Strong damping and low-temperature anomalies for the harmonic oscillator

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We consider Ullersma's model of a damped harmonic oscillator interacting with a heat bath. We show that for large damping the oscillator does not undergo Brownian motion at any temperature. For high temperatures non-Markovian effects show up in initial slips only. For low temperatures we find, as further anomalies, power-law decay of time-dependent expectation values as well as a strong squeezing of the displacement and momentum uncertainties; again these anomalies are most strongly pronounced for strong damping.

I. INTRODUCTION

The simplest systems for which the origin of irreversible behavior can be studied quantitatively on a microscopic basis are linear ones. Of special interest is a harmonic oscillator linearly coupled to a heat bath which itself consists of harmonic oscillators.[1,2] For the characterization of this prototypical system the following five parameters are needed. Most importantly, we have the complex frequency $\Omega+i\Gamma$ into which the unperturbed real frequency ω_0 of the oscillator is shifted by the heat bath. With the heat-bath temperature T there is associated a thermal frequency $k_BT/\hbar$ which sets a time scale typical for quantum effects. Finally, we must consider a rate constant α to represent the response characteristics of the heat bath variable to which the oscillator is coupled in the interaction Hamiltonian. This rate constant, usually related to an ultraviolet cutoff in the spectrum of eigenfrequencies of the bath oscillators, must be larger than $|\Gamma+i\Omega|$ if the heat bath is to deserve its name.

In view of the abundance of treatments of the damped harmonic oscillator it is quite astonishing that until the recent phenomenological approach of Ref. 3 and the microscopic investigation[4(a)] a satisfactory understanding had been reached only in the classical case and for the weak-coupling limit[5]

$$\Gamma \ll \omega_0 \approx \Omega \ll \alpha\ , \quad \Gamma \ll k_BT/\hbar\ . \tag{1.1}$$

In that case the mean displacement and the mean momentum of the "central" oscillator undergo a slowly damped harmonic oscillation corresponding to the complex frequency $\Omega+i\Gamma$. The mean energy of the oscillator, on the other hand, relaxes towards the equilibrium value

$$E(\Omega,T)=\tfrac{1}{2}\hbar\Omega\coth(\hbar\Omega/2k_BT) \tag{1.2}$$

which is the thermal excitation energy of a harmonic oscillator with frequency Ω at temperature T. In the classical limit, $\hbar\Omega \ll k_BT$, this excitation energy of course takes on the value k_BT. As for fluctuations, the density operator of the central oscillator may be represented by the Wigner function[6] and is thus revealed to undergo an Ornstein-Uhlenbeck process.[7]

Corrections to the ideal weak-damping behavior just described arise in first order in the small dimensionless ratios Γ/Ω, Ω/α, etc., defined by the limit (1.1). It is remarkable that the ideal weak-damping behavior is universal inasmuch as it does not explicitly involve the rate α nor any other characteristics of the heat bath beyond the ones manifest in the small difference between the unperturbed frequency ω_0 and the observable complex frequency $\Omega+i\Gamma$.

We propose to show, in the following, that the linear system in question displays a more complex and less universal behavior if the heat bath is held at low temperatures

$$k_BT \ll \hbar\Gamma \tag{1.3}$$

and/or is designed such as to impart strong damping

$$\Gamma \ll \Omega \tag{1.4}$$

to the oscillator.

In the low-temperature regime (1.3) we encounter anomalies for various observables of the central oscillator. The mean displacement and the mean momentum still approach vanishing equilibrium values through damped oscillations, but the temporal behavior depends sensitively on the coupling to the heat bath and may deviate considerably from simple linear damping. Expectation values of powers and products of these operators do acquire very nonclassical and unexpected features both in their relaxation towards equilibrium and in their equilibrium values. As for their time dependence, exponentials decaying with integer multiples of the thermal decay rate $k_BT/\hbar$ begin to outlive the mechanical transients like $\exp(-\Gamma t)$. In the extreme quantum limit $k_BT \ll \hbar\Gamma$ the multiples of $k_BT/\hbar$ tend to behave, in their effects with respect to the time scale $1/\Gamma$, like a continuum and then give rise to an inverse power-law falloff in expectation values and correlation functions, a result consistent with that in Ref. 3.

As a most interesting low-temperature anomaly in the equilibrium state of the central oscillator we shall find that, in contrast to the weak-damping regime (1.1), the mean squared displacement and the mean squared momentum have a ratio rather different from that of a free oscillator with frequency Ω. The kinetic energy of the oscillator is even dramatically afflicted by the bath. As the number of bath oscillators goes to infinity the spectrum of their frequencies must be provided with an

ultraviolet cutoff for the mean kinetic energy of the central oscillator to remain finite; compare Refs. 3 and 8.

The low-temperature anomalies just mentioned become especially well pronounced for a strongly damped or even overdamped oscillator. Inverse power-law decay of equilibrium correlation functions and of nonequilibrium expectation values then tend to acquire weights comparable to those of exponential transients. Moreover, the equilibrium uncertainties of the displacement and the momentum display a considerable amount of "squeezing."[9]

While the central oscillator can be said to undergo an Ornstein-Uhlenbeck process in the weak-coupling regime (1.1) there is no Markovian stochastic process we could associate with the behavior at low temperatures and for strong damping. However, the Wigner function of the central oscillator still displays a simple Gaussian behavior provided only the heat bath is in some sort of thermal equilibrium initially such that the Wigner function of the whole system is a Gaussian with respect to the displacements and momenta of the bath oscillators. This is the case, due to the harmonicity of the Hamiltonian, for any of the following physically relevant initial states: (i) thermal equilibrium of the whole system, (ii) thermal equilibrium of the heat bath with the coupling to the central oscillator disregarded and without any correlation to the central oscillator, the latter in any arbitrary state, and (iii) global thermal equilibrium constrained by prescribed initial expectation values for any linear or quadratic function of the displacement of the central oscillator. For all of these initial conditions we find the Wigner function of the central oscillator to obey a simple second-order partial differential equation. There are, in fact, only two important differences between the general equation of motion and the Fokker-Planck equation of the Ornstein-Uhlenbeck process. First, there is an additional diffusion coefficient (vanishing in the classical limit) which unfortunately generates a negative eigenvalue for the diffusion matrix. Second, both the drift and the diffusion coefficients carry an explicit time dependence; they become stationary only for times larger than both the bath response time $1/\alpha$ and the thermal relaxation time $\hbar/k_BT$. It is thus only in the limit

$$\alpha, k_BT/\hbar \gg \Gamma \tag{1.5}$$

that the behavior of the Wigner function on the time scale $1/\Gamma$ can be described by a time-independent generator l of infinitesimal time translations. In all other cases the drift or the diffusion coefficients approach stationary limits no faster than the observables of the central oscillator.

The existence of a time-independent generator l for $k_BT \gg \hbar\Gamma$ does not, of course, imply Markovian behavior. Rather, the exact time-dependent generator $l(t)$ and its long-time limit $l(\infty)\equiv l$ can and in general do go with different initial conditions for the Wigner function. The effective initial Wigner function $W_{\rm as}(0)$ to be used together with l may be defined through

$$W(t)=\left[\exp\int_0^t dt' l(t')\right]_+ W(0)\to e^{lt}W_{\rm as}(0) \quad \text{for } t\gg 1/\alpha,\hbar/k_BT, \tag{1.6}$$

where $(\cdots)_+$ means a time-ordered product. The difference $W(0)-W_{\rm as}(0)$, a so-called initial slip,[10] constitutes a non-Markovian effect. We shall show that slip to be large except for very weak damping.

We shall in the following mostly employ Ullersma's notation.[2] In fact, our paper may be considered as an extension of Ullersma's work to include large damping and low temperatures. Similar to our approach are the recent ones by Lindenberg and West[4] and by Riseborough, Hänggi, and Weiss.[11] Some of our results on low-temperatures effects are also implicit in the papers of Caldeira and Legget[8] and of Grabert, Weiss, and Talkner.[3] A preliminary version of our work was presented at the seminar on "Fundamentals on Quantum Optics" in Ref. 12.

II. THE MODEL AND ITS EXACT SOLUTION

We denote the displacement and momentum operators of the central oscillator by Q_0 and P_0 and the corresponding operators for the N bath oscillators by Q_i,P_i, $i=1,2,\ldots,N$. Whenever convenient we shall use Greek indices running over all $N+1$ oscillators and write Q_ν,P_ν with $\nu=0,1,2,\ldots,N$. Ullersma's Hamiltonian then reads

$$H=\tfrac{1}{2}\sum_{\nu=0}^{N}(P_\nu^2+\omega_\nu^2Q_\nu^2)+\sum_{n=1}^{N}\epsilon_nQ_0Q_n\ . \tag{2.1}$$

For H to have a finite lower bound the coupling constants ϵ_n and the unperturbed eigenfrequencies have to fulfill the "positivity" condition[13]

$$\omega_0^2-\sum_{n=1}^{N}\frac{\epsilon_n^2}{\omega_n^2}\geq 0\ . \tag{2.2}$$

The Hamiltonian (2.1) being a quadratic form in the Q_ν and P_ν the time-dependent displacements and momenta are linearly related to their initial values as

$$\begin{aligned} Q_\mu(t)&=\sum_{\nu=0}^{N}[\dot A_{\mu\nu}(t)Q_\nu(0)+A_{\mu\nu}(t)P_\nu(0)]\ ,\\ P_\mu(t)&=\dot Q_\mu(t)\ . \end{aligned} \tag{2.3}$$

The matrix elements $A_{\mu\nu}(t)$ are easily found with the help of the orthogonal matrix $X_{\mu\nu}$ which diagonalizes the Hamiltonian (2.1) as

$$\begin{aligned} Q_\mu&=\sum_{\nu=0}^{N}X_{\mu\nu}Q'_\nu\ ,\\ P_\mu&=\sum_{\nu=0}^{N}X_{\mu\nu}P'_\nu\ ,\\ H&=\sum_{\nu=0}^{N}\tfrac{1}{2}[(P'_\nu)^2+z_\nu^2(Q'_\nu)^2]\ . \end{aligned} \tag{2.4}$$

The $N+1$ eigenfrequencies z_ν are the positive zeros of the function[15]

$$g(z)=z^2-\omega_0^2-\sum_n\frac{\epsilon_n^2}{z^2-\omega_n^2} \tag{2.5}$$

while the matrix $X_{\mu\nu}$ is determined by

$$X_{0\nu}=\left[\left[\frac{1}{2z}\frac{dg(z)}{dz}\right]_{z=z_\nu}\right]^{-1/2}, \tag{2.6}$$

$$X_{n\nu}=\frac{\epsilon_n}{z_\nu^2-\omega_n^2}X_{0\nu}\ . \tag{2.7}$$

By first solving the initial-value problem for each normal mode we immediately find the matrix $A_{\mu\nu}(t)$ as

$$A_{\mu\nu}(t)=\sum_{\rho=0}^{N}X_{\mu\rho}X_{\nu\rho}\frac{1}{z_\rho}\sin(z_\rho t)\ . \tag{2.8}$$

Since the N bath oscillators are to behave as a heat bath they must be large in number and their unperturbed eigenfrequencies ω_n must be densely spaced. We may therefore simplify the function $g(z)$ by introducing a spectral strength function $\gamma(\omega)$ as

$$\gamma(\omega)\Delta\omega=\sum_{\omega<\omega_n<\omega+\Delta\omega}\epsilon_n^2 \tag{2.9}$$

and by replacing the sum in (2.5) by an integral[16]

$$g(z)=z^2-\omega_0^2-\int_0^\infty d\omega\frac{\gamma(\omega)}{z^2-\omega^2}\ . \tag{2.10}$$

Similarly, the positivity condition (2.2) can be written as

$$\omega_0^2-\int_0^\infty d\omega\frac{\gamma(\omega)}{\omega^2}\geq 0\ . \tag{2.11}$$

For any given spectral strength $\gamma(\omega)$ we now have, up to some frequency integrals, the complete solution of the initial value problem for the Hamiltonian (2.1).

