Exact solution of the Hu-Paz-Zhang master equation

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The Hu-Paz-Zhang equation is a master equation for an oscillator coupled to a linear passive bath. It is exact within the assumption that the oscillator and bath are initially uncoupled. Here an exact general solution is obtained in the form of an expression for the Wigner function at time t in terms of the initial Wigner function. The result is applied to the motion of a Gaussian wave packet and to that of a pair of such wave packets. A serious divergence arising from the assumption of an initially uncoupled state is found to be due to the zero-point oscillations of the bath and not removed in a cutoff model. As a consequence, worthwhile results for the equation can only be obtained in the high temperature limit, where zero-point oscillations are neglected. In that limit closed form expressions for wave packet spreading and attenuation of coherence are obtained. These results agree within a numerical factor with those appearing in the literature, which apply for the case of a particle at zero temperature that is suddenly coupled to a bath at high temperature. On the other hand very different results are obtained for the physically consistent case in which the initial particle temperature is arranged to coincide with that of the bath.

I. INTRODUCTION

The Hu-Paz-Zhang equation is a master equation with time-dependent coefficients for a harmonic oscillator interacting with a linear passive heat bath of oscillators. The equation is exact and general within the assumption that in the initial state the bath is in equilibrium and not coupled to the oscillator. It was first derived in generality using path integral methods by Hu, Paz and Zhang [1], although equivalent equations had been obtained earlier for the case of an Ohmic bath [2,3]. See also [4]. Later a derivation in the form of an equation for the Wigner function was given by Halliwell and Yu [5], who corrected a misprint in the earlier publication. Using the notation of these last authors, the equation has the form

$$\frac{\partial W}{\partial t} = -\frac{1}{m} p \frac{\partial W}{\partial q} + m\Omega^2(t) q \frac{\partial W}{\partial p} + 2\Gamma(t) \frac{\partial p\, W}{\partial p}$$
$$+ \hbar m \Gamma(t) h(t) \frac{\partial^2 W}{\partial p^2} + \hbar \Gamma(t) f(t) \frac{\partial^2 W}{\partial q \partial p}, \quad (1.1)$$

where $\Omega^2(t)$, $2\Gamma(t)$, $h(t)$, and $f(t)$ are time-dependent parameters for which one has explicit expressions [see Eqs. (2.19) and (3.8) below].

The integration of this equation, with its time-dependent coefficients, appears to be a formidable problem. Indeed, earlier discussions have generally used numerical methods. Our purpose here is, first of all, to present an exact general solution of this equation. This solution can be evaluated in explicit, closed form for many problems of interest. In particular, we exhibit the solution for two such problems: an initial

state corresponding to a Gaussian minimum uncertainty wave packet and an initial state corresponding to a widely separated pair of such wave packets. We use these results to accomplish our second purpose, which is to critically examine the assumption of an uncoupled initial state. We find that there is a serious difficulty arising from this assumption: the zero-point oscillations of the bath give rise to a divergence that leads to an instantaneous spread of a wave packet to infinite width. In effect, the state instantaneously disappears. The result is that meaningful results can be obtained only in the high temperature limit, where one conventionally neglects the zero-point oscillations. Even in this limit, we find significant difficulties arising from the fact that translational invariance is broken. Nevertheless, we find for short times expressions for wave packet spreading and attenuation of coherence that are consistent with those found by earlier authors. On the other hand, by adjusting the initial temperature of the particle to be the same as that of the bath, we find in the high temperature Ohmic limit results consistent with exact calculations which take into account entanglement at all times [6,7].

The plan of this paper is as follows. The basis for our discussion is the quantum Langevin equation, so we begin in Sec. II with a description of that equation and its solution, first for the stationary case, then for the initial value case, and finally for the form local in time. Next in a short Sec. III we give a simple derivation of the exact master equation (1.1). Then in Sec. IV we derive our general solution. The key result, given in Eq. (4.15), is an explicit expression for the Wigner function at time t in terms of the initial Wigner function. A particularly useful result, given in Eq. (4.24), is an expression for the probability distribution at time t. In Sec. V we first evaluate this expression to find the probability distribution corresponding to an initial Gaussian wave packet. There we find the divergence mentioned above, which in the Appendix is shown to be present even in a model with a high frequency cutoff. Also in Sec. V we consider the motion of a pair of Gaussian wave packets (Schrö-

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dinger "cat" state) and obtain an explicit expression for the attenuation of coherence. For the case of a particle at temperature zero suddenly coupled to a bath at high temperature T, this leads to an expression for the decoherence time equivalent with that appearing in many places in the literature. But for a consistent initial state in which the temperature of the particle is adjusted to coincide with that of the bath, a very different expression for the decoherence time is obtained, an expression corresponding to decoherence without dissipation [7]. Finally, in Sec. VI we summarize our results and make some concluding remarks.

II. THE LANGEVIN EQUATION

A. Stationary process

The Langevin equation is a Heisenberg equation of motion for $x(t)$, the dynamical variable corresponding to the coordinate of a Brownian particle in equilibrium with a linear passive heat bath. For the case of a particle in an external oscillator potential, this equation for the stationary process has the well known form [8]

$$m\ddot{x} + \int_{-\infty}^{t} dt' \mu(t-t')\dot{x}(t') + Kx = F(t), \qquad (2.1)$$

where $\mu(t)$ is the memory function, K is the oscillator force constant and $F(t)$ is a fluctuating operator force with mean $\langle F(t)\rangle = 0$, and whose correlation and commutator are given by

$$\frac{1}{2}\langle F(t')F(t) + F(t)F(t')\rangle$$

$$= \frac{1}{\pi}\int_{0}^{\infty} d\omega \, \mathrm{Re}\{\tilde{\mu}(\omega+i0^+)\}\hbar\omega$$

$$\times \coth\frac{\hbar\omega}{2kT}\cos\omega(t-t'),$$

$$(2.2)$$

$$[F(t),F(t')] = \frac{2\hbar}{i\pi}\int_{0}^{\infty} d\omega \, \mathrm{Re}\{\tilde{\mu}(\omega+i0^+)\}\omega$$

$$\times \sin\omega(t-t').$$

Here $\tilde{\mu}(z)$ is the Fourier transform of the memory function:

$$\tilde{\mu}(z) = \int_{0}^{\infty} dt \mu(t)e^{izt}. \qquad (2.3)$$

As a consequence of the second law of thermodynamics, $\tilde{\mu}(z)$ must be what is called a positive real function: analytic and with a real part positive in the upper half plane. In particular, $\tilde{\mu}(z)$ can be represented in terms of the real part of its boundary value on the real axis through the Stieltjes inversion theorem

$$\tilde{\mu}(z) = -icz + \frac{2iz}{\pi}\int_{0}^{\infty} d\omega\frac{\mathrm{Re}\{\tilde{\mu}(\omega+i0^+)\}}{z^2-\omega^2}, \qquad (2.4)$$

where c is a positive constant.

The solution of the Langevin equation (2.1) can be written

$$x_s(t) = \int_{-\infty}^{t} dt' G(t-t')F(t'), \qquad (2.5)$$

where $G(t)$, the Green function, is given by

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\alpha(\omega+i0^+)e^{-i\omega t}, \qquad (2.6)$$

with $\alpha(z)$ the familiar response function

$$\alpha(z) = \frac{1}{-mz^2 - iz\tilde{\mu}(z) + K}. \qquad (2.7)$$

Here we have introduced a subscript s to emphasize that $x_s(t)$ is a stationary operator-process, in the sense that correlations, probability distributions, etc. for this dynamical variable are invariant under time-translation $(t\rightarrow t+t_0)$. In particular, the correlation,

$$\frac{1}{2}\langle x_s(t)x_s(t') + x_s(t')x_s(t)\rangle$$

$$= \frac{\hbar}{\pi}\int_{0}^{\infty} d\omega \, \mathrm{Im}\{\alpha(\omega+i0^+)\}\coth\frac{\hbar\omega}{2kT}\cos\omega(t-t'),$$

$$(2.8)$$

is a function only of the time-difference $t-t'$. In addition, for the free particle, where $K=0$, the process is invariant under space translation $(x\rightarrow x+a)$.

