Quantum Theory of the Damped Harmonic Oscillator

Hermann Grabert and Ulrich Weiss
Institut für Theoretische Physik, Universität Stuttgart,
Federal Republic of Germany

Peter Talkner
Institut für Physik, Universität Basel, Switzerland

A phenomenological stochastic modelling of the process of thermal and quantal fluctuations of a damped harmonic oscillator is presented. The divergence of the momentum dispersion associated with the Markovian limit is removed by a Drude regularization. The variances of position and momentum are evaluated in closed form at arbitrary temperature and for arbitrary damping. Properties of real and imaginary time correlation functions are discussed, and a spectral decomposition of the equilibrium density matrix is given.

1. Introduction

There has been renewed interest recently in the theory of quantum mechanical stochastic processes. About two decades ago, the problem to describe damping of a quantum system has been investigated in detail, mainly in the context of quantum optics and spin relaxation theory. The results of these studies have been presented in various books and review articles [1–4]. However, apart from formal work, most of the results were restricted to very weakly damped systems, where the relaxation times are long compared with the periods of the reversible motion and also long compared with the "thermal time" $\hbar/k_B T$. Therefore, these methods cannot be used to treat systems at low temperature.

On the other hand, progress in cryogenic engineering has motivated recent work on the influence of damping on low temperature quantum systems [5, 6]. Numerous further articles are quoted in the paper by Caldeira and Leggett [6] which also may serve as a general introduction into the field. Most of these approaches originate from the functional integral techniques developed by Feynman [7, 8]. While these sophisticated methods are very powerful indeed, several interesting properties of quantum stochastic processes at low temperature can be obtained by extending the phenomenological methods familiar from the theory of classical stochastic processes [9] to the quantum regime.

In this article, we investigate the quantum dynamics of a damped harmonic oscillator. A detailed review of previous work on this problem has been given by Dekker [10]. Most of the phenomenological models are in contradiction with general principles, and those derived from microscopic models are based on approximations that cannot be made at arbitrary temperature. In Sect. 2 we present a consistent stochastic modelling of the process of thermal and quantal fluctuation using phenomenological considerations. The resulting position autocorrelation function of the damped harmonic oscillator is discussed in Sect. 3.

In the theory of classical Markov processes it is well known that higher order sum rules are divergent. In the quantal case, such a divergence is already met with the sum rule for the momentum dispersion [6]. In Sect. 4 we study in detail a regularization of this divergence. This is necessary in order to have a well-defined equilibrium state, the properties of which are discussed in Sect. 5. It is shown that the ground state of a damped oscillator is not a pure state. Finally, in Sect. 6 we present our conclusions.

2. Stochastic Modelling

For classical systems whose deterministic irreversible equations of motion are known, a stochastic theory including thermal fluctuations can be formulated on the basis of phenomenological considerations [9, 11]. This stochastic modelling of classical irreversible processes is possible because of the intimate connection between thermal fluctuations and dissipation [12, 13]. For quantum systems a general method for the formulation of the stochastic theory has only been given in the limit of a weak damping [1-4]. In this case one has

$$\gamma \ll \omega_0 \tag{2.1}$$

and

$$\hbar\gamma \ll k_B T \tag{2.2}$$

where γ is a typical damping constant (inverse relaxation time) and ω_0 is a typical frequency of the reversible motion. These inequalities do not exclude quantum phenomena since we may have $\hbar\omega_0 > k_B T$. However, they do exclude an application of the approach to low temperature phenomena. If the inequality (2.2) ceases to hold, there arises a complicated interplay between thermal and quantal fluctuations which seems to require a statistical-mechanical treatment in general.

On the other hand, a damped harmonic oscillator is a system simple enough to enable a study of its quantum-mechanical stochastic process by using only phenomenological considerations for the whole range of the dimensionless parameters

$$\kappa = \frac{\gamma}{2\omega_0} \tag{2.3}$$

and

$$\sigma = \frac{\hbar\omega_0}{k_B T}. \tag{2.4}$$

We base the stochastic modelling upon the following three principles:

(i) The mean values obey the classical equations of motion according to the *Ehrenfest theorem.*

(ii) The response functions and the equilibrium correlation functions are related by the *fluctuation-dissipation theorem* (FDT).

(iii) The stochastic process is a *stationary Gaussian process.*

While the first two principles are of general nature, the Gaussian assumption can only be made for linear systems with linear damping.

