right)}. \tag{30}$$

This result leaves a prefactor undetermined which for the thermodynamical equilibrium quantities is irrelevant. The temperature dependence, however, agrees with the result obtained by means of other techniques, e.g. the path integral approach.

5 The missing mass of bath oscillators

In the previous section, we have found that a negative specific heat occurs provided the condition (24) is satisfied. This rather formal condition can be given a physical meaning. In order to avoid an infrared divergence in the limit of vanishing argument z, we first express the Laplace transform of the damping kernel (8) as

$$\hat{\gamma}(z) = \hat{\gamma}(0) + \frac{2}{\pi}\int_0^\infty d\omega \left(\frac{J(\omega)}{M\omega} - \hat{\gamma}(0)\right)\frac{z}{\omega^2+z^2}. \quad (31)$$

With (24) and (31) the condition for a negative specific heat then becomes

$$\frac{2}{\pi}\int_0^\infty d\omega \frac{M\hat{\gamma}(0)\omega - J(\omega)}{\omega^3} > M. \quad (32)$$

Observing that according to (7) the total mass of the bath oscillators can be obtained from the spectral density of bath oscillators $J(\omega)$ as [40,41]

$$\mathcal{M} = \sum_{n=1}^{\infty} m_n = \frac{2}{\pi}\int_0^\infty d\omega \frac{J(\omega)}{\omega^3} \quad (33)$$

the condition (32) can be expressed as

$$\Delta\mathcal{M}_{\mathrm{B}} > M. \quad (34)$$

Here, $\Delta\mathcal{M}_{\mathrm{B}}$ is defined by the left-hand side of (32) and refers to the total mass of oscillators which are missing in the actual bath with respect to a strictly Ohmic reference bath where $J(\omega) = M\hat{\gamma}(0)\omega$ for all frequencies. We note that while due to the infrared divergence mentioned above the total mass is infinite for both baths, the difference $\Delta\mathcal{M}_{\mathrm{B}}$ is finite.

We thus arrive at the following interpretation. Coupling a system degree of freedom of zero frequency to the bath oscillators tends to shift the frequencies of the latter to larger values. However, for a strictly Ohmic environment, i.e. in the absence of a finite cutoff in the spectral density of bath oscillators, the ensemble of bath oscillators resists a reduction of the spectral density of eigenmodes at low frequencies. A suppression only becomes possible if one eliminates a number of bath oscillator with a total mass at least as large as the mass associated with the system degree of freedom. The bath then is no longer able to resist the "pressure" of the system degree of freedom pushing the eigenmodes to higher frequencies.

6 Conclusions

In order to achieve a better understanding of the unusual thermodynamic properties of a free Brownian quantum particle, we have employed a somewhat uncommon approach to the analysis of dissipative quantum systems by taking the perspective of the environment. This approach is, however, quite natural if thermodynamic quantities are defined in terms of a reduced partition function of the system because they actually refer to the change of these quantities when the system degree of freedom is coupled to the heat bath.

We have analyzed the modification of the bath spectrum induced by the coupling to the system degree of freedom. Interestingly, the spectral density of bath oscillators is sufficient to describe the change in the bath spectrum. As a consequence the latter depends only on properties of the damped system as has been exemplified by means of a Drude-type damping. Starting from the change in the bath spectrum, expressions for the specific heat, the internal energy and the reduced partition function obtained previously from a system-based approach have been reproduced.

The low-temperature behavior of the specific heat of the free damped particle is determined by the shift of the low-frequency environmental oscillators induced by the coupling to the system degree of freedom. If the ratio of cutoff frequency and damping strength is sufficiently small, the system degree of freedom succeeds in suppressing the spectral density of eigenmodes at low frequencies by shifting the bath modes to higher frequencies. As a result, at low temperatures the specific heat of the heat bath is lowered if the system degree of freedom is attached. In contrast, for larger cutoff frequencies, the high-frequency oscillators of the environment act against the tendency of the system to shift the bath modes to higher frequencies. Then, the specific heat remains positive for all frequencies.

The condition to be satisfied by the environment to allow for a negative specific heat at low temperatures has been shown to have a physical interpretation. The anomaly in the specific heat appears if the mass missing in the environment with respect to a strictly Ohmic reference bath exceeds the mass associated with the system degree of freedom. Then, the bath oscillators are not strong enough to resist the zero-frequency degree of freedom which, when coupled to the environment, tends to increase their frequencies. Otherwise the spectrum of bath modes is sufficiently stiff to prevent the spectral density of eigenmodes from being reduced.

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