B. Langevin equation for the initial value problem

The description of the system given by the Langevin equation can be realized by a bath of harmonic oscillators. Perhaps the simplest such system, and the one we use as the basis of our discussion of the Hu-Paz-Zhang equation and its solution, is the independent oscillator model, for which the Hamiltonian is [9,8]

$$H = \frac{p^2}{2m} + \frac{1}{2}Kx^2 + \sum_{j}\left\{\frac{p_j^2}{2m_j} + \frac{1}{2}m_j\omega_j^2(q_j-x)^2\right\}. \qquad (2.9)$$

Writing the equations of motion and then eliminating the bath variables in terms of their initial values, one obtains the Langevin equation for the oscillator with given initial values [10],

$$m\ddot{x} + \int_{0}^{t} dt' \mu(t-t')\dot{x}(t') + Kx = -\mu(t)x(0) + F(t), \qquad (2.10)$$

where the memory function is given by

$$\mu(t) = \sum_{j} m_j\omega_j^2\cos\omega_j t\,\theta(t), \qquad (2.11)$$

while the random force is given in terms of the initial bath variables by

$$F(t) = \sum_j \{ q_j(0) m_j \omega_j^2 \cos \omega_j t + p_j(0) \omega_j \sin \omega_j t \}. \tag{2.12}$$

To express the solution of this equation, we first note that the Green function (2.6) vanishes for negative times and for positive times is the solution of the homogeneous equation,

$$m\ddot{G} + \int_0^t dt' \, \mu(t-t') \dot{G}(t') + KG = 0, \tag{2.13}$$

with the initial conditions

$$G(0) = 0, \quad \dot{G}(0) = \frac{1}{m}. \tag{2.14}$$

With this, we can show that the general solution of the initial value Langevin equation (2.10) is given by

$$x(t) = m\dot{G}(t)x(0) + mG(t)\dot{x}(0) + X(t)$$
$$\dot{x}(t) = m\ddot{G}(t)x(0) + m\dot{G}(t)\dot{x}(0) + \dot{X}(t), \tag{2.15}$$

where we have introduced the fluctuating position operator,

$$X(t) = \int_0^t dt' \, G(t-t') F(t'). \tag{2.16}$$

In our subsequent discussion we assume that at $t=0$ the system is in a state in which the oscillator is not coupled to the bath and that the bath is in equilibrium at temperature T. In particular this means that the initial coordinates of the oscillator are not correlated with those of the bath, i.e., $\langle x(0)F(t) \rangle = \langle \dot{x}(0)F(t) \rangle = 0$. On the other hand, with regard to the bath, the equilibrium is with respect to the bath Hamiltonian, H_{bath}, obtained by setting the oscillator variables x and p equal to zero in Eq. (2.9),

$$H_{\text{bath}} = \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 q_j^2 \right). \tag{2.17}$$

With this we find $\langle F(t) \rangle = 0$, and the correlation and commutator are the same as those for the stationary equation, given in Eqs. (2.2).

Typically, the memory function $\mu(t)$ falls to zero in a very short time τ, called the relaxation time of the bath. For times long compared with this bath relaxation time, the extra term on the right hand side of Eq. (2.10) vanishes, but only for much longer times, times long compared with the oscillator decay time, will this equation become the stationary equation, with the lower limit on the integration taken to be $-\infty$. To be more specific, we note from the general expression (2.6) for the Green function that, so long as the oscillator force constant K is not zero, the Green function will vanish exponentially for long times. This follows from the Tauberian theorem: the asymptotic behavior of a function

depends upon the low frequency behavior of its Fourier transform. It follows that, for long times, the dependence upon the initial coordinates in Eqs. (2.15) disappears and, from a comparison of Eq. (2.16) with the expression (2.5) for $x_s(t)$, that $X(t)$ becomes the solution of the stationary Langevin equation (2.1).

C. Form local in time

We want now to write the Langevin equation (2.10) in the form of an equation that is local in time with time-dependent coefficients. To get this form, we first invert Eqs. (2.15) to express the initial variables in terms of those at time t. We next form the time derivative of the second of Eqs. (2.15) and then insert these expressions for the initial variables in the right hand side. We can write the result in the form

$$\ddot{x} + 2\Gamma(t)\dot{x} + \Omega^2(t)x = \frac{1}{m} F(t), \tag{2.18}$$

where we have introduced the quantities

$$2\Gamma(t) = \frac{G(t)\dddot{G}(t) - \dot{G}(t)\ddot{G}(t)}{\dot{G}^2(t) - G(t)\ddot{G}(t)} = -\frac{d \log(\dot{G}^2 - G\ddot{G})}{dt},$$
$$\Omega^2(t) = \frac{\ddot{G}^2(t) - \dot{G}(t)\dddot{G}(t)}{\dot{G}^2(t) - G(t)\ddot{G}(t)}. \tag{2.19}$$

This equation is the local form we seek. In obtaining this form we have used the fact that $X(t)$ is the solution of the inhomogeneous equation (2.10) with the initial conditions $X(0) = 0$ and $\dot{X}(0) = 0$. It follows that $X(t)$ is also the solution of the local equation (2.18) with the same initial conditions. The fact that the symbols used for the quantities (2.19) also appear in the exact master equation (1.1) is not accidental, as we shall see in the next section, where we give a derivation of that equation.

III. THE TIME-DEPENDENT MASTER EQUATION

The strategy for deriving the exact master equation is to obtain expressions for the first and second moments, first from Eq. (1.1) and then from the local Langevin equation (2.18). From a comparison, we obtain explicit expressions for the time-dependent parameters in the Hu-Paz-Zhang equation (1.1).

In forming the moments of Eq. (1.1), we take note of the relations [11]

$$x\rho \leftrightarrow \left(q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) W, \quad \rho x \leftrightarrow \left(q - \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) W,$$
$$p\rho \leftrightarrow \left(p - \frac{i\hbar}{2} \frac{\partial}{\partial q} \right) W, \quad \rho p \leftrightarrow \left(p + \frac{i\hbar}{2} \frac{\partial}{\partial q} \right) W. \tag{3.1}$$

Here on the left x and p are the position and momentum operators for the oscillator, while ρ is the density matrix

operator. On the right, q and p are the c-number variables of the Wigner function $W(q,p;t)$. Thus, for example,

$$\langle x \rangle \equiv \text{Tr}\{x\rho\} = \int_{-\infty}^{\infty} dq \int_{-\infty}^{\infty} dp \left(q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) W. \quad (3.2)$$

In this way, forming the first moments of Eq. (1.1), we find

$$\langle \dot{x} \rangle = \frac{1}{m}\langle p \rangle, \quad \langle \dot{p} \rangle = -2\Gamma(t)\langle p \rangle - m\Omega^2(t)\langle x \rangle. \quad (3.3)$$

Eliminating $\langle p \rangle$, we find

$$\langle \ddot{x} \rangle + 2\Gamma(t)\langle \dot{x} \rangle + \Omega^2(t)\langle x \rangle = 0. \quad (3.4)$$

If now, we form the mean of the local Langevin equation (2.18), using the fact that $\langle X(t) \rangle = 0$, we get exactly the same equation, but with now the quantities $2\Gamma(t)$ and $\Omega^2(t)$ given by the expressions (2.19).

