

Wigner distribution function approach to dissipative problems in quantum mechanics with emphasis on decoherence and measurement theory

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Abstract

We first review the usefulness of the Wigner distribution functions (WDFs), associated with Lindblad and pre-master equations, for analysing a host of problems in quantum optics where dissipation plays a major role, an arena where weak coupling and long-time approximations are valid. However, we also show their limitations for the discussion of decoherence, which is generally a short-time phenomenon with decay rates typically much smaller than typical dissipative decay rates. We discuss two approaches to the problem both of which use a quantum Langevin equation as a starting-point: (a) use of a reduced WDF but in the context of an exact master equation (b) use of a WDF for the complete system corresponding to entanglement at all times.

Keywords: Dissipation, decoherence, Wigner distribution

1. Introduction

In recent years, there has been widespread interest in dissipative problems arising in a variety of areas in physics. Historically, particularly in quantum optics and NMR (where weak coupling and long-time approximations are valid), master equations for the time evolution of the density matrix have been extensively utilized in analysing such problems [1–6] and it has also been found useful to re-express such equations in terms of the Wigner distribution function (WDF) [1, 4]. However, with the recent burgeoning interest in decoherence, which is generally a short-time phenomenon with decay rates much smaller than typical dissipative decay rates, a new element arises. Recognizing that conventional master equation approaches are often not adequate, some investigators have used path integral methods [3]. However, we have found that the simplest and most physically appealing approach to the problem is via use of generalized quantum Langevin equations (QLEs) [7], supplemented by use of WDFs [8]. Our focus is on quantum Brownian motion: a quantum particle interacting with a heat bath and moving in an arbitrary external potential. For the investigation of decoherence phenomena, we have found [9, 10] that it is important to distinguish

between two different physical scenarios: namely (a) complete entanglement between the quantum particle and the heat bath at all times and (b) the system in a state in which the oscillator is not coupled to the bath at, say, $t = 0$ and such that the bath is in equilibrium at temperature T . Thus, it takes a characteristic time of the order of γ^{-1} (where γ is a typical dissipative decay time) for the complete coupling to occur and for the whole system to come into thermal equilibrium.

Scenario (b), with the assumption of an uncoupled initial state is that used in the derivation of master equations, including the exact master equation of Hu *et al* [23]. However, this scenario is inappropriate for the calculation of very short decoherence decay times and, in general, one must abandon master equation methods for this purpose. For analysis of scenario (a), by its nature, it is necessary to abandon master equation methods. Instead, we have employed [9] a more general method due to Ford and Lewis [11]. Finally, the presence of a classical external force $f(t)$ brings a new dimension to the problem.

The familiar master equation of quantum optics is in Lindblad form [2], which guarantees that the density matrix is always positive definite during time evolution. In the derivation of this equation [1, 6], rapidly oscillating terms are

omitted by the method of coarse-graining in time; the high frequencies correspond to the oscillator frequency ω_0 and, in the usual weak coupling limit, $\omega_0 \gg \gamma$, where γ is a typical decay constant.

We have referred to the equations obtained prior to coarse-graining in time as pre-master (or pre-Lindblad) equations [6, 12] and such equations have been used extensively in other areas of physics [3, 4]; other authors have simply referred to them as master equations but, to avoid confusion, we reserve the latter term for equations in Lindblad form. Pre-master equations, like the master equation, describe an approach to the equilibrium state. This equilibrium state is the same in either case [12], but with pre-master (non-Lindblad) equations the approach can be through non-physical states of negative probability. However, as we demonstrate here, pre-master equations have other advantages *vis à vis* master equations:

- (a) they lead to the exact expression for the mean value of $x(t)$ (as obtained from the exact Langevin equation for the problem),
- (b) they lead, in the classical limit ($\hbar \rightarrow 0$), to the familiar Fokker–Planck equation of classical probability,
- (c) the exact master equation [23] is for long times of pre-master form, positivity being preserved through the time dependence of the coefficients.

However, the pre-master equations can exhibit different forms, depending on whether momentum or coordinate coupling forms of H have been used.

It is thus clear that there are many facets to the overall question of analysing dissipative systems. Our purpose is to delineate the strengths and weaknesses of the various approaches. As will become apparent, one common thread which will permeate the discussion is the usefulness of the Wigner distribution for all scenarios.

As already indicated, there is an important dividing line between long-time ($t \gg \gamma^{-1}$) and short-time ($t \ll \gamma^{-1}$) phenomena. Thus, in section 2, we discuss the QLE for scenario (a), which describes quantum particle and bath entanglement at all times, and we consider in turn both the stationary process (corresponding to the absence of an external force $f(t)$ in which case we are dealing with the system in thermal equilibrium) and then the case of $f(t) \neq 0$. This naturally leads us to a comparison of the Langevin equations of motion with those derived (in the ohmic limit and for an oscillator) using the conventional master equation techniques of quantum optics and NMR. Thus, as a starting-point, in section 3 we write down the QLE for the ohmic model. In addition, we present, in the interaction representation, the two forms (momentum coupling and coordinate coupling) of the weak coupling pre-master equations as well as the corresponding master equation (which is the same for both couplings [12]).

Then in section 4, we consider in detail the momentum and coordinate coupling forms, respectively, of the pre-master equations as well as the master equation. In section 5, we discuss the corresponding Wigner quantum probability distributions and their classical limit.

To incorporate short-time phenomena, a more sophisticated analysis is required, requiring both the Langevin equation discussed in section 2 as well as a generalization to a

Langevin equation for the initial value problem, which is the theme of section 6. First, we present the solution of this equation in terms of the solution of the stationary equation, the corresponding Green function and the fluctuation force. Next, we write this solution in a form local in time. Moreover, we point out that the equivalent master equation, as distinct from those discussed in sections 3–5, is exact in that the coefficients are time-dependent for which explicit expressions are readily determined using the aforementioned solution of the Langevin equation. Then, in section 7, with a view toward calculation of quantum probability functions for superposition states and the corresponding decay of the interference term (decoherence) and developing a framework which will accommodate many different possibilities, we are led again to a consideration of WDFs, both for the whole system of quantum particle and bath and also (after averaging over the bath variables) for the reduced system. We also show that it is sometimes useful to express the solution for the Wigner function at time t in the form of an integral of a transition probability acting on the initial Wigner function; in particular, we are led to a generalization of the classical Kramers equation, in the sense that it is quantum, applies to an arbitrary heat bath and allows for a time dependence in the external force. In sections 6 and 7, we confine ourselves to $f(t) = 0$ and in section 8 we show how these various results can be applied to the calculation of decoherence, both for the case of (a) entanglement at all times and (b) the initial value problem where the system and bath are initially decoupled. In addition to our detailed discussion of decoherence in coordinate space, we also comment on results obtained for decoherence in both phase space and momentum space. The case of $f(t) \neq 0$ is also considered.