For a harmonic oscillator of mass M, coordinate q, and momentum p, which is damped by a frictional force $-\gamma p$, the classical equations of motions read

$$\dot{q} = \frac{1}{M} p \tag{2.5}$$

$$\dot{p} = -M\omega_0^2 q - \gamma p.$$

Thus, by virtue of Ehrenfest's theorem, we obtain for the average position $\langle q(t)\rangle$ of a damped quantum oscillator the equation of motion

$$\langle \ddot{q}(t)\rangle + \gamma\langle \dot{q}(t)\rangle + \omega_0^2\langle q(t)\rangle = \frac{1}{M} F(t) \tag{2.6}$$

where we have added an external force $F(t)$. The response of $\langle q(t)\rangle$ to this force is given by

$$\langle q(t)\rangle = \int_{-\infty}^{+\infty} ds\, \chi(t-s)\, F(s) \tag{2.7}$$

where

$$\chi(t) = \theta(t)\, \frac{1}{M\zeta}\, e^{-\frac{\gamma}{2}t} \sinh(\zeta t) \tag{2.8}$$

is the response function. Here $\theta(t)$ is the unit step function

$$\theta(t) = \begin{cases} 1 & \text{for } t>0 \\ 0 & \text{for } t<0 \end{cases} \tag{2.9}$$

and

$$\zeta = \sqrt{\tfrac{1}{4}\gamma^2 - \omega_0^2}. \tag{2.10}$$

As is well-known, the response function (2.8) of the quantum oscillator coincides with the classical response function [6].

The dynamic susceptibility

$$\chi(\omega) = \int_0^{\infty} dt\, e^{i\omega t} \chi(t) \tag{2.11}$$

takes the form

$$\chi(\omega) = \frac{1}{M} \frac{1}{\omega_0^2 - \omega^2 - i\gamma\omega} = \chi'(\omega) + i\chi''(\omega). \tag{2.12}$$

Its imaginary part

$$\chi''(\omega) = \frac{1}{M} \frac{\gamma\omega}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2} \tag{2.13}$$

is related to the spectral density

$$J(\omega) = \int_{-\infty}^{+\infty} dt\, e^{i\omega t} \langle q(t)\, q(0)\rangle \tag{2.14}$$

of the position fluctuations in thermal equilibrium by the FDT [14]

$$\chi''(\omega) = \frac{1}{2\hbar}\left(1 - e^{-\beta\hbar\omega}\right) J(\omega) \tag{2.15}$$

where $\beta = 1/k_B T$.

From (2.14-15) we can determine the position autocorrelation function, and find that it may be written

$$\langle q(t)\,q(0)\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi}\, \chi''(\omega)\, \frac{\hbar e^{-i\omega t}}{1-e^{-\beta\hbar\omega}} \tag{2.16}$$

which combines with (2.13) to yield

$$\langle q(t)\,q(0)\rangle = \frac{\hbar}{M} \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\, \frac{\gamma\omega}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\, \frac{e^{-i\omega t}}{1-e^{-\beta\hbar\omega}}. \tag{2.17}$$

Because of $\dot{q}=p/M$, the other pair correlation functions are given by

$$\begin{aligned} \langle p(t)\,q(0)\rangle &= M \frac{\partial}{\partial t} \langle q(t)\,q(0)\rangle \\ \langle q(t)\,p(0)\rangle &= -M \frac{\partial}{\partial t} \langle q(t)\,q(0)\rangle \\ \langle p(t)\,p(0)\rangle &= -M^2 \frac{\partial^2}{\partial t^2} \langle q(t)\,q(0)\rangle \end{aligned} \tag{2.18}$$

where we have made use of $\langle q(t)\,\dot{q}(0)\rangle = -\langle \dot{q}(t)\,q(0)\rangle$ which is a consequence of the stationarity of the stochastic process, that is

$$\langle q(t)\,q(t')\rangle = \langle q(t-t')\,q(0)\rangle. \tag{2.19}$$

In view of the Gaussian property, correlation functions of an odd number of position and momentum variables are vanishing, while correlation functions of an even number are given by the sum of all factorized pair correlation functions where the order of the variables of each pair has to be preserved [15]. For example:

$$\begin{aligned} \langle q(t)\,p(t')\,q(t'')\,p(0)\rangle &= \langle q(t)\,p(t')\rangle \langle q(t'')\,p(0)\rangle \\ &+ \langle q(t)\,q(t'')\rangle \langle p(t')\,p(0)\rangle \\ &+ \langle q(t)\,p(0)\rangle \langle p(t')\,q(t'')\rangle. \end{aligned} \tag{2.20}$$

Hence, the quantum-mechanical stochastic process of the damped harmonic oscillator is determined completely by the aforementioned principles.

3. The Position Autocorrelation Function

In the quantal case, the position autocorrelation function

$$J(t) = \langle q(t)\,q(0)\rangle \tag{3.1}$$

is a complex valued quantity. From (2.16) we see that $J(t)$ can analytically be continued to complex times $\tau = t - i\hbar\alpha$ where $0 \leqq \alpha \leqq \beta$. The integral

$$J(\tau) = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi}\, \frac{\hbar\chi''(\omega)\, e^{-i\omega\tau}}{1-e^{-\beta\hbar\omega}} \tag{3.2}$$

may be evaluated by contour integration. In the lower half-plane, $\chi''(\omega)$ has two poles at $\omega = -i\lambda_{1,2}$ where

$$\lambda_{1,2} = \frac{\gamma}{2} \pm \zeta \tag{3.3}$$

are the roots of the characteristic equation of the damped oscillator, while $[1-e^{-\beta\hbar\omega}]^{-1}$ has an infinite sequence of poles at $\omega = -i\nu_n$ $(n=1,2,\ldots)$ where