Next, forming the second moments of Eq. (1.1), we find

$$\frac{d\langle x^2 \rangle}{dt} = \frac{1}{m}\langle xp + px \rangle,$$

$$\frac{d\langle xp + px \rangle}{dt} = \frac{2}{m}\langle p^2 \rangle - 2m\Omega^2\langle x^2 \rangle$$

$$- 2\Gamma\langle xp + px \rangle + 2\hbar\Gamma f, \quad (3.5)$$

$$\frac{d\langle p^2 \rangle}{dt} = -m\Omega^2\langle xp + px \rangle - 4\Gamma\langle p^2 \rangle + 2\hbar m\Gamma h.$$

On the other hand, using the local Langevin equation (2.18), we find

$$\frac{d\langle x^2 \rangle}{dt} = \langle x\dot{x} + \dot{x}x \rangle,$$

$$\frac{d\langle x\dot{x} + \dot{x}x \rangle}{dt} = 2\langle \dot{x}^2 \rangle + \langle x\ddot{x} + \ddot{x}x \rangle$$

$$= 2\langle \dot{x}^2 \rangle - 2\Omega^2(t)\langle x^2 \rangle - 2\Gamma(t)\langle x\dot{x} + \dot{x}x \rangle$$

$$+ \frac{1}{m}\langle x(t)F(t) + F(t)x(t) \rangle, \quad (3.6)$$

$$\frac{d\langle \dot{x}^2 \rangle}{dt} = \langle \dot{x}\ddot{x} + \ddot{x}\dot{x} \rangle$$

$$= -\Omega^2(t)\langle x\dot{x} + \dot{x}x \rangle - 4\Gamma(t)\langle \dot{x}^2 \rangle$$

$$+ \frac{1}{m}\langle \dot{x}(t)F(t) + F(t)\dot{x}(t) \rangle.$$

Now, in the right-hand side of the second of these equations we use the fact $x(t) - X(t)$ is not correlated with $F(t)$ This should be clear since, as we see from Eqs. (2.15), this combination depends only upon the initial coordinates of the oscillator. Therefore we can replace $x(t)$ with $X(t)$ in the cor-

relations of x with F. Using the same argument in the last of these equations, we see that after a little rearrangement we can write

$$\frac{d\langle x^2 \rangle}{dt} = \langle x\dot{x} + \dot{x}x \rangle,$$

$$\frac{d\langle x\dot{x} + \dot{x}x \rangle}{dt} = 2\langle \dot{x}^2 \rangle - 2\Omega^2(t)\langle x^2 \rangle - 2\Gamma(t)\langle x\dot{x} + \dot{x}x \rangle$$

$$+ \frac{1}{m}\langle X(t)F(t) + F(t)X(t) \rangle, \quad (3.7)$$

$$\frac{d\langle \dot{x}^2 \rangle}{dt} = -\Omega^2(t)\langle x\dot{x} + \dot{x}x \rangle - 4\Gamma(t)\langle \dot{x}^2 \rangle$$

$$+ \frac{1}{m}\langle \dot{X}(t)F(t) + F(t)\dot{X}(t) \rangle.$$

We now compare these equations with Eqs. (3.5) obtained from Eq. (1.1). In doing so we must interpret $p = m\dot{x}$. We see then that we can identify

$$2\hbar\Gamma(t)f(t) = \langle X(t)F(t) + F(t)X(t) \rangle,$$

$$2\hbar\Gamma(t)h(t) = \langle \dot{X}(t)F(t) + F(t)\dot{X}(t) \rangle. \quad (3.8)$$

This completes the derivation of the exact master equation (1.1), with explicit expressions for the time-dependent coefficients.

IV. GENERAL SOLUTION OF THE TIME-DEPENDENT MASTER EQUATION

The task of solving Eq. (1.1), with its time-dependent coefficients given by the complicated expressions (2.19) and (3.8), appears formidable. Indeed, if one were presented with the equation with no idea of the origin of the coefficients its solution would be very difficult. But we have in Eqs. (2.15) an explicit solution of the Langevin equation describing the underlying motion. This will allow us to construct the general solution of the equation.

To begin, we remind ourselves Eq. (1.1) is an equation for the reduced density matrix, given by the partial trace over the bath coordinates. That is,

$$W(q,p;t) = \int d\mathbf{q} \int d\mathbf{p} W_{\text{system}}(q,p;\mathbf{q},\mathbf{p};t). \quad (4.1)$$

Here W_{system} is the Wigner function for the system of oscillator and bath, with $\mathbf{q} = (q_1, q_2, \cdots)$ and $\mathbf{p} = (p_1, p_2, \cdots)$ the bath coordinates and momenta. Now, the system is one of coupled oscillators and for such a system the solution of the equation of motion is formally identical to that for the corresponding classical system. That is, the Wigner function for the system at time t is related to that at time $t = 0$ through the relation

$$W_{\text{system}}(q,p;\mathbf{q},\mathbf{p};t) = W_{\text{system}}(q(0),p(0);\mathbf{q}(0),\mathbf{p}(0);0), \quad (4.2)$$

where $q(0), p(0); \mathbf{q}(0), \mathbf{p}(0)$ are the initial values for which the solution of the equations of motion is such that $q(t) = q$, $p(t) = p$, $\mathbf{q}(t) = \mathbf{q}$, $\mathbf{p}(t) = \mathbf{p}$. Finally, we remind ourselves that for the Hu-Paz-Zhang equation the initial state is a product state corresponding to a Wigner function of the form [11]

$$W_{\text{system}}(q, p; \mathbf{q}, \mathbf{p}; 0) = W(q, p; 0) \prod_j w_j(q_j, p_j). \quad (4.3)$$

Here, on the right $W(q, p; 0)$ is the initial Wigner function for the oscillator and the product is the Wigner function for the bath, in which $w_j(q_j, p_j)$ is the Wigner function for a single oscillator of mass m_j and frequency ω_j,

$$w_j(q_j, p_j) = \frac{1}{\pi \hbar \coth(\hbar \omega_j / 2kT)}$$

$$\times \exp \left\{ -\frac{p_j^2 + m_j^2 \omega_j^2 q_j^2}{m_j \hbar \omega_j \coth(\hbar \omega_j / 2kT)} \right\}. \quad (4.4)$$

Combining these results, we see that the reduced density matrix at time t is given by

$$W(q, p; t)$$

$$= \int d\mathbf{q} \int d\mathbf{p} W(q(0), p(0); 0) \prod_j w_j(q_j(0), p_j(0)).$$

$$(4.5)$$

This reduced density matrix is the solution that we seek. So far, however, all we have done is to carefully indicate the definition of this quantity, we must now carry out the indicated operations to obtain an explicit expression.

As a first step we transform the integration to the initial bath coordinates, holding q and p fixed. Under this transformation,

$$dq d\mathbf{p} = \frac{\partial(q, p; \mathbf{q}, \mathbf{p})}{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))} d\mathbf{q}(0) d\mathbf{p}(0), \quad (4.6)$$

where the factor is the Jacobian of the transformation, for which we have used the notation of Landau and Lifshitz [12]. But,

$$\frac{\partial(q, p; \mathbf{q}, \mathbf{p})}{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))} = \frac{\partial(q, p; \mathbf{q}, \mathbf{p})}{\partial(q(0), p(0); \mathbf{q}(0), \mathbf{p}(0))}$$

$$\times \frac{\partial(q(0), p(0); \mathbf{q}(0), \mathbf{p}(0))}{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))}$$

$$= \frac{\partial(q(0), p(0); \mathbf{q}(0), \mathbf{p}(0))}{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))}$$

$$= \left(\frac{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))}{\partial(q(0), p(0); \mathbf{q}(0), \mathbf{p}(0))} \right)^{-1}$$

$$= \left(\frac{\partial q}{\partial q(0)} \frac{\partial p}{\partial p(0)} - \frac{\partial q}{\partial p(0)} \frac{\partial p}{\partial q(0)} \right)^{-1}.$$

$$(4.7)$$

Here, we use in the first line the fact that the Jacobian of two successive transformations is the product of the Jacobians, in

the second line the fact that the motion of the system corresponds to a canonical transformation for which the Jacobian is unity, in the third line the fact that the Jacobian of the inverse transformation is the reciprocal of that of the direct transformation, and finally in the last line the definition of the Jacobian as the determinant of the matrix of partial derivatives. Now, to evaluate this Jacobian we use the solution (2.15), which we write in the form

$$q \equiv q(t) = m \dot{G}(t) q(0) + G(t) p(0) + X(t),$$

$$(4.8)$$

$$p \equiv p(t) = m^2 \ddot{G}(t) q(0) + m \dot{G}(t) p(0) + m \dot{X}(t).$$

Here we recall, from the definitions (2.16) of $X(t)$ and the expression (2.12) for $F(t)$ that $X(t)$ depends only on the initial coordinates of the bath, which are held fixed in forming the partial derivatives in the last line of Eq. (4.7). Therefore, we see that

$$\frac{\partial(q, p; \mathbf{q}, \mathbf{p})}{\partial(q, p; \mathbf{q}(0), \mathbf{p}(0))} = \frac{1}{m^2 (\dot{G}^2 - G\ddot{G})} \quad (4.9)$$

and, using Eq. (4.6) we can write Eq. (4.5) in the form

$$W(q, p; t) = \frac{\langle W(q(0), p(0); 0) \rangle}{m^2 (\dot{G}^2 - G\ddot{G})}, \quad (4.10)$$

where the brackets represent the average over the initial equilibrium distribution of the bath. Again, we remind ourselves that in the integrand $q(0)$ and $p(0)$ are obtained by inverting Eqs. (4.8). That is,

$$q(0) = \frac{m \dot{G}(q - X) - G(p - m \dot{X})}{m^2 (\dot{G}^2 - G\ddot{G})},$$

$$(4.11)$$

$$p(0) = \frac{-m^2 \ddot{G}(q - X) + m \dot{G}(p - m \dot{X})}{m^2 (\dot{G}^2 - G\ddot{G})}.$$

Since X is linear in the initial bath variables, its average has the Gaussian property: averages of all moments can be expressed in terms of those of the second moment.