III. THERMAL EQUILIBRIUM

Since we are dealing with a macroscopic system we may describe its equilibrium statistics by employing the canonical density operator

$$\rho\sim e^{-\beta H},\quad \beta=1/k_BT\ . \tag{3.1}$$

Due to the harmonicity of the Hamiltonian (2.1) this is a Gaussian ensemble.

To describe temporal correlations in equilibrium we consider the symmetrized autocorrelation function

$$\begin{aligned}C(t)&=\langle\tfrac{1}{2}[Q_0(t)Q_0(0)+Q_0(0)Q_0(t)]\rangle\\&\equiv\langle\{Q_0(t),Q_0(0)\}\rangle\ .\end{aligned} \tag{3.2}$$

By using (2.3) and (2.6) we find

$$\begin{aligned}C(t)&=\sum_{\nu=0}^{N}X_{0\nu}^2E(z_\nu,T)\frac{1}{z_\nu^2}\cos(z_\nu t)\\&=\frac{1}{2\pi i}\oint dz\frac{z}{g(z)}\frac{E(z,T)}{z^2}\cos(zt)\ ,\end{aligned} \tag{3.3}$$

provided the closed contour in the complex z plane encircles all $2(N+1)$ zeros of $g(z)$ in the positive sense but none of the poles of $E(z,T)$ except the one at $z=0$. We shall discuss complex integrals of this type below.

The function $C(t)$ completely defines the Gaussian process undergone by the central oscillator since it has the other symmetrized two-point correlation functions as its time derivatives,

$$\dot{C}(t)=\langle\{P_0(t),Q_0(0)\}\rangle=-\langle\{Q_0(t),P_0(0)\}\rangle\ , \tag{3.4}$$

$$\ddot{C}(t)=-\langle\{P_0(t),P_0(0)\}\rangle\ , \tag{3.5}$$

and contains the second- and first-order static moments as initial values and as limiting values for $t\to\infty$, respectively. Also, through the fluctuation-dissipation theorem[17] it determines the linear response of the displacement of the central oscillator to an external force acting on its displacement.

IV. PARTIAL EQUILIBRIUM

As a simple nonequilibrium situation we now imagine the set of bath oscillators to be decoupled from the central oscillator and in thermal equilibrium according to the canonical operator

$$\rho_{\text{bath}}\sim\exp\left[-\beta\sum_{n=1}^{N}\tfrac{1}{2}(P_n^2+\omega_n^2Q_n^2)\right]\ . \tag{4.1}$$

The central oscillator we imagine prepared separately, so as to bear no correlations with the bath and to be represented by some initial density operator ρ_0. If the two subsystems are then brought into contact sufficiently fast and without any further perturbation we can describe the subsequent process by the Hamiltonian (2.1) and the "initial" density operator

$$\rho(0)=\rho_0\otimes\rho_{\text{bath}}\ . \tag{4.2}$$

Clearly, this does not correspond to a stationary ensemble with respect to the Hamiltonian (2.1). Moreover, due to the arbitrariness of ρ_0 we are now in general facing a non-Gaussian problem, at least for finite times.

We shall investigate the time-dependent first and second moments for the central oscillator. Since for the ensemble (4.2) we have $\langle P_n(0)\rangle=\langle Q_n(0)\rangle=0$ the mean displacement now reads

$$\langle Q_0(t)\rangle=\dot{A}(t)\langle Q_0(0)\rangle+A(t)\langle P_0(0)\rangle\ , \tag{4.3}$$

where we have introduced the shorthand $A(t)$ for the matrix element $A_{00}(t)$. Similar to the equilibrium correlation function $C(t)$, we can transform the sum defining the amplitude $A(t)$ [see (2.8)] into a complex integral,

$$A(t)\equiv A_{00}(t)=\frac{1}{2\pi i}\oint dz\frac{1}{g(z)}\sin(zt)\ . \tag{4.4}$$

By recalling that the zeros of $g(z)$ are the $N+1$ real pairs $\pm z_\nu$ we easily verify that $A(t)$ is the inverse Laplace transform of

$$\tilde{A}(z)=\int_0^\infty dt\,e^{-zt}A(t)=-\frac{1}{g(-iz)}\ . \tag{4.5}$$

As for the second moments, we have the initial values

$$\begin{aligned}&\langle\{Q_n(0),P_n(0)\}\rangle=0\ ,\\&\langle[P_n(0)]^2\rangle=\omega_n^2\langle[Q_n(0)]^2\rangle=E(\omega_n,T)\end{aligned} \tag{4.6}$$

and obtain

$$\langle [Q_0(t)]^2\rangle = \dot{A}(t)^2\langle [Q_0(0)]^2\rangle + 2\dot{A}(t)A(t)\langle \{Q_0(0),P_0(0)\}\rangle + A(t)^2\langle [P_0(0)]^2\rangle + X(t) , \tag{4.7}$$

$$\langle [P_0(t)]^2\rangle = \ddot{A}(t)^2\langle [Q_0(0)]^2\rangle + 2\ddot{A}(t)\dot{A}(t)\langle \{Q_0(0),P_0(0)\}\rangle + \dot{A}(t)^2\langle [P_0(0)]^2\rangle + Y(t) , \tag{4.8}$$

$$\langle \{Q_0(t),P_0(t)\}\rangle = \frac{1}{2}\frac{d}{dt}\langle [Q_0(t)]^2\rangle , \tag{4.9}$$

where we have defined the new auxiliary quantities

$$X(t) = \sum_{n=1}^{N} \{[\dot{A}_{n0}(t)]^2/\omega_n^2 + [A_{n0}(t)]^2\} E(\omega_n,T) ,$$
$$Y(t) = \sum_{n=1}^{N} \{[\ddot{A}_{n0}(t)]^2/\omega_n^2 + [\dot{A}_{n0}(t)]^2\} E(\omega_n,T) . \tag{4.10}$$

Since the amplitude decays to zero as $t\to\infty$ the functions $X(t)$ and $Y(t)$ must approach the stationary mean squares $\langle [Q_0(\infty)]^2\rangle$ and $\langle [P_0(\infty)]^2\rangle$, respectively. We shall show presently that these are actually the equilibrium expectation values.

In order to bring the quantities $X(t)$ and $Y(t)$ into manageable form we recall the results (2.7) and (2.8) for the matrix elements $X_{n\nu}$ and A_{n0} which imply that the amplitudes $A_{n0}(t)$ can be looked upon as driven oscillations according to

$$\ddot{A}_{n0}(t) + \omega_n^2 A_{n0}(t) = -\epsilon_n A(t) . \tag{4.11}$$

Using this to express $A_{n0}(t)$ and its derivatives by $A(t)$ we can carry out the sums in (4.10) in the sense of (2.9) and obtain

$$X(t) = \int_0^\infty d\omega \frac{\gamma(\omega)}{\omega^2} \left| \int_0^t dt' e^{i\omega t'} A(t') \right|^2 E(\omega,T) ,$$
$$Y(t) = \int_0^\infty d\omega \frac{\gamma(\omega)}{\omega^2} \left| \int_0^t dt' e^{i\omega t'} \dot{A}(t') \right|^2 E(\omega,T) . \tag{4.12}$$

V. CONSTRAINED EQUILIBRIUM

Another nonequilibrium situation of physical interest arises if we impose by some external means fixed expectation values of the displacement and the momentum of the central oscillator. After allowing the coupled system to equilibrate otherwise, the constraints are relaxed at some moment of time to be referred to as $t=0$. We obtain the appropriate initial density operator, a generalized canonical operator, by maximizing the entropy of the system described by the Hamiltonian (2.1), accounting for the constraints

$$\langle Q_0(0)\rangle = Q , \quad \langle P_0(0)\rangle = P \tag{5.1}$$

beyond the usual ones of fixed mean energy and normalization. The density operator then reads

$$\rho(0) = Z^{-1} e^{-\beta(H+\xi Q_0+\eta P_0)} \tag{5.2}$$

with additional Lagrange parameters ξ and η to be fixed by the constraints (5.1).

The exponent in (5.2) being a quadratic form in the $N+1$ pairs P_ν, Q_ν we are again, as for the canonical operator (3.1), facing a Gaussian ensemble. Moreover, both density operators are diagonalized by the same matrix $X_{\mu\nu}$. The normal coordinates appropriate for (5.2), Q_ν'' and P_ν'', are related to Q_ν and P_ν by

$$P_\mu = \sum_{\nu=0}^{N} X_{\mu\nu} P_\nu'' - \eta\delta_{\mu 0} ,$$
$$Q_\mu = \sum_{\nu=0}^{N} X_{\mu\nu} Q_\nu'' - \xi \sum_{\nu=0}^{N} X_{0\nu} X_{\mu\nu}/z_\nu^2 . \tag{5.3}$$

This transformation allows for the determination of the Lagrange parameters as

$$\xi = -Q\Omega_1^2 , \quad \eta = -P , \tag{5.4}$$

$$\Omega_1^{-2} = \sum_{\lambda=0}^{N} X_{0\lambda}^2/z_\lambda^2 = \frac{1}{2\pi i}\oint dz \frac{1}{zg(z)} . \tag{5.5}$$

Note that the frequency Ω_1 would reduce to the unperturbed eigenfrequency ω_0 of the central oscillator if the couplings ϵ_n were all switched off. We shall meet this quantity several times below.