Figures 1 and 2 present an overview of the paper which should hopefully enable the reader to ‘see the wood from the trees’. In particular, in figure 1, we see that specification of the complete Hamiltonian H leads immediately to a QLE, the exact form for which depends on whether one is considering entanglement at all times or an initial value problem. From this equation, one is led to Wigner quantum probability distributions from which one may obtain, in particular, probabilities in either coordinate space or momentum space. These are the tools necessary for consideration of various problems such as decoherence phenomena. Figure 2 deals with the weak coupling limit of exact master equations and delineates their shortcomings.

2. Generalized quantum Langevin equation: entanglement for all time

In recent years, there has been widespread interest in dissipative problems arising in a variety of areas in physics. As it turns out, solutions of many of these problems are encompassed by a generalization of Langevin’s equation to encompass quantum, memory, and non-Markovian effects, as well as arbitrary temperature and the presence of an external potential $V(x)$. As in [7], we refer to this as the generalized QLE

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

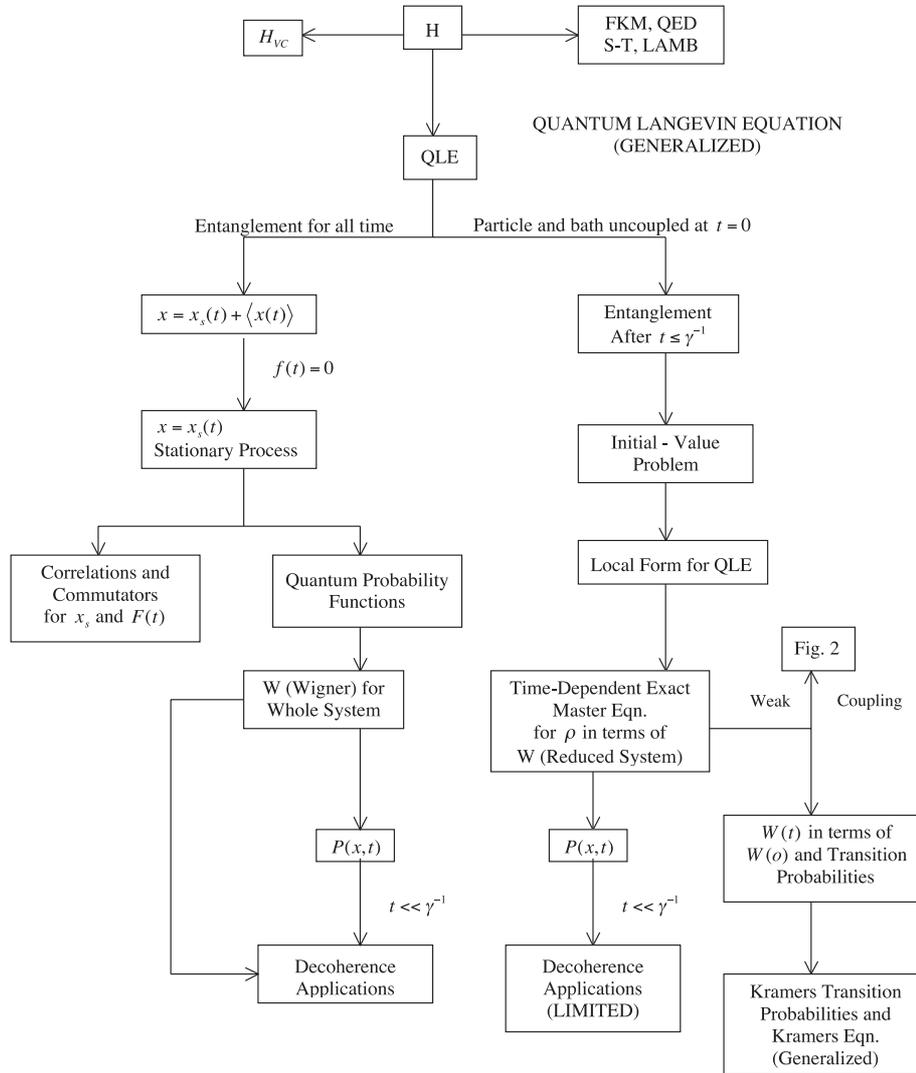


Figure 1. QLE, exact master equations and WDFs.

where $V'(x) = dV(x)/dx$ is the negative of the time-independent external force and $\mu(t)$ is the so-called memory function. $F(t)$ is the random (fluctuation or noise) force and $f(t)$ is a c -number external force. In addition, it should be strongly emphasized that ‘the description is more general than the language’ [7] in that $x(t)$ can be a generalized displacement operator (such as the phase difference of the superconducting wavefunction across a Josephson junction).

A detailed discussion of (2.1) appears in [7]. In particular, it was pointed out the QLE corresponds to a macroscopic description of a quantum system interacting with a quantum mechanical heat bath and that this description can be precisely formulated, using such general principles as causality and the second law of thermodynamics. We also stressed that this is a model-independent description. However, the most general QLE can be realized with a simple and convenient model, namely the independent-oscillator (IO) model. The Hamiltonian of the IO system is

$$H = \frac{p^2}{2m} + V(x) + \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 (q_j - x)^2 \right) - x f(t). \quad (2.2)$$

Here m is the mass of the quantum particle while m_j and ω_j refer to the mass and frequency of heat bath oscillator j . In addition, x and p are the coordinate and momentum operators for the quantum particle and q_j and p_j are the corresponding quantities for the heat bath oscillators.

The infinity of choices for the m_j and ω_j give this model its great generality [7]. In particular, it can describe nonrelativistic quantum electrodynamics (QED) [7], the Schwabl–Thirring (ST) model [13], the Ford–Kac–Mazur (FKM) model [14], and the Lamb model [15].