We can carry out this average if we introduce the Fourier transform of the initial Wigner function, writing

$$W(q, p; 0) = \frac{1}{(2\pi\hbar)^2} \int_{-\infty}^{\infty} dQ \int_{-\infty}^{\infty} dP \tilde{W}(Q, P; 0) e^{i(Pq + Qp)/\hbar}.$$

$$(4.12)$$

Inserting this in Eq. (4.10), we can write

$$W(q, p; t) = \frac{1}{(2\pi\hbar m)^2 (\dot{G}^2 - G\ddot{G})} \int_{-\infty}^{\infty} dQ \int_{-\infty}^{\infty} dP \tilde{W}(Q, P; 0)$$

$$\times \langle \exp\{i[Pq(0) + Qp(0)]/\hbar\} \rangle. \quad (4.13)$$

The form of this result can be made a bit simpler if we introduce a transformation to variables r and s, defined by

$$Q = m\dot{G}r + Gs, \quad P = m^2\ddot{G}r + m\dot{G}s. \quad (4.14)$$

We then find that $Pq(0) + Qp(0) = r(p - m\dot{X}) + s(q - X)$ and $dQ\,dP = m^2(\dot{G}^2 - G\ddot{G})dr\,ds$, so that Eq. (4.13) becomes

$$W(q,p;t) = \frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{\infty}dr\int_{-\infty}^{\infty}ds\,\widetilde{W}(m\dot{G}r + Gs,$$

$$m^2\ddot{G}r + m\dot{G}s;0)e^{i(rp+sq)/\hbar}$$

$$\times e^{-(1/2\hbar^2)(m^2\langle\dot{X}^2\rangle r^2 + m\langle X\dot{X}+\dot{X}X\rangle rs + \langle X^2\rangle s^2)}, \quad (4.15)$$

where we have used the Gaussian property to write

$$\langle e^{-i(m\dot{X}r + Xs)/\hbar}\rangle = e^{-(1/2\hbar^2)(m^2\langle\dot{X}^2\rangle r^2 + m\langle X\dot{X}+\dot{X}X\rangle rs + \langle X^2\rangle s^2)}. \quad (4.16)$$

This is the form of the solution that is perhaps most useful. In its evaluation, the Green function $G(t)$ is given by Eq. (2.6), while $X(t)$ is given by Eq. (2.16) and its correlations are evaluated using Eqs. (2.2).

While we find Eq. (4.15) to be the most useful form of the solution, one can insert the inverse of the Fourier transform (4.12) to express the solution in the form of a transition operator acting on the initial Wigner function,

$$W(q,p;t) = \int_{-\infty}^{\infty}dq'\int_{-\infty}^{\infty}dp'\,P(q,p;q',p';t)W(q',p';0). \quad (4.17)$$

Here $P(q,p;q',p';t)$, called the transition probability, can be written

$$P(q,p;q',p';t) = \frac{1}{2\pi\sqrt{\det\mathbf{A}}}\exp\{-\tfrac{1}{2}\mathbf{R}\cdot\mathbf{A}^{-1}\cdot\mathbf{R}\}, \quad (4.18)$$

where we have used a dyadic notation with

$$\mathbf{A}(t) = \begin{pmatrix} m^2\langle\dot{X}^2\rangle & \dfrac{m}{2}\langle X\dot{X}+\dot{X}X\rangle \\[2mm] \dfrac{m}{2}\langle X\dot{X}+\dot{X}X\rangle & \langle X^2\rangle \end{pmatrix},$$

$$\mathbf{R}(t) = \begin{pmatrix} p - \langle p(t)\rangle \\ q - \langle q(t)\rangle \end{pmatrix}. \quad (4.19)$$

Here, in $\mathbf{R}$, the quantities $\langle q(t)\rangle$ and $\langle p(t)\rangle$ correspond to the mean of the initial value solution (2.15) with initial values q' and p'. That is,

$$\langle q(t)\rangle = m\dot{G}(t)q' + G(t)p',$$

$$\langle p(t)\rangle = m^2\ddot{G}(t)q' + m\dot{G}(t)p'. \quad (4.20)$$

It is of interest that this expression (4.18) for the transition probability is formally the same as that for the classical Kramers equation [13]. The difference is that the Green function and the mean square of the fluctuating position and velocity operators here are for a quantum oscillator interacting with an arbitrary heat bath, while in the classical solution of the Kramers equation they are for a classical oscillator interacting with an Ohmic bath. Another significant difference is that the solution (4.20) is that of the mean of the initial value Langevin equation (2.10), with the term $-\mu(t)x(0)$ on the right-hand side. The classical solution of the Kramers equation corresponds to dropping this term, since it is describing the classical stationary process.

As a first illustration of the utility of the form (4.15), we show how the equilibrium solution arises for long times. First we recall that, so long as the oscillator force constant K is not zero, the Green function will vanish as $t\to\infty$. Next, we recall that, again as $t\to\infty$, $X(t)\to x_s(t)$, the solution (2.5) of the stationary Langevin equation (2.1). Thus, we see almost by inspection that

$$W(q,p;t) \xrightarrow[t\to\infty]{} \frac{1}{2\pi m\sqrt{\langle x_s^2\rangle\langle\dot{x}_s^2\rangle}}$$

$$\times\exp\left\{-\frac{p^2}{2m^2\langle\dot{x}_s^2\rangle} - \frac{q^2}{2\langle x_s^2\rangle}\right\}, \quad (4.21)$$

where $\langle x_s^2\rangle$ and $\langle\dot{x}_s^2\rangle$ are the equilibrium values of the mean square position and velocity, given by the fluctuation-dissipation theorem,

$$\langle x_s^2\rangle = \frac{\hbar}{\pi}\int_0^{\infty}d\omega\,\mathrm{Im}\{\alpha(\omega+i0^+)\}\coth\frac{\hbar\omega}{2kT}, \quad (4.22)$$

$$\langle\dot{x}_s^2\rangle = \frac{\hbar}{\pi}\int_0^{\infty}d\omega\,\omega^2\mathrm{Im}\{\alpha(\omega+i0^+)\}\coth\frac{\hbar\omega}{2kT}.$$

This result is perhaps more familiar in the weak coupling limit, where $\mathrm{Im}\{\alpha(\omega+i0^+)\}\to\pi\delta(\omega-\omega_0)/2m\omega_0$ with $\omega_0 = \sqrt{K/m}$. Then $\langle\dot{x}_s^2\rangle = \omega_0^2\langle x_s^2\rangle = (\hbar\omega_0/2m)\coth(\hbar\omega_0/2kT)$ and (4.21) becomes the familiar equilibrium form of the Wigner function for the uncoupled oscillator [11].