We also infer from (5.3) the initial mean displacements and momenta of the bath oscillators and thus find the time-dependent mean displacement of the central oscillator as

$$\langle Q_0(t)\rangle = a(t)Q + A(t)P , \quad \langle P_0(t)\rangle = \frac{d}{dt}\langle Q_0(t)\rangle , \tag{5.6}$$

$$a(t) = 1 - \Omega_1^2 \int_0^t dt' A(t') . \tag{5.7}$$

Since the constraints (5.1) do not involve any moments beyond first-order ones the variances must take their equilibrium values at all times $t\geq 0$. We can therefore find the second moments of $Q_0(t)$ and $P_0(t)$ without any new calculations as

$$\langle [Q_0(t)]^2\rangle = \langle Q_0(t)\rangle^2 + \langle Q_0^2\rangle_{\rm eq} ,$$
$$\langle [P_0(t)]^2\rangle = \langle P_0(t)\rangle^2 + \langle P_0^2\rangle_{\rm eq} ,$$
$$\langle \{Q_0(t),P_0(t)\}\rangle = \langle Q_0(t)\rangle\langle P_0(t)\rangle . \tag{5.8}$$

VI. FREQUENCY INTEGRALS

We now turn to the problem of evaluating the complex integrals (3.4), (4.4), and (5.5) which are all of the structure

$$\sum_{\nu=0}^{N} X_{0\nu}^2 f(z_\nu) = \frac{1}{2\pi i}\oint dz \frac{z}{g(z)} f(z) \equiv I(\{f\}) \tag{6.1}$$

with suitable functions $f(z)$. As already mentioned in Sec. II the closed contour encircles the $2(N+1)$ zeros of $f(z)$ in the positive sense but leaves eventual singularities of $f(z)$ (save for a possible pole at the origin) outside. In the limit of a dense spectrum of bath frequencies these poles merge to a cut along the real z axis. We can thus place the contour along the edges of the cut where the

function $g(z)$ takes the values

$$g_{\pm}(x)=g(x\pm i0^{+})$$
$$=x^2-\omega_0^2+\mathrm{P}\int_0^{\infty}d\omega\frac{\gamma(\omega)}{\omega^2-x^2}\pm i\pi\frac{\gamma(|x|)}{2x}\ . \tag{6.2}$$

The integrals (6.1) can then be written as

$$I(\{f\})=\tfrac{1}{2}\int_{-\infty}^{+\infty}dx\frac{f(x)\gamma(|x|)}{g_+(x)g_-(x)}\ . \tag{6.3}$$

In exploiting the identity (6.3) we assign to the amplitude $A(t)$ and to the correlation function $C(t)$ the following Fourier integrals:

$$A(t)=\int_0^{\infty}d\omega\frac{\gamma(\omega)}{g_+(\omega)g_-(\omega)\omega}\sin(\omega t)\ , \tag{6.4}$$

$$C(t)=\int_0^{\infty}d\omega\frac{\gamma(\omega)E(\omega,T)}{g_+(\omega)g_-(\omega)\omega^2}\cos(\omega t)\ . \tag{6.5}$$

Similarly, we may bring the definition (5.5) of the shifted frequency to the form

$$\Omega_1^{-2}=\int_0^{\infty}d\omega\frac{\gamma(\omega)}{\omega^2 g_+(\omega)g_-(\omega)}\ . \tag{6.6}$$

Finally, we would like to remark that the identity (6.3), together with (4.12) and (4.5), can be used to prove that the nonequilibrium mean squares $\langle Q_0(t)^2\rangle$ and $\langle P_0(t)^2\rangle$ as given in (4.7), (4.8), and (4.12) relax to the equilibrium ones, i.e.,

$$\langle Q_0^2\rangle_{\mathrm{eq}}=C(0)=X(\infty)\ ,$$
$$\langle P_0^2\rangle_{\mathrm{eq}}=-\ddot{C}(0)=Y(\infty)\ . \tag{6.7}$$

Having replaced the original frequency sums by integrals in the quantities Ω_1, $\langle Q_0^2\rangle_{\mathrm{eq}}$, $\langle P_0^2\rangle_{\mathrm{eq}}$, $A(t)$, $C(t)$, $X(t)$, and $Y(t)$ we are in effect facing an infinite number of degrees of freedom. It is therefore worthwhile to check that the integrals in question are free of both infrared and ultraviolet divergencies. Indeed, any spectral strength $\gamma(\omega)$ consistent with the positivity condition (2.11) leads to integrable behavior of $\gamma(\omega)/\omega^2$ near $\omega=0$ and $\omega\to\infty$. It follows that $(g_+g_-)^{-1}$ approaches a finite constant at zero frequency and falls off as ω^{-4} for large ω. The convergence of the integrals representing the amplitude $A(t)$ and the shifted frequency Ω_1 is thus obvious. The temperature-dependent quantities $C(t)$ given in (6.5), and $\langle Q_0^2\rangle_{\mathrm{eq}}$ and $\langle P_0^2\rangle_{\mathrm{eq}}$ given in (6.7), on the other hand, also converge since $E(\omega,T)\to k_BT$ for $\omega\to 0$ and $E(\omega,T)\to\omega$ for $\omega\to\infty$. General statements about the quantities $X(t),Y(t)$ at finite times are more difficult to achieve.

VII. ULLERSMA'S SPECTRAL STRENGTH

Ullersma[2] has given some physical motivation for a particular choice of the spectral strength,[18]

$$\gamma(\omega)=\frac{2}{\pi}\frac{\kappa\alpha^2\omega^2}{\alpha^2+\omega^2}\ . \tag{7.1}$$

The two parameters involved, κ and α, both have the dimension of a frequency. They are restricted to obey

$$\alpha\kappa\le\omega_0^2 \tag{7.2}$$

by the positivity condition (2.11). The combination $\kappa\alpha^2$ obviously measures the overall strength of the coupling of the central oscillator to the heat bath. The meaning of α can be inferred from the response function

$$\phi_{\mathrm{bath}}(t)=\frac{i}{\hbar}\left\langle\left[\sum_{n=1}^{N}\epsilon_n Q_n(t),\sum_{m=1}^{N}\epsilon_m Q_m(0)\right]\right\rangle \tag{7.3}$$

with the time dependence according to the free bath Hamiltonian ($\epsilon_n=0$). In the continuum limit and with the spectral strength (7.1) we have

$$\phi_{\mathrm{bath}}(t)=\int_0^{\infty}d\omega\,\gamma(\omega)\frac{1}{\omega}\sin(\omega t)=\kappa\alpha^2e^{-\alpha t} \tag{7.4}$$

and thus recognize α^{-1} as the response time of the bath observable to which the displacement of the central oscillator is coupled in the Hamiltonian (2.1).

The most important virtue of (7.1) is that it allows for closed-form expressions for all of the frequency integrals encountered above. Especially the functions $g_{\pm}(\omega)$ take the form

$$g_{\pm}(\omega)=\omega^2-\omega_0^2+\frac{\kappa\alpha^3}{\alpha^2+\omega^2}\pm i\frac{\kappa\alpha^2\omega}{\alpha^2+\omega^2}\ , \tag{7.5}$$

where the shifted frequency comes out as

$$\Omega_1^2=\omega_0^2-\alpha\kappa\ . \tag{7.6}$$

Due to (7.2) Ω_1^2 is non-negative.

Before turning to the other frequency integrals it is instructive to discuss the zeros of the denominator in the integrand in (6.3) in some detail. There are obviously three pairs of complex conjugate zeros. Of the three roots with positive imaginary parts one is always purely imaginary and will be denoted as $i\lambda$. The other two roots are either also purely imaginary ($i\Gamma_{\pm}$) or lie symmetrically to the imaginary axis ($i\Gamma\pm\Omega$). The three roots with positive imaginary parts obey the identities

$$0=\lambda-\alpha+2\Gamma\ , \tag{7.7}$$

$$\omega_0^2=\Omega^2+\Gamma^2+2\lambda\Gamma\ , \tag{7.8}$$

$$\Omega_1^2=(\Omega^2+\Gamma^2)(\lambda/\alpha)\ . \tag{7.9}$$

These remain correct in the overdamped case in which Ω is imaginary.

Figure 1 shows how the pair $i\Gamma\pm\Omega$ moves in the complex plane as $\kappa\alpha/\omega_0^2$ is varied for $\alpha/\omega_0=10$. For small values of $\kappa\alpha/\omega_0^2$ we have $\Gamma\ll\Omega$. Upon increasing $\kappa\alpha/\omega_0^2$ we find Γ to grow and Ω to decrease until, at $\kappa\alpha/\omega_0^2\approx 0.99$, the two roots $i\Gamma\pm\Omega$ meet on the imaginary axis. For yet higher coupling Ω becomes imaginary so that $i\Gamma\pm\Omega$ turn into a pair of purely imaginary zeros, $i\Gamma_{\pm}=i(\Gamma\pm|\Omega|)$. We shall show presently that the fate of the two roots just described reflects the transition from weak damping to overdamping of the mean displacement of the central oscillator.[19] As a further illustration we display, in Fig. 2, the ratio $\Gamma/(\Omega^2+\Gamma^2)^{1/2}$ as a function of $\kappa\alpha/\omega_0^2$ for various fixed values of α/Ω_0. The plot shows that the case of overdamping, $\Omega^2\le 0$, is possible only for $\alpha/\omega_0\ge\sqrt{3}$.

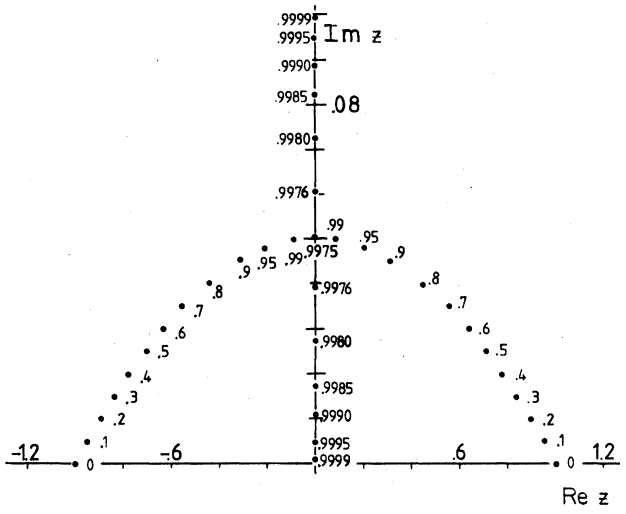

FIG. 1. The two roots $i\Gamma\pm\Omega$ are represented by dots in the complex plane, labeled by the corresponding values of the parameter $\kappa\alpha/\omega_0^2$. Ratio α/ω_0 was chosen as 10.

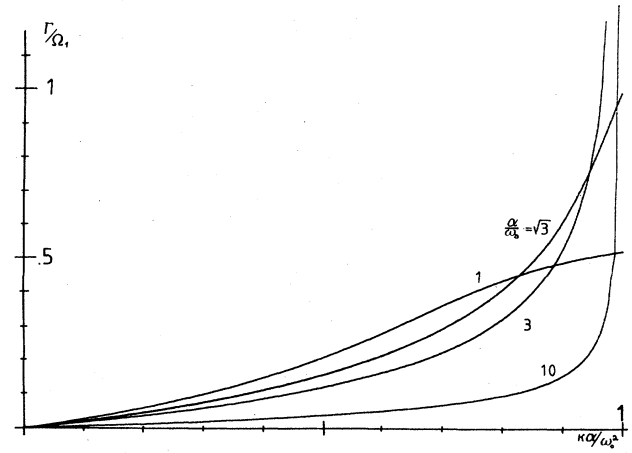

FIG. 2. Ratio $\Gamma/(\Omega^2+\Gamma^2)^{1/2}$ as a function of $\kappa\alpha/\omega_0^2$. Curves pertain to different value of the parameter α/ω_0.