In this context, it should be noted that, whereas H in (2.2) has been put into a form in which all the heat bath oscillators interact with the central oscillator of interest but not with each other, we have shown that this is the most general H one can write down to describe most types of dissipation encountered in the literature; in particular, it is unitarily equivalent to the FKM model in which all the oscillators are coupled (as discussed in section 5.5 of [7]). Also of interest, in connection with our later discussions, is the velocity-coupling model in which the coupling is through the particle momentum (as distinct from the particle coordinate as in (2.2) corresponding to the Hamiltonian

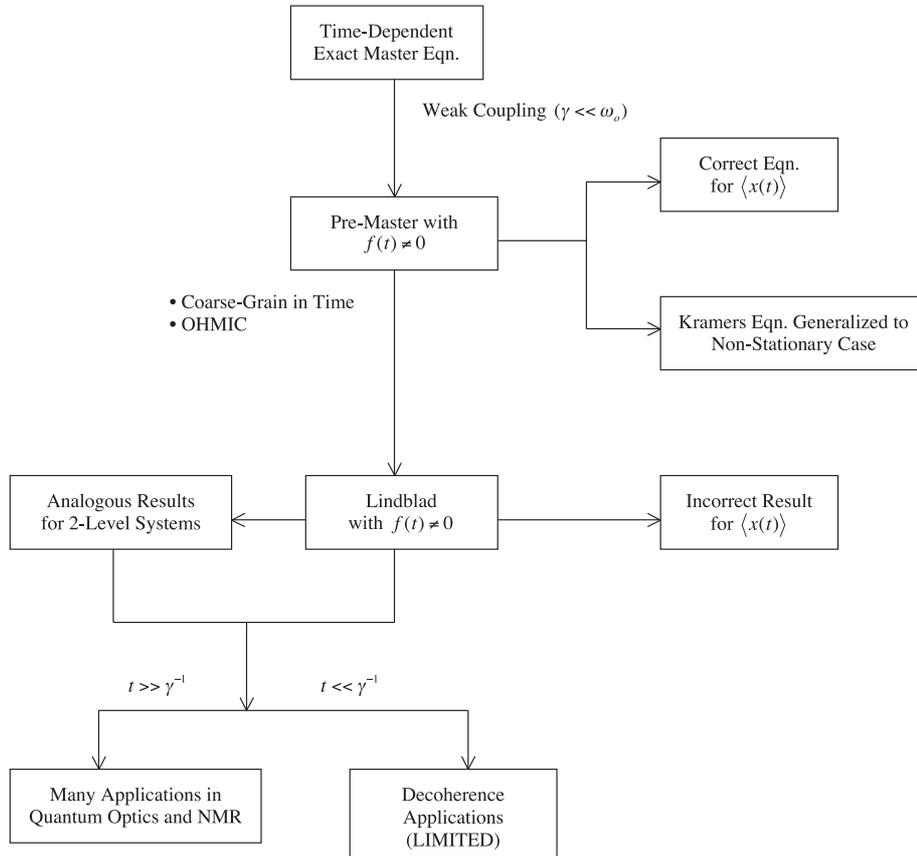


Figure 2. Pre-master and master equations for a driven oscillator in the weak coupling limit.

$$H_{VC} = \frac{1}{2m} \left(p + \sum_j m_j \omega_j q_j \right)^2 + V(x) + \sum_j \left(\frac{p_j^2}{2m_j} + \frac{1}{2} m_j \omega_j^2 q_j^2 \right) - x f(t). \tag{2.3}$$

As shown explicitly in [7], H_{VC} is obtained from H by means of two unitary transformations which change the p , p_j , and q_j but which do not change the coordinate x . We have refrained from putting primes on the changed variables since the context will always ensure that no confusion will arise. However, for future purposes, we note that, in proceeding from (2.2) to (2.3),

$$p \rightarrow p - \sum_j m_j \omega_j q_j. \tag{2.4}$$

Thus, it is not surprising that both the IO model and the vector coupling model lead to the same identical GLE (2.1). Moreover, since both Hamiltonians (2.2) and (2.3) are unitarily equivalent to the Hamiltonian of non-relativistic QED we see the close analogy with the equivalence of the $\vec{x} \cdot \vec{E}$ and $\vec{p} \cdot \vec{A}$ couplings in QED. Whereas most of our previous work has used the IO form of the Hamiltonian, we found it convenient in [6] to use the VC form for the derivation of a non-Markovian master equation.

Use of the Heisenberg equations of motion leads to the GLE (2.1) describing the time development of the particle motion, where

$$\mu(t) = \sum_j m_j \omega_j^2 \cos(\omega_j t) \theta(t), \tag{2.5}$$

is the memory function, with $\theta(t)$ the Heaviside step function. Also

$$F(t) = \sum_j m_j \omega_j^2 q_j^h(t), \tag{2.6}$$

is a fluctuating operator force with mean $\langle F(t) \rangle = 0$, where $q^h(t)$ denotes the general solution of the homogeneous equation for the heat bath oscillators (corresponding to no interaction). These results were used to obtain the results for the (symmetric) autocorrelation and commutator of $F(t)$, namely

$$\frac{1}{2} \langle F(t) F(t') + F(t') F(t) \rangle = \frac{1}{\pi} \int_0^\infty d\omega \operatorname{Re}[\tilde{\mu}(\omega + i0^+)] \hbar \omega \times \coth(\hbar\omega/2kT) \cos[\omega(t - t')] \tag{2.7}$$

$$[F(t), F(t')] = \frac{2\hbar}{i\pi} \int_0^\infty d\omega \operatorname{Re}\{\tilde{\mu}(\omega + i0^+)\} \omega \sin \omega(t - t'). \tag{2.8}$$

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

$$\tilde{\mu}(z) = \int_0^\infty dt \mu(t) e^{izt}. \tag{2.9}$$

Equation (2.7) is referred to by Kubo [16] as the second fluctuation-dissipation theorem and we note that it can be written down explicitly once the GLE is obtained. Also, its evaluation requires only knowledge of $\operatorname{Re} \tilde{\mu}(\omega)$. On the other hand, the first fluctuation-dissipation theorem is an equation involving the autocorrelation of $x(t)$ and its explicit evaluation requires a knowledge of the generalized susceptibility $\alpha(\omega)$ (to

be defined below) which is equivalent to knowing the solution to the GLE and also requires knowledge of both $\text{Re } \tilde{\mu}(\omega)$ and $\text{Im } \tilde{\mu}(\omega)$. This solution is readily obtained when $V(x) = 0$, corresponding to the original Brownian motion problem [17]. As shown by FLO [7], a solution is also possible in the case of an oscillator. Taking $V(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega_0^2x^2$, these authors obtained the solution of the Langevin equation (2.1) in the form

$$x(t) = \int_{-\infty}^t dt' G(t-t')\{F(t') + f(t')\}, \quad (2.10)$$

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

$$G(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \alpha(\omega + i0^+) e^{-i\omega t}, \quad (2.11)$$

