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Non-Markovian Irreversible Behavior in a Simple Model

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The soluble model of an oscillator coupled to a scalar field is used as an example of irreversible behavior. By studying the reduced density operator for the oscillator, a generalized Fokker-Planck-Kramers-Chandrasekhar equation for the Wigner distribution function is derived. The diagonal matrix elements of the reduced density operator satisfy a generalized non-Markovian master equation. By application of a time-averaged method, the ordinary Pauli master equation is derived. The time evolution of the occupation probabilities of the oscillator levels has been numerically computed, and compared with the solutions of the Pauli equation.

I. INTRODUCTION

Great progress in the understanding of irreversible phenomena in quantum statistics was made by van Hove and his co-workers,[1] and by Prigogine and his school.[2] An important landmark in this context was the derivation by these workers of the generalized master equation (GME). This equation governs the time evolution of the probability distribution of the system over states of the unperturbed Hamiltonian H_0. For infinite systems, it predicts the evolution towards statistical equilibrium.[1,2]

The GME, an equation to infinite order in the perturbation, is a direct consequence of the Schrödinger equation,[3] and the only statistical hypothesis used in its derivation is the assumption of random phases at the initial time.

It is known that in the weak-coupling limit, the GME goes over into the much simpler Pauli master equation (PME), which has been solved for a number of different physical situations. The GME, on the other hand, has been explicitly written down and solved only in very few cases.[4,5] As a consequence, very little is known to date about the time evolution of the probability distribution for arbitrary coupling strength. It would seem then that a number of simple examples are still needed in order to clarify and illustrate the general features of the approach to equilibrium in cases where the coupling constant cannot be considered small.

We present here a study of irreversible behavior for the simple model of an harmonic oscillator linearly coupled to a scalar field.[6,7] Similar models have been considered by other authors.[8-11]

The dynamical equations for the system can be exactly solved, and this fact has been exploited throughout. We take the density operator at the initial time as the product of a canonical ensemble density operator for the field and an arbitrary density operator for the oscillator. Consequently the approach to equilibrium described by the model is meant in a restricted sense, because at the initial time all but one of the degrees of freedom are already in equilibrium. As has been pointed out elsewhere,[7] irreversible behavior in this model is essentially determined by the infinite extension of the system, which makes the recurrence period infinitely long.

In Sec. II, we briefly review the most important properties of the solution of the equation of motion and how a connection with the phenomenological theory of Brownian motion can be established by means of a Langevin equation.

In Sec. III, we give the Green functions for the oscillator and the corresponding spectral density function, which illustrates the fact that the interaction causes a frequency renormalization and leads to a finite width of the oscillator levels.

Using a complete set of Weyl operators,[12,13] in Sec. IV we make an operator Fourier analysis of the reduced density operator (RDO) for the oscillator. The ensuing Fourier amplitude is the dynamical characteristic function (DCF).[12] The ordinary Fourier transform of the DCF is the Wigner distribution function.[14] We show that this distribution function obeys a partial differential equation, which can be seen to be a generalization of an equation first derived by Kramers and Chandrasekhar in the theory of Brownian motion.[15,16] In going over to the limit of classical statistical mechanics, it can be shown from the properties of the autocorrelation function for the stochastical force in the Langevin equation that the model describes Markovian processes. In this case, our dynamical equation coincides with the equation of Kramers and Chandrasekhar.

In Sec. V, we establish a connection between the DCF and the matrix elements of the reduced density operator (RDO), taken between eigenstates of an oscillator Hamiltonian with the frequency renormalized by the interaction. This allows us to derive an equation for the rate of change of the matrix elements of the RDO. This equation connects diagonal and off-diagonal matrix elements taken at the same time and is somewhat similar to the matrix equation with a tetradic Liouville operator derived by Zwanzig.[17] Elimination of the off-diagonal elements gives then the GME for the model. Since we work with states of a renormalized Hamiltonian, thus separating transient and permanent effects of the perturbation,[1] our master equation falls somewhat outside of the usual formulations.[1,2,17]

At the end of Sec. V we show how an application of the *method of averaging*[18] and the consideration of the small-coupling limit allows us to obtain the PME for the model. This coincides with an equation previously derived by Montroll[9,19] for an oscillator interacting with a thermostat through the exchange of radiation.

In Sec. VI, we find an explicit form for the occupation probabilities of the oscillator levels as a function of time. A computer calculation of these occupation probabilities has been performed and the results are compared with the solution of the PME. The relevant fact here is the oscillating character of the exact solutions, which contrasts with the smooth behavior of the approximate solutions.[4] This oscillator character of the time evolution of occupation probabilities thus seems to be a general feature of the approach to equilibrium in any nonweak-coupling theory.[4,17]

Another general feature of irreversible behavior, which also shows up in this simple model, is the existence of three time scales measured, respectively, by a "collision" time, a quantum correlation time $\hbar/kT$, and a relaxation time, determined by the coupling parameter.[1,9,17] Throughout this paper we have systematically neglected the "collision" time; it can be shown that the neglected corrections can be accounted for by means of a power-series expansion. This will be a question for future study.