The amplitude governing the relaxation of the means $\langle Q_0(t)\rangle$ and $\langle P_0(t)\rangle$ can now be written as[2]

$$A(t)=\frac{2\Gamma}{\lambda^2+\Omega^2+\Gamma^2-2\lambda\Gamma}[e^{-\lambda t}-e^{-\Gamma t}\cos(\Omega t)] + \frac{\lambda^2+\Omega^2-\Gamma^2}{\lambda^2+\Omega^2+\Gamma^2-2\Gamma\lambda}\frac{1}{\Omega}e^{-\Gamma t}\sin(\Omega t)\,. \quad (7.10)$$

The equilibrium correlation function $C(t)$ takes a more complicated form due to the poles of $E(\omega,T)$ in the complex ω plane at integer multiples of $i\nu$ where

$$\nu=2\pi k_B T/\hbar \quad (7.11)$$

has the meaning of a thermal relaxation time. We find[11,20]

$$C(t)=\frac{k_B T\lambda^2}{\lambda^2+\Omega^2+\Gamma^2-2\lambda\Gamma}\left\{\frac{e^{-\Gamma t}}{\Omega^2+\Gamma^2}\left[\left[1+\frac{\Omega^2-3\Gamma^2}{\lambda^2}\right]\cos(\Omega t)+\frac{\Gamma}{\Omega}\left[1+\frac{3\Omega^2-\Gamma^2}{\lambda^2}\right]\sin(\Omega t)\right]\right.$$
$$+\sum_{l=1}^{\infty}\left[\frac{4\Gamma}{\nu\lambda^2}\mathrm{Re}\left[\frac{(\lambda/\nu)e^{-\lambda t}-le^{-\nu lt}}{(\lambda/\nu)^2-l^2}-\frac{(1/\nu)(\Gamma+i\Omega)e^{-(\Gamma+i\Omega)t}-le^{-\nu lt}}{(\Gamma+i\Omega)^2/\nu^2-l^2}\right]\right.$$
$$\left.\left.-\frac{2}{\Omega\nu}\left[1+\frac{\Omega^2-\Gamma^2}{\lambda^2}\right]\mathrm{Im}\left[\frac{(1/\nu)(\Gamma+i\Omega)e^{-(\Gamma+i\Omega)t}-le^{\nu lt}}{(\Gamma+i\Omega)^2/\nu^2-l^2}\right]\right]\right\}. \quad (7.12)$$

From this result we finally obtain the equilibrium mean squares $\langle Q_0^2\rangle_{\mathrm{eq}}$ and $\langle P_0^2\rangle_{\mathrm{eq}}$ as $C(0)$ and $-\ddot{C}(0)$, respectively. We can even sum up the contributions from the thermal poles to expressions involving the digamma function ψ,

$$\langle Q_0^2\rangle_{\mathrm{eq}}=\frac{k_B T\lambda^2}{\lambda^2+\Omega^2+\Gamma^2-2\lambda\Gamma}\left[\frac{1+\lambda^{-2}(\Omega^2-3\Gamma^2)}{\Omega^2+\Gamma^2}+\frac{2\Gamma}{\lambda^3}-\frac{4\Gamma}{\nu\lambda^2}\mathrm{Re}[\psi(1+\lambda/\nu)-\psi(1+(\Gamma+i\Omega)/\nu)]\right.$$
$$\left.+\frac{2}{\Omega\nu}\left[1+\frac{\Omega^2-\Gamma^2}{\lambda^2}\right]\mathrm{Im}\psi(1+(\Gamma+i\Omega)/\nu)\right], \quad (7.13)$$

$$\langle P_0^2\rangle_{\mathrm{eq}}=\frac{k_B T\lambda^2}{\lambda^2+\Omega^2+\Gamma^2-2\lambda\Gamma}\left[1+\frac{\Omega^2-3\Gamma^2}{\lambda^2}-\frac{2\Gamma}{\lambda}-\frac{4\Gamma}{\nu}\mathrm{Re}[\psi(1+\lambda/\nu)-\psi(1+(\Gamma+i\Omega)/\nu)]\right.$$
$$\left.+\frac{2}{\nu\Omega}\left[\Omega^2-\Gamma^2+\frac{(\Omega^2+\Gamma^2)^2}{\lambda^2}\right]\mathrm{Im}\psi(1+(\Gamma+i\Omega)/\nu)\right]. \quad (7.14)$$

We shall not write down, for the moment being, the even lengthier closed-form expressions for the quantities $X(t)$ and $Y(t)$ which describe the relaxation of the mean squares $\langle[Q_0(t)]^2\rangle$ and $\langle[P_0(t)]^2\rangle$ into equilibrium.

In discussing these exact results special interest is due to the instant response

$$\alpha,\lambda \gg |\Gamma+i\Omega| \ . \tag{7.15}$$

The bath oscillators cannot constitute a heat bath unless the inequality (7.15) holds, i.e., unless the response time of $\sum_n \epsilon_n Q_n(t)$ in the free bath is much smaller than the time constants of the central oscillator. For times larger than $1/\lambda$ and apart from corrections of order $|\Gamma+i\Omega|/\lambda$ the amplitudes $A(t)$ and $a(t)$ then simply undergo damped oscillations with the complex frequency $\Omega+i\Gamma$,

$$\begin{aligned} A(t) &\overset{t>1/\lambda}{\longrightarrow} A_{\rm as}(t)=\frac{1}{\Omega}e^{-\Gamma t}\sin(\Omega t) \ , \\ a(t) &\overset{t>1/\lambda}{\longrightarrow} a_{\rm as}(t)=e^{-\Gamma t}\left[\cos(\Omega t)+\frac{\Gamma}{\Omega}\sin(\Omega t)\right] \ . \end{aligned} \tag{7.16}$$

For imaginary Ω the result (7.16) remains correct, too, but A and a then creep to zero as for an overdamped oscillator.

We should note that in the limit (7.15) the damping constant Γ can be evaluated explicitly as

$$\Gamma=\kappa/2 \tag{7.17}$$

while the shifted frequency Ω_1 becomes the modulus of the complex frequency $\Omega+i\Gamma$,

$$\Omega_1^2=\Omega^2+\Gamma^2 \ . \tag{7.18}$$

We should note that the replacement (7.16) corresponds to the formal limit $\lambda\to\infty$ in (7.10) and (5.7). It will be important below that this limit is uniform in time for $a(t)$, $A(t)$, and $\dot{A}(t)$. However, $\ddot{A}(t)$ is not uniformly in time approximated by $\ddot{A}_{\rm as}(t)$; for $t>0$ (7.16) does give the right limit as $\lambda\to\infty$, but the initial values $\ddot{A}(0)$ and $\ddot{A}_{\rm as}(0)$ differ; we have $\ddot{A}(0)=0$ but $\ddot{A}_{\rm as}(0)=-2\Gamma$. We shall come back to such "initial slip" effects in Sec. X.

According to (4.3), (5.6), and (7.16) the mean value $\langle Q_0(t)\rangle$ tends, for $t>1/\lambda$, to behave like the displacement of a classical damped harmonic oscillator, i.e., obeys the differential equation[2]

$$\langle\ddot{Q}_0(t)\rangle_{\rm as}+2\Gamma\langle\dot{Q}_0(t)\rangle_{\rm as}+\Omega_1^2\langle Q_0(t)\rangle_{\rm as}=0 \ . \tag{7.19}$$

The temperature-dependent quantities $C(t)$, $\langle Q_0^2\rangle_{\rm eq}$, $\langle P_0^2\rangle_{\rm eq}$, $X(t)$, and $Y(t)$, on the other hand, take especially simple and well known[2] forms in the classical limit

$$k_BT/\hbar \gg \alpha \ , \lambda \gg |\Gamma+i\Omega| \tag{7.20}$$

in which the lifetime of thermal fluctuations of the bath observable $\sum_n \epsilon_n q_n(t)$ is smaller yet than the response time $1/\alpha$. For $t>1/\lambda$, the classical expressions read

$$C_{\rm as}(t)=\frac{k_BT}{\Omega_1^2}e^{-\Gamma t}\left[\cos(\Omega t)+\frac{\Gamma}{\Omega}\sin(\Omega t)\right] \ , \tag{7.21a}$$

$$\Omega_1^2\langle Q_0^2\rangle_{\rm eq}=\langle P_0^2\rangle_{\rm eq}=k_BT \ , \tag{7.21b}$$

$$X_{\rm as}(t)=(k_BT/\Omega_1^2)\{1-[a_{\rm as}(t)]^2-\Omega_1^2[A_{\rm as}(t)]^2\} \ , \tag{7.21c}$$

$$Y_{\rm as}(t)=k_BT\{1-[\dot{A}_{\rm as}(t)]^2-\Omega_1^2[A_{\rm as}(t)]^2\} \ . \tag{7.21d}$$

We should note that the results (7.16) and (7.21) are correct regardless of the ratio Γ/Ω. Especially, their region of validity includes the cases of strong damping ($\Gamma\approx\Omega$) and overdamping (Ω imaginary).

VIII. QUANTUM EFFECTS

Nonclassical behavior arises if the bath response is fast with regard to the thermal relaxation time,

$$\alpha,\lambda \gg \nu, |\Gamma+i\Omega| \ , \tag{8.1}$$

irrespective of the relative magnitudes of ν, Γ, and Ω. Our exact results then take the asymptotic forms, for $t>1/\lambda$,

$$\begin{aligned} C_{\rm as}(t)=(k_BT/\Omega_1^2)e^{-\Gamma t}&\left[\cos(\Omega t)+\frac{\Gamma}{\Omega}\sin(\Omega t)\right] \\ &+\frac{\hbar}{2\pi\Omega}\mathrm{Im}\{e^{-(\Gamma+i\Omega)t}[\psi(1+(\Gamma+i\Omega)/\nu) \\ &\qquad -\psi(1-(\Gamma+i\Omega)/\nu)]\} \\ &+\frac{\hbar}{\pi\Omega}\mathrm{Im}\sum_{l=1}^{\infty}\frac{le^{-l\nu t}}{(\Gamma+i\Omega)^2/\nu^2-l^2} \ , \end{aligned} \tag{8.2}$$

$$\langle Q_0^2\rangle_{\rm eq}=C(0)=\frac{k_BT}{\Omega_1^2}+\frac{\hbar}{\pi\Omega}\mathrm{Im}\psi(1+(\Gamma+i\Omega)/\nu) \ , \tag{8.3}$$

$$\begin{aligned} \langle P_0^2\rangle_{\rm eq}=k_BT&+\frac{2}{\pi}\hbar\Gamma\,\mathrm{Re}\left[\ln\frac{\lambda}{\nu}-\psi(1+(\Gamma+i\Omega)/\nu)\right] \\ &+\frac{\hbar(\Omega^2-\Gamma^2)}{\pi\Omega}\mathrm{Im}\psi(1+(\Gamma+i\Omega)/\nu) \ . \end{aligned} \tag{8.4}$$

Note that (8.2) and (8.3) formally result from (7.12) and (7.13) by taking the limit $\lambda\to\infty$. In obtaining (8.4) we have also neglected corrections of order $|\Gamma+i\Omega|/\lambda$ and ν/λ; we could not simply let $\lambda\to\infty$, however, because of a logarithmic divergence we would incur in the digamma function,

$$\psi(1+\lambda/\nu)\to\ln\frac{\lambda}{\nu}+O(\nu/\lambda) \ . \tag{8.5}$$

We should also note that (8.4) cannot be derived from (8.2) as $-\ddot{C}_{\rm as}(0)$ because by taking two time derivatives in (8.2) we do not obtain an approximation for $\ddot{C}(t)$ which is uniform in time. We are again facing an initial-slip phenomenon here.