$$\nu_n = \frac{2\pi}{\hbar\beta}\, n. \tag{3.4}$$

By summing up the residues, we find for $t>0$

$$J(\tau) = \frac{i\hbar}{2M\zeta} \left(\frac{e^{-\lambda_1\tau}}{1-e^{i\beta\hbar\lambda_1}} - \frac{e^{-\lambda_2\tau}}{1-e^{i\beta\hbar\lambda_2}} \right) - \frac{2\gamma}{M\beta} \sum_{n=1}^{\infty} \frac{\nu_n e^{-\nu_n\tau}}{(\nu_n^2-\lambda_1^2)(\nu_n^2-\lambda_2^2)}. \tag{3.5}$$

Since $\chi''(-\omega) = -\chi''(\omega)$, it is readily seen from (3.2) that

$$J(t-i\hbar\beta) = J(-t) = \langle q(0)\,q(t)\rangle. \tag{3.6}$$

Furthermore, (3.2) gives

$$J(\tau) = J(-\tau^*)^*. \tag{3.7}$$

Hence, for imaginary times $\tau = -i\hbar\alpha$, the correlation function $J(\tau)$ is real and periodic, $J(-i\hbar\beta) = J(0)$, and it can be expanded into a Fourier series. The last term in (3.5) is already of this form, while the remaining terms may be written

$$\frac{i\hbar}{2M\zeta} \left(\frac{e^{-\lambda_1\tau}}{1-e^{i\beta\hbar\lambda_1}} - \frac{e^{-\lambda_2\tau}}{1-e^{i\beta\hbar\lambda_2}} \right) = \frac{1}{M\beta} \sum_{n=-\infty}^{+\infty} \frac{e^{-\nu_n\tau}}{(\nu_n-\lambda_1)(\nu_n-\lambda_2)} \tag{3.8}$$

which combines with (3.5) to yield

$$J(\tau) = \frac{1}{M\beta} \sum_{n=-\infty}^{+\infty} \frac{e^{-\nu_n\tau}}{\omega_0^2+\nu_n^2+\gamma|\nu_n|} \tag{3.9}$$

for $\tau = -i\hbar\alpha$, $0 \leqq \alpha \leqq \beta$. The Fourier coefficients

$$J(\nu_n) = \frac{1}{M\beta}\, \frac{1}{\omega_0^2+\nu_n^2+\gamma|\nu_n|} \tag{3.10}$$

of the imaginary time correlation function can be related directly to the dynamic susceptibility $\chi(\omega)$. From (3.2) we have

$$\begin{aligned} J(\nu_n) &= \frac{1}{\beta} \int_0^{\beta} d\alpha\, e^{-i\nu_n\hbar\alpha} J(-i\hbar\alpha) = \frac{1}{\beta} \int_{-\infty}^{+\infty} \frac{d\omega}{\pi}\, \frac{\chi''(\omega)}{\omega+i\nu_n} \\ &= \frac{1}{\beta}\, \mathrm{Im} \int_{-\infty}^{+\infty} \frac{d\omega}{\pi}\, \frac{\omega\chi(\omega)}{\omega^2+\nu_n^2} \end{aligned} \tag{3.11}$$

where we have made use of $\chi''(\omega) = -\chi''(-\omega)$. The last integral may be evaluated by contour integration. Since $\chi(\omega)$ is analytic on the upper half-plane, we have

$$J(v_n) = J(-v_n) = \frac{1}{\beta}\,\chi(i v_n) \tag{3.12}$$

for $v_n \geqq 0$.
The real time correlation function $J(t)$ is conveniently written as

$$J(t) = S(t) + i A(t). \tag{3.13}$$

In view of (3.7), the real part $S(t)$ is the symmetrized correlation function

$$S(t) = S(-t) = \tfrac{1}{2}\langle q(t)\,q(0) + q(0)\,q(t)\rangle \tag{3.14}$$

while the imaginary part is connected with the expectation of the commutator

$$A(t) = -A(-t) = \frac{1}{2i}\,\langle [q(t), q(0)]\rangle. \tag{3.15}$$

Because of

$$\frac{1}{1-e^{-\beta\hbar\omega}} = \frac{1}{2} + \frac{1}{2}\coth\left(\frac{1}{2}\beta\hbar\omega\right) \tag{3.16}$$

and $\chi''(-\omega) = -\chi''(\omega)$, we find from (2.16)

$$S(t) = \frac{\hbar}{2}\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\,\chi''(\omega)\coth\left(\frac{1}{2}\beta\hbar\omega\right)\cos(\omega t) \tag{3.17}$$

and

$$A(t) = -\frac{\hbar}{2}\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\,\chi''(\omega)\sin(\omega t). \tag{3.18}$$