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

$$\alpha(z) = \frac{1}{-mz^2 - iz\tilde{\mu}(z) + K}. \quad (2.12)$$

It is often convenient to write (2.10) in the form

$$x(t) = x_s(t) + x_d, \quad (2.13)$$

where x_d is the ‘driven’ contribution [18] due to the external force $f(t)$ and x_s is the contribution due to the fluctuation force $F(t)$. 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

$$\begin{aligned} C_o(t-t') &\equiv \frac{1}{2}(x_s(t)x_s(t') + x_s(t')x_s(t)) \\ &= \frac{\hbar}{\pi} \int_0^{\infty} d\omega \text{Im}\{\alpha(\omega + i0^+)\} \coth \frac{\hbar\omega}{2kT} \cos \omega(t-t'), \end{aligned} \quad (2.14)$$

is a function only of the time difference $t-t'$. Furthermore, [18]

$$\begin{aligned} C_d(t, t') &\equiv \frac{1}{2}(x(t)x(t') + x(t')x(t)) \\ &= C_o(t-t') + \langle x(t) \rangle \langle x(t') \rangle, \end{aligned} \quad (2.15)$$

where $\langle x(t) \rangle$ is the steady mean of the driven motion.

Also, taking the Fourier transform of (2.10), we obtain

$$\tilde{x}(\omega) = \alpha(\omega)\{\tilde{F}(\omega) + \tilde{f}(\omega)\}, \quad (2.16)$$

where the tilde is used to denote the Fourier transform. Thus, $\tilde{x}(\omega)$ is the Fourier transform of the operator $x(t)$:

$$\tilde{x}(\omega) = \int_{-\infty}^{\infty} dt x(t) e^{i\omega t}. \quad (2.17)$$

We have now all the tools we need to calculate observable quantities.

3. Quantum Langevin equation for the ohmic model and corresponding weak coupling master equations

As a special case of (2.1), we see that in the particular case of an oscillator with spring constant K , the Langevin equation for ohmic coupling (constant γ), has the form

$$m\ddot{x} + m\gamma\dot{x} + Kx = F(t) + f(t), \quad (3.1)$$

Moreover,

$$\langle \dot{x}(t) \rangle = \frac{\langle p(t) \rangle}{m}, \quad \langle \dot{p}(t) \rangle = -\gamma \langle p(t) \rangle - K \langle x(t) \rangle + f(t). \quad (3.2)$$

These are exact results. In the weak coupling limit, the corresponding pre-master and master equations for the density matrix may be obtained. First, a word about notation [6]. In the Schrödinger representation, the density matrix for the whole system (quantum oscillator plus heat bath) is denoted by ρ whereas $\tilde{\rho}$ denotes the reduced density matrix, obtained after a partial trace has been carried out over the heat bath variables (which, in effect, eliminates the very rapid stochastic fluctuations). The equation for $\tilde{\rho}$ is what we refer to as a pre-master equation and it includes high-frequency oscillating terms $\exp\{\pm 2i\omega_0 t\}$, where ω_0 is the oscillator frequency. If the equation for $\tilde{\rho}$ is time-averaged (which is equivalent to discarding the high-frequency oscillating terms) then the resulting equation is called a master equation for the time-averaged density matrix which is denoted by $\bar{\rho}$. The corresponding quantities in the interaction representation are σ , $\tilde{\sigma}$ and $\bar{\sigma}$. Explicitly [6], in the interaction representation,

$$\sigma = \exp\left\{\frac{iHt}{\hbar}\right\} \rho \exp\left\{-\frac{iHt}{\hbar}\right\}, \quad (3.3)$$

$$\tilde{\sigma}(t) = \text{Tr}_R\{\sigma(t)\}, \quad (3.4)$$

(where Tr_R refers to the trace over the reservoir),

$$\frac{\partial \bar{\sigma}}{\partial t} = \frac{\partial \tilde{\sigma}}{\partial t} + \exp\{\pm 2i\omega_0 t\} \text{ terms}, \quad (3.5)$$

and we have corresponding equations in the Schrödinger representation.

Moreover, the form of any of these density matrix equations depends on whether one is using the momentum or the coordinate coupling forms. In the interaction representation [6, 12] the momentum coupling form can be written

$$\begin{aligned} \frac{\partial \tilde{\sigma}}{\partial t} &= -\frac{\gamma}{2\hbar} \left\{ \frac{1}{m\omega_0} \coth \frac{\hbar\omega_0}{2kT} [p(t), [p(t), \tilde{\sigma}]] \right. \\ &\quad \left. - i[p(t), x(t)\tilde{\sigma} + \tilde{\sigma}x(t)] \right\}, \end{aligned} \quad (3.6)$$

while the coordinate coupling form can be written

$$\begin{aligned} \frac{\partial \tilde{\sigma}}{\partial t} &= -\frac{\gamma}{2\hbar} \left\{ m\omega_0 \coth \frac{\hbar\omega_0}{2kT} [x(t), [x(t), \tilde{\sigma}]] \right. \\ &\quad \left. + i[x(t), p(t)\tilde{\sigma} + \tilde{\sigma}p(t)] \right\}. \end{aligned} \quad (3.7)$$

From either of these equations one obtains the same master equation by discarding the terms explicitly oscillating at frequency $2\omega_0$ (often referred to as the rotating-wave approximation (RWA)) and this is best achieved by transforming from the variables x, p to a and a^\dagger [6].

The corresponding master equation is [12]

$$\begin{aligned} \frac{\partial \bar{\sigma}}{\partial t} &= -\frac{\gamma}{4\hbar} \left\{ \coth \frac{\hbar\omega_0}{2kT} \left(\frac{1}{m\omega_0} [p, [p, \bar{\sigma}]] + m\omega_0 [x, [x, \bar{\sigma}]] \right) \right. \\ &\quad \left. + i([x, p\bar{\sigma} + \bar{\sigma}p] - [p, x\bar{\sigma} + \bar{\sigma}x]) \right\} \end{aligned} \quad (3.8)$$

and it is a simple matter to verify that this has the Lindblad form of the master equation familiar in quantum

optics [1, 5, 6]. On the other hand, outside this community, the pre-master equations have been used extensively by Caldeira and Leggett [3] and others. We wish to emphasize that all three of the above equations lead to the same equilibrium state: $\rho_{cq} = \exp\{-H_0/kT\}$; i.e. detailed balance is obeyed. The difference is in the *approach* to equilibrium. For the pre-Lindblad equations this can be through (unphysical) states in which ρ is not positive definite. Note that this form of the equilibrium state holds only if H_0 is the free oscillator Hamiltonian (given below in (4.3)).