II. PROPERTIES OF THE MODEL

In this section, we shall briefly review the most important properties of the dynamical model, as have been discussed in Refs. 6 and 7. The equations of motion are

$$\left(\frac{d^2}{dt^2}+\omega_0^2\right)Q=\int d^3k\, g(\vec{k})\phi(\vec{k}) \quad , \tag{1}$$

$$\left(\frac{\partial^2}{\partial t^2}+k^2\right)\phi(\vec{k})=g(\vec{k})Q \quad , \tag{2}$$

where Q is the coordinate of the oscillator and ϕ represents the field amplitude. The coupling function is

$$g(\vec{k})=gM(M^2+k^2)^{-1/2} \quad ,$$

and will eventually be considered in the limit $M\to\infty$; we shall henceforth refer to this as the M limit. This amounts to neglecting the collision time in an ordinary kinetic problem.[11]

The solution of the initial-value problem for Eqs. (1) and (2) can be put into the form

$$Q=Q_1+Q_2\,,\quad \phi(\vec{k})=\phi_1(\vec{k})+\phi_2(\vec{k}) \quad , \tag{3}$$

where the indices 1 and 2 refer to quantities which depend upon the initial values of the oscillator and the field variables, respectively. Explicitly we have[6,7]

$$Q_1(t)=\dot{S}(\tau)Q_0+S(\tau)\dot{Q}_0 \quad , \tag{4}$$

$$Q_2(t)=\int d^3k\,[\dot{N}(\vec{k},\tau)\phi_0(k)+N(\vec{k},\tau)\dot{\phi}_0(\vec{k})] \quad ,$$

$$\phi_1(\vec{k},t)=\dot{N}(\vec{k},\tau)Q_0+N(\vec{k},\tau)\dot{Q}_0 \quad ,$$

$$\phi_2(\vec{k},t)=\int d^3k'[\dot{Y}(\vec{k},\vec{k}',\tau)\phi_0(\vec{k}') \tag{5}$$

$$+Y(\vec{k},\vec{k}',\tau)\phi_0(\vec{k}')] , \quad \tau = t - t_0 ,$$

with $S(t) = \int d^3q \, |f(\vec{q})|^2(\sin qt/q)$,

$$N(\vec{k},t) = \int d^3q \, (\vec{k}|\Omega|\vec{q}) f(\vec{q})(\sin qt/q) , \quad (6a)$$

$$Y(\vec{k},\vec{k}',t) = \int d^3q \, (\vec{k}|\Omega|\vec{q})(\vec{q}|\Omega^+|\vec{k}')(\sin qt/q) ,$$

and $f(\vec{q}) = g(\vec{q})D^{-1}(\vec{q})$,

$$(\vec{k}|\Omega|\vec{q}) = \delta(\vec{k}-\vec{q}) + [g(\vec{k})/(k^2-q^2)]f(\vec{q}) , \quad (6b)$$

$$D(\vec{q}) = \omega_0^2 - q^2 + \int d^3k [|g(\vec{k})|^2/(q^2-k^2)] .$$

The functions (6) have been explicitly given in Ref. 7.

The dynamical variables can be used as operators in quantum mechanics, assuming the following commutations relations:

$$[Q,\dot{Q}] = i\hbar, \quad [\phi(\vec{r},t), \dot{\phi}(\vec{r}',t)] = i\hbar\delta(\vec{r}-\vec{r}') , \quad (7)$$

where $\hbar$ is Dirac's constant expressed in suitable units.

We want to study the evolution of the system starting from an initial state which describes the field as a thermal bath of temperature T, and the oscillator in an arbitrary state. We thus assume the following density matrix at the initial time:

$$\rho(t_0) = \rho_1(t_0)\rho_2(t_0) , \quad (8)$$

where $\rho_2(t_0) = e^{F-\beta H_2}$,

where H_2 is the Hamiltonian of the free field. $\rho_1(t_0)$ gives the initial condition for the oscillator.

The model can be related to the theory of Brownian Motion[7,10-13] by showing that Langevin's equation can be derived from Eq. (1),

$$\ddot{Q} + \bar{\omega}^2 Q + 2\Gamma\dot{Q} = K(t) , \quad (9)$$

where $\bar{\omega}^2 = \omega_0^2 - 2\Gamma M, \quad \Gamma = \pi^2 g^2$.

We assume ω_0 adjusted so that $\bar{\omega}^2 > 0$.

We recall here that the stochastical force $K(t)$ satisfies, in the phenomenological theory, the two relations

$$\bar{K}(t) = 0, \quad \overline{K(t)K(t')} \sim \delta(t-t') . \quad (10a)$$

Calculating the ensemble average of $K(t)$ and $K(t)K(t')$ with the density matrix (8), and considering times $t \gg 1/M$, we get[7]

$$\langle K(t) \rangle = 0 , \quad (10b)$$

$$\langle K(t)K(t') \rangle = \frac{2\Gamma\hbar}{\pi}\left\{ \frac{1}{\tau^2} - \frac{\pi}{\hbar\beta^2}\,\mathrm{csch}^2\,\frac{\pi\tau}{\hbar\beta} + \frac{\partial}{\partial\tau}\left[\frac{P}{\tau} + i\pi\delta(\tau)\right]\right\} , \quad (10c)$$

with $\tau = t - t'$. The term containing the derivative tends to zero as $h \to 0$, so that it describes a kind of quantum correlation.