In order to obtain the asymptotic versions of the quantities $X(t)$ and $Y(t)$ we use the exact result (7.10) for both $A(t)$ and $\dot{A}(t)$ in (4.12). After performing the time and frequency integrals we extract the leading terms in $1/\lambda$. Again for $t>1/\lambda$, we have

$$\begin{aligned} X_{\rm as}(t)=\{1+[a_{\rm as}(t)]^2\}\langle Q_0^2\rangle_{\rm eq}&+[A_{\rm as}(t)]^2\langle P_0^2\rangle_{\rm eq} \\ &+2[A(t)\dot{C}(t)-a(t)C(t)]_{\rm as} \ , \end{aligned} \tag{8.6}$$

$$Y_{\rm as}(t)=\Omega_1^4[A_{\rm as}(t)]^2\langle Q_0^2\rangle_{\rm eq}+\{1+[\dot{A}_{\rm as}(t)]^2\}\langle P_0^2\rangle_{\rm eq}$$
$$+2[\Omega_1^2 A(t)\dot{C}(t)+\dot{A}(t)\ddot{C}(t)]_{\rm as}\ . \qquad (8.7)$$

These remarkably simple expressions generalize the classical results (7.21). They correctly imply $X(\infty)=\langle Q_0\rangle_{\rm eq}$ and $Y(\infty)=\langle P_0^2\rangle_{\rm eq}$ as well as the initial values $X(0)=Y(0)=0$. We should emphasize again, however, that we may use (8.2) to obtain $\dot{C}(t)$ and $\ddot{C}(t)$ for $t>1/\lambda$ only. To ensure $Y(0)=0$ from (8.7) we must use the correct initial value $\ddot{C}(0)=-\langle Q_0^2\rangle_{\rm eq}$.

It is instructive to further specialize the above results for the various order-of-magnitude relations between $k_BT/\hbar$, Γ, and Ω or $|\Omega|$ which are compatible with the instant-response limit (8.1).

For applications in quantum optics, for instance, one is mostly interested in the case of short-lived thermal transients, $\Gamma\ll\nu$. In that regime, it makes sense to restrict the consideration to times larger than $1/\nu$, i.e., to neglect the thermal transients in the expression (8.2) for the correlation function $C_{\rm as}(t)$. Of course, we thus incur an initial slip since the resulting expression does not extrapolate back to $\langle Q_0^2\rangle_{\rm eq}$ at $t=0$. If we use (8.9a) in the results (8.6) and (8.7) the initial slip in $C(t)$ carries over to the quantities $X(t)$ and $Y(t)$. By expanding the digamma functions in powers of Γ/ν we reveal the slip effects in question as of relative order Γ/ν.

Figure 3 illustrates the behavior of the equilibrium second moments (8.3) and (8.4) for $\Gamma/\nu=0.01$, a case marginally compatible with the limit $\Gamma\ll\nu$. Note the considerable difference between $\langle P_0^2\rangle_{\rm eq}$ and the unperturbed thermal energy $E(\Omega_1)$. That difference becomes negligible only for much smaller values of Γ/ν.

Often, one is even confronted with weak damping such that $\Gamma\ll\nu$ is sharpened to $\Gamma\ll\nu,\Omega$. It is appropriate, then, to neglect Γ against ν and Ω everywhere except in the exponentials $\exp(-\Gamma t)$. We thus recover the ideal weak-damping behavior characterized in the Introduction. There might, on the other hand, be situations in which corrections of first order in Γ/Ω or Γ/ν are observable. Such corrections are immediately obtained by expanding

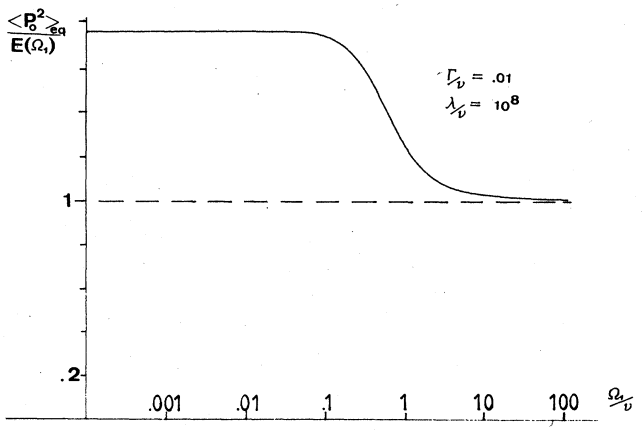

FIG. 3. Equilibrium expectation values $\langle P_0^2\rangle_{\rm eq}$ (solid line) and $\Omega_1^2\langle Q_0^2\rangle$ (dashed line) according to (8.3) and (8.4). Note the large difference between these two quantities.

the expressions given in (8.2)–(8.4). Of special interest may be the logarithmic anomaly $\sim\Gamma\ln(\lambda/\nu)$ in (8.4).

Quantum effects become much more pronounced when the temperature is sufficiently low for the lifetime $1/\nu$ of the thermal transients to be larger than the relaxation time $1/\Gamma$ and the period $1/\Omega$,

$$\nu\ll\Gamma,\Omega\ . \qquad (8.8)$$

In writing down the corresponding asymptotic results for the static mean squares we must distinguish the case of real Ω (damped oscillation),

$$\langle Q_0^2\rangle_{\rm eq}=\frac{\hbar}{\pi\Omega}\arctan\left[\frac{\Omega}{\Gamma}\right]+\frac{2\pi}{3}(k_BT)^2\frac{\Gamma}{\hbar\Omega_1^4}+O(T^3)\ , \qquad (8.9a)$$

$$\langle P_0^2\rangle_{\rm eq}=\frac{\hbar}{\pi\Omega}(\Omega^2-\Gamma^2)\arctan\left[\frac{\Omega}{\Gamma}\right]$$
$$+\frac{2}{\pi}\hbar\Gamma\ln\left[\frac{\alpha}{\Omega_1}\right]+O(T^3)\ , \qquad (8.9b)$$

from the case of overdamping (imaginary Ω),

$$\langle Q_0^2\rangle_{\rm eq}=\frac{\hbar}{\pi(\Gamma_+-\Gamma_-)}\ln\left[\frac{\Gamma_+}{\Gamma_-}\right]$$
$$+\frac{\pi}{3}(k_BT)^2\frac{\Gamma_++\Gamma_-}{\hbar(\Gamma_+\Gamma_-)^2}+O(T^3)\ , \qquad (8.9c)$$

$$\langle P_0^2\rangle_{\rm eq}=\frac{\hbar}{\pi}(\Gamma_++\Gamma_-)\ln\left[\frac{\alpha}{\sqrt{\Gamma_+\Gamma_-}}\right]$$
$$-\frac{\hbar}{2\pi}\frac{\Gamma_+^2+\Gamma_-^2}{\Gamma_+-\Gamma_-}\ln\left[\frac{\Gamma_+}{\Gamma_-}\right]+O(T^3)\ . \qquad (8.9d)$$

These expressions are equivalent to the results of Ref. 3. For strong damping ($\Gamma\lesssim\Omega$) and for the case of overdamping these mean squares differ radically from the corresponding ones of a free harmonic oscillator ($\Gamma=0$) at low temperatures (see Fig. 4). Especially noteworthy may be the strong asymmetry between $\Omega_1^2\langle Q_0^2\rangle_{\rm eq}$ and $\langle P_0^2\rangle_{\rm eq}$ at zero temperature. Such asymmetries or squeezing effects are of potential relevance for displacement measurements of high resolution.[9]

Finally, the correlation function $C_{\rm as}(t)$ as given by (8.2) also simplifies in the low-temperature limit (8.8). Especially, the sum over thermal transients,

$$\delta C(t)=\frac{\hbar}{\pi\Omega}\mathrm{Im}\left[\sum_{l=1}^{\infty}\frac{le^{-l\nu t}}{(\Gamma+i\Omega)^2/\nu^2-l^2}\right]\ , \qquad (8.10)$$

is then well approximated by an integral as

$$\sum_{l=1}^{\infty}\rightarrow\frac{1}{\nu}\int_0^{\infty}d\omega\ . \qquad (8.9e)$$

We find, for real Q, the result to be given in terms of the exponential integral as

$$\delta C(t)=\frac{\hbar}{\pi\Omega}\mathrm{Im}\left[\int_0^\infty d\omega\frac{\omega e^{-\omega t}}{(\Gamma+i\Omega)^2-\omega^2}\right]$$

$$=\frac{\hbar}{2\pi\Omega}\mathrm{Im}\{e^{-(\Gamma+i\Omega)t}\mathrm{Ei}[(\Gamma+i\Omega)t]$$

$$+e^{+(\Gamma+i\Omega)t}\mathrm{Ei}[-(\Gamma+i\Omega)t]\}\ . \qquad (8.9f)$$

The most remarkable property of $\delta C(t)$ is its nonexponential decay at large times[9,11]

$$\delta C(t)\to-\frac{2\hbar\Gamma^3}{\pi\Omega_1^4}\left[\frac{1}{\Gamma t}\right]^2 . \qquad (8.9g)$$

Clearly, this "long-time tail" will tend to outweigh the exponentially decaying part of $C(t)$. In the case of strong damping the contribution (8.9g) to the correlation function can even be comparable in magnitude to the initial value $\langle Q_0^2\rangle$.

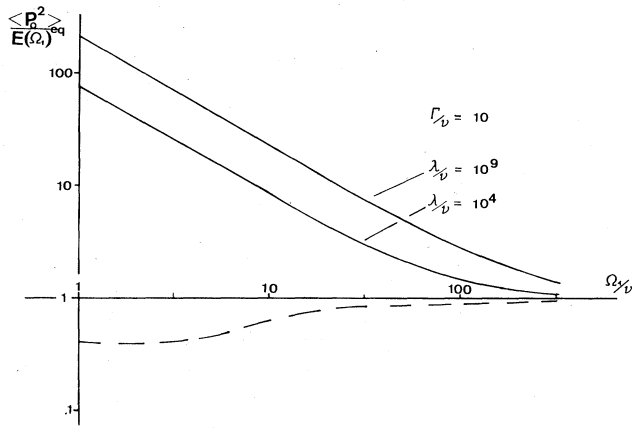

FIG. 4. This plot characterizes situations of strong squeezing. While $\Omega_1^2\langle Q_0^2\rangle_{\mathrm{eq}}$ (dashed curve) is independent of λ and remains of order unity, the kinetic energy is sensitive to λ and can acquire large values.

