Non-rotating-wave master equation

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There has been much recent discussion of problems or unphysical results occurring from the study of the non-rotating-wave (NRW) master equations. Much of this discussion has centered on the quantum Brownian motion master equation, one particular NRW master equation. These anomalous results can occur because the (NRW) master equation is not of the ''Lindblad form.'' In this paper we discuss the limitations of the NRW master equation. Two specific examples are considered, the first being a closely spaced two-level system, while the second is the classical damped free particle.

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I. INTRODUCTION

The introduction of the concept of a quantum-mechanical master equation during the past 30 years has led to a relatively straightforward and very useful method of treating damped quantum systems [1–5]. The most notable field in which master equations are used is in quantum optics, where the calculations carried out have now been verified experimentally so many times that there can be no doubt about the validity and practicality of the method. The rotating-wave quantum optical master equation gives a description of a system interacting with a heat bath—usually the radiation field—in which the effect of the heat bath is to cause transitions between well-defined energy levels of the system, which are also consequently broadened by an amount that is much less than the spacing between them. However, there are situations in quantum optics where this does not pertain.

Central to the success of the rotating-wave master equations of quantum optics is the fact that they are of the ''Lindblad form'' [3,6,7], that is, there is an equation of motion for the density operator of the system under study, which can be written in the form

$$\frac{d\rho}{dt}=-\frac{i}{\hbar}[H,\rho]+\sum_J \{2A_J^\dagger \rho A_J-\rho A_J A_J^\dagger - A_J A_J^\dagger \rho\}, \qquad (1.1)$$

where H is some (Hermitian) Hamiltonian operator and the A_J are certain operators that depend upon the problem under consideration. The form (1.1) was shown by Lindblad [6] to be the only possible form of the first-order linear differential equation for ρ that will preserve the positive semidefinite nature of ρ, that is, the property that $\langle\varphi|\rho|\varphi\rangle \geq 0$ for all $|\varphi\rangle$ as ρ evolves in time.

Although the form of (1.1) is thus rendered very attractive, from the point of view of physics it is *not* an exact equation. Its validity for quantum optical situations arises because in such systems we have a description in terms of well-defined energy levels, coupled rather weakly to the myriads of modes of the electromagnetic field. The derivations of equations of this form [1–4,8,9] make it clear that the equation for ρ is valid only on a coarse-grained time scale, which can average over many cycles of the optical electromagnetic field. This is the ''rotating-wave approximation'' in which the damping is very slow compared to the motion at optical frequencies.

In practice, the Hamiltonian part of the quantum optical master equation can be written

$$H=H_0+H_I, \qquad (1.2)$$

where H_I is a small perturbation to H_0 and

$$[H_0,A_J]=\hbar\omega_J A_J. \qquad (1.3)$$

The requirement means that H_0 is the Hamiltonian that describes the energy levels of the system and the operators A_J are transition operators, which take the system from one energy level to another.

In order to extend the success of the master-equation approach to more general situations it is possible to consider situations in which H_0 is not overwhelmingly the dominant term in the equation of motion for ρ. This allows consideration of strongly damped systems or systems with closely spaced energy levels. Recently Suominen, Garraway, and Stenholm[10] considered a two-level physical setup, as depicted in Fig. 1. Here we have two atoms separated by a distance x and the figure depicts the two energy levels corresponding to bonding and antibonding wave functions. In this model a laser pulse excites the ground state 1 to an excited (antibonding) state 2, in a wave function that is still

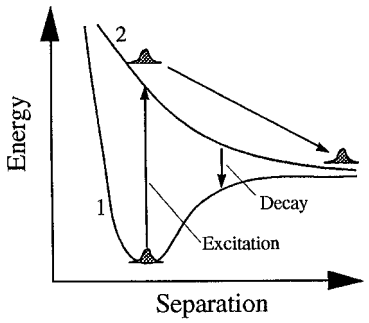

FIG. 1. Schematic representation of an ultrashort laser pulse exciting a wave packet from the lower level 1 to the upper level 2. The pulse then begins to slide down surface 2, which can bring it close to surface 1.

localized at the mean position of the bonding state. This wave packet then begins sliding down the slope to a position where the two energy levels are quite close together. The description of the process of increasing separation is handled semiclassically, so that the possible decay from the upper to the lower level should be described by a master equation whose form depends parametrically on the separation. However, in the region in which the levels are rather close together (large separation) we would not expect the rotating-wave approximation to be true. In such a regime we do not necessarily have well-defined energy levels and the approximations present in the derivation of the optical master equation may be violated.