The other two terms yield

$$\lim_{\hbar/kT \to 0} \langle K(t)K(t') \rangle = (4\Gamma kT/m)\delta(\tau) .$$

III. GREEN FUNCTIONS DESCRIPTION

It is illustrative to look at the spectral density function which one obtains by solving for the Green functions. We define

$$D_{11}(t,t') = i\langle TQ(t)Q(t') \rangle ,$$
$$D_{22}(\vec{k}t, \vec{k}'t') = i\langle T\phi(\vec{k},t)\phi(\vec{k}',t') \rangle , \quad (11)$$
$$D_{12}(t,\vec{k}'t') = i\langle TQ(t)\phi(\vec{k}',t') \rangle ,$$

where T is the time-ordering operator. These Green functions obey the following equations of motion:

$$\left(\frac{\partial^2}{\partial t^2} + \omega_0^2\right) D_{11}(t,t') = \delta(t-t') + \int d^3k\, g(\vec{k}) D_{12}(t,\vec{k}t') ,$$

$$\left(\frac{\partial^2}{\partial t^2} + \omega_0^2\right) D_{12}(t,\vec{k}'t') = \int d^3k\, g(\vec{k}) D_{22}(\vec{k}t,\vec{k}'t') ,$$

$$\left(\frac{\partial^2}{\partial t^2} + k^2\right) D_{22}(\vec{k}t,\vec{k}'t') = \delta(\vec{k}-\vec{k}')\delta(t-t') + g(\vec{k})D_{12}(t,\vec{k}'t') , \quad (12)$$

$$\left(\frac{\partial^2}{\partial t^2} + k^2\right) D_{12}(t',\vec{k}t') = g(\vec{k}) D_{11}(t,t') .$$

From these equations, the following Dyson equation for D_{11} can be easily obtained:

$$D_{11}(t,t') = D_0(\omega_0, t-t') + \int dt_1\, dt_2\, D_0(\omega_0, t-t_1) \times \Sigma(t_1-t_2) D_{11}(t_2-t') .$$

The self-energy function Σ is defined by

$$\Sigma(t-t') = \int d^3q\, |g(\vec{q})|^2 D_0(q, t-t') .$$

The zeroth-order functions $D_0(q,t)$ are the solutions of

$$\left(\frac{\partial^2}{\partial t^2} + q^2\right) D_0(q,t) = \delta(t) .$$

The self-energy function can be explicitly evaluated. For the zero-temperature case we obtain

$$\Sigma(\omega) = \Sigma_1(\omega) + i\Sigma_2(\omega) ,$$

where $\Sigma_1(\omega) = 2\Gamma M^3(M^2+\omega^2)^{-1}$, $\Sigma_2(\omega) = 2i\Gamma|\omega|$.

In the M limit, the Fourier transform of the Green function D_{11} becomes

$$D_{11}(\omega) = (\bar{\omega}^2 - \omega^2 - 2i\Gamma|\omega|)^{-1}, \quad \bar{\omega}^2 = \omega_0^2 - 2\Gamma M .$$

The corresponding spectral density function, giving the number of oscillator modes per unit frequency range, is

$$\rho(\omega) = (\omega/\pi)\,\mathrm{Im}D_{11}(\omega) = 2\pi\omega^2|f(\omega)|^2$$

$$= (2\Gamma/\pi)\omega^2/[(\bar{\omega}^2-\omega^2)^2+4\Gamma^2\omega^2] \quad . \tag{13}$$

We see that it has a Lorentzian form, centered around $\bar{\omega}$ and of width Γ.

IV. DISTRIBUTION FUNCTIONS AND FOKKER-PLANCK EQUATION

We shall base our discussion of the time development of the density matrix on an operator Fourier analysis of the RDO

$$\rho_1(t) = \mathrm{Tr}_2\rho(t) \quad . \tag{14}$$

This is done by expanding $\rho_1(t)$ in the complete set of Weyl operators[9,14]

$$\Omega(\xi,\eta) = \exp i(\xi Q_0 + \eta \dot{Q}_0) \tag{15}$$

in the form

$$\rho_1(t) = (\hbar/2\pi)\int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\eta\, R(\xi,\eta,t)\Omega(\xi,\eta) \quad .$$

The Fourier amplitude, usually called the dynamical characteristic function DCF, is

$$R(\xi,\eta,t) = \mathrm{Tr}_1[\rho_1(t)\Omega^+(\xi,\eta)]$$
$$= \mathrm{Tr}[\rho(0)\Omega^+(\xi,\eta,t)] \quad , \tag{16}$$

where $\Omega(\xi,\eta,t) = \exp i[\xi Q(t) + \eta \dot{Q}(t)]$.