IX. THE WIGNER FUNCTION

For a full characterization of the statistics of the central oscillator it is not sufficient to discuss the means and the mean squares of the displacement and the momentum. We should either evaluate the means of all symmetrized products $\langle\{Q_0(t)^nP_0(t)^m\}\rangle$ or, rather more conveniently, calculate the Wigner function which has these mean values as its moments.

By associating c-number variables q_μ and p_μ with the operators Q_μ and P_μ, respectively, we can write the equation of motion for the Wigner function $W(\{q_\mu,p_\mu\},t)$ of the $N+1$ oscillators as the partial differential equation[21]

$$\dot W=LW\ , \qquad (9.1)$$

$$L=\sum_{\mu=0}^{N}\left[-\frac{\partial}{\partial q_\mu}p_\mu+\frac{\partial}{\partial p_\mu}\omega_\mu^2 q_\mu\right]$$

$$+\sum_{n=1}^{N}\epsilon_n\left[\frac{\partial}{\partial p_\mu}q_0+\frac{\partial}{\partial p_0}p_\mu\right] .$$

The method of characteristics yields the solution originating from an initial distribution $W_0(\{q_\mu,p_\mu\})$ as

$$W(\{q_\mu,p_\mu\},t)=W_0\left[\left\{\sum_\nu[\dot A_{\mu\nu}(t)q_\nu-A_{\mu\nu}(t)p_\nu]\ ,\sum_\nu[-\ddot A_{\mu\nu}(t)q_\nu+\dot A_{\mu\nu}(t)p_\nu]\right\}\right] . \qquad (9.2)$$

The reduced Wigner function $W(q_0,p_0,t)$ for the central oscillator finally obtained as the $2N$-fold integral of $W(\{q_\mu,p_\mu\},t)$ over the bath coordinates $\{q_n,p_n\}$. Fortunately, that integral can be evaluated for the two initial ensembles introduced in Secs. IV and V. The corresponding initial distributions W_0 can be constructed from the well-known Wigner function of a free harmonic oscillator of frequency ω in canonical equilibrium at the temperature T,

$$\overline{W}(q,p)=[2\pi E(\omega,T)/\omega]^{-1}\exp[-H/E(\omega,T)]\ ,$$
$$H=\tfrac{1}{2}(p^2+\omega^2q^2)\ . \qquad (9.3)$$

The partial-equilibrium density operator of (4.1) and (4.2) corresponds to a $W_0(\{q_\nu,p_\nu\})$ which is a product of $N+1$ functions. Each bath oscillator is represented by a thermal Wigner function of the form (9.3) as a factor while the central oscillator contributes an unspecified Wigner function $W_0(q_0,p_0)$,

$$W_0(\{q_\nu,p_\nu\})=W_0(q_0,p_0)\prod_{n=1}^{N}\overline{W}(q_n,p_n)\ . \qquad (9.4)$$

The constrained-equilibrium density operator (5.2), on the other hand, is associated with a product of $N+1$ thermal Wigner functions, one for each of the normal modes defined in (5.3),

$$W_0(\{q_\nu,p_\nu\})=\prod_{\nu=0}^{N}\overline{W}(q_n'',p_n'')\ . \qquad (9.5)$$

Since both functions given in (9.4) and (9.5) are Gaussians with respect to the bath coordinates we can carry out the integrals over the q_n and p_n explicitly. We shall sketch the calculation for the case of partial equilibrium.

We first extend the $2N$-fold integral defining the reduced Wigner function $W(q,p,t)$ to a $2(N+1)$-fold one as

$$W(q,p,t)=\int\left[\prod_{\nu=0}^{N}dq_\nu\,dp_\nu\right]\delta(q-q_0)\delta(p-p_0)$$

$$\times W(\{q_\mu,p_\mu\},t) \qquad (9.6)$$

and represent the delta functions by Fourier integrals. After inserting (9.2) and (9.3) we change the $2(N+1)$ integration variables q_ν,p_ν to

$$q_\mu^0=\sum_\nu[\dot A_{\mu\nu}(t)q_\nu-A_{\mu\nu}(t)p_\nu]\ ,$$
$$p_\mu^0=\sum_\nu[-\ddot A_{\mu\nu}(t)q_\nu+\dot A_{\mu\nu}(t)p_\nu]\ . \tag{9.7}$$

This transformation is interpretable as the inverse of the time evolution (2.3); it is thus unitary and has a Jacobian equal to unity. The integral (9.6) then reads

$$W(q,p,t)=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}e^{-kq+ik'p}\int dq_0^0dp_0^0\exp[-iq_0^0(k\dot A+k\ddot A)-ip_0^0(kA+k\dot A)]W_0(q_0^0,p_0^0)$$
$$\times\int\left[\prod_{n=1}^N\int dq_n^0dp_n^0\exp[-iq_n^0(k\dot A_{0n}+k'\ddot A_{0n})-ip_n^0(kA_{0n}+k'\dot A_{0n})]\overline{W}(q_n^0,p_n^0)\right]. \tag{9.8}$$

Note that the twofold integral over q_0^0 and p_0^0 now involves the Fourier transform $\tilde W_0(k\dot A+k\ddot A,kA-k'\dot A)$ of the initial Wigner function of the central oscillator. Similarly, the nth bath oscillator contributes the Fourier transform $\tilde{\overline{W}}(k\dot A_{0n}+k\ddot A_{0n},kA_{0n}+k'\dot A_{0n})$ of its thermal Wigner function (9.3),

$$\tilde{\overline{W}}(k,k')=\int dq_n^0dp_n^0e^{ikq_n^0-ik'p_n^0}\overline{W}(q_n^0,p_n^0)$$
$$=\exp\{-[k^2/\omega_0^2+(k')^2]E(\omega_nT)/2\}\ . \tag{9.9}$$

The reduced Wigner function therefore takes the form of a Fourier integral,

$$W(q,p,t)=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}e^{i(kq+k'p)}\times\tilde W_0(k\dot A(t)+k'\ddot A(t),ka(t)+k'\dot A(t))\times\exp\{-[k^2X(t)+k'^2Y(t)+kk'\dot X(t)]/2\}\ . \tag{9.4'}$$

The three functions $A(t)$, $X(t)$, and $Y(t)$ which determine the first and second moments according to (4.3), (4.7), and (4.8) are now revealed as determining the evolution in time of the whole Wigner function. This simple behavior is, of course, due to the harmonicity of the Hamiltonian (2.1) and the Gaussian initial statistics of the bath assumed in (9.4).

In the constrained-equilibrium case (9.5) we can obtain, after a similar reasoning, an even more explicit result. As we have already noted at the end of Sec. V, the constraints (5.1) do not affect the variances of the observables Q_0 and P_0 which therefore take on their equilibrium values at all times $t\geq0$. For the same reason we must expect and do indeed find a Wigner function yielding thermal, i.e., vanishing cumulants of third and higher orders; i.e., the Gaussian

$$W(q,p,t)=\frac{1}{2\pi(\langle Q_0^2\rangle_{\rm eq}\langle P_0^2\rangle_{\rm eq})^{1/2}}\times\exp\{-[q-\langle Q_0(t)\rangle]^2/2\langle Q_0^2\rangle_{\rm eq}-[p-\langle P_0(t)\rangle]^2/2\langle P_0^2\rangle_{\rm eq}\} \tag{9.5'}$$

with the first moments given by (5.6) and the equilibrium mean squares by (6.4) and (6.5).

Both Wigner functions, (9.4') and (8.5'), relax, as $t\to\infty$, to a stationary distribution which is of the form (9.5') with $\langle Q_0(t)\rangle\to0$ and $\langle P_0(t)\rangle\to0$. In the partial-equilibrium case (9.4') this statement is easily verified from $A(t)\to0$, $X(t)\to\langle Q_0^2\rangle_{\rm eq}$, $Y(t)\to\langle P_0^2\rangle_{\rm eq}$, and the normalization condition $\tilde W_0(0,0)=1$.

In order to make contact with the classical theory of random processes we now propose to discuss the equations of motion obeyed by the Wigner functions (9.4') and (9.5'). By simply differentiating these functions it is easily checked that in both cases the equation of motion is a second-order partial differential equation of the form[22]

$$\dot W(q,p,t)=lW(q,p,t)\ ,$$
$$l=-\frac{\partial}{\partial q}p-\frac{\partial}{\partial p}[f_{pq}(t)q+f_{pp}(t)p]+\frac{\partial^2}{\partial p^2}d_{pp}(t)+\frac{\partial^2}{\partial p\,\partial q}d_{pq}(t)\ . \tag{9.10}$$

The drift coefficients $f_{pq}(t)$,$f_{pp}(t)$ and the diffusion coefficients $d_{pp}(t)$,$d_{pq}(t)$ come out as

$$f_{pq}(t)=-(\ddot A^2-\dot A A)/(\dot A^2-A\ddot A)\ ,$$
$$f_{pp}(t)=-(A^2-\dot A\ddot A)/(\dot A^2-A\ddot A)\ ,$$
$$d_{pp}(t)=\tfrac12\dot Y-\tfrac12f_{pq}\dot X-f_{pp}Y\ ,$$
$$d_{pq}(t)=-Y-\tfrac12\ddot X-\tfrac12f_{pp}\dot X-f_{pq}X \tag{9.4''}$$

for the partial-equilibrium ensemble and as

$$f_{pq}(t)=-(\dot A^2-A\ddot A)/(A^2+\dot Aa/\Omega_1^2)\ ,$$
$$f_{pp}(t)=(A\dot A+\ddot Aa/\Omega_1^2)/(A^2+\dot Aa/\Omega_1^2)\ ,$$
$$d_{pp}(t)=-\langle P_0^2\rangle_{\rm eq}f_{pp}(t)\ ,$$
$$d_{pq}(t)=-\langle Q_0^2\rangle_{\rm eq}f_{pq}(t)-\langle P_0^2\rangle_{\rm eq} \tag{9.5''}$$

for the constrained-equilibrium ensemble.