In this case of closely spaced energy levels, the approximations used to derive the master equation are of quite a different kind and what we will call the non-rotating-wave (NRW) master equation [4,11–14] in the quantum Brownian motion (QBM) limit, which takes the form

$$\frac{\partial\rho(t)}{\partial t}=-\frac{i}{\hbar}[H_{\rm sys},\rho(t)]-\frac{i\gamma}{2\hbar}[X,[\dot{X},\rho]_+]-\frac{\gamma kT}{\hbar^2}[X,[X,\rho(t)]] \tag{1.4}$$

in which

$$\dot{X}=\frac{i}{\hbar}[H_{\rm sys},X] \tag{1.5}$$

and $H_{\rm sys}$ and X are in principle arbitrary. The particular form written in (1.4) assumes coupling to a heat bath of temperature T. (This is often called the ''quantum Brownian motion'' master equation, but our terminology is less misleading since its applicability is much wider.)

The point of immediate interest is that the NRW master equation given by (1.4) is not of the Lindblad form [14–16] and this must inevitably lead to situations in which an unphysical density operator will arise. This is not necessarily a reason to abandon this equation, but it does mean that we must face the fact that in applying the equation, more care must be taken than is necessary when using the rotating-wave quantum optical master equation. In order to put the problem in perspective, one should point out that the basic situation is this: if one uses the quantum optical master equation outside the region of validity of its derivation, one will get incorrect results, but not unphysical results such as negative probabilities; on the other hand, using the NRW master equation outside the region of validity of its derivation, the results may be both incorrect and unphysical.

The aim of this paper is to gain an understanding of the limitations of the NRW master equation. To do this we first review the derivation of the NRW master equation given by Gardiner [8]. We follow this derivation with several specific examples of the kind of unphysical solution that may be obtained, investigating in particular two extreme cases. The first model we consider is a simple two-level system, which perhaps might model a bistable superconducting quantum interference device system [17,18]. We can show that unphysical results will be obtained for all temperatures provided that an appropriate initial condition is chosen. The second system considered is a particle for which $H_{\rm sys}$ is purely a kinetic term.

II. DERIVATION AND VALIDITY OF THE NON-ROTATING-WAVE MASTER EQUATION

There have been many approaches used to derive the NRW master equation. The approach we will take in this derivation will be to use the Langevin equation, the particular form used having been presented by Gardiner *et al.* [8,19,20,21]. There are other approaches such as projection operator techniques that can be used to derive the master equation[22]. We choose to use an approach that uses the Langevin equation explicitly with the cumulant expansion [22,23] as this technique clearly demonstrates the assumption in the derivation.

A. Equations of motion

Let us consider our heat bath as an ensemble of harmonic oscillators. For a general system where we have a coupling between the system and the heat bath, we may write the Hamiltonian as

$$H=H_{\rm sys}(\mathbf{Z})+\frac{1}{2}\sum_n\{(p_n-\kappa_nX)^2+\omega_n^2q_n^2\}, \tag{2.1}$$

where $H_{\rm sys}(\mathbf{Z})$ represents the system Hamiltonian. At this stage the system Hamiltonian is left arbitrary. We write the system variables as the vector $\mathbf{Z}$. X is one of the particular system operators $\mathbf{Z}$. The coupling between the system and bath is achieved by harmonically binding the q_n to the X.

The equation of motion for an arbitrary system operator Y is

$$\dot{Y}=\frac{i}{\hbar}[H_{\rm sys},Y]+\frac{i}{2\hbar}\sum_n[[Y,\kappa_nX],p_n-\kappa_nX]_+, \tag{2.2}$$

where the $+$ sign at the end of Eq. (2.2) is used to represent an anticommutation relation. In the limit $t_0\to-\infty$ the general quantum Langevin equation becomes

$$\dot{Y}=\frac{i}{\hbar}[H_{\rm sys},Y]-\frac{i}{2\hbar}[[X,Y],\xi(t)]_+-\frac{i}{2\hbar}\left[[X,Y],\int_{t_0}^{t}f(t-t')\dot{X}(t')dt'\right]_+, \tag{2.3}$$

where X is the particular system operator harmonically bound to the heat bath, Y is an arbitrary system operator, $\dot{X}$ is given by (1.5), and $H_{\rm sys}$ is the system Hamiltonian. $\xi(t)$ is an operator function of time given by

$$\xi(t)=\sum_n\kappa_n\sqrt{\frac{\hbar\omega_n}{2}}\left[\frac{p_n(t_0)}{2\hbar\omega_n}\cos[\omega_n(t-t_0)]-\frac{q_n(t_0)}{2\hbar}\sin[\omega_n(t-t_0)]\right]. \tag{2.4}$$

We note that $\xi(t)$ is not, however, a system operator, but an externally specified operator determined by the initial values

of the bath variables [$p_n(t_0)$ and $q_n(t_0)$]. Since $\xi(t)$ is determined directly in terms of heat bath operators at a time t_0, the nature of the bath is significant. Generally the heat bath is assumed to be thermal in nature.