It can be shown that the ordinary Fourier transform of the DCF is the Wigner distribution function

$$W(p,q,t) = \frac{1}{(2\pi)^2}\int d\xi \int d\eta\, R(\xi,\eta,t)\exp i(\xi q + \eta q)$$
$$= [1/(2\pi)^2]\int d\xi\, d\eta\, \langle \exp i[\xi(q-Q(t)) + \eta(p-\dot{Q}(t))]\rangle_0 \quad , \tag{17}$$

where $\langle\,\rangle_0$ means the mean value with the density matrix at $t=0$. It is known that $W(p,q,t)$ is the quantum-mechanical analogue of the distribution function in phase space. To illustrate the meaning of W in the present case, we can evaluate it explicitly. For this, we take $\rho_1(0)$ as a Gaussian combination of coherent states, which allows us to retain a statistical distribution of the initial coordinates, even in the classical limit. Thus let

$$\rho_1(0) = \int d^2\alpha\, F(\alpha)|\alpha\rangle\langle\alpha| \quad , \tag{18}$$

where $|\alpha\rangle$ is a coherent state,[20,21] $\alpha = (2\hbar/\bar{\omega})^{1/2} \times (x + i\bar{\omega}y)$,

$$F(\alpha) = \frac{1}{4\pi\Delta x\Delta y}\exp - \left(\frac{(x-Q_0)^2}{2\Delta x^2} + \frac{(y-\dot{Q}_0)^2}{2\Delta y^2}\right),$$

and $F(\alpha)$ satisfies

$$\int d^2\alpha\, F(\alpha) = 1 \quad .$$

Equation (18) is a generalization of Glauber's Gaussian density operator.[21] Using the explicit form of the density operator, it is possible to evaluate the DCF and the Wigner distribution function. For the latter we obtain

$$W(p,q,t) = \frac{1}{2\pi(\Delta Q^2\Delta\dot{Q}^2-\Delta^2)^{1/2}}\exp - \frac{\Delta Q^2[p-p(t)]^2 + \Delta\dot{Q}^2[q-q(t)]^2 - 2\Delta[q-q(t)][p-p(t)]}{2(\Delta Q^2\Delta\dot{Q}^2-\Delta^2)} \quad , \tag{19a}$$

where

$$\Delta Q^2 = \Delta Q_0^2\dot{S}^2 + \Delta\dot{Q}_0^2 S^2 + \hbar\int (d^3k/k)\,(n_k+\tfrac{1}{2})(\dot{N}^2 + k^2N^2) \quad ,$$
$$\Delta\dot{Q}^2 = \Delta Q_0^2\ddot{S}^2 + \Delta\dot{Q}_0^2\dot{S}^2 + \hbar\int (d^3k/k)\,(n_k+\tfrac{1}{2})(\ddot{N}^2 + k^2\dot{N}^2) \quad ,$$
$$\Delta^2 = \Delta Q_0^2\dot{S}\ddot{S} + \Delta\dot{Q}_0^2 S\dot{S} + \hbar\int (d^3k/k)(n_k+\tfrac{1}{2})\dot{N}(\ddot{N}+k^2N) \quad , \tag{19b}$$

$$\Delta Q_0^2 = \Delta x^2 + \hbar/2\bar{\omega}, \quad \Delta\dot{Q}_0^2 = \Delta y^2 + \tfrac{1}{2}\hbar\bar{\omega} \quad ,$$
$$p(t) = \langle Q(t)\rangle, \qquad q(t) = \langle Q(t)\rangle \quad .$$

The distribution function Eq. (19a) has the same form as the solution of the Kramers-Chandrasekhar equation,[15,16] given, for instance, by Prigogine.[2,22,23] The difference can be seen to lie in the dispersions Eq. (19b). Particularly the dependence on the bath temperature, contained here in the factor n_k, can be seen to be directly related to the spectral-density function $|f(k)|^2$.

The next step in comparing this particular model with general theories of irreversible behavior is to look at the equation obeyed by $W(p,q,t)$. The derivation is given in Appendix A, and it is

$$\left(\frac{\partial}{\partial t} - \bar{\omega}^2 q\frac{\partial}{\partial q} + p\frac{\partial}{\partial q}\right)W = \frac{\partial}{\partial p}(2\Gamma pW) + a'(t)\frac{\partial^2 W}{\partial p^2} + b'(t)\frac{\partial^2 W}{\partial p\,\partial q} \quad , \tag{20}$$

where
$$a'(t) = \tfrac{1}{2}\langle K(t)\dot{Q}(t) + \dot{Q}(t)K(t)\rangle \quad ,$$
$$b'(t) = \tfrac{1}{2}\langle K(t)Q(t) + Q(t)K(t)\rangle \quad . \tag{21}$$

In the classical limit, when $K(t)$ satisfies the conditions (10a) of the phenomenological theory, Eqs. (21) give

$$a'(t) = 2\Gamma kt, \quad b'(t) = 0 \quad ,$$

and Eq. (20) becomes exactly equal to the Kramers-

Chandrasekhar equation.[15,16] We note briefly that the left-hand side of Eq. (20) should be interpreted as the usual left-hand side of the Boltzmann equation, while the right-hand side contains the effect of "collisions." Working with the RDO makes the left-hand side of the kinetic equation (20) time dependent; this fact will prevail in the GME to be obtained in Sec. V.