Finally, we remark that the interest is most often in the probability density at time t, given by

$$P(x;t) = \int_{-\infty}^{\infty}dp\,W(x,p;t). \quad (4.23)$$

Using the solution (4.15), the integral over p gives a δ-function in r. With this we can perform the r integration to obtain the result

$$P(x;t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} ds\, \tilde{W}(Gs, m\dot{G}s; 0)$$

$$\times \exp\left\{-\frac{1}{2\hbar^2}\langle X^2 \rangle s^2 + i\frac{x}{\hbar}s\right\}. \quad (4.24)$$

In the next section, we evaluate this probability density for some problems of interest.

V. EXAMPLES

In this section we consider the evaluation of the general result (4.24) for the case of a free particle ($K=0$) interacting with an Ohmic bath. We have chosen the Ohmic model since it is that used most extensively, almost universally, in discussions of dissipative systems. Newtonian drag is Ohmic, as is the Stokes force and, of course, classical Brownian motion. In quantum electrodynamics, the Weisskopf-Wigner approximation is an Ohmic model. In addition, our results take their simplest form for that model. In the Appendix we present selected results for the more general single relaxation time model.

The examples are intended, first of all, to illustrate the power and utility of our exact solution. They are chosen since they appear in a truly large number of recent papers, where approximate methods were used. They are also the examples discussed, by numerical methods, in the original Hu-Paz-Zhang paper as well as in the earlier papers we have cited.

A. Preliminary formulas

For the Ohmic bath the memory function has the form

$$\mu(t) = 2\zeta\delta(t), \quad (5.1)$$

where ζ is the Newtonian friction constant (the factor 2 is because the integral in the Langevin equation is over only half the delta-function). In this case Eq. (2.10) is already in local form. With the form (5.1) for the memory function and with $K=0$, the response function (2.7) takes the simple form

$$\alpha(z) = \frac{1}{-mz^2 - iz\zeta}. \quad (5.2)$$

The Green function (2.6) is then

$$G(t) = \frac{1 - e^{-\zeta t/m}}{\zeta}. \quad (5.3)$$

If we form the quantities (2.19) with this Green function, we find

$$2\Gamma(t) = \frac{\zeta}{m}, \quad \Omega^2(t) = \frac{2\zeta}{m}\delta(t). \quad (5.4)$$

For any finite time these expressions follow trivially. The delta function is not so easy to see, although it should be obvious from the form (2.10) of the Langevin equation. In

the Appendix, this result is derived explicitly in the Ohmic limit of the single relaxation time model.

The only other quantity that we need to evaluate the general result is $\langle X^2(t) \rangle$, the mean square of the fluctuating position operator. In this connection, it is a simple matter, comparing the stationary solution (2.5) with the definition (2.16) of $X(t)$, to obtain the general relation

$$X(t) = x_s(t) - x_s(0) + \int_{-\infty}^{0} dt'\{G(-t') - G(t-t')\}F(t'). \quad (5.5)$$

In discussing this operator, in particular the mean of its square, we shall make use of the mean square displacement for the stationary process,

$$s(t) \equiv \langle [x_s(t) - x_s(0)]^2 \rangle$$

$$= \frac{2\hbar}{\pi} \int_0^{\infty} d\omega\, \mathrm{Im}\{\alpha(\omega + i0^+)\}\coth\frac{\hbar\omega}{2kT}(1 - \cos\omega t). \quad (5.6)$$

The discussion in the previous paragraph has been general, applying to an oscillator interacting with an arbitrary heat bath. We now specialize to the current case of a free particle interacting with an Ohmic bath. The Green function is then given by Eq. (5.3), from which we see that $G(-t') - G(t-t') = -mG(t)\dot{G}(-t')$ and Eq. (5.5) becomes

$$X(t) = x_s(t) - x_s(0) - mG(t)\dot{x}_s(0). \quad (5.7)$$

Forming the mean square, we can write

$$\langle X^2(t) \rangle = s(t) - mG(t)\dot{s}(t) + \frac{1}{2}m^2 G^2(t)\ddot{s}(0). \quad (5.8)$$

In the same way we find

$$\langle \dot{X}^2(t) \rangle = \frac{1}{2}[1 + m^2\dot{G}^2]\ddot{s}(0) - m\dot{G}(t)\ddot{s}(t). \quad (5.9)$$

For this Ohmic case, using the form (5.2) for the response function in the expression (5.6) for the mean square displacement, we find

$$s(t) = \frac{2\hbar\zeta}{\pi} \int_0^{\infty} d\omega\, \frac{\coth\dfrac{\hbar\omega}{2kT}}{\omega(m^2\omega^2 + \zeta^2)}(1 - \cos\omega t). \quad (5.10)$$

1. High temperature limit

In the high temperature limit ($kT \gg \hbar\zeta/m$) we replace the hyperbolic cotangent in Eq. (5.10) by the reciprocal of its argument (thus, neglecting the zero-point oscillations). The result takes the form [14]

$$s(t) = \frac{2kT}{\zeta}\left(t - m\frac{1 - e^{-\zeta t/m}}{\zeta}\right). \quad (5.11)$$

With this in the expression (5.8) for the mean square of the fluctuating displacement, we see that, still in the high temperature limit,

$$\langle X^2(t)\rangle = \frac{kT}{\zeta}\left(2t - 2m\frac{1-e^{-\zeta t/m}}{\zeta} - m\frac{(1-e^{-\zeta t/m})^2}{\zeta}\right). \tag{5.12}$$

2. Zero temperature

At zero temperature, we replace the hyperbolic cotangent in Eq. (5.10) by unity. The result can be written

$$s(t) = \frac{2\hbar}{\pi\zeta}I\left(\frac{\zeta t}{m}\right), \tag{5.13}$$

where [14]

$$I(x) = \int_0^\infty dy\,\frac{x^2}{y(y^2+x^2)}(1-\cos y)$$

$$= \log x + \gamma - \frac{1}{2}[e^{-x}\overline{\mathrm{Ei}}(x) + e^x\mathrm{Ei}(-x)]. \tag{5.14}$$

Here $\gamma = 0.577215665$ is Euler's constant. Note the expansions [15], for small x,

$$I(x) = -(\log x + \gamma)(\cosh x - 1)$$

$$- \frac{1}{2}\left[e^{-x}\sum_{n=1}^\infty \frac{x^n}{n!n} + e^x\sum_{n=1}^\infty \frac{(-x)^n}{n!n}\right], \tag{5.15}$$

and, asymptotically, for large x,

$$I(x) \sim \log x + \gamma - \frac{1}{x^2} - \frac{3!}{x^4} - \frac{5!}{x^6} - \cdots. \tag{5.16}$$

Here we see that there is a serious concern: for small x the second derivative $I''(x) \cong -\log x$ and therefore the term involving $\ddot{s}(0)$ in the expression (5.8) for $\langle X^2(t)\rangle$ is logarithmically divergent. This divergence persists for long times, where

$$\langle X^2(t)\rangle \sim \frac{2\hbar}{\pi\zeta}\log\zeta t - \frac{\hbar}{\pi\zeta}\log 0^+, \tag{5.17}$$

in which the neglected quantity is of the order of a finite constant. This divergence for the Ohmic case has, of course, been noted by earlier authors [3,1], but it does not seem to be known that this divergence persists in a model with a high frequency cutoff. In the Appendix we show this explicitly for the single relaxation time model.