In Eq. (2.3), the memory function $f(t)$ is defined by

$$f(\tau)=\sum_n \kappa_n^2 \cos[\omega_n \tau]. \tag{2.5}$$

The most extreme form, often referred to as the Ohmic dissipation limit, that can be chosen for this memory function is

$$f(\tau)=\delta(\tau), \tag{2.6}$$

this being the limit required for the NRW master equation (or more generally all Markovian master equations). The importance of this choice of memory function is that our Langevin equation reduces to a simple first-order differential equation. All the future time dependence of the operators is determined simply by the present system operators and the noise. However, the equations of motion for various averages do depend on their values in the past because of the fact that $\xi(t)$ has a nonzero correlation time.

The Ohmic assumption is not necessary when the rotating-wave approximation is made in the derivation of the quantum optical master equation. Here only the nature of the couplings within a narrow bandwidth of transition frequencies are involved in the damping constants.

B. The Adjoint equation

The conversion of the Langevin equation to the master equation has been done previously [8]. Let us define the adjoint operator $\mu(t)$ by

$$\mu(t)=\sum_i \mathrm{Tr}_{\mathrm{sys}}\{e_i(t)\rho_{sys}\}e_i^\dagger, \tag{2.7}$$

where e_i represents a complete set of Schrödinger picture system projection operators and $e_i(t)$ are the corresponding Heisenberg picture system operators. The adjoint equation obtained from Eq. (2.3) is

$$\frac{\partial \mu}{\partial t}=[A_0+\alpha(t)A_1]\mu(t), \tag{2.8}$$

where

$$A_0\mu(t)=-\frac{i}{\hbar}[H_{\mathrm{sys}},\mu(t)]+\frac{i}{2\hbar}[[\dot{X},\mu(t)]_+,Xb], \tag{2.9}$$

$$A_1\mu(t)=-\frac{i}{\hbar}[\mu(t),X], \tag{2.10}$$

and $\alpha(t)$ is defined by the relation

$$\alpha(t)\mu(t')=(1/2)[\xi(t),\mu(t')]_+. \tag{2.11}$$

The anticommutator correlation function is given by

$$\langle[\xi(t),\xi(t')]_+\rangle=\frac{2\gamma\hbar}{\pi}\int_0^\infty d\omega\,\omega\,\coth\left(\frac{\hbar\omega}{2kT}\right)\cos\omega(t-t'). \tag{2.12}$$

C. The NRW master equation

Applying van Kampen's cumulant expansion to Eq. (2.8), we obtain an equation of motion for $\rho(t)=\langle\mu(t)\rangle$ in the form of a perturbation expansion in a smallness parameter $||\alpha||\,||A_1||\tau_c$, where $||\alpha||$ is the root-mean-square amplitude of $\alpha(t)$, $||A_1||$ is a measure of the magnitude of the operator A_1, and τ_c is the correlation time of α_c. The master equation to second order in this smallness parameter is

$$\frac{\partial\rho(t)}{\partial t}=A_0\rho(t)+\int_0^t d\tau\langle\alpha(t)A_1\exp[A_0\tau]\alpha(t-\tau)A_1 \times\exp[-A_0\tau]\rangle\rho(t) \tag{2.13}$$

Next we resolve the operator X [in Eqs. (2.9) and (2.10)] into eigenoperators of H_{sys},

$$X=\sum_n (X_n^+ + X_n^-), \tag{2.14}$$

where

$$[H_{\mathrm{sys}},X_n^\pm]=\pm\hbar\omega_n X_n^\pm. \tag{2.15}$$

Considering the specific case where all the ω_n are much larger that γ, we can then omit the γ dependence in A_0 present in the terms $\exp(\pm A_0\tau)$. Hence it is possible to make the replacement

$$\exp(\pm A_0\tau)X_n^\pm\rightarrow\exp(\pm i\omega_n\tau)X_n^\pm\exp(\pm A_0\tau) \tag{2.16}$$

in Eq. (2.13). Using the correlation function defined by (2.12), we find that the NRW quantum optical master equation can be written as

$$\begin{aligned}\frac{\partial\rho(t)}{\partial t}=&-\frac{i}{\hbar}[H_{\mathrm{sys}},\rho(t)]-\sum_n\frac{\pi\omega_n}{2\hbar}[\bar{N}(\omega_n)+1]\kappa(\omega_n)^2[\rho X_n^+ - X_n^-\rho,X]\\&-\sum_n\frac{\pi\omega_n}{2\hbar}\bar{N}(\omega_n)\kappa(\omega_n)^2[\rho X_n^- - X_n^+\rho,X]\\&+\frac{i}{2\hbar}\sum_n \mathrm{P}\int_{-\infty}^{\infty}\frac{d\omega\,\kappa(\omega)^2}{\omega_n-\omega}\omega\left(\bar{N}(\omega)+\frac{1}{2}\right)[[\rho,X_n^+ - X_n^-],X]\\&+\frac{i}{4\hbar}\sum_n \mathrm{P}\int_{-\infty}^{\infty}\frac{d\omega\,\kappa(\omega)^2}{\omega_n-\omega}\times\omega_m[[\rho,X_n^+ + X_n^-]_+,X],\end{aligned} \tag{2.17}$$