V. MATRIX ELEMENTS OF REDUCED DENSITY OPERATOR AND MASTER EQUATION

There is a simple relation between the DCF $R(\xi,\eta,t)$ and the matrix elements of $\rho_1(t)$, taken between eigenstates of the renormalized oscillator Hamiltonian:

$$R(\xi,\eta,t)=\mathrm{Tr}_1[\rho_1(t)\Omega^+(\xi,\eta)]=\sum_{mn}\langle m|\rho_1(t)|n\rangle\langle n|\Omega^+|m\rangle=\sum_{mn}p_{mn}(t)\langle n|\Omega^+|m\rangle \ .$$

This can in turn be written

$$R(\xi,\eta,t)=R_{\mathrm{d.}}(\xi,\eta,t)+R_{\mathrm{o.d.}}(\xi,\eta,t) \ ,$$

with $R_{\mathrm{d.}}(\xi,\eta,t)=\sum_n p_n(t)\langle n|\Omega^+|n\rangle$,

$$R_{\mathrm{o.d.}}(\xi,\eta,t)=\sum_{n,m}{}' p_{mn}(t)\langle n|\Omega^+|m\rangle \ ,$$

where $\sum'$ means that the terms with $n=m$ are excluded and where d. and o.d. stand for diagonal and off-diagonal, respectively. Using the explicit form[12] of the matrix elements $\langle m|\Omega|n\rangle$, introducing polar coordinates in the (ξ,η) plane

$r=(\hbar/2\overline{\omega})(\xi^2+\overline{\omega}^2\eta^2)$, $\varphi=\arctan(\omega\eta\xi^{-1})$

and the indices $\nu=n-m$, $N=n+m$, we can show that

$$P_{mn}(t)=P_N^\nu(t)=(1/2\pi)\int_0^{2\pi}d\varphi\int_0^\infty dr\,e^{-i\nu\varphi}\times\left(\frac{\frac{1}{2}(N-\nu)!}{\frac{1}{2}(N+\nu)!}\right)^{1/2}(e^{-i\pi}r)^{\nu/2}l_{(N-\nu)/2}(r)R(r,\varphi,t) \ , \tag{22}$$

where $l_N^\nu(x)=e^{-x/2}L_N^\nu(x)$ is the Laguerre function.

It is shown in Appendix A how the projection rules Eq. (22) allow us to transform the differential equation for R into an equation for P_N^ν which is of the form

$$\dot{P}_N^\nu=\sum_{\nu'N'}M_{NN'}^{\nu\nu'}P_{N'}^{\nu'} \ . \tag{23}$$

The nonvanishing matrix elements of M are

$$M_{NN}^{\nu\nu}=\Gamma-(N+1)a+i\nu\overline{\omega} \ ,$$

$$M_{NN}^{\nu\nu\pm2}=\tfrac{1}{2}(a\mp ib)(N\mp\nu)^{1/2}(N\pm\nu+2)^{1/2}\times(1+\delta_{\pm2,\nu}+\delta_{\mp1,\nu}) \ ,$$

$$M_{NN+2}^{\nu\nu\pm2}=-\tfrac{1}{4}(a\mp ib+\Gamma)(N\pm\nu+4)^{1/2}(N\pm\nu+2)^{1/2}\times(1+\delta_{\mp2,\nu}+\delta_{\mp1,\nu}) \ , \tag{24}$$

$$M_{NN-2}^{\nu\nu\pm2}=-\tfrac{1}{4}(a\mp ib-\Gamma)(N\mp\nu)^{1/2}(N\mp\nu-2)^{1/2}\times(1+\delta_{\mp2,\nu}+\delta_{\mp1,\nu}) \ ,$$

$$M_{NN\pm2}^{\nu\nu}=\tfrac{1}{2}(a\pm\Gamma)(N+\nu+1\pm1)^{1/2}(N-\nu+1\pm1)^{1/2} \ ,$$

where $a=(\hbar\overline{\omega})^{-1}a'$, $b=\hbar^{-1}b'$.

For a given N, ν varies between $-N$ and N, so we can arrange P_N^ν as a column vector (written horizontally for typographical reasons)

$$P=[P_0^0,P_1^{-1},P_1^1,P_2^{-2},P_2^0,P_2^2,\ldots] \ .$$

It follows from Eq. (24) that M' does not couple N's of different parity, so that in Eq. (23) we actually have two uncoupled sets of equations. Since eventually we shall be interested in a diagonal GME, we can restrict ourselves in what follows to consider only those elements of P which contain even N's. Defining a matrix D such that multiplied by P it gives the diagonal elements[17] $P_{\mathrm{d.}}=DP$: the off-diagonal elements are contained in $P_{\mathrm{o.d.}}=(1-D)P$. We have the obvious relation $P=P_{\mathrm{d.}}+P_{\mathrm{o.d.}}$.