In the instant-response limit (7.16) of Ullersma's spectral strength (7.1), where the amplitudes $A(t)$ and $a(t)$ are given by (7.17), the drift coefficients for the two cases (9.4″) and (9.5″) become equal to one another and independent of the time,

$$f_{pq}=-\Omega_1^2,\ f_{pp}=-2\Gamma\ . \tag{9.11}$$

The diffusion coefficients, however, remain different for the two initial ensembles. In the case of partial equilibrium we obtain for $t>0$

$$d_{pp}(t)=2\Gamma\langle P_0^2\rangle_{\rm eq}+\frac{2\pi\hbar\nu^2}{\Gamma\Omega}e^{-\Gamma t}{\rm Re}\left[e^{i\Omega t}\sum_{l=1}^{\infty}\frac{il[\Omega_1^2+l\nu(i\Omega-\Gamma)]e^{-l\nu t}}{(\Omega+il\nu)^2+\Gamma^2}\right],$$
$$d_{pq}(t)=\Omega_1^2\langle Q_0^2\rangle_{\rm eq}-\langle P_0^2\rangle_{\rm eq}+\frac{2\pi\hbar\nu^2}{\Gamma\Omega}e^{-\Gamma t}{\rm Re}\left[e^{i\Omega t}\sum_{l=1}^{\infty}\frac{l(\Omega+i\Gamma+il\nu)e^{-l\nu t}}{(\Omega+il\nu)^2+\Gamma^2}\right]. \tag{9.4‴}$$

For the constrained-equilibrium case, on the other hand, the diffusion coefficients contain no thermal transients and read

$$d_{pp}=2\Gamma\langle P_0^2\rangle_{\rm eq}\ ,$$
$$d_{pq}=\Omega_1^2\langle Q_0^2\rangle_{\rm eq}-\langle P_0^2\rangle_{\rm eq}\ . \tag{9.5‴}$$

We should accompany the presentation of the asymptotic results (9.11), (9.4‴), and (9.5‴) with a warning, however. Due to the noncommutativity of the limits $t\to 0$ and $\lambda\to\infty$ in $\ddot{A}(t)$ and $A(t)$ with $A(t)$ given by (7.10), the above asymptotic results hold for $t>0$ only. Their indiscriminate use in solving initial-value problems for the evolution equation (9.10) can amount to tampering with initial slips and lead to errors.

In the classical limit (7.20) we easily infer from (7.21) that for both initial ensembles $d_{pp}=2\Gamma k_BT$ and $d_{pq}=0$. The evolution equation thus turns out to be the Fokker-Planck equation for the Ornstein-Uhlenbeck process[5] with the asymptotic ($t>1/\lambda>1/\nu$) generator

$$l=-\frac{\partial}{\partial q}p+\frac{\partial}{\partial p}(2\Gamma p+\Omega_1^2q)+\frac{\partial^2}{\partial p^2}2\Gamma k_BT\ . \tag{9.12}$$

The only other case with a time independent generator is the one of short-lived thermal transients, $\Gamma\ll\nu$. For $T>1/\nu>1/\lambda$ we have, again for both initial ensembles,

$$l=-\frac{\partial}{\partial q}p+\frac{\partial}{\partial p}(2\Gamma p+\Omega_1^2q)+\frac{\partial^2}{\partial p^2}2\Gamma\langle P_0^2\rangle_{\rm eq}+\frac{\partial^2}{\partial p\,\partial q}(\Omega_1^2\langle Q_0^2\rangle_{\rm eq}-\langle P_0^2\rangle_{\rm eq}) \tag{9.13}$$

with the equilibrium moments given in (8.3) and (8.4). We should note that the diffusion matrix has one negative eigenvalue, due to the off-diagonal matrix element d_{pq}. The potential relevance of the off-diagonal element d_{pq} is obvious from Fig. 3. It is only in zeroth order in Γ that the generator (9.13) becomes a genuine Fokker-Planck operator which is, in fact, of the classical form (9.12) save for the replacement of the classical thermal energy k_BT by the quantum expression $E(\Omega,T)$.[2,23]

No useful analogy to any classical stochastic process survives in the low-temperature limit (8.8). Not only is the diffusion matrix nonpositive because of $d_{pq}(t)\neq 0$. Worse yet, the difference of the diffusion coefficients (9.4‴) and (9.5‴) shows that the diffusion matrix depends on the initial preparation of the heat bath. We should also emphasize that the thermal transients in the diffusion coefficients (9.4‴) live as long as the ones in the mean squares $\langle Q_0(t)^2\rangle$ and $\langle P_0(t)^2\rangle$.

X. INITIAL SLIPS

By dropping fast "mechanical" ($\sim e^{-\lambda t}$) and thermal ($\sim e^{-\nu t}$) transients from the quantities $A(t)$, $a(t)$, $C(t)$, $X(t)$, and $Y(t)$ and their time derivatives we incur important initial slips whenever the limits $\lambda\to\infty$ and $\nu\to\infty$ are not uniform in time. We have, e.g.,

$$\ddot{A}(0)=0\neq\ddot{A}_{\rm as}(0)=-2\Gamma\ . \tag{10.1}$$

Assume, now, the partial equilibrium state of (4.1), and (4.2) with given initial means $\langle Q_0(0)\rangle$ and $\langle P_0(0)\rangle$. Suppose we want to calculate the time-dependent means $\langle Q_0(t)\rangle$ and $\langle P_0(t)\rangle$ for $t>1/\lambda$, i.e., the asymptotic versions $\langle Q_0(t)\rangle_{\rm as}$ and $\langle P_0(t)\rangle_{\rm as}$. We may, of course, use the exact results (4.4) and (7.11) and let $\lambda\to\infty$ therein. We thus obtain $\langle P_0(t)\rangle_{\rm as}=(d/dt)\langle Q_0(t)\rangle_{\rm as}$ and

$$\langle P_0(t)\rangle_{\rm as}=\ddot{A}_{\rm as}(t)\langle Q_0(0)\rangle+\dot{A}_{\rm as}(t)\langle P_0(0)\rangle \tag{10.2}$$

and conclude, with the help of (10.1), that the asymptotic means extrapolation back to the effective initial values

$$\langle P_0(0)\rangle a_{\rm as}=-2\Gamma\langle Q_0(0)+\langle P_0(0)\rangle\ ,$$
$$\langle Q_0(0)\rangle_{\rm as}=\langle Q_0(0)\rangle\ . \tag{10.3}$$

Instead of employing exact results we can solve the asymptotic equation of motion (7.16). We must then, in order to recover (10.2), use the effective initial data (10.3).

Similar considerations apply to higher-order moments, to the density operator, or the Wigner function of the central oscillator whenever asymptotic equations of motion are available. We have seen asymptotic evolution equations to arise both in the classical limit and for $\Gamma\ll\nu$. For such asymptotic equations of motion to be useful they must be accompanied with effective initial data.[10]

The effective initial values for the asymptotic second moments can be read off the exact results (4.7)—(4.9),

$$\langle Q_0^2(0)\rangle_{\rm as}=\langle[Q_0(0)]^2\rangle+X_{\rm as}(0)\ ,$$

$$\langle P_0^2(0)\rangle_{\rm as}=4\Gamma^2\langle[Q_0(0)]^2\rangle-2\Gamma\langle\{Q_0(0),P_0(0)\}\rangle+\langle[P_0(0)]^2\rangle+Y_{\rm as}(0)\ , \tag{10.4}$$

$$\langle\{Q_0(0),P_0(0)\}\rangle_{\rm as}=-2\Gamma\langle[Q_0(0)]^2\rangle+\dot{X}_{\rm as}(0)\ .$$

The terms proportional to Γ are related to the slips we have found for the first moments. No additional slips arise in the classical case, as is clear from (7.21c) and (7.21d) and the uniform convergence of $a(t)$, $A(t)$, and $\dot{A}(t)$ with $\lambda\to\infty$. In the case of short-lived thermal transients ($\Gamma\ll\nu$), however, we do incur "thermal" slips since the formal limit $\nu\to\infty$ is nonuniform in time for $X(t)$ and $Y(t)$. From (8.2), (8.6), and (7.16) we determine

$$X_{\rm as}(0)=-\frac{4}{\pi}\frac{\hbar\Gamma}{\nu^2}\rho\left[\frac{\Omega}{\nu}\right]<0\ ,$$
$$\rho(x)=\sum_{l=1}^{\infty}\frac{l}{(l^2+x^2)^2}\ , \tag{10.5}$$

and a similar result for $Y_{\rm as}(0)$. It is only in zeroth order in Γ that no slips at all appear. We should recall that to that order the asymptotic evolution equation is of the Ornstein-Uhlenbeck form, with $E(\Omega,T)$ as the equilibrium energy.

The second moments $\langle Q^2\rangle$, $\langle P^2\rangle$, $\langle QP\rangle=\langle\{Q,P\}\rangle+i\hbar/2$, and $\langle PQ\rangle=\langle\{QP\}\rangle-i\hbar/2$ form a non-negative 2×2 matrix at all times $t\geq0$. However, the corresponding effective initial matrix, being an auxiliary quantity rather than an observable one, may have negative eigenvalues. As an example, consider a squeezed coherent initial state such that

$$\langle[Q_0(0)]^2\rangle=\hbar^2/4\sigma^2,\quad\langle[P_0(0)]^2\rangle=\sigma^2,$$
$$\langle\{Q_0(0),P_0(0)\}\rangle=0\ . \tag{10.6}$$

For a sufficient degree of squeezing, i.e., for sufficiently large σ^2, the effective initial mean $\langle[Q_0(0)]^2\rangle$ as given by (10.4) and (10.5) becomes negative. Conversely, the effective initial matrix is restricted by the positivity of the observable initial matrix. It is quite easy to identify forbidden effective initial data which would imply, through (10.4), negative eigenvalues for the observable initial matrix. We should mention once more that the asymptotic means $\langle[Q_0(t)]^2\rangle$, etc., take on a physical meaning for times larger than $1/\lambda$ and $1/\nu$; they meet all positivity requirements then, of course. For instance, the quantity $X_{\rm as}(t)$ is easily seen, from (8.9e), to turn positive at a time of the order $1/\nu$.

Finally, the asymptotic Wigner function can also be obtained from an asymptotic initial-value problem as

$$W_{\rm as}(q,p,t)=e^{lt}W_{\rm as}(q,p,0)\ , \tag{10.7}$$

provided there is an asymptotic time-independent generator like (9.12) or (9.13). The effective initial distribution $W_{\rm as}(q,p,0)$ can be read off (9.4′), assuming the partial equilibrium ensemble,

$$W_{\rm as}(q,p,0)=\int\frac{dk}{2\pi}\int\frac{dk'}{2\pi}e^{(ikq+k'p)}\tilde{W}_0(k-2\Gamma k',k')\times\exp\{-[k^2X_{\rm as}(0)+(k')^2Y_{\rm as}(0)]/2\}\ . \tag{10.8}$$

In the classical case this reduces to

$$W_{\rm as}(q,p,0)=W_0(q,p+2\Gamma q),\quad k_BT/\hbar\gg\lambda\gg|\Gamma+i\Omega| \tag{10.9}$$

while in zeroth order in Γ, i.e., for the extreme weak-damping limit we find the ideal no-slip case

$$W_{\rm as}(q,p,0)=W_0(q,p)+O(\Gamma)\ ,\quad\lambda\gg\Omega,\ k_BT/\hbar\gg\Gamma\ . \tag{10.10}$$

The asymptotic initial weight $W_{\rm as}(q,p,0)$ is not admitted to all of the function space accessible to a genuine Wigner function since the initial Wigner function $W_0(q,p)$ related to $W_{\rm as}(q,p,0)$ by (10.8) must have a positive matrix of second moments. On the other hand, for the integral in (10.8) to exist at all the initial Wigner function W_0 must be sufficiently sharply peaked in k space to compensate the growth of $\exp[-\frac{1}{2}k^2X_{\rm as}(0)]$ at large k.