where $N(\omega_n)$ is given by $N(\omega_n)=\coth(\hbar\omega_n/2kT)-1/2$. The symbol $\mathrm{P}\int$ means the Cauchy principal value of that integral. This is the generalized NRW (Markovian) master equation for an arbitrary system with system operators **Z** coupled via one particular system operator X to heat bath of harmonic oscillators.

D. The NRW master equation in the QBM limit

A much more simple form of the NRW master equation occurs in the QBM limit. We do not explicitly resolve X in terms of the eigenoperators of H_{sys}. Instead we assume that

there exists a correlation time τ_c such that $\exp[A_0\tau]\sim 1$. In this limit $\kappa(\omega)\rightarrow\kappa$ (independent of ω) Eq. (2.13) can be simplified to

$$\frac{\partial\rho(t)}{\partial t}=-\frac{i}{\hbar}[H_{\rm sys},\rho(t)]-\frac{i\gamma}{2\hbar}b[X,[\dot{X},\rho]_+b] - \frac{\gamma kT}{\hbar^2}[X,[X,\rho(t)]], \tag{2.18}$$

where $\int_0^\infty d\tau\langle\alpha(t)\alpha(t-\tau)\rangle$ is obtained from Eq. (2.12).

E. Validity of the NRW master equation

We must make several comments about the NRW master equation and the application of van Kampen's cumulant expansion.

(i) First, the cumulant expansion [22,23] uses a perturbative expansion in the smallness parameter defined by

$$||\alpha||\ ||A_1||\tau_c, \tag{2.19}$$

which should always be much less than one. To an intuitive feel about the size of this smallness parameter, let us consider a Brownian particle bound in a potential well as an example. In this case the thermal correlation time is given by

$$\tau_c=\frac{\hbar}{2\pi kT}, \tag{2.20}$$

while the root-mean-square amplitude of α is given by $||\alpha||=2kT\sqrt{\gamma\pi/\hbar}$, the square root of the coefficient of the exponential in the asymptotic form for the correlation function [8]. Noting these are very problem specific, an estimate for the magnitude of A_1 for a Brownian particle near thermal equilibrium is [8]

$$||A_1||=\frac{1}{2\sqrt{mkT}}. \tag{2.21}$$

With these estimates we find that the smallness parameter may be expressed as $||\alpha||\ ||A_1||\tau_c=\sqrt{\gamma\hbar/4\pi mkT}$ and the requirement for the validity of the cumulant expansion for the Brownian particle is

$$\frac{\hbar\gamma}{m}\ll kT\ \ (\text{or}\ \ \tau_c\ll\tau_D\equiv\gamma/m), \tag{2.22}$$

where τ_D is the damping constant of the system. Examining Eq. (2.22), we could interpret γ/m as an imaginary "frequency" and hence this equation means that the thermal energy given by kT must be much greater than the quantum of energy associated with the imaginary frequency for the cumulant expansion to be value.

In our general derivation of the master equation from a Langevin equation, only second-order terms in the cumulant expansion were retained. If the quantity $A_1\alpha\tau$ becomes large (this can occur as $T\rightarrow 0$), then the perturbative approach can break down and hence higher-order terms in the perturbation need to be included. A NRW master equation including fourth-order terms has been derived by Collett.

(ii) In the derivation of the NRW master equation in the QBM limit we made the approximation $\exp[A_0\tau]\sim 1$. As long as the correlation time τ_c is short this is quite a reasonable assumption. However, the thermal correlation time, given by 2.20, can become large as the temperature approaches zero. In this case it is no longer valid to use this approximation and a more appropriate approximation may be $\exp[A_0\tau]$ by $\exp[A_{\rm sys}\tau]$.

(iii) To derive the master equations we have considered it has been necessary to assume that the system and bath are initially statistically independent and noninteracting. This allows a factorization of the total density operator ρ into system and bath parts. In some quantum-mechanical cases, however, the system and bath are initially interlinked and hence there is no natural way of generating a factorized density operator. Assuming a factorized initial density operator in these cases will cause initial transient behaviors, which we, however, drop. Without this initial factorization the Markovian master equation cannot be derived.