Multiplying Eq. (23) alternately by D and by $(1-D)$, we have the two equations

$$\dot{P}_{\mathrm{d.}}=DMP_{\mathrm{d.}}+DMP_{\mathrm{o.d.}} \ , \tag{25a}$$

$$\dot{P}_{\mathrm{o.d.}}=(1-D)MP_{\mathrm{d.}}+(1-D)MP_{\mathrm{o.d.}} \ . \tag{25b}$$

Defining $U(t,t')$ as the solution of $dU/dt=(1-D)MU$, with the initial condition $U(t,t)=1$, and assuming $P_{\mathrm{o.d.}}(0)=0$ (random phases), we can obtain from Eqs. (25) the following diagonal GME:

$$\frac{d}{dt}P_{\mathrm{d.}}(t)=DM(t)P_{\mathrm{d.}}(t)+\int_0^t dt'\,U(t,t')\times(1-D)M(t')P_{\mathrm{d.}}(t') \ . \tag{26}$$

It should be noticed that the general relation between matrix elements Eqs. (23) and (25) are instantaneous; they do not contain any memory term. This appears upon elimination of the off-diagonal terms $P_{\mathrm{o.d.}}$. As opposed to what happens with the complete master equations,[1,3] which refer to the full density matrix, the kernel in Eq. (26) does not depend only on the difference $t-t'$, but rather it depends on t and t' separately.

Ford[18] has used the *method of averaging* to derive the Boltzmann equation starting from the Liouville equation. We will see that this method also provides a link between Eqs. (25) and (26) on one hand, and the PME on the other hand. We recall here that the *method of averaging* is designed to systematically separate, in an equation such as (23) above, the slow from the rapid time variation of the solutions. Accordingly, we go back to Eq. (23) and write it as $\dot{P}=\epsilon MP$, where ϵ is a parameter which will eventually be set equal to one. We propose the following series expansion for $P(t)$:

$$P(t)=[1+\epsilon A^{(2)}(t)+\epsilon^2 A^{(2)}(t)+\cdots]Y(t), \tag{27}$$

where $Y(t)$ is assumed to satisfy the following equation:

$$\dot{Y}(t)=(\epsilon B^{(1)}+\epsilon^2 B^{(2)}+\cdots)Y(t) \quad . \tag{28}$$

Here $B^{(n)}$ is taken as time independent; this is the prescription that will make $Y(t)$ a slowly varying function. Replacing Eqs. (27) and (28) in (23), we are led to the following set of equations:

$$\dot{A}^{(1)}+B^{(1)}=M, \quad \dot{A}^{(2)}+B^{(2)}=MA^{(1)}-A^{(1)}B^{(1)} . \tag{29}$$

For $A^{(1)}(t)$ to describe only the rapid fluctuations, we take

$$B^{(1)}=\overline{M}(t)=\lim_{t\to\infty}(1/t)\int_0^t M(t')\,dt' \quad . \tag{30}$$

Upon imposing the initial condition

$$P(0)=Y(0) \quad , \tag{31}$$

we immediately obtain

$$A^{(1)}(t)=\int_0^t dt'\,[M(t')-\overline{M}] \quad . \tag{32}$$

To first order in ϵ, we thus have

$$\dot{Y}=\overline{M}Y \quad . \tag{33}$$

Equation (33) still contains diagonal and off-diagonal matrix elements of Y. The elimination of the off-diagonal elements can be done in exactly the same way as it was done for P, Eqs. (25) above. To lowest order in ϵ, we thus have $\dot{Y}_{\text{d.}}=D\overline{M}Y_{\text{d.}}$, or explicitly

$$\frac{dY_n}{dt}=(\overline{a}-\Gamma)nY_{n-1}+(\overline{a}+\Gamma)(n+1)Y_{n+1} +[\Gamma-(2n+1)\overline{a}]Y_n \quad . \tag{34}$$

This is the lowest-order approximation produced by the method of averaging, but it still contains the coupling parameter Γ to all orders, through the quantity $\overline{a}$. In fact, we have

$$\overline{a}=2\Gamma\hbar\int d^3k\,k\,|f(k)|^2(n_k+\tfrac{1}{2}) \quad . \tag{35}$$

Using the property

$$\lim_{\Gamma\to 0}|f(k)|^2=\lim_{\Gamma\to 0}\frac{1}{\pi^2}\frac{\Gamma}{(\overline{\omega}^2-k^2)^2+4\Gamma^2k^2} =\frac{1}{2\pi k}\,\delta(\overline{\omega}^2-k^2) \quad , \tag{36}$$

we obtain the following lowest-order approximation in Γ:

$$\frac{dY_n}{dt}=\frac{2\Gamma}{1-e^{-\theta}}\{(n+1)Y_{n+1}-[(n+1)e^{-\theta}+n]Y_n+ne^{-\theta}Y_{n-1}\}, \tag{37}$$

where $\theta=\hbar\overline{\omega}/kT$. This explicit form of the PME was first obtained by Montroll[9, 19] for a system of oscillators interacting with a thermostat through the exchange of radiation. Here we found that for this dynamical model, it follows from the GME by considering the lowest-order approximation to the slowly varying part of $P_n(t)$.

VI. SOLUTION OF THE MASTER EQUATION

Assuming the initial condition

$$Y_n(0)=P_n(0)=\delta_{nN} \quad , \tag{38}$$

the solution of the PME (37) can be put in the form

$$Y_n(t)=\left(\frac{e^{\theta}-1}{e^{\theta}-e^{-\tau}}\right)\left(\frac{1-e^{-\tau}}{e^{\theta}-e^{-\tau}}\right)^{n+N}e^{\theta N}{}_2F_1(-N,-n;1;x) , \tag{39}$$

where $\quad x=\sinh^2\tfrac{1}{2}\theta/\sinh^2\tfrac{1}{2}\tau, \quad \tau=2\Gamma t$,

and ${}_2F_1$ is the hypergeometric function, which in this case reduces to a polynomial of order equal to the smallest of the integers N and n. The properties of the solution (39) have been thoroughly discussed in Ref. 19.