The last integral gives

$$A(t) = -A(-t) = -\frac{\hbar}{2}\,\chi(t) \tag{3.19}$$

for $t \geqq 0$. From (3.15) and (3.19) we see that the response function $\chi(t)$ is related to the expectation of the commutator $[q(t), q(0)]$ in the familiar way

$$\chi(t) = \theta(t)\,\frac{i}{\hbar}\,\langle [q(t), q(0)]\rangle. \tag{3.20}$$

For $\tau = t > 0$, the real part of (3.5) gives for the symmetrized correlation function

$$S(t) = \frac{i\hbar}{4M\zeta}\left[\coth\left(\frac{i}{2}\beta\hbar\lambda_2\right)e^{-\lambda_2 t} - \coth\left(\frac{i}{2}\beta\hbar\lambda_1\right)e^{-\lambda_1 t}\right] - \Gamma(t) \tag{3.21}$$

where

$$\Gamma(t) = \frac{2\gamma}{M\beta}\sum_{n=1}^{\infty}\frac{v_n e^{-v_n t}}{(v_n^2-\lambda_1^2)(v_n^2-\lambda_2^2)}. \tag{3.22}$$

The RHS of (3.21) is real since λ_1 and λ_2 are real or complex conjugate quantities, respectively.
At finite temperatures, $\Gamma(t)$ decays as $\exp(-v_1 t)$. Hence, for $\hbar\gamma \ll k_B T$ it decays much faster than the remaining terms and may be disregarded. On the other hand, since $v_1 = 2\pi k_B T/\hbar$, the part $\Gamma(t)$ dominates the long time behaviour of $S(t)$ at very low temperatures. In particular at $T=0$ an asymptotic analysis shows that

$$S(t) \sim -\frac{\hbar\gamma}{\pi M\omega_0^4}\,\frac{1}{t^2} \quad \text{for } t\to\infty. \tag{3.23}$$

This algebraic decay for long times is an interesting quantum phenomenon.

4. Dispersion and Drude Regularization

The dispersion of the position in the equilibrium state is given by

$$\langle q^2\rangle = J(0) = \frac{1}{M\beta}\sum_{n=-\infty}^{+\infty}\frac{1}{\omega_0^2 + v_n^2 + \gamma|v_n|} \tag{4.1}$$

where we have made use of (3.9). This may be transformed to read

$$\langle q^2\rangle = \frac{1}{M\beta\omega_0^2} + \frac{1}{M\beta\zeta}\sum_{n=1}^{\infty}\left(\frac{1}{v_n+\lambda_2} - \frac{1}{v_n+\lambda_1}\right). \tag{4.2}$$

Now, by use of the formula [16]

$$\sum_{n=0}^{\infty}\left(\frac{1}{n+z_1} - \frac{1}{n+z_2}\right) = \psi(z_2) - \psi(z_1), \tag{4.3}$$

where the psi function is the logarithmic derivative of the gamma function, we obtain from (4.2)

$$\langle q^2\rangle = \frac{1}{M\beta\omega_0^2} + \frac{\hbar}{2\pi M\zeta}\,[\psi(1+\lambda_1/v) - \psi(1+\lambda_2/v)] \tag{4.4}$$

where $v = v_1 = 2\pi/\hbar\beta$.
From (2.10) and (3.3) we have

$$\beta\hbar\lambda_{1,2} = \sigma(\kappa \pm \sqrt{\kappa^2 - 1}) \tag{4.5}$$

where the dimensionless parameters κ and σ have been introduced previously. Thus, for high temperatures ($\sigma = \beta\hbar\omega_0 \ll 1$, $\sigma\kappa = \frac{1}{2}\beta\hbar\gamma \ll 1$), we may expand the psi functions in (4.4) about 1 to yield

$$\langle q^2\rangle = \frac{k_B T}{M\omega_0^2}\left[1 + \frac{1}{12}\sigma^2 + O(\sigma^3)\right]. \tag{4.6}$$

On the other hand, for low temperatures ($\sigma, \sigma\kappa \gg 1$) we may use the asymptotic expansion of the psi function to find

$$\langle q^2\rangle = \frac{\hbar}{2M\omega_0}\left[\frac{1}{\pi}\,\frac{\ln\dfrac{\kappa+\sqrt{\kappa^2-1}}{\kappa-\sqrt{\kappa^2-1}}}{\sqrt{\kappa^2-1}} + \frac{4\pi\kappa}{3\sigma^2} + O\left(\frac{1}{\sigma^3}\right)\right]. \tag{4.7}$$

The zero temperature ($\sigma=\infty$) result for $\langle q^2\rangle$ has also been given by Caldeira and Leggett [6]. We note that for $\kappa<1$

$$\frac{1}{\pi}\,\frac{\ln[(\kappa+\sqrt{\kappa^2-1})/(\kappa-\sqrt{\kappa^2-1})]}{\sqrt{\kappa^2-1}} = \frac{1}{\sqrt{1-\kappa^2}}\left(1-\frac{2}{\pi}\arctan\frac{\kappa}{\sqrt{1-\kappa^2}}\right) \tag{4.8}$$

so that (4.7) gives the correct dispersion $\langle q^2\rangle = \hbar/2M\omega_0$ of the position of an undamped oscillator ($\kappa=0$) in its ground state. For finite κ the dispersion $\langle q^2\rangle$ is diminished.