We would like to conclude by touching upon a rather subtle but conceptually important point. By transforming the c-number evolution equation (9.10) into a master equation for the density operator ρ of the central operator we find

$$\dot{\rho}(t)=\hat{l}(t)\rho(t)$$
$$=-\frac{i}{\hbar}[\tfrac{1}{2}P_0^2-\tfrac{1}{2}f_{pq}(t)Q_0^2,\rho(t)]+\frac{i}{\hbar}f_{pp}(t)[Q_0,\{P_0,\rho(t)\}]$$
$$-\frac{1}{\hbar^2}d_{pp}(t)[Q_0,[Q_0,\rho(t)]]+\frac{1}{\hbar^2}d_{pq}(t)[P_0,[Q_0,\rho(t)]]\ . \tag{10.11}$$

This being a rigorous equation of motion for both initial ensembles considered, the positivity of the density operator $\rho(t)$ is maintained at all times if given initially.

For both the classical limit and the weak-damping case we may, as above, restrict our consideration to times larger than $1/\lambda$ and $1/\nu$. The generator $\hat{l}(t)$ then takes an asymptotic time-independent form $\hat{l}$ and the asymptotic density operator can be written as

$$\rho_{\rm as}(t)=e^{\hat{l}t}\rho_{\rm as}(0) \tag{10.12}$$

with an effective initial operator corresponding to the Wigner function (10.8). For $t>1/\lambda,1/\nu$ the asymptotic density operator (10.12) approaches the exact one $\rho(t)$ and is positive. Neither the effective initial operator $\rho_{\rm as}(0)$ nor

the operator $\rho_{as}(t)$ for $t<1/\lambda,1/\nu$ need be positive. It is even known that generators $\hat{l}$ of the form as in (10.11) with time-independent drift and diffusion coefficients can transform positive into nonpositive operators.[24]

For axiomatic approaches to master equations it would be quite a challenge to identify the class of operators (containing nonpositive ones) which are turned into positive density operators by "nonpositive" generators $\hat{l}$ according to the transformation (10.12) for sufficiently long times. In microscopic treatments no conceptual difficulties arise as long as $\hat{l}$ and $\rho_{as}(0)$ are consistently calculated and correctly interpreted. Our exactly diagonizable Hamiltonian (2.1) combined with Ullersma's spectral strength (7.1) has the special virtue of allowing for a rigorous determination of $\hat{l}$ and ρ_{as}.

XI. REMARKS ON UNIVERSALITY

As was already shown by Ullersma,[2] the behavior of the central oscillator is insensitive to the choice of the strength function $\gamma(\omega)$ in the weak-coupling limit in which $\Gamma\ll\Omega,\nu$ and $\Omega\approx\omega_0$. In fact, corrections to the ideal weak-coupling behavior [$\Gamma=0$ everywhere in $A,\dot{A},\ddot{A},C$ except in the exponentials $\exp(-\Gamma t)$] arise only in first order in $\Gamma\gamma'(\omega_0)/\gamma(\omega_0)$. The latter parameter, given by Γ/ω_0 for the special spectral strength (7.1), obviously measures the relative variation of the strength function across the resonance at $\Omega\approx\omega_0$.

For strong damping, however, we encounter a less universal behavior. To illustrate it we propose to replace Ullersma's strength (7.1) with

$$\gamma(\omega)=\frac{2\kappa\alpha^3\omega^3}{(\alpha^2+\omega^2)^2}\ . \tag{11.1}$$

The positivity condition (2.11) again implies

$$\alpha\kappa\le\omega_0^2\ . \tag{11.2}$$

In order to evaluate the frequency integral (6.3) we must discuss the principal-value integral in (6.2),

$$\mathrm{P}\int_0^\infty d\omega\frac{\gamma(\omega)}{\omega^2-x^2}=\frac{\kappa\alpha^3}{\alpha^2+x^2}\left[1+\frac{x^2}{\alpha^2+x^2}\ln\left[\frac{x^2}{\alpha^2}\right]\right]\ . \tag{11.3}$$

As the frequency x changes from zero to infinity, this integral decreases monotonically from $\kappa\alpha$ to zero. For $x=\alpha$ the decrease has gone half way, to $\kappa\alpha/2$. Since the physically interesting special cases [(6.4), (6.5), (6.8), and (6.9)] of (6.3) draw their important contributions from frequencies much smaller than the cutoff α we may, accepting relative errors of the order $|\Gamma+i\Omega|/\alpha$, replace the principal-value integral (11.3) by its value for $x=0$, i.e., by $\kappa\alpha$.

Thus simplified, the frequency integral (6.3) takes the form

$$I(\{f\})=\frac{\kappa\alpha}{\alpha^2+\pi^2\kappa^2}\int_{-\infty}^{+\infty}dx\frac{|x|^3f(x)}{|x^2-(\Omega+i\Gamma)^2|^2}\ , \tag{11.4}$$

where the complex frequency $\Omega+i\Gamma$ is given by

$$\Omega+i\Gamma=[(\omega_0^2-\kappa\alpha)/(1-i\pi\kappa/\alpha)]^{-1/2}\ . \tag{11.5}$$

While the case of imaginary Ω [overdamping in $A(t)$] cannot appear it is obviously possible to realize, by suitably choosing ω_0, κ, and α, any value for the ratio Γ/Ω without violating the inequality $|\Omega+i\Gamma|\ll\alpha$.

It is now quite straightforward to confirm Ullersma's general result for $\Gamma/\Omega\ll1$. For the strongly damped oscillator, on the other hand, more complicated expressions arise. It suffices , for our purpose, to note the following limiting results. The temperature-independent amplitude $A(t)$ is obtained from (11.4) and (6.8) as displaying an algebraic decay,

$$A(t)=\frac{\kappa\alpha}{\alpha^2+\pi^2\kappa^2}\frac{4}{(\Gamma t)^3}\quad\text{for } t>1/\Gamma\ . \tag{11.6}$$

The power law in (11.6) is due to the factor $|x|^3$ in the integrand in (11.4) which has a discontinuous third derivative at $x=0$.

For the temperature-dependent quantities $\langle Q_0^2\rangle_{eq}$ and $C(t)$ we employ (11.4), (6.4), and (6.9). At high temperatures $k_BT\gg\hbar\Gamma\approx\hbar\Omega$, we have

$$\begin{aligned}\langle Q_0^2\rangle_{eq}&=\frac{k_BT}{\Gamma^2}\frac{\kappa\alpha}{\alpha^2+\pi^2\kappa^2}\ ,\\ C(t)&=\langle Q_0^2\rangle_{eq}\frac{2}{(\Gamma t)^2}\quad\text{for}t>1/\Gamma\end{aligned} \tag{11.7}$$

while the low-temperature results ($k_BT\ll\hbar\Gamma\approx\hbar\Omega$) read

$$\begin{aligned}\langle Q_0^2\rangle_{eq}&=\frac{\hbar}{\Gamma}\frac{\pi\kappa\alpha}{4(\alpha^2+\pi^2\kappa^2)}\ ,\\ C(t)&=\langle Q_0^2\rangle_{eq}e^{-\Gamma t}[\Omega\cos(\Omega t)-\Gamma\sin(\Omega t)]\ .\end{aligned} \tag{11.8}$$

The reason for the algebraic decay of the correlation function at high temperatures is the same as in the case of the amplitude $A(t)$. At zero temperature, on the other hand, the integrand in the frequency integral representing $C(t)$ is regular at $x=0$ since $|x|^3E(x,T)\to\hbar x^4/2$ for $T\to0$; this is the reason for the exponential behavior of $C(t)$ in (11.8). Of course, there are algebraic tails in the temperature-dependent corrections to $C(t)$ in (11.8).

We must conclude that the strong-damping anomalies depend rather critically on the spectral strength $\gamma(\omega)$. Interestingly enough, both the "ultraviolet" ($\omega\gtrsim\alpha$) and the "infrared" ($\omega\to0$) properties of $\gamma(\omega)$ enter sensitively. It also follows from the above discussion that either the amplitude $A(t)$ or the correlation function $C(t)$ at low temperatures must decay algebraically provided $\gamma(\omega)\sim\omega^n$ with n integer as $\omega\to0$.[25]

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[13]Alternatively, we could start with the manifestly positive Hamiltonian

$$\tilde{H}=\tfrac{1}{2}(\tilde{p}_0+\textstyle\sum_n \tilde{\epsilon}_n\tilde{q}_n)^2+\tfrac{1}{2}\tilde{\omega}_0^2\tilde{q}_0^2+\tfrac{1}{2}\textstyle\sum_n(\tilde{p}_n^2+\tilde{\omega}_n^2\tilde{q}_n^2)$$

which has been studied by Rzążewski *et al.* (Ref. 14). This "minimal-coupling" Hamiltonian can be reduced to the one in (2.1) by a unitary transformation.

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[15]Our function $g(z)$ is related to Ullersma's $G(z)$ as $g(z)=G(z^2)$.

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[18]This choice is equivalent to the Drude regularization often used in phenomenological approaches (Ref. 3).

[19]The case of overdamping might look like an exotic exception since it requires $\alpha\kappa$ to lie very close to the upper end of the allowable interval, $0<\alpha\kappa<\omega_0^2$. It looks rather more natural a case if one starts with the minimal coupling Hamiltonian $\tilde{H}$ mentioned in Ref. 12. It is possible to show that a strength function $\tilde{\gamma}(\omega)=(2\tilde{\kappa}/\pi)\omega^2\tilde{\alpha}^2/(\omega^2+\tilde{\alpha}^2)$ pertaining to $\tilde{H}$ is equivalent to Ullersma's strength function pertaining to our H with $\alpha\kappa=\omega_0^2\tilde{\alpha}\tilde{\kappa}/(1+\tilde{\alpha}\tilde{\kappa})$. The parameter $\alpha\kappa$ takes on values near ω_0^2 for $\tilde{\alpha}\tilde{\kappa}$ in the interval $1\ll\tilde{\alpha}\tilde{\kappa}<\infty$. Strong damping and, in fact, overdamping thus appear as typical strong-coupling effects.

[20]In the case of imaginary Ω the expressions $\mathrm{Re}f(\Gamma+i\Omega)$ and $\mathrm{Im}(\Gamma+i\Omega)$ must be understood as $\frac{1}{2}[f(\Gamma_+)\pm f(\Gamma_-)]$.

[21]From the Schrödinger equation one switches to the Liouville operator by $\hat{q}\hat{X}\to[q+(i/2\hbar)\partial_p]X$, $\hat{X}\hat{q}\to[q-(i/2\hbar)\partial_p]X$; $\hat{p}\hat{X}\to[p-(i/2\hbar)\partial_q]X$, and $\hat{X}\hat{p}\to[p+(i/2\hbar)\partial_q]X$.

[22]An alternative derivation of (9.11) is sketched in Ref. 12.

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[25]It seems not uncommon that strong damping and nonexponential decay show up together. A nice example is provided by certain autoionizing states in atoms (Ref. 26).

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