Using the definition (16) we can find the explicit form of the function $R(\xi,\eta,t)$ for the initial conditions (38). The projection rules Eqs. (22) allow us then to find the diagonal elements $P_n(t)$. In this form, we obtain

$$\begin{aligned}P_n(t)&=\langle n|\rho_1(t)|n\rangle\\ &=(1/\pi)\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dy\,L_N(ux^2+vy^2+2wxy)\\ &\quad\times L_n(x^2+y^2)\exp[-(\alpha x^2+\beta y^2+2\gamma xy)] ,\end{aligned} \tag{40}$$

where $L_n(x)$ is the Laguerre polynomial of degree n, and the functions u, v, w, α, β, γ are defined as follows:

$$\begin{aligned}u(t)&=\dot{S}^2(t)+\overline{\omega}^2S^2(t) \quad ,\\ v(t)&=S^2(t)+(1/\overline{\omega}^2)\ddot{S}^2(t) \quad ,\\ w(t)&=\dot{S}(t)[\overline{\omega}S(t)+(1/\overline{\omega})\ddot{S}(t)] \quad ,\\ \alpha(t)&=\tfrac{1}{2}[1+u(t)]+\overline{\omega}\int(d^3k/k)\,(n_k+\tfrac{1}{2})(\dot{N}^2+k^2N^2) \quad ,\\ \beta(t)&=\tfrac{1}{2}[1+v(t)]+(1/\overline{\omega})\int(d^3k/k)\,(n_k+\tfrac{1}{2})(\ddot{N}^2+k^2\dot{N}^2) \quad ,\\ \gamma(t)&=\tfrac{1}{2}w(t)+\int d^3k\,(n_k+\tfrac{1}{2})\dot{N}(\ddot{N}+k^2N) \quad .\end{aligned} \tag{41}$$

In Appendix C we show how this expression can be further transformed so that finally we obtain $P_n(t)$ as a finite sum of terms where

$$P_n(t)=\frac{n!N!}{(n+N)!}\sum_{j=0}^{\min(n,N)}4^{j+1}\frac{[F(t)-G(t)]^{N-j}G(t)^j}{F(t)^{N+j+1}}\sum_{a_1+a_2+\cdots a_8=n+N}\frac{(-)^{a_8}}{a_1!a_2!\cdots a_8!}$$

$$\times\frac{j!(n-j)!(N-j)!(n+N+a_8)!}{(j-a_1)!(n-j-a_2)!(n-j-a_3)!(N-j-a_4)!(N-j-a_5)!}\frac{1}{(j-a_6)!(j-a_7)!}z_1^{j-a_1}(z_1-A_1)^{n-j-a_2}$$

$$\times(z_1-A_2)^{n-j-a_3}(z_1-B_1)^{N-j-a_4}(z_1-B_2)^{N-j-a_5}(z_1-M_1)^{j-a_6}(z_1-M_2)^{j-a_7}(z_1-z_2)^{-(n+N+a_8+1)}, \quad (42)$$

where $F(t)=\alpha-\beta-2i\gamma$, $G(t)=u-v-2iw$, and $A_{1,2}$, $B_{1,2}$, $M_{1,2}$, and $z_{1,2}$ are the roots of the following quadratic equations:

$$\begin{aligned} &F(t)z^2+2(\alpha+\beta-2)z+F^*(t)=0 \ , \\ &[F(t)-G(t)]z^2+2(\alpha+\beta-u-v)z+F^*(t)-G^*(t)=0 \ , \\ &G(t)z^2+2(u+v)z+G^*(t)=0 \ , \\ &F(t)z^2+2(\alpha+\beta)z+F^*(t)=0 \ , \end{aligned} \quad (43)$$

respectively. z_1 is chosen such that $|z_1|<|z_2|$.

In order to visualize the relevant features of the time evolution of the probabilities, a computer calculation of Eq. (42) has been performed. As is well known,[19] the solution $Y_n(t)$ of the PME has a smooth time variation; in fact, it can always be expressed as a finite sum of real exponentials. The computed values of $P_n(t)$ show rapid fluctuations; Fig. 1 is a plot of $\Delta P_n(t)=Y_n(t)-P_n(t)$ as a function of $2\Gamma t$.