In Secs. III and IV we consider two specific examples that show anomalous behavior. For computational simplicity we use the NRW master equation in the QBM limit instead of the more general NRW master equation given by (2.17).

III. TWO-LEVEL SYSTEM

Probably the simplest quantum optical example that we could consider is the two-level system. The two-level atom is commonly used to model many atomic systems in quantum optics. Generally here though, the upper and lower level are well separated and the damping is weak compared with the coupling between the levels. Recently, however, Parkins and Gardiner [17,18] applied a two-level system to the study of macroscopic quantum coherence. They considered a quantum system in which a symmetric double-well potential yields two closely spaced low-lying states, which are well separated from the remaining higher-energy states. Parkins and Gardiner assumed that the higher-energy states were not significantly populated and modeled the system as being composed of only two levels. Because of the narrowly spaced levels, the standard quantum optical master equation could not be used and a NRW master equation in the QBM limit approach was taken. In fact, the authors did not explicitly use the NRW master equation, but instead directly simulated the adjoint equation (2.8).

For the two-level atom we may choose a basis for the system as $|1/2\rangle$ and $|-1/2\rangle$, where $|1/2\rangle$ represents the excited state and $|-1/2\rangle$ represent the ground state. The density matrix may then be defined by $\rho_{n,m}=\langle n|\rho|m\rangle$, with $n,m=\pm\frac{1}{2}$. The states $\rho_{-1/2,-1/2}$ and $\rho_{1/2,1/2}$ represent the diagonal elements of the density-matrix and are constrained by the requirement $\rho_{-1/2,-1/2}+\rho_{1/2,1/2}=1$. The off-diagonal elements are $\rho_{-1/2,1/2}$ and $\rho_{1/2,-1/2}$. These density matrix elements are related to the Pauli spin matrices by the standard relations.

Choosing the system operator $X=\sqrt{\hbar/\Omega}\sigma_x$ to couple to bath, we can show that the density-matrix element $\rho_{n,m}(t)$ evolves as

$$\left\langle n\left|\frac{d\rho}{dt}\right|m\right\rangle = -\frac{i}{2}\Omega\langle n|[\sigma_z,\rho]|m\rangle - \frac{i\gamma}{2}\langle n|[\sigma_x,[\sigma_y,\rho]_+]|m\rangle - \frac{\gamma kT}{\hbar\Omega}\langle n|[\sigma_x,[\sigma_x,\rho]]|m\rangle. \tag{3.1}$$

Here the system Hamiltonian is given by $H_{\rm sys}=\frac{1}{2}\hbar\Omega\sigma_z$. $\dot{X}$ is given by

$$\dot{X}=\frac{i}{\hbar}[H_{\rm sys},X]=-\sqrt{\hbar\Omega}\sigma_y. \tag{3.2}$$

Equation (3.1) contains two decoupled sets of differential equations, one for the diagonal elements and one for the off-diagonal elements. Explicitly solving for the diagonal elements, we have

$$\rho_{-\frac{1}{2},-\frac{1}{2}}(t)=\left\{\frac{1}{2}\left(\frac{\hbar\Omega}{2kT}+1\right)\left[1-\exp\left(-\frac{4\gamma kT}{\hbar\Omega}t\right)\right]+\rho_{-1/2,-1/2}\exp\left(-\frac{4\gamma kT}{\hbar\Omega}t\right)\right\}, \tag{3.3}$$

$$\rho_{1/2,1/2}(t)=1-\rho_{-1/2,-1/2}(t). \tag{3.4}$$

The off-diagonal elements have the solution

$$\rho_{-1/2,1/2}(t)=\exp\left[-\frac{2\gamma kT}{\hbar\Omega}t\right]\left[\frac{I\Omega}{\Theta}\sinh(\Theta t)+\cosh(\Theta t)\right]\rho_{-1/2,1/2}+\frac{2\gamma kT}{\hbar\Omega\Theta}\times\exp\left[-\frac{2\gamma kT}{\hbar\Omega}t\right]\sinh(\Theta t)\rho_{1/2,-1/2}, \tag{3.5}$$

$$\rho_{1/2,-1/2}(t)=\rho_{-1/2\,,\,1/2}(t)^* \tag{3.6}$$

where Θ is defined

$$\Theta=\sqrt{\left(\frac{2\gamma kT}{\hbar\Omega}\right)^2-\Omega^2}. \tag{3.7}$$

The initial density-matrix elements are given by $\rho_{-1/2,-1/2}$, $\rho_{1/2,-1/2}$, and $\rho_{-1/2,1/2}$.