B. Gaussian wave packet

To begin, we note that in evaluating the solution we make repeated use of the standard Gaussian integral:

$$\int_{-\infty}^\infty dx\,\exp\left\{-\frac{1}{2}ax^2 + ibx\right\} = \sqrt{\frac{2\pi}{a}}\exp\left\{-\frac{b^2}{2a}\right\}. \tag{5.18}$$

We consider an initial state corresponding to a Gaussian wave packet of the form,

$$\psi(x,0) = \frac{1}{(2\pi\sigma^2)^{1/4}}\exp\left\{-\frac{(x-x_0)^2}{4\sigma^2}\right\}. \tag{5.19}$$

This is a so-called minimum uncertainty wave packet, centered at $\langle x(0)\rangle = x_0$ and with variance $\langle\Delta x^2(0)\rangle \equiv \langle[x(0) - \langle x(0)\rangle]^2\rangle = \sigma^2$. The corresponding mean momentum is $\langle p(0)\rangle = m\langle\dot{x}(0)\rangle = 0$ and the momentum variance (corresponding to minimum uncertainty) is $\langle\Delta p^2(0)\rangle = m^2\langle[\dot{x}(0) - \langle\dot{x}(0)\rangle]^2\rangle = \hbar^2/4\sigma^2$. The Wigner function corresponding to this state is

$$W(q,p;0) = \frac{1}{2\pi\hbar}\int_{-\infty}^\infty du\,e^{iup/\hbar}\psi\left(q-\frac{u}{2},0\right)\psi^*\left(q+\frac{u}{2},0\right)$$

$$= \frac{1}{\pi\hbar}\exp\left\{-\frac{(q-x_0)^2}{2\sigma^2} - \frac{2\sigma^2 p^2}{\hbar^2}\right\}. \tag{5.20}$$

Its Fourier transform is

$$\widetilde{W}(Q,P;0) = \int_{-\infty}^\infty dq\int_{-\infty}^\infty dp\,e^{-i(Pq+Qp)/\hbar}W(q,p;0)$$

$$= \int_{-\infty}^\infty dq\,e^{-iPq/\hbar}\psi\left(q-\frac{Q}{2},0\right)\psi^*\left(q+\frac{Q}{2},0\right)$$

$$= \exp\left\{-\frac{Q^2}{8\sigma^2} - \frac{\sigma^2 P^2}{2\hbar^2} - i\frac{x_0 P}{\hbar}\right\}. \tag{5.21}$$

Putting this in the expression (4.24) for the probability density at time t, we find

$$P(x;t) = \frac{1}{\sqrt{2\pi\langle\Delta x^2(t)\rangle}}\exp\left\{-\frac{[x-m\dot{G}(t)x_0]^2}{2\langle\Delta x^2(t)\rangle}\right\}, \tag{5.22}$$

where $\langle\Delta x^2(t)\rangle$ is the variance of the position, given by

$$\langle\Delta x^2(t)\rangle = m^2\dot{G}^2(t)\sigma^2 + \frac{\hbar^2 G^2(t)}{4\sigma^2} + \langle X^2(t)\rangle. \tag{5.23}$$

This is a general result, valid for any heat bath. For the Ohmic case the Green function is given in Eq. (5.3) and $\langle X^2(t)\rangle$ is given by Eq. (5.8). For the single relaxation time model, the corresponding results are given in Eqs. (A4) and (A9).

The first thing that should strike us in this result is that the variance is in fact infinite, due to the divergence found in the expression (5.8) for $\langle X^2(t)\rangle$ at zero temperature. This divergence arises from the zero-point oscillations and is therefore always present, although conventionally one neglects the

zero-point oscillations in the high temperature limit. This is a serious difficulty, since it tells us that an initial wave packet spreads instantly to infinite width. In effect, the state vanishes. We emphasize that the problem here is not with the Hu-Paz-Zhang equation or its solution, which are perfectly correct, but with the assumption of an uncorrelated initial state. Unease with this assumption has been expressed by many authors (we note in particular the remarks in the concluding Discussion section of the Hu-Paz-Zhang paper [1]) but it does not seem to have been realized how serious are its consequences. Indeed, the only meaningful results for the equation are for the high temperature limit, and we confine our discussion in the following to that limit.

In the high temperature limit, using the expression (5.3) for the Green function in the Ohmic case, the probability density (5.22) becomes

$$P(x;t) = \frac{1}{\sqrt{2\pi\langle\Delta x^2(t)\rangle}}\exp\left\{-\frac{(x-x_0 e^{-\zeta t/m})^2}{2\langle\Delta x^2(t)\rangle}\right\}, \quad (5.24)$$

where, evaluating the expression (5.8) for $\langle X^2(t)\rangle$ with the high-temperature expression (5.11) for the mean square displacement, the variance is given by

$$\langle\Delta x^2(t)\rangle = \sigma^2 e^{-2\zeta t/m} + \frac{\hbar^2(1-e^{-\zeta t/m})^2}{4\zeta^2\sigma^2}$$

$$+\frac{kT}{\zeta}\left(2t-2m\frac{1-e^{-\zeta t/m}}{\zeta}-m\frac{(1-e^{-\zeta t/m})^2}{\zeta}\right). \quad (5.25)$$

A difficulty with this result is that the center of the wave packet drifts to the origin. Since for a free particle the origin cannot be a special point, we see from this that the translational invariance of the problem is broken by the assumption that the initial state corresponds to an uncoupled system. Indeed, the system Hamiltonian (2.9) is invariant under simultaneous translation of the particle and bath coordinates $(x\to x+d, q_j\to q_j+d)$ and the time-dependent master equation (1.1) correctly describes the dynamics of the system with regard to this Hamiltonian. But the bath Hamiltonian (2.17) does not possess this invariance and the initial state is one in which the bath is in equilibrium with respect to this Hamiltonian. Another way to see this effect is to note that for a free particle interacting with an Ohmic bath the mean motion described (1.1) satisfies the equation

$$m\langle\ddot{x}\rangle + \zeta\langle\dot{x}\rangle = -2\zeta\delta(t)\langle x(0)\rangle. \quad (5.26)$$

That is, the particle receives an initial impulse $-\zeta\langle x(0)\rangle$, directed toward the origin and with a magnitude such that in the course of time the particle arrives at the origin. Another difficulty, which in fact has the same origin as the first, is that in the expression (5.25) for the variance the first term, which corresponds to the initial variance, decays in time. But the initial variance should persist and not decay.

A further difficulty is seen if we look at the variance (5.25) for times short compared with the Ohmic decay time,

$$\langle\Delta x^2(t)\rangle \cong \sigma^2 + \frac{\hbar^2 t^2}{4m^2\sigma^2}, \quad \zeta t/m \ll 1. \quad (5.27)$$

But this is exactly the formula for the RMS width of a wave packet as obtained from elementary quantum mechanics [16]. It therefore corresponds to temperature zero and the thermal spreading one should expect at high temperature is absent [17,6,7]. Now this last is not a difficulty with the equation or our solution, but with the initial state we have chosen, which corresponds to a particle at temperature zero. Instead we should choose a state corresponding to a wave packet at temperature T, obtained by averaging the initial Wigner function (5.20) over a thermal distribution of initial velocities.

To accomplish this, we note first that the initial state (5.19) corresponds to a particle at rest (i.e., at $T=0$). To obtain the state corresponding to a particle with velocity v, we simply multiply with a factor $e^{imvx/\hbar}$. With this, we see that the Fourier transform of the corresponding Wigner function is obtained by multiplying Eq. (5.21) by $e^{-imvQ/\hbar}$. The thermal average of this factor is

$$\sqrt{\frac{m}{2\pi kT}}\int_{-\infty}^{\infty}dv\,\exp\left\{-\frac{mv^2}{2kT}-i\frac{mQ}{\hbar}v\right\} = \exp\left\{-\frac{Q^2}{2\bar{\lambda}^2}\right\}, \quad (5.28)$$

where $\bar{\lambda}$ is the thermal de Broglie wavelength,

$$\bar{\lambda} = \frac{\hbar}{\sqrt{mkT}}. \quad (5.29)$$

Therefore, we see that for a particle at temperature T the Fourier transform of the initial Wigner function is obtained by multiplying the corresponding function at $T=0$ by the factor (5.28). Multiplying Eq. (5.21) by this factor we obtain

$$\tilde{W}_T(Q,P;0) = \exp\left\{-\left(\frac{1}{8\sigma^2}+\frac{1}{2\bar{\lambda}^2}\right)Q^2-\frac{\sigma^2 P^2}{2\hbar^2}-i\frac{x_0 P}{\hbar}\right\}, \quad (5.30)$$

where we indicate that this corresponds to temperature T by the subscript. Using this in Eq. (4.24) we find for the probability distribution at temperature T the result

$$P_T(x;t) = \frac{1}{\sqrt{2\pi\langle\Delta x^2\rangle_T}}\exp\left\{-\frac{(x-x_0 e^{-\zeta t/m})^2}{2\langle\Delta x^2\rangle_T}\right\}, \quad (5.31)$$

where we have introduced

$$\langle\Delta x^2\rangle_T = \langle\Delta x^2\rangle + \frac{\hbar^2}{\bar{\lambda}^2\zeta^2}(1-e^{-\zeta t/m})^2$$

$$= \sigma^2 e^{-2\zeta t/m} + \frac{\hbar^2(1-e^{-\zeta t/m})^2}{4\zeta^2\sigma^2}$$

$$+\langle X^2(t)\rangle_T, \quad (5.32)$$

in which

$$\langle X^2(t)\rangle_T = \frac{kT}{\zeta}\left(2t - 2m\frac{1 - e^{-\zeta t/m}}{\zeta}\right). \quad (5.33)$$

Note that now the variance for very short times includes the thermal spreading [6,7],

$$\langle \Delta x^2\rangle_T \cong \sigma^2 + \frac{\hbar^2 t^2}{4m^2\sigma^2} + \frac{kT}{m}t^2, \quad \zeta t/m \ll 1. \quad (5.34)$$

However, the long time drift of the wave packet center and the shrinking of the initial variance remain.