Using (2.18) and (3.2), we find that the dispersion of the momentum in the equilibrium state is given by the sum rule

$$\langle p^2\rangle = -M^2\frac{\partial^2}{\partial t^2}J(t)|_{t=0} = M^2\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\,\frac{\hbar\omega^2\chi''(\omega)}{1-e^{-\beta\hbar\omega}}. \tag{4.9}$$

The integral is logarithmically divergent which is a consequence of the fact that we have treated a Markovian model with frequency-independent damping. In reality, the damping coefficient approaches zero at high frequencies. In the following, we shall treat a Drude-model with the frequency-dependent damping coefficient

$$\gamma(\omega) = \frac{\gamma\omega_D}{\omega_D - i\omega} \tag{4.10}$$

which is associated with the classical equation of motion

$$\ddot{q}(t) + \omega_0^2 q(t) + \gamma\int_{-\infty}^{t} ds\,\omega_D e^{-\omega_D(t-s)}\dot{q}(s) = \frac{1}{M}F(t). \tag{4.11}$$

The Drude frequency ω_D is supposed to be much larger than ω_0 and γ so that the memory is short on the time scale of interest.

The line of reasoning followed in the preceeding sections can easily be transferred to the case of frequency-dependent damping. The dynamic susceptibility now takes the form

$$\chi(\omega) = \frac{1}{M}\,\frac{1}{\omega_0^2-\omega^2-i\omega\gamma(\omega)}. \tag{4.12}$$

For the Drude model (4.10), $\chi(\omega)$ has three poles in the lower half-plane at $\omega=-i\lambda_k$ ($k=1,2,3$), where the λ_k are the roots of the cubic equation

$$\lambda^3 - \omega_D\lambda^2 + (\omega_0^2+\gamma\omega_D)\lambda - \omega_D\omega_0^2 = 0. \tag{4.13}$$

These roots satisfy the relations

$$\begin{aligned}&\lambda_1+\lambda_2+\lambda_3=\omega_D\\ &\lambda_1\lambda_2+\lambda_2\lambda_3+\lambda_3\lambda_1=\omega_0^2+\gamma\omega_D\\ &\lambda_1\lambda_2\lambda_3=\omega_D\omega_0^2.\end{aligned} \tag{4.14}$$

For $\omega_D \gg \omega_0, \gamma$, one finds that the roots are approximately given by

$$\begin{aligned}&\lambda_1=\frac{\gamma}{2}+\zeta\\ &\lambda_2=\frac{\gamma}{2}-\zeta\\ &\lambda_3=\omega_D-\gamma\end{aligned} \tag{4.15}$$

where terms of order ω_0/ω_D and γ/ω_D have been disregarded.

By virtue of (3.12), the imaginary time position autocorrelation function may be written

$$J(\tau) = \frac{1}{M\beta}\sum_{n=-\infty}^{+\infty}\frac{e^{-\nu_n\tau}}{\omega_0^2+\nu_n^2+\gamma\omega_D|\nu_n|/(\omega_D+|\nu_n|)} \tag{4.16}$$

where $\tau=-i\hbar\alpha$, $0\leqq\alpha\leqq\beta$. From (4.16) we obtain for the dispersion of the position in the ground state

$$\langle q^2\rangle = \frac{1}{M\beta}\sum_{n=-\infty}^{+\infty}\frac{1}{\omega_0^2+\nu_n^2+\gamma\omega_D|\nu_n|/(\omega_D+|\nu_n|)}. \tag{4.17}$$

This sum may be written

$$\langle q^2\rangle = -\frac{1}{M\beta\omega_0}\,\frac{\partial}{\partial\omega_0}\ln Z' \tag{4.18}$$

where

$$Z' = \frac{1}{\hbar\beta\omega_0}\prod_{n=1}^{\infty}\frac{\nu_n^2}{\omega_0^2+\nu_n^2+\gamma\omega_D|\nu_n|/(\omega_D+|\nu_n|)}. \tag{4.19}$$

Furthermore, by means of an infinite-product representation of the gamma function [16] and the relations (4.14), we find

$$Z' = \frac{\hbar\beta\omega_0}{4\pi^2}\,\frac{\Gamma(\lambda_1/\nu)\,\Gamma(\lambda_2/\nu)\,\Gamma(\lambda_3/\nu)}{\Gamma(\omega_D/\nu)}. \tag{4.20}$$

Using the approximate roots (4.15), one may easily show that (4.18) and (4.20) yield for $\langle q^2\rangle$ the previous result (4.4) apart from corrections of order ω_0/ω_D and γ/ω_D.