With explicit solutions for the various density-matrix elements in the two-level atom, can we determine if these elements violate the properties of the density operator? In order for the density matrix to be positive semidefinite, we must have

$$\det\rho(t)>0. \tag{3.8}$$

A. Initial transients

To examine the short-time regime of (3.8) we expand the determinant as a power series in time. To first order in t, we have

$$\det\rho(t)=\frac{4\gamma kT}{\hbar\Omega}t\left[2\rho^2_{-1/2,-1/2}-\rho_{-1/2,-1/2}\left(2+\frac{\hbar\Omega}{2kT}\right)+\frac{1}{2}\left(1+\frac{\hbar\Omega}{2kT}\right)\right], \tag{3.9}$$

where we have assumed that the initial conditions are chosen such that the density matrix elements satisfy $|\rho_{-1/2,1/2}|^2=\rho_{-1/2,-1/2}\rho_{1/2,1/2}$. These choices for the density-matrix elements mean that the initial determinant is zero.

It can be clearly seen from Eq. (3.9) that the determinant is negative for $1/2<\rho_{-1/2,-1/2}<1/2+\hbar\Omega/4kT$, with the minimum value occurring at $\rho_{-1/2\,,-1/2}=1/2+\hbar\Omega/8kT$. At this minimum the determinant to first order in time is given by $\det\rho(t)=-\gamma\hbar\Omega/4kT\,t$. What is more interesting is that these unphysical result occurs for all temperatures, but the determinant $\det\rho(t)$ becomes asymptotic to zero in the high-temperature (or classical) limit.

B. Validity of the cumulant expansion for the two-level atom

We have observed unphysical results can occur in the short-time regime. It is necessary, however, to confirm whether the cumulant expansion is valid in this limit. Using Eq. (2.19) with an estimate for the magnitude of $||A_1||$ as

$$||A_1||\sim\frac{1}{\sqrt{\hbar\Omega}}, \tag{3.10}$$

we have the criteria for the validity of the expansion as

$$\frac{\gamma}{\Omega}\ll 1. \tag{3.11}$$

This indicates that the cumulant expansion is only valid in the weak damping limit, the opposite limit to which we are studying. In the next section we consider a second example that shows similar anomalous behavior.

IV. DAMPED FREE PARTICLE

The second example we consider is the motion of a free damped particle [24]. In this case the system Hamiltonian may be described by

$$H_{\rm sys}\rightarrow\frac{p^2}{2m}. \tag{4.1}$$

Choosing the position operator x as the operator coupled to the environment, the NRW master equation is

$$\frac{d\rho}{dt}=-\frac{i}{\hbar}[H_{\rm sys},\rho]-\frac{i\gamma}{2\hbar m}[x,[p,\rho]_+]-\frac{\gamma kT}{\hbar^2}[x,[x,\rho]]. \tag{4.2}$$

If we consider our system to be initially in a pure state $|\varphi\rangle$, then initially the expectation value is

$$\langle\varphi|\rho(0)|\varphi\rangle=1. \tag{4.3}$$

Initially at $t=0$, the expectation value of $\rho(t)$ evolves as

$$\left\langle \varphi\left|\frac{d\rho}{dt}\right|\varphi\right\rangle\Bigg|_{t=0}=\frac{\gamma}{2m}\langle\varphi|\rho|\varphi\rangle\Bigg|_{t=0}-\frac{\gamma kT}{\hbar^2}[\langle\varphi|x^2|\varphi\rangle -\langle\varphi|x|\varphi\rangle^2]\Bigg|_{t=0}, \tag{4.4}$$

where the second part, proportional to $[\langle\varphi|x^2|\varphi\rangle-\langle\varphi|x|\varphi\rangle^2]$, must always be negative. If we consider our system to be in a near eigenstate of position, that is, $[\langle\varphi|x^2|\varphi\rangle-\langle\varphi|x|\varphi\rangle^2]$ is very small, then the first term in Eq. (4.4) dominates. It is always possible to choose $|\varphi\rangle$ so that the second term is less than the first and under these circumstances, $\langle\varphi|\rho(t)|\varphi\rangle$ will initially increase past one [since $\langle\varphi|\rho(0)|\varphi\rangle=1$], yielding an unphysical result. More specifically if we were to consider that the system is in a near thermal equilibrium minimum-uncertainty state with the variance in the momentum given by $\langle\Delta p^2\rangle=mkT$, then the expectation value of $\rho(t)$ must initially evolve as

$$\left\langle \varphi\left|\frac{d\rho}{dt}\right|\varphi\right\rangle\Bigg|_{t=0}=\frac{\gamma}{4m} \tag{4.5}$$

for all temperatures.

The above behavior is only a transient behavior, as can be seen from the following argument. When the system is in a near position eigenstate (little uncertainty in x) and because the uncertainty principle requires $\Delta x\Delta p=i\hbar$, we must have a very large uncertainty in the momentum. The position operator x evolves as

$$x\rightarrow x+p/mdt, \tag{4.6}$$

which, because of the large uncertainty in p, will drive the system from its near position eigenstate. Hence the second term in Eq. (4.4) proportional to γkT will make a larger contribution and this will force the expectation valve of $\rho(t)$ rapidly back below one.