As already alluded to, whereas the Lindblad form of the master equation has the merit of ensuring a positive definite matrix element at all times (in contrast to pre-master equations) it has the disadvantage of being subject to the RWA. On the other hand, there are undesirable features associated with the non-positivity associated with the pre-master equations [19] but it should be remarked that all master equations give an incorrect form for very short times, as can be shown most simply by calculating the mean-square displacement, defined in (8.8) below, by means of both an exact calculation and a master equation approach. On the other hand, after a short initial time of the order of the 'bath relaxation time' (zero for the ohmic case, τ for the single relaxation time case) the exact equation has the pre-master form. This can be seen from [10], where in equation (5.4) we gave explicit expressions for the ohmic case or in equation (A5) for the single relaxation time case. Another point is that the pre-master equation gives the exact equation of motion for the mean motion, the master equation does not.

4. Mean values for the various forms of the density matrix

4.1. The momentum coupling form of the pre-master equation

In the Schrödinger representation (3.6) becomes [6]

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{i\hbar}[H_d, \tilde{\rho}] - \frac{\gamma}{2\hbar} \left\{ \frac{1}{m\omega_0} \coth \frac{\hbar\omega_0}{2kT} [p, [p, \tilde{\rho}]] - i[p, x\tilde{\rho} + \tilde{\rho}x] \right\}, \quad (4.1)$$

where H_d , the Hamiltonian for the driven oscillator, is given by

$$H_d = H_o - xf(t) \quad (4.2)$$

and where

$$H_o = \frac{p^2}{2m} + \frac{1}{2}Kx^2, \quad (4.3)$$

is the free oscillator Hamiltonian [18].

The corresponding equations for the mean of x and p are

$$\frac{d}{dt}\langle x \rangle = \frac{\langle p \rangle}{m} - \gamma\langle x \rangle, \quad \frac{d}{dt}\langle p \rangle = -m\omega_0^2\langle x \rangle + f(t). \quad (4.4)$$

If we eliminate $\langle p \rangle$ between these two equations, we get

$$\frac{d^2\langle x \rangle}{dt^2} + \gamma \frac{d\langle x \rangle}{dt} + \omega_0^2\langle x \rangle = f(t). \quad (4.5)$$

This, of course, is just what we would get from the QLE.

4.2. The coordinate coupling form of the pre-master equation

In the Schrödinger representation (3.7) becomes

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{i\hbar}[H_d, \tilde{\rho}] - \frac{\gamma}{2\hbar} \left\{ m\omega_0 \coth \frac{\hbar\omega_0}{2kT} [x, [x, \tilde{\rho}]] + i[x, p\tilde{\rho} + \tilde{\rho}p] \right\}. \quad (4.6)$$

Here, and also below, we neglect the small energy shifts because they are of no consequence as far as the present discussion is concerned. The corresponding equations for the mean of x and p are

$$\frac{d}{dt}\langle x \rangle = \frac{\langle p \rangle}{m}, \quad \frac{d}{dt}\langle p \rangle = -m\omega_0^2\langle x \rangle - \gamma\langle p \rangle + f(t). \quad (4.7)$$

If again we eliminate $\langle p \rangle$ between these two equations, we get the same equation (4.5) as in the momentum-coupling case. In other words, both forms of the pre-master equation lead to what we would get from the exact QLE.

4.3. The master equation

In the Schrödinger representation (3.8) becomes

$$\frac{\partial \tilde{\rho}}{\partial t} = \frac{1}{i\hbar}[H_d, \tilde{\rho}] - \frac{\gamma}{4\hbar} \left\{ \coth \frac{\hbar\omega_0}{2kT} \times \left(\frac{1}{m\omega_0} [p, [p, \tilde{\rho}]] + m\omega_0 [x, [x, \tilde{\rho}]] \right) + i([x, p\tilde{\rho} + \tilde{\rho}p] - [p, x\tilde{\rho} + \tilde{\rho}x]) \right\}. \quad (4.8)$$

The corresponding equations for the mean of x and p are [18]

$$\frac{d\langle x \rangle}{dt} = \frac{\langle p \rangle}{m} - \frac{\gamma}{2}\langle x \rangle, \quad \frac{d\langle p \rangle}{dt} = -m\omega_0^2\langle x \rangle - \frac{\gamma}{2}\langle p \rangle + f(t). \quad (4.9)$$

Eliminating $\langle p \rangle$ between these two equations, we get

$$\frac{d^2\langle x \rangle}{dt^2} + \gamma \frac{d\langle x \rangle}{dt} + \left(\omega_0^2 + \frac{\gamma^2}{4} \right) \langle x \rangle = \frac{f(t)}{m}. \quad (4.10)$$

Because of the spurious $(\gamma^2/4)$ term, this is *not* the equation one gets from the QLE. In fact, this equation is identical with the equation obtained from use of an RWA approximation to the exact Hamiltonian [20].

5. Quantum probability distributions

These are most simply obtained by using the Wigner function which is defined by the relation [8]

$$W(q, p; t) \equiv \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} du e^{iup/\hbar} \rho \left(q - \frac{u}{2}, q + \frac{u}{2}; t \right). \quad (5.1)$$

The translation from the operator equation for ρ to the quasi-classical equation for the Wigner function is most easily carried out by use of the Bopp operators [8], as a result of which we get the correspondence

$$\begin{aligned} x\rho &\leftrightarrow \left(q + \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) W, & \rho x &\leftrightarrow \left(q - \frac{i\hbar}{2} \frac{\partial}{\partial p} \right) W, \\ p\rho &\leftrightarrow \left(p - \frac{i\hbar}{2} \frac{\partial}{\partial q} \right) W, & \rho p &\leftrightarrow \left(p + \frac{i\hbar}{2} \frac{\partial}{\partial q} \right) W. \end{aligned} \quad (5.2)$$

It follows that the corresponding equation for the Wigner function is

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{p}{m} \frac{\partial W}{\partial q} + m\omega_0^2 q \frac{\partial W}{\partial p} - f(t) \frac{\partial W}{\partial p} \\ & + \frac{\gamma}{2} \left\{ (1+\lambda) \frac{\partial q W}{\partial q} + (1-\lambda) \frac{\partial p W}{\partial p} \right\} + \gamma \left(N + \frac{1}{2} \right) \\ & \times \left\{ (1+\lambda) \frac{\hbar}{2m\omega_0} \frac{\partial^2 W}{\partial q^2} + (1-\lambda) \frac{m\hbar\omega_0}{2} \frac{\partial^2 W}{\partial p^2} \right\}, \end{aligned} \quad (5.3)$$

where $\lambda = 0, 1$ and -1 correspond to the master, momentum coupling pre-master and coordinate coupling pre-master equations, respectively, and where

$$2\left(N + \frac{1}{2}\right) = \coth(\hbar\omega_0/2kT). \quad (5.4)$$

As a check, we note that the equilibrium distribution,

$$W_0(q, p) = \frac{1}{(2N+1)\pi} \exp\left\{-\frac{p^2 + m^2\omega_0^2 q^2}{(2N+1)m\hbar\omega_0}\right\}, \quad (5.5)$$

satisfies this equation for any value of λ if $f(t) = 0$. It is also instructive to write (5.3) explicitly for each value of λ .