C. Pair of Gaussian wave packets

We consider now an initial state corresponding to two separated Gaussian wave packets. The corresponding wave function has the form

$$\psi(x,0) = \frac{1}{(8\pi\sigma^2)^{1/4}(1 + e^{-d^2/8\sigma^2})^{1/2}}\left(\exp\left\{-\frac{\left(x - \frac{d}{2}\right)^2}{4\sigma^2}\right\}\right.$$
$$\left. + \exp\left\{-\frac{\left(x + \frac{d}{2}\right)^2}{4\sigma^2}\right\}\right), \quad (5.35)$$

where d is the separation and σ is the width of each packet. Using Eq. (5.21) we see that the Fourier transform of the initial Wigner function is given by

$$\widetilde{W}(Q,P;0) = \frac{1}{1 + e^{-d^2/8\sigma^2}}\exp\left\{-\frac{Q^2}{8\sigma^2} - \frac{\sigma^2 P^2}{2\hbar^2}\right\}$$
$$\times\left(\cos\frac{Pd}{2\hbar} + e^{-d^2/8\sigma^2}\cosh\frac{Qd}{4\sigma^2}\right). \quad (5.36)$$

Putting this in the expression (4.24) for the probability density at time t, we find

$$P(x;t) = \frac{1}{2(1 + e^{-d^2/2\sigma^2})\sqrt{2\pi\langle\Delta x^2\rangle}}$$
$$\times\left(\exp\left\{-\frac{\left(x - \frac{d}{2}e^{-\zeta t/m}\right)^2}{2\langle\Delta x^2\rangle}\right\}\right.$$
$$+ \exp\left\{-\frac{\left(x + \frac{d}{2}e^{-\zeta t/m}\right)^2}{2\langle\Delta x^2\rangle}\right\} + 2\exp\left\{-\frac{x^2}{2\langle\Delta x^2\rangle}\right\}$$
$$\left. -\frac{d^2}{8\sigma^2} + \frac{(1 - e^{-\zeta t/m})^2\hbar^2 d^2}{32\zeta^2\sigma^4\langle\Delta x^2\rangle}\right\}\cos\frac{G\hbar dx}{4\sigma^2\langle\Delta x^2\rangle}\right). \quad (5.37)$$

Here the first two terms in the parentheses correspond to a pair of Gaussian wave packets of the form (5.22), initially centered at $x = \pm d/2$ and drifting toward the origin. The third term, that with the cosine, is an interference term. The attenuation factor $a(t)$ is the ratio of the coefficient of the cosine term divided by twice the geometric mean of the first two terms. We find

$$a(t) = \exp\left\{-\frac{\langle X^2(t)\rangle}{8\sigma^2\langle\Delta x^2(t)\rangle}d^2\right\}, \quad (5.38)$$

where at high temperature $\langle X^2(t)\rangle$ is given in Eq. (5.12) and $\langle\Delta x^2(t)\rangle$ in Eq. (5.25).

For times long compared with the Ohmic decay time, $t \gg m/\zeta$, we see that $\langle X^2(t)\rangle$ and $\langle\Delta x^2\rangle$ become asymptotically equal, growing linearly with t. For such long times the attenuation coefficient (5.38) therefore approaches a very small constant, $a(t) \sim \exp\{-d^2/8\sigma^2\}$. For times short compared with the Ohmic decay time, $t \ll m/\zeta$, we see that $\langle X^2(t)\rangle \cong (2\zeta kT/3m^2)t^3$ while $\langle\Delta x^2(t)\rangle \cong \sigma^2 + (\hbar^2 t^2/4m^2\sigma^2)$ and therefore

$$a(t) \cong \exp\left\{-\frac{\zeta kTd^2 t^3}{12m^2\sigma^4 + 3\hbar^2 t^2}\right\}, \quad t \ll m/\zeta. \quad (5.39)$$

If we suppose that the slit width is negligibly small, we find $a(t) \cong \exp\{-t/\tau_d\}$ where $\tau_d = 3\hbar^2/\zeta kTd^2$. This, except for a factor of 6 is exactly the decoherence time that often appears in the literature [18]. But, as we have seen above, this result corresponds to a particle in an initial state that is effectively at temperature zero, which is suddenly coupled to a heat bath at high temperature. The result is therefore unphysical in the sense that the initial state does not correspond to that envisioned when we speak of a system at temperature T.

Now, just as in our discussion of the spreading of a single Gaussian wave packet, this difficulty can be repaired by choosing the initial temperature of the particle to be the same as that of the heat bath. The prescription for accomplishing this is very simple: multiply $\widetilde{W}(Q,P;0)$, given in Eq. (5.36), by the factor given in Eq. (5.28). The result is to replace Eq. (5.36) by

$$\widetilde{W}_T(Q,P;0) = \frac{1}{1 + e^{-d^2/8\sigma^2}}\exp\left\{-\left(\frac{1}{8\sigma^2} + \frac{1}{2\overline{\lambda}^2}\right)Q^2\right.$$
$$\left. -\frac{\sigma^2 P^2}{2\hbar^2}\right\}\left(\cos\frac{Pd}{2\hbar} + e^{-d^2/8\sigma^2}\cosh\frac{Qd}{4\sigma^2}\right). \quad (5.40)$$

Putting this in the expression (4.24) for the probability density at time t, we find, in place of Eq. (5.37)

$$P_{\rm T}(x;t) = \frac{1}{2(1+e^{-d^2/2\sigma^2})\sqrt{2\pi\langle\Delta x^2\rangle_{\rm T}}}$$

$$\times\left(\exp\left\{-\frac{\left(x-\frac{d}{2}e^{-\zeta t/m}\right)^2}{2\langle\Delta x^2\rangle_{\rm T}}\right\}\right.$$

$$+\exp\left\{-\frac{\left(x+\frac{d}{2}e^{-\zeta t/m}\right)^2}{2\langle\Delta x^2\rangle_{\rm T}}\right\}+2\exp\left\{-\frac{x^2}{2\langle\Delta x^2\rangle_{\rm T}}\right.$$

$$\left.-\frac{d^2}{8\sigma^2}+\frac{(1-e^{-\zeta t/m})^2\hbar^2 d^2}{32\zeta^2\sigma^4\langle\Delta x^2\rangle_{\rm T}}\right\}\cos\frac{G\hbar dx}{4\sigma^2\langle\Delta x^2\rangle_{\rm T}}\right),$$

$$(5.41)$$

where $\langle\Delta x^2\rangle_{\rm T}$ is given in Eq. (5.32). With this, we find that the attenuation coefficient is given by

$$a_{\rm T}(t)=\exp\left\{-\frac{\langle X^2(t)\rangle_{\rm T}}{8\sigma^2\langle\Delta x^2(t)\rangle_{\rm T}}d^2\right\}. \qquad (5.42)$$

Here we recall that $\langle\Delta x^2(t)\rangle_{\rm T}$ and $\langle X^2(t)\rangle_{\rm T}$ are given in Eqs. (5.32) and (5.33).