A. The Wigner function

Our analysis given above is valid only in the limit $t\rightarrow 0$. An alternative approach by which the time evolution of the system can be studied is to consider the Wigner function. Defining the Wigner function by [8]

$$W(x,p)=\frac{1}{\hbar\pi}\int dy\langle x+y|\rho|x-y\rangle\exp[-2iyp/\hbar], \tag{4.7}$$

the free particle NRW master equation in the QBM limit can be converted to the following equation of motion for the Wigner function:

$$\frac{\partial W}{\partial t}=\left\{-\frac{\partial}{\partial x}\frac{p}{m}+\frac{\partial}{\partial p}\gamma\frac{p}{m}+\gamma kT\frac{\partial^2}{\partial p^2}\right\}W. \tag{4.8}$$

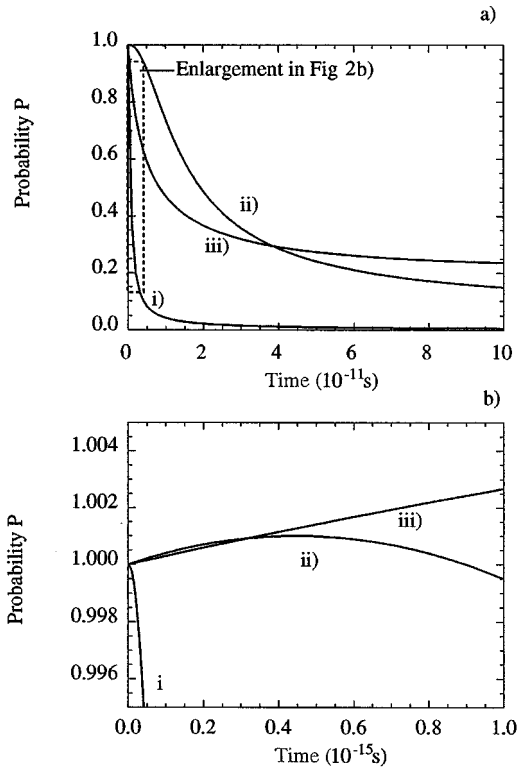

FIG. 2. Plot of the probability P versus time for the damped free particle with $T=1$ K, $\gamma\sim 10^{-15}$ kg s^{-1}, and $m\sim 10^{-26}$ kg. For these parameters $||A_1||\,||\alpha||\tau_c\sim 0.2$. (a) is plotted on a picosecond time scale and (b) on a femtosecond time scale for (i) $\sigma=10^{-11}$ m, (ii) $\sigma=5\times 10^{-11}$ m, and (iii) $\sigma=10^{-10}$ m.

This is identical to the corresponding classical Fokker-Planck equation [8]. The probability of the system being in the state $|\varphi\rangle$ is given by

$$P=\langle\varphi|\rho(t)|\varphi\rangle=\int\phi(x)\phi^*(y)\langle x|\rho|y\rangle dxdy\leqslant 1, \tag{4.9}$$

where $\phi(x)$ is the initial position wave function and $\langle x|\rho|y\rangle$ is determined from the Fourier transform of the Wigner function given by (4.7).

There are exact Gaussian solutions to Eq. (4.8). The time evolution of the Wigner function is specified by the covariance matrix, which can be obtained from the solution of the various equations of motion for the second-order moments. With these solutions the Wigner function can be specified and hence $\langle x|\rho(t)|y\rangle$ determined. Performing the integration present in (4.9), the probability can be determined provided that the initial position and momentum wave functions have well known variances.

B. Numerical solutions

We choose our system to be in a minimum-uncertainty state, with the variance in the position specified by $\langle\Delta x^2\rangle=\sigma^2$. Performing the procedure discussed above, we present in Fig. (2) our results for various initial σ. Two explicit times scales are shown. The first set of results [Fig. 2(a)] is plotted on a time scale associated with the damping

constant τ_D. It is difficult here to determine whether the probability does exceed one for any time, the results for that time scale indicating $P<1$ for all t. However, if we plot on a much finer time scale Fig. 2(b), then we clearly observe that P does exceed one provided $\sigma^2 \leqslant \hbar^2/2mkT$. We note that the second time scale we have considered is even shorter than the thermal correlation time for the system and that the probability is not much greater than one.

It is also worthwhile reconsidering our case considered in Sec. IV A, where we considered the system is in a near thermal equilibrium minimum-uncertainty state with the variance in the momentum given by $\langle \Delta p^2 \rangle = mkT$. For this specific set of parameters, the probability can exceed one, but for reasonable temperatures this only gives rise to a very rapid and rather small transient.