From (4.16), the imaginary time momentum correlation function is found to read

$$J_p(\tau) = -M^2 \frac{\partial^2 J(\tau)}{\partial \tau^2}$$
$$= -\frac{M}{\beta} \sum_{n=-\infty}^{+\infty} \frac{\nu_n^2 e^{-\nu_n \tau}}{\omega_0^2 + \nu_n^2 + \gamma \omega_D |\nu_n| / (\omega_D + |\nu_n|)} \tag{4.21}$$

for $\tau = -i\hbar\alpha$, $0 < \alpha < \beta$. The Fourier series (4.16) continues the correlation function $J(\tau)$ periodically to all imaginary times $\tau = -i\hbar\alpha$, while it provides an analytical continuation of the real time correlation function in the interval $0 \leqq \alpha \leqq \beta$, only. As a consequence of this continuation beyond the physical region, $J(\tau)$ has cusp singularities at $\tau = i\hbar\beta n$, ($n=0, \pm 1, \pm 2, \ldots$) which lead to δ-function singularities of $J_p(\tau)$. To obtain the dispersion of the momentum in the equilibrium state, we must take the limit

$$\langle p^2 \rangle = \lim_{\alpha \to 0^+} J_p(-i\hbar\alpha) \tag{4.22}$$

which gives

$$\langle p^2 \rangle = \frac{M}{\beta} \sum_{n=-\infty}^{+\infty} \frac{\omega_0^2 + \gamma \omega_D |\nu_n| / (\omega_D + |\nu_n|)}{\omega_0^2 + \nu_n^2 + \gamma \omega_D |\nu_n| / (\omega_D + |\nu_n|)}. \tag{4.23}$$

The same result can be obtained from (4.9) by contour integration.

From (4.17) and (4.19), one easily shows that (4.23) may be written

$$\langle p^2 \rangle = M^2 \omega_0^2 \langle q^2 \rangle + \Delta \tag{4.24}$$

where

$$\Delta = -\frac{2M\gamma}{\beta} \frac{\partial}{\partial \gamma} \ln Z'. \tag{4.25}$$

Using the approximate roots (4.15), one obtains from (4.20) and (4.24)

$$\Delta = \frac{\hbar \gamma M}{2\pi} \left[2\psi(1 + \lambda_3/\nu) - \left(1 + \frac{\gamma}{2\zeta}\right) \psi(1 + \lambda_1/\nu) - \left(1 - \frac{\gamma}{2\zeta}\right) \psi(1 + \lambda_2/\nu) \right] \tag{4.26}$$

where terms of order ω_0/ω_D and γ/ω_D have been disregarded. For very high temperatures ($\beta\hbar\omega_D \ll 1$) one can expand the psi functions about 1 to give in leading order

$$\Delta = \frac{\hbar^2 \gamma M \omega_D}{12 k_B T}. \tag{4.27}$$

Thus Δ vanishes at high temperatures, and the correct classical ratio of $\langle p^2 \rangle$ and $\langle q^2 \rangle$ is recovered from (4.24). For lower temperatures where $\beta\hbar\omega_D \gg 1$, the main contribution to Δ comes from the first term in (4.26) and it reads

$$\Delta \approx \frac{\hbar \gamma M}{\pi} \ln(\beta \hbar \omega_D). \tag{4.28}$$

Note that (4.28) may be the dominant contribution to $\langle p^2 \rangle$ even for temperatures where $\langle q^2 \rangle$ is still in the classical region. This is the case in the temperature range where $\beta\hbar\omega_D$ is large while $\beta\hbar\omega_0$ and $\beta\hbar\gamma$ are small, except for systems where the damping is so weak that

$$\beta \hbar \gamma \ln(\beta \hbar \omega_D) \ll 1. \tag{4.29}$$

This gives a further restriction of the range of validity of the weak coupling approximation.

At very low temperatures, where $\beta\hbar\omega_0 \gg 1$ and $\beta\hbar\gamma \gg 1$, one can use the asymptotic expansion of all psi functions in (4.26) to give

$$\Delta = \frac{\hbar \gamma M}{\pi} \ln \frac{\omega_D}{\omega_0} - \frac{\hbar \gamma^2 M}{4\pi\zeta} \ln \frac{\lambda_1}{\lambda_2} - \frac{\pi \hbar \gamma M}{3\sigma^2} + O\left(\frac{1}{\sigma^3}\right) \tag{4.30}$$

where terms of order ω_0/ω_D, γ/ω_D and $k_B T/\hbar\omega_D$ have been disregarded. (4.30) combines with (4.7) and (4.24) to yield at zero temperature

$$\langle p^2 \rangle = \tfrac{1}{2} \hbar M \omega_0 \left[(1 - 2\kappa^2) \frac{\ln \dfrac{\kappa + \sqrt{\kappa^2 - 1}}{\kappa - \sqrt{\kappa^2 - 1}}}{\pi \sqrt{\kappa^2 - 1}} + \frac{4\kappa}{\pi} \ln \left(\frac{\omega_D}{\omega_0}\right) \right]. \tag{4.31}$$

The lowest finite temperature corrections are proportional to T^3. By virtue of (4.8) it is easy to show that (4.31) reduces for $\kappa = 0$ to the correct momentum dispersion $\langle p^2 \rangle = \frac{1}{2}\hbar M \omega_0$ of an undamped oscillator in its ground state.