Now, for times short compared with the Ohmic decay time we find

$$a_{\rm T}(t)\cong\exp\left\{-\frac{\frac{kT}{m}t^2}{8\left(\sigma^4+\sigma^2\frac{kT}{m}t^2+\frac{\hbar^2}{4m^2}t^2\right)}d^2\right\}, \quad t\ll m/\zeta.$$

$$(5.43)$$

This is exactly the form of the attenuation coefficient for a free particle [7], which for very short times is of the form $a_{\rm T}(t)\cong\exp\{-t^2/\tau_d^2\}$, where the decoherence time is

$$\tau_d=\frac{\sqrt{8}\sigma^2}{\bar{v}d}, \qquad (5.44)$$

in which $\bar{v}=\sqrt{kT/m}$ is the mean thermal velocity.

VI. CONCLUDING REMARKS

The system we are discussing is that of an oscillator coupled to a linear passive heat bath, with a microscopic Hamiltonian of the form (2.9). The long time equilibrium state of this system is entangled, in the sense that the normal modes correspond to coupled motion of the oscillator and the bath. The Hu-Paz-Zhang equation is an exact master equation describing how this entangled equilibrium state arises from an initial state in which the bath and the oscillator are not coupled. We should perhaps emphasize that this assumption of a decoupled initial state is common to all derivations of a master equation, going back at least to the work of Wangness and Bloch [19], who phrased it as an assumption

that at any instant of time the system is approximately decoupled. Indeed, such an assumption is essential for the introduction of the notion of partial trace, i.e., the trace over states of the uncoupled bath as in Eq. (4.1), key to the existence of any master equation. Now, our exact solution has allowed us to see more clearly how serious is that assumption. In particular, we have seen that within this assumption an exact solution leads to meaningful results only in the high temperature limit. Here we hasten to add that this remark does not apply to the many successful applications of master equations in the weak coupling approximation.

For the most part, previous discussions have been made under the restriction that the initial state of the particle is a pure state, effectively at zero temperature, while the bath is at a high temperature T. There has even been an approximate experimental realization of such a state [20]. However, we would argue that such a state is unphysical in the sense that it does not correspond to what is envisioned when one speaks of a system at temperature T. Rather, the initial time dependence is then dominated by the "warming up" of the particle, which occurs on a time scale of order the decay time m/ζ. On the other hand, as we have shown, the restriction to such a state is not necessary, one can, within the assumption of an uncoupled initial state, choose the particle state to be at the same temperature as the bath.

In order to describe a state of the system that is entangled at all times, including the initial time, it is necessary to abandon master equation methods. Some time ago, a more general method applicable to such systems was described by Ford and Lewis [21]. In their method, a system in equilibrium is put into an initial state (e.g., a wave-packet state) by a measurement and then at a later time is sampled by a second measurement. This method of successive measurements has recently been applied to obtain exact results for the problems of wave packet spreading and decoherence [6]. For the wave packet spreading one finds in place of Eqs. (5.22) or (5.31) the result

$$P(x;t)=\exp\left\{-\frac{(x-x_0)^2}{2w^2(t)}\right\}, \qquad (6.1)$$

where the variance is now given by

$$w^2(t)=\sigma^2+s(t)-\frac{[x(t),x(0)]^2}{4\sigma^2}. \qquad (6.2)$$

An equivalent result for wave packet spreading in the Ohmic case has been obtained by Hakim and Ambegaokar [17], who used functional integration methods. For the decoherence problem, one obtains in place of Eqs. (5.38) or (5.42) the result

$$a(t)=\exp\left\{-\frac{s(t)}{8\sigma^2 w^2(t)}\right\}. \qquad (6.3)$$

Note that these results are finite at any temperature and apply to an arbitrary heat bath and for all times. At short times, the results (5.34) and (5.43) are in agreement with these exact results.

APPENDIX: SINGLE RELAXATION TIME MODEL

Here we consider the single relaxation time model for the case of a free particle ($K=0$). This model corresponds to a memory function of the form

$$\mu(t) = \frac{\zeta}{\tau} e^{-t/\tau} \theta(t), \qquad (A1)$$

where θ is the Heaviside function. Note that in the limit $\tau \to 0$ this becomes the Ohmic memory function (5.1). With this form of the memory function and with $K=0$, the response function (2.7) takes the form

$$\alpha(z) = \frac{1}{-mz^2 - iz \dfrac{\zeta}{1 - iz\tau}}$$

$$= \frac{z + i(\gamma_+ + \gamma_-)}{-mz(z + i\gamma_+)(z + i\gamma_-)}, \qquad (A2)$$

where we have introduced

$$\gamma_\pm = \frac{1 \pm \sqrt{1 - \dfrac{4\zeta\tau}{m}}}{2\tau}. \qquad (A3)$$

Note that in the Ohmic limit $\gamma_+ \to \tau^{-1} \to \infty$ and $\gamma_- \to \zeta/m$ and we recover the form (5.2) of the response function.

With this form of the response function, the Green function (2.6) can be written in the form

$$G(t) = \frac{\gamma_+^2(1 - e^{-\gamma_- t}) - \gamma_-^2(1 - e^{-\gamma_+ t})}{m\gamma_-\gamma_+(\gamma_+ - \gamma_-)}, \qquad (A4)$$

If we form the quantities (2.19) with this Green function, we find

$$2\Gamma(t) = \gamma_- - \frac{(\gamma_+ - \gamma_-)[(\gamma_+ + \gamma_-)e^{\gamma_- t} - \gamma_+]}{(\gamma_+ + \gamma_-)(e^{\gamma_+ t} - e^{\gamma_- t}) + \gamma_+ - \gamma_-}, \qquad (A5)$$

$$\Omega^2(t) = \frac{\gamma_-\gamma_+(\gamma_+ - \gamma_-)}{(\gamma_+ + \gamma_-)(e^{\gamma_+ t} - e^{\gamma_- t}) + \gamma_+ - \gamma_-}.$$

In the Ohmic limit, it is clear that for any finite time, $2\Gamma(t) \to \gamma_- \to \zeta/m$ and $\Omega^2(t) \to 0$. On the other hand

$2\Gamma(0) = 0$ and $\Omega^2(0) = \gamma_-\gamma_+ \to (\zeta/m\tau) \to \infty$. For t of order τ we see that in this Ohmic limit

$$\Omega^2(t) \cong \frac{\zeta}{m\tau} e^{-t/\tau} \to \frac{2\zeta}{m} \delta(t). \qquad (A6)$$

This justifies the assertion made in Eqs. (5.4).

Next, we consider the fluctuating position operator, $X(t)$, for the single relaxation time model. With the Green function (A4) it is a simple matter to verify the relation

$$G(-t') - G(t - t') = -mG(t)\dot{G}(-t')$$

$$- \frac{1 - m\dot{G}(t)}{\gamma_+\gamma_-}\ddot{G}(-t'). \qquad (A7)$$

Putting this in Eq. (5.5) we find in place of Eq. (5.7),

$$X(t) = x_s(t) - x_s(0) - mG(t)\dot{x}_s(0) - \frac{m\tau}{\zeta}[1 - m\dot{G}(t)]\ddot{x}_s(0). \qquad (A8)$$

Forming the mean square, we can write

$$\langle X^2(t) \rangle = s(t) - mG(t)\dot{s}(t) + \frac{1}{2}m^2 G^2(t)\ddot{s}(0)$$

$$- \frac{m\tau}{\zeta}[1 - m\dot{G}(t)][\ddot{s}(t) - \ddot{s}(0)]$$

$$- \frac{m^2\tau^2}{2\zeta^2}[1 - m\dot{G}(t)]^2 s^{(4)}(0). \qquad (A9)$$

The interest here is in the zero temperature limit. With the response function given by Eq. (A2) and with $T=0$, the expression (5.6) for the mean square displacement can be put in the form

$$s(t) = \frac{2\hbar}{\pi\zeta} \frac{\gamma_+^2 I(\gamma_- t) - \gamma_-^2 I(\gamma_+ t)}{\gamma_+^2 - \gamma_-^2}, \qquad (A10)$$

where $I(x)$ is given by Eq. (5.14). We see now that $\ddot{s}(0)$ is finite, but the fourth derivative $s^{(4)}(0)$ is logarithmically divergent. Indeed the divergence is the same as in the Ohmic case, with the same long time form (5.17).

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