C. Validity of the cumulant expansion for the free particle

The results above indicate that, provided that a well-localized initial position wave function is chosen ($\sigma^2 \leqslant \hbar^2/2mkT$), the probability can exceed one for short times. However, in deriving the master equation we applied a perturbation expansion to second order in a smallness parameter $|A_1 \alpha \tau_c|$. For the validity of the cumulant expansion we require the smallness parameter to be much less than one. For the Brownian particle in near thermal equilibrium as discussed previously, we require $\sqrt{\gamma\hbar/4\pi mkT} \ll 1$. For the parameters chosen in Fig. 2 we have $|A_1 \alpha \tau_c| \sim 0.2$. If we choose this smallness much smaller by, say, increasing the temperature, then the probability of the system being in the state $|\varphi\rangle$ can still exceed one, but it does so on a much shorter time, and the magnitude of the violation is smaller.

V. MODIFYING THE NRW MASTER EQUATION

In Secs. III and IV we considered two specific situations in which the NRW master equation showed anomalous behavior in the short-time regime. Various authors have proposed that modifying this master equation may alleviate this problem. Two specific approaches have been considered.

(i) The first is an *ad hoc* method by which the necessary terms are added to make the master equation of the Lindblad form [25]. A term of the form

$$\frac{\gamma}{4\eta kT} b[\dot{X},[\dot{X},\rho]b] \tag{5.1}$$

added to Eq. (1.4) will give the Lindblad master equation

$$\begin{aligned}\frac{\partial \rho(t)}{\partial t} = &-\frac{i}{\hbar}\left[H_{\rm sys} + \frac{\gamma}{2}\dot{X}X, \rho(t)\right] - \frac{\gamma kT(1-\eta)}{\hbar^2}[X,[X,\rho(t)]] \\ &-\left[\sqrt{\frac{\gamma}{4\eta kT}}\,\dot{X} - i\sqrt{\frac{\gamma\eta kT}{\hbar^2}}X, \left[\sqrt{\frac{\gamma}{4\eta kT}}\,\dot{X}\right.\right. \\ &\left.\left. + i\sqrt{\frac{\gamma\eta kT}{\hbar^2}}X, \rho(t)\right]\right].\end{aligned} \tag{5.2}$$

Here η is an arbitrary constant that must be less than 1. If we let η be very small in (5.1), then its contribution can be small for reasonable temperatures. It is hard, however, to explain the physical significance of this additional term. Recently, Stenholm [16] has pointed out that the addition of terms of the form $[p,[p,\rho]]$ can mean that the variance in the momentum increases with time and hence this can lead to uncontrolled heating of the system. This is physically unacceptable.

(ii) The second method is based on altering the physical model. We modify the physical picture to make it look more like the rotating-wave quantum optical master equation. In particular, work by Collett [14] and us have included higher-order terms in the cumulant expansion (up to sixth order in α). In this approach anomalous results still occur for certain parameters.

An alternative approach to this problem was considered by Hakim and Ambegaokar [24], who considered a quantum theory of a free particle interacting with a linearly dissipative medium. These authors considered nonfactorized initial conditions for the system and bath. More explicitly, the case was examined in which the initial off-diagonal coherence of the density matrix was comparable to that in the state of thermal equilibrium of the coupled system. Transients are still present for this nonfactorized initial condition.

VI. CONCLUSION

This paper has explored various aspects of non-rotating-wave master equations. In particular, like many other authors, we have pointed out that the NRW master equation is not of the Lindblad form. To many physicists this may be seen as a minor problem; however, as we have discussed, there are physical systems that can be modeled by such a master equation, which would give anomalous or unphysical results. In particular we considered two extreme cases: (i) simple two-level system modeled the system Hamiltonian $H_{\rm sys} = (1/2)\hbar\Omega$ and (ii) particle in which $H_{\rm sys}$ is purely a kinetic term.

In both of these cases we found that under appropriate initial conditions, very rapid and rather small transients can occur (anomalous results for other systems in these transient time regimes have been discussed previously by Ambegaokar and others [8,26–29,]). Two particular assumptions may be being violated. The first is that the cumulant expansion smallness parameter is not much much less than one, while the second is due to the initial factorization of system and bath. Recent, work by Gardiner [8] and Collett [30], however, suggest that this transient behavior may be due to the unrealistic factorization of the system and bath's density operator. Factorizing the system and bath may put the total system into a higher-energy state than it was initially in. Disregarding this phenomenon causes a small but rapid initial transient. Hence, in the NRW master equation there is little validity to considering time scales shorter than the thermal correlation time because of the coarse-grain time-scale approach used in its derivation.

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