The two curves shown correspond to $\bar{\omega}=5\Gamma$ and to the two values $\theta=7.84$ and 2. As is apparent from Fig. 1, the difference between the Pauli approximation and the exact results is bigger for small times, which should be expected. For long times, ΔP_n does not approach zero because the equilibrium values $P_n(\infty)$ of the dynamical model differ from the Boltzmann distribution predicted by the PME. We can see from Eq. (42) that

$$P_n(\infty)=[4n!/\alpha(\infty)-\beta(\infty)] \times\sum_{a_1+a_2+a_3=n}\frac{(-)^{a_8}(n+a_3)!}{a_1!a_2!a_3!(n-a_1)!(n-a_2)!} \times\frac{[z_1(\infty)-A_1(\infty)]^{n-a_1}[z_1(\infty)-A_2(\infty)]^{n-a_2}}{[z_1(\infty)-z_2(\infty)]^{n+a_3+1}} \ . \quad (44)$$

The quantities $z_{1,2}(\infty)$, $A_{1,2}(\infty)$ may be evaluated from (43) using the fact that for $t=\infty$ we have $\gamma=u=v=w=0$ and

$$\begin{aligned} \alpha(\infty)&=\tfrac{1}{2}+\bar{\omega}\int(d^3k/k)\,|f(k)|^2(n_k+\tfrac{1}{2}) \ , \\ \beta(\infty)&=\tfrac{1}{2}+(1/\bar{\omega})\int d^3k\,k\,|f(k)|^2(n_k+\tfrac{1}{2}) \ . \end{aligned} \quad (45)$$

In the weak-coupling limit it follows straightforwardly from Eq. (44) that

$$Y_n(\infty)=(1-e^{-\beta\hbar\bar{\omega}})e^{-n\beta\hbar\bar{\omega}} \ . \quad (46)$$

Figure 2 gives the equilibrium occupation probabilities for the oscillator levels in logarithmic scale. In all cases we have taken $\theta=7.84$. It should be noted how the probability for the ground state decreases with decreasing $\bar{\omega}/\Gamma$, while the

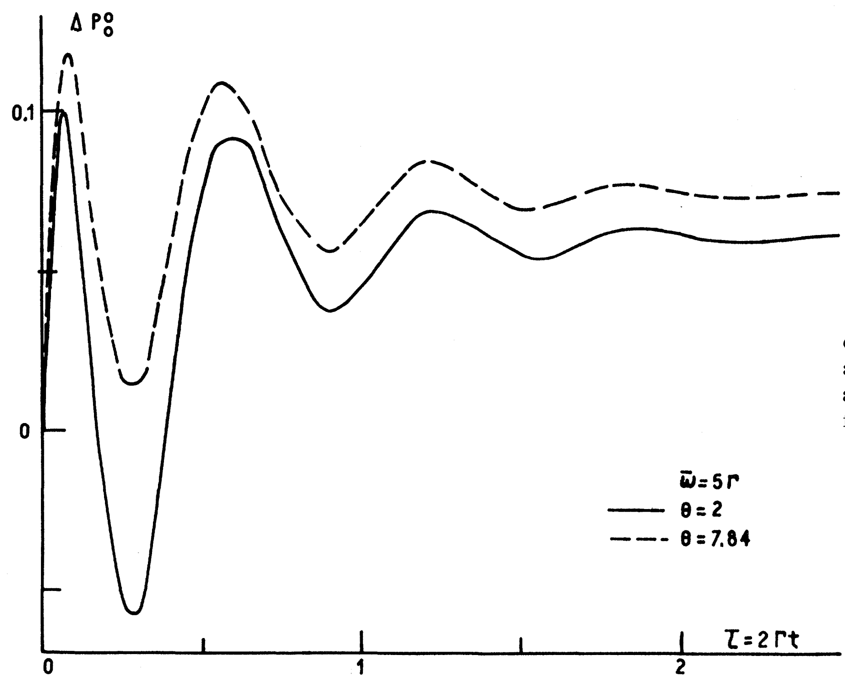

FIG. 1. Difference between the exact solution for the occupation probabilities and the Pauli approximation as a function of time. Solid line is for $\theta=7.84$ and dotted line for $\theta=2$.

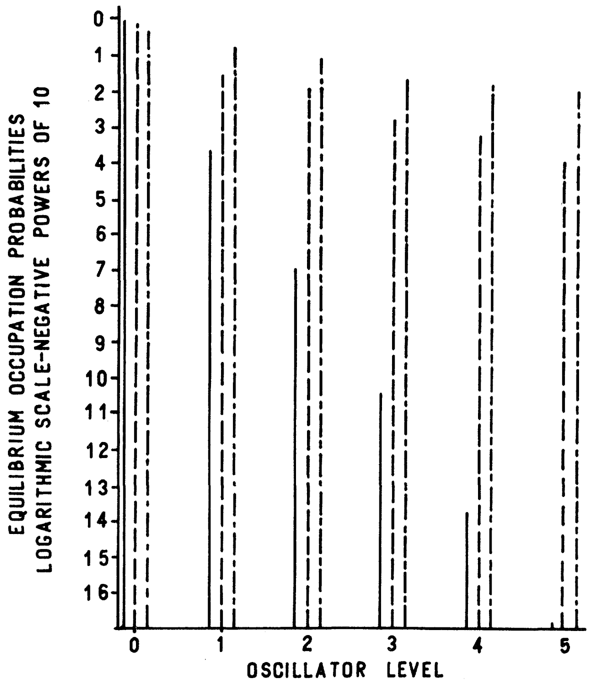

FIG. 2. Equilibrium values of the occupation probabilities for the oscillator levels. All cases correspond to $\theta = 7.84$. The solid line is the Boltzmann distribution $\bar{\omega} = 5\Gamma$, the dashed line is $\bar{\omega} = 5\Gamma$, and the dot-dashed line is $\bar{\omega} = 2\Gamma$.

probability