(a) Momentum coupling pre-master ($\lambda = 1$)

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{p}{m} \frac{\partial W}{\partial q} + m\omega_0^2 q \frac{\partial W}{\partial p} - f(t) \frac{\partial W}{\partial p} \\ & + \gamma \frac{\partial q W}{\partial q} + \gamma \left(N + \frac{1}{2} \right) \frac{\hbar}{m\omega_0} \frac{\partial^2 W}{\partial q^2}. \end{aligned} \quad (5.6)$$

(b) Coordinate coupling pre-master ($\lambda = -1$)

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{p}{m} \frac{\partial W}{\partial q} + m\omega_0^2 q \frac{\partial W}{\partial p} - f(t) \frac{\partial W}{\partial p} \\ & + \gamma \frac{\partial p W}{\partial p} + \gamma \left(N + \frac{1}{2} \right) m\hbar\omega_0 \frac{\partial^2 W}{\partial p^2}. \end{aligned} \quad (5.7)$$

(c) Master ($\lambda = 0$)

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{p}{m} \frac{\partial W}{\partial q} + m\omega_0^2 q \frac{\partial W}{\partial p} - f(t) \frac{\partial W}{\partial p} \\ & + \frac{\gamma}{2} \left\{ \frac{\partial q W}{\partial q} + \frac{\partial p W}{\partial p} \right\} \\ & + \gamma \left(N + \frac{1}{2} \right) \left\{ \frac{\hbar}{2m\omega_0} \frac{\partial^2 W}{\partial q^2} + \frac{m\hbar\omega_0}{2} \frac{\partial^2 W}{\partial p^2} \right\}. \end{aligned} \quad (5.8)$$

We note that, in the high-temperature limit, (5.7) reduces to the well-known classical Kramers equation [21], generalized to include time dependence in the external force. Actually, (5.6) is not inconsistent with (5.7) since the values of the momentum p appearing in both equations are not the same, as discussed in the introduction (while emphasizing that q is the same in both equations). On the other hand, (5.8) does not reduce to the correct classical result. Earlier discussions of different forms of the master and Fokker–Planck equations may be found in [4] and [22]. In the next section, we will show how the exact master equation is obtained from the solution of the initial value QLE. As above, it is found to be desirable to express the result in the form of an equation for the corresponding Wigner distribution (see (6.7) below).

6. Quantum Langevin equation: initial value problem

In this and the following section, we will take $f(t) = 0$. The Langevin equation for the oscillator with given initial values is given by [10]

$$m\ddot{x} + \int_0^t dt' \mu(t-t')\dot{x}(t') + Kx = -\mu(t)x(0) + F(t), \quad (6.1)$$

and the general solution is given by

$$x(t) = m\dot{G}(t)x(0) + mG(t)\dot{x}(0) + X(t) \quad (6.2)$$

where we have introduced the fluctuating position operator,

$$X(t) = \int_0^t dt' G(t-t')F(t'). \quad (6.3)$$

If 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 , we find that the correlation and commutator are the same as those for the stationary equation. Also, the Green function is the solution of the homogeneous equation

$$m\ddot{G} + \int_0^t dt' \mu(t-t')\dot{G}(t') + KG = 0, \quad (6.4)$$

with the initial conditions

$$G(0) = 0, \quad \dot{G}(0) = \frac{1}{m}. \quad (6.5)$$

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 (6.1) 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 $-\infty$. It was then possible to show [10] that one could write the Langevin equation (6.1) in the form of an equation that is local in time with time-dependent coefficients:

$$\ddot{x} + 2\Gamma(t)\dot{x} + \Omega^2(t)x = \frac{1}{m}F(t), \quad (6.6)$$

where explicit expressions for $\Gamma(t)$ and $\Omega(t)$ were obtained in terms of $G(t)$. Furthermore, it was shown that these results constitute in essence a derivation of the HPZ exact master equation [23] with explicit expressions for the time-dependent coefficients.

The HPZ equation is perhaps best displayed in the form of its corresponding Wigner function equation. Using (5.2), we obtained [10]

$$\begin{aligned} \frac{\partial W}{\partial t} = & -\frac{1}{m}p \frac{\partial W}{\partial q} + m\Omega^2(t)q \frac{\partial W}{\partial p} + 2\Gamma(t) \frac{\partial p W}{\partial p} \\ & + \hbar m\Gamma(t)h(t) \frac{\partial^2 W}{\partial p^2} + \hbar\Gamma(t)f(t) \frac{\partial^2 W}{\partial q \partial p}, \end{aligned} \quad (6.7)$$

where $\Omega^2(t)$, $2\Gamma(t)$, $h(t)$, and $f(t)$ are time-dependent parameters for which we obtained explicit expressions in terms of $X(t)$, $F(t)$ and $G(t)$. Since these are rather cumbersome, we

simply refer to equations (2.19) and (3.8) of [10]. It should also be noted that equations equivalent to the HPZ equation have been obtained in [24–26] and in [27, 28] for the particular case of an ohmic bath.

The solution of this exact master equation will be addressed in the next section. However, it is prudent to point out a serious caveat at this stage: 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 [10].