5. The Equilibrium Density Matrix

Because of the Gaussian property, the equilibrium state is completely determined by $\langle p^2 \rangle$ and $\langle q^2 \rangle$. The equilibrium density matrix ρ_β may be written

$$\rho_\beta = \frac{1}{Z} e^{-\beta H_{\mathrm{eff}}} \tag{5.1}$$

where Z is a normalization factor, and

$$H_{\mathrm{eff}} = \frac{1}{2M_{\mathrm{eff}}} p^2 + \tfrac{1}{2} M_{\mathrm{eff}} \omega_{\mathrm{eff}}^2 q^2 \tag{5.2}$$

is an effective Hamiltonian. The effective frequency

ω_{eff} reads

$$\omega_{\text{eff}}=\frac{1}{\hbar\beta}\ln\frac{\sqrt{\langle p^2\rangle\langle q^2\rangle}+\frac{\hbar}{2}}{\sqrt{\langle p^2\rangle\langle q^2\rangle}-\frac{\hbar}{2}}$$

$$=\frac{2}{\hbar\beta}\operatorname{Ar\,coth}\left(\frac{2}{\hbar}\sqrt{\langle p^2\rangle\langle q^2\rangle}\right), \tag{5.3}$$

and the effective mass M_{eff} is given by

$$M_{\text{eff}}=\frac{1}{\omega_{\text{eff}}}\sqrt{\frac{\langle p^2\rangle}{\langle q^2\rangle}}. \tag{5.4}$$

Since ω_{eff} and M_{eff} depend on temperature, H_{eff} might more appropriately be called the free energy operator of the oscillator.

The density matrix (5.1) can be diagonalized in the usual way

$$\rho_\beta=\sum_{n=0}^{\infty}p_n|n\rangle\langle n| \tag{5.5}$$

where we have introduced the eigenstates $|n\rangle$ of the effective Hamiltonian (5.2)

$$H_{\text{eff}}|n\rangle=E_n|n\rangle, \tag{5.6}$$

with the eigenvalues

$$E_n=\hbar\omega_{\text{eff}}(n+\tfrac{1}{2}), \tag{5.7}$$

and where

$$p_n=\frac{1}{Z}e^{-\beta E_n} \tag{5.8}$$

are the occupation probabilities of these states. In coordinate representation we have

$$\langle q|n\rangle=\left(\frac{1}{\pi}\right)^{\frac{1}{4}}\left(\frac{c}{2^n n!}\right)^{\frac{1}{2}}e^{-\frac{1}{2}c^2q^2}H_n(cq) \tag{5.9}$$

where the H_n are Hermite polynomials, and where

$$c=\sqrt{\frac{M_{\text{eff}}\,\omega_{\text{eff}}}{\hbar}}=\left(\frac{\langle p^2\rangle}{\hbar^2\langle q^2\rangle}\right)^{\frac{1}{4}}. \tag{5.10}$$

Finally, the partition function Z reads

$$Z=\frac{1}{2\sinh(\frac{1}{2}\beta\hbar\omega_{\text{eff}})}=\sqrt{\frac{1}{\hbar^2}\langle p^2\rangle\langle q^2\rangle-\frac{1}{4}}. \tag{5.11}$$

For a damped system, Z differs from the quantity Z' which has been introduced previously.

The coordinate representation of the density matrix is given by [8]

$$\langle q|\rho_\beta|q'\rangle$$
$$=\frac{c}{Z\sqrt{2\pi\sinh\Omega}}\,e^{-\frac{c^2}{2\sinh\Omega}[(q^2+q'^2)\cosh\Omega-2qq']} \tag{5.12}$$

where

$$\Omega=\beta\hbar\omega_{\text{eff}}. \tag{5.13}$$

By virtue of (5.3), (5.10) and (5.11), we find that (5.12) may be transformed to read

$$\langle q|\rho_\beta|q'\rangle=\frac{1}{\sqrt{2\pi\langle q^2\rangle}}\,e^{-\frac{1}{2}\left[\frac{(q+q')^2}{4\langle q^2\rangle}+\hbar^{-2}\langle p^2\rangle(q-q')^2\right]} \tag{5.14}$$

which clearly gives the correct variances of p and q.

At high temperatures, the effective quantitites ω_{eff} and M_{eff} approach their bare values ω and M, while at low temperatures they undergo strong modifications caused by the damping. Using (4.7) and (4.31) we obtain from (5.3) for the effective frequency near zero temperature

$$\hbar\omega_{\text{eff}}=2k_BT\operatorname{Ar\,coth}\sqrt{f(\kappa)\left[\frac{4\kappa}{\pi}\ln\left(\frac{\omega_D}{\omega_0}\right)+(1-2\kappa^2)f(\kappa)\right]} \tag{5.15}$$

where

$$f(\kappa)=\frac{1}{\pi}\frac{\ln[(\kappa+\sqrt{\kappa^2-1})/(\kappa-\sqrt{\kappa^2-1})]}{\sqrt{\kappa^2-1}}. \tag{5.16}$$

Hence, for a damped oscillator, the energy levels (5.7) becomes very narrowly spaced near zero temperature, and the occupation probabilities (5.8) remain finite in the limit $T\to 0$. This shows that the ground state is not a pure state but a mixture.

6. Conclusions

Starting from basic principles we have examined the process of spontaneous thermal and quantal fluctuations of a simple damped harmonic oscillator. No assumptions about the strength of the damping and the range of temperature have been made. Some of the results have also been obtained by Schmid [5], Caldeira and Leggett [6], and Zwerger [17]. We have removed the divergence of the momentum dispersion by treating the non-Markovian case of frequency-dependent damping, and explicit results have been deduced for a Drude model. The equilibrium state has been shown to be characterized by an effective Hamiltonian which has the form of the Hamiltonian of the undamped oscillator with modified mass and frequency.

For high temperatures ($k_B T \gg \hbar\omega_0$, $k_B T \gg \hbar\gamma$, $k_B T \gg \hbar\sqrt{\gamma\omega_D}$), one can easily see from (3.21), (4.6), (4.24) and (4.27) that the quantum stochastic process reduces to the classical Fokker-Planck process of a damped harmonic oscillator [9]. On the other hand, for sufficiently weak damping ($\gamma \ll \omega_0$, $\hbar\gamma \ll k_B T$, $\gamma \ln(\beta\hbar\omega_D) \ll \omega_0$, $\hbar\gamma \ln(\beta\hbar\omega_D) \ll k_B T$) a connection between our results and those of the weak coupling theory of the damped harmonic oscillator [1–4] can be established.

In a previous study [18], we have determined the canonical position autocorrelation function of a damped harmonic oscillator by means of a quantum master equation based on a kinetic model. Using well-known relations between the various types of quantum correlation functions [13], it may easily be shown that the properties of the position autocorrelation function discussed in Sect. 3 likewise emerge from the result in [18]. On the other hand, the simple approximation for the operator Λ used in [18] is not accurate enough to calculate higher order correlation functions directly from the master equation unless $\hbar\gamma/k_B T$ is small. The connection between the present work and the master equation approach will be discussed in greater detail elsewhere.

While the approach to dissipative quantum systems presented here is very simple, it is at present restricted to linear systems. However, if the nonlinearities of a system are entirely due to its reversible motion, the same dissipative mechanism as in linear systems can be adopted. This makes an extension of the approach possible which we hope to discuss in the near future.

We wish to thank P. Hänggi and H. Thomas for helpful discussions, and are grateful to A.J. Leggett for communicating to us his unpublished results. One of us (H.G.) acknowledges the warm hospitality of the Physics Department of the University of Basel where an important part of this work was carried out. Support was provided by the Swiss National Science Foundation and the Deutsche Forschungsgemeinschaft.

References

1. Haken, H.: Light and matter Ic. In: Handbuch der Physik, Vol. XXV/2c. Berlin, Heidelberg, New York: Springer 1969
2. Haake, F.: Statistical treatment of open systems by generalized master equations. In: Springer Tracts in Modern Physics. Vol. 66. Berlin, Heidelberg, New York: Springer 1973
3. Haken, H.: Rev. Mod. Phys. **47**, 67 (1975)
4. Davies, E.B.: Quantum theory of open systems. London: Academic Press 1976
5. Schmid, A.: J. Low. Temp. Phys. **49**, 609 (1982)
6. Caldeira, A.O., Leggett, A.J.: Ann. Phys. (NY) **149**, 374 (1983)
7. Feynman, R.P., Hibbs, A.R.: Quantum mechanics and path integrals. New York: McGraw-Hill 1965
8. Feynman, R.P.: Statistical mechanics. Reading: Benjamin 1972
9. Hänggi, P., Thomas, H.: Phys. Rep. **88**, 207 (1982)
10. Dekker, H.: Phys. Rep. **80**, 1 (1981)
11. Grabert, H., Graham, R., Green, M.S.: Phys. Rev. **21**, 2136 (1980)
12. Green, M.S.: J. Chem. Phys. **20**, 1281 (1952)
13. Kubo, R.: Rep. Prog. Phys. (London) **29**, 255 (1966)
14. Callen, H.B., Welton, T.A.: Phys. Rev. **83**, 34 (1951)
15. Talkner, P.: Z. Phys. B – Condensed Matter **41**, 365 (1981)
16. Gradshteyn, I.S., Ryzhik, I.M.: Tables of integrals, series, and products. London: Academic Press 1965
17. Zwerger, W.: Z. Phys. B – Condensed Matter **51**, 301 (1983)
18. Grabert, H., Talkner, P.: Phys. Rev. Lett. **50**, 1335 (1983)

Hermann Grabert
Ulrich Weiss
Institut für Theoretische Physik Universität Stuttgart
Pfaffenwaldring 57/III
D-7000 Stuttgart 80
Federal Republic of Germany

Peter Talkner
Institut für Physik
Universität Basel
Klingelbergstrasse 82
CH-4056 Basel
Switzerland