7. Wigner distributions for the initial value problem

Our explicit solution (6.2) of the Langevin equation, together with use of Wigner functions enables us to construct the general solution of the exact master equation. Since the latter is an equation for the reduced density matrix, it was natural to proceed by writing

$$W(q, p; t) = \int dq \int dp W_{\text{system}}(q, p; q, p; t). \quad (7.1)$$

Here W_{system} is the Wigner function for the system of oscillator and bath, with $q = (q_1, q_2 \dots)$ and $p = (p_1, p_2 \dots)$ the bath coordinates and momenta. Also, since the initial state for the HPZ equation is a product state, it follows that the corresponding Wigner function is of the form

$$W_{\text{system}}(q, p; q, p; 0) = W(q, p; 0) \prod_j w_j(q_j, p_j). \quad (7.2)$$

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 ,

$$w_j(q_j, p_j) = \frac{1}{\pi \hbar \coth(\hbar \omega_j / 2kT)} \times \exp \left\{ -\frac{p_j^2 + m_j^2 \omega_j^2 q_j^2}{m_j \hbar \omega_j \coth(\hbar \omega_j / 2kT)} \right\}. \quad (7.3)$$

After some algebra, we were able to write the solution in the form of a transition operator acting on the initial Wigner function,

$$W(q, p; t) = \int_{-\infty}^{\infty} dq' \int_{-\infty}^{\infty} dp' P(q, p; q', p'; t) W(q', p'; 0). \quad (7.4)$$

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

$$P(q, p; q', p'; t) = \frac{1}{2\pi \sqrt{\det \mathbf{A}}} \exp \left\{ -\frac{1}{2} \mathbf{R} \cdot \mathbf{A}^{-1} \cdot \mathbf{R} \right\}, \quad (7.5)$$

where we have used a dyadic notation with

$$\mathbf{A}(t) = \begin{pmatrix} m^2 \langle \dot{X}^2 \rangle & \frac{m}{2} \langle X \dot{X} + \dot{X} X \rangle \\ \frac{m}{2} \langle X \dot{X} + \dot{X} X \rangle & \langle X^2 \rangle \end{pmatrix} \quad (7.6)$$

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

Here, in \mathbf{R} , the quantities $\langle q(t) \rangle$ and $\langle p(t) \rangle$ correspond to the mean of the initial value solution with initial values q' and p' . We refer to [10] for further details. We also note that transition probabilities are also discussed in [29].

In fact, the expression (7.4) for the transition probability is formally the same as that for the classical Kramers equation [21]. 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. Also, the classical solution of the Kramers equation corresponds to taking the stationary limit.

Finally, it should be emphasized that the key results we obtained in [10], some of which will be discussed below, depended only on our solution of the initial value Langevin equation, in the course of which we showed equivalence with the HPZ equation.

8. Decoherence

The problem of decoherence in quantum systems has been of considerable recent interest [9, 10, 30–35]. Decoherence refers to the destruction of a quantum interference pattern and is relevant to the many experiments that depend on achieving and maintaining entangled states. Examples of such efforts are in the areas of quantum teleportation [36], quantum information and computation [37, 38], entangled states [39], Schrödinger cats [40], and the quantum–classical interface [41]. For an overview of many of the interesting experiments involving decoherence, we refer to [39] and [42].

Much of the discussion of decoherence has been in terms of a particle moving in one dimension that is placed in an initial superposition state (a Schrödinger ‘cat’ state) corresponding to two widely separated wavepackets (see equation (8.3) below) so that the packets are separated by a distance d . Decoherence is said to occur when the long-time interference pattern is destroyed. The key questions asked are, first, under what conditions does decoherence occur and, second, what is the decoherence time? In broad outline, the problem is that of a quantum particle in a superposition state and interacting with the environment and two distinct physical scenarios present themselves depending on whether the particle is initially decoupled from the environment or, alternatively, in thermal equilibrium with the environment at the time it is put into the initial state by a measurement. We will now examine each situation in turn, using the results developed in sections 6 and 7.

8.1. Initial decoupling of particle and environment

This has been the situation which has been examined by most previous investigators and the tools of choice are either the Feynman–Vernon influence functional techniques [30] or master equation techniques [10, 31–33]. It has now become clear that, in general, the Lindblad and other weak coupling master equations are not adequate because they cannot properly handle the short times associated with decoherence phenomena [10]. We have recently given an exact treatment of the problem based on our exact solution of the Langevin equation for the initial value problem and concomitantly, the

exact solution of the HPZ master equation [10]. As discussed in section 7, the solution is best presented as a Wigner function for the reduced density matrix. We recall that the HPZ 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. 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 [43], 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, key to the existence of any master equation. The bath at $t = 0$ is in equilibrium at temperature T whereas, for the oscillator, we have the freedom to decide its initial state. More often, the initial temperature of the bath is taken to be zero or T but it is important to emphasize that, depending on the choice, different predictions ensue [10]. Hence, we will examine both situations in turn. In both cases, we need as a starting-point the probability density at time t , given by

$$P(x; t) = \int_{-\infty}^{\infty} dp W(x, p; t), \quad (8.1)$$

where $W(x, p, t)$ is the reduced Wigner function. This enables us to obtain the general result [10]

$$P(x; t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} ds \tilde{W}(Gs, m\dot{G}s; 0) \times \exp\left\{-\frac{1}{2\hbar^2} \langle X^2 \rangle s^2 + i\frac{x}{\hbar} s\right\}, \quad (8.2)$$

where \tilde{W} is the Fourier transform of the Wigner function.

8.1.1. Particle initially at zero temperature. This is the only case where one can start with a pure Schrödinger superposition ('cat') state, undisturbed by temperature or environmental effects (albeit difficult to achieve in practice). When this state at temperature zero is suddenly coupled to the heat bath at temperature T , 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 γ^{-1} . However, since γ^{-1} is generally very much greater than the decoherence decay time τ_d , decoherence will have occurred before the particle has reached the bath temperature, as a result of which an important contribution to τ_d is missed. To see this explicitly, we considered an initial state corresponding to two separated Gaussian wavepackets. The corresponding wavefunction has the form

$$\psi(x, 0) = \frac{1}{(8\pi\sigma^2)^{1/4} [1 + \exp(-\frac{d^2}{8\sigma^2})]^{1/2}} \times \left(\exp\left\{-\frac{(x - \frac{d}{2})^2}{4\sigma^2}\right\} + \exp\left\{-\frac{(x + \frac{d}{2})^2}{4\sigma^2}\right\} \right), \quad (8.3)$$

where d is the separation and σ is the width of each packet. Next, using (8.1), we obtain an expression for the probability distribution which consists of three terms, the first two of which correspond to the individual wavepackets whereas the third is an interference term, which consists of a cosine term multiplied

by a time-dependent factor. 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, for an ohmic bath, high T and $t \ll \gamma^{-1}$ [10]

$$a(t) \cong \exp\left\{-\frac{\zeta kT d^2 t^3}{12m^2\sigma^4 + 3\hbar^2 t^2}\right\}, \quad (8.4)$$

where $\zeta = m\gamma$. If we suppose that σ is negligibly small, we find $a(t) \cong \exp\{-t/\tau_d\}$ where $\tau_d = \frac{3\hbar^2}{\zeta kT d^2}$. This, except for a factor of six, is exactly the decoherence time that often appears in the literature [32, 44] for the off-diagonal terms of the density matrix (as distinct from the spatial probability discussed here, which is of more interest because it is a measurable quantity). On the other hand, if the σ term in the denominator dominates, then decoherence occurs on a time scale $\sim t^3$. 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 .

8.1.2. Particle initially at the bath temperature T . In this case, when the particle and bath are suddenly coupled, the whole system is immediately in equilibrium at temperature T . In order to analyse this scenario, we simply generalize to a state corresponding to a particle with a random velocity v due to the temperature environment. Next, we obtain the corresponding Wigner function which we average over a thermal environment. This leads to the result [9, 10]

$$a_T(t) \cong \exp\left\{-\frac{\frac{kT}{m} t^2}{8(\sigma^4 + \sigma^2 \frac{kT}{m} t^2 + \frac{\hbar^2}{4m^2} t^2)} d^2\right\}, \quad t \ll \gamma^{-1}, \quad (8.5)$$

which for very short times is of the form $a_T(t) \cong \exp\{-t^2/\tau_d^2\}$, where the decoherence time is

$$\tau_d = \frac{\sqrt{8}\sigma^2}{\bar{v}d}, \quad (8.6)$$

in which $\bar{v} = \sqrt{kT/m}$ is the mean thermal velocity. In fact, as we have shown [34, 35], the latter result can be obtained solely within the framework of elementary quantum mechanics and equilibrium statistical mechanics. In particular, since τ_d is independent of the parameters of the heat bath, the result given in (8.5) exhibits 'decoherence without dissipation' [9, 34, 35]. Thus, very different results are obtained than for case (i). Moreover, it is clear that a similar procedure can be carried out for the case of a particle initially in a very general state different from that of zero temperature.

However, as mentioned previously, all of these calculations are subject to a serious caveat connected with the assumption of an initially uncoupled state: namely we found [10] a serious persistent divergence related to the zero-point oscillations of the bath, which are 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. Such problems do not arise in case (b), which we will now examine.

8.2. Particle and environment entangled at all times

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 [11]. In their method, a system in equilibrium is put into an initial state (e.g. a wavepacket 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 wavepacket spreading and decoherence [9]. For the decoherence problem, one obtains the result [9]

$$a(t) = \exp\left\{-\frac{s(t)}{8\sigma^2 w^2(t)}\right\}, \quad (8.7)$$

for a free particle initially in the state given by (8.3), where $s(t)$ is the mean square displacement. For $f(t) = 0$, we have $s(t) \equiv \langle [x_s(t) - x_s(0)]^2 \rangle$

$$= \frac{2\hbar}{\pi} \int_0^\infty d\omega \operatorname{Im}\{\alpha(\omega + i0^+)\} \coth \frac{\hbar\omega}{2kT} (1 - \cos \omega t), \quad (8.8)$$

is the mean square displacement for the stationary process and where the variance is given by

$$w^2(t) = \sigma^2 + s(t) - \frac{[x(t), x(0)]^2}{4\sigma^2}. \quad (8.9)$$

The calculations leading to these results were based on the quantum probability functions, introduced by Ford and Lewis [11], and which may be shown to be closely related to WDFs. In the high-temperature limit, (8.7) reduces to the same result given in (8.5). This is not very surprising since (8.5) corresponds to the particle and bath both being at the same temperature, albeit uncoupled, at $t = 0$ (case 8.1.2). However, when they are suddenly coupled, they immediately become entangled, as distinct from case 8.1.1, where the particle temperature is initially zero so that it takes a time $\approx \gamma^{-1}$ for entanglement to occur.

In our view, this scenario is the most physically realistic one because at all times the particle is coupled to the bath. Moreover, we have obtained exact results, for all t , which incorporate both arbitrary temperature and arbitrary dissipation and, in particular, contains non-trivial t dependences in both numerator and denominator, especially in the case where $kT \approx \hbar\gamma$. Also, even at $T = 0$, writing $a(t) = \exp\{-b(t)\}$, we find that $b(t) \sim -t^2 \log(\gamma\tau)$ for the single relaxation time model with $(t/\tau) \ll 1$ [10, 47].

While our calculations of $a(t)$ have concentrated on the time decay of the interference term in the probability distributions, they were derived from Wigner distributions or closely related quantities [9, 10] from which other measures of decoherence are readily calculated, leading to similar conclusions.

In order to calculate decoherence in phase space, we start by considering *any* quantum state consisting of two identical components separated by a distance d . Then, it is not difficult to show that the corresponding WDF, $W^{(2)}(q, p)$ at time $t = 0$, say, is given by

$$W^{(2)}(q, p, 0) = N_0 \left\{ W\left(q + \frac{d}{2}, p, 0\right) + W\left(q - \frac{d}{2}, p, 0\right) + 2 \cos\left(\frac{pd}{\hbar}\right) W(q, p, 0) \right\}, \quad (8.10)$$

where $W(q, p, 0)$ is the Wigner function for one of the pairs at $t = 0$ and N_0 is a normalization factor. Applying this result to the two-Gaussian superposition, we concluded that there is no decoherence in either phase space or momentum space i.e. decoherence is only manifest in coordinate space [45].

The effect of an external classical force $f(t)$ on decoherence has also been considered [46]. In the absence of dissipation and for negligibly low temperature (which approximates the experimental conditions discussed in [42]) we obtained [46]

$$a(t) = \exp\left\{-\frac{s_d(t)d^2}{8\sigma^2[\sigma^2 + s_d(t)] + \frac{2\hbar^2 t^2}{m^2}}\right\}, \quad (8.11)$$

where

$$s_d(t) = \langle x_d^2(t) \rangle = \int_0^t dt' \int_0^{t'} dt'' G(t-t')G(t-t'')g(t'-t''), \quad (8.12)$$

is the mean-square displacement due to the driving force with

$$g(t' - t'') = \langle f(t')f(t'') \rangle. \quad (8.13)$$

In the case of a random delta-correlated force so that

$$g(t' - t'') = g\delta(t' - t'') \quad (8.14)$$

where g is time-independent, we obtained, for small times characteristic of decoherence phenomena,

$$s_d = \frac{gt^3}{3m^2} (\omega_0 t \ll 1). \quad (8.15)$$

In summary, we have shown that the WDF is an invaluable tool for analysing dissipative problems in quantum mechanics including investigations dealing with decoherence. Also, with regard to the latter, we demonstrated that very different results may ensue depending on the choice of whether the particle is initially decoupled from the environment or, alternatively, in thermal equilibrium with the environment at the time it is put into the initial state by a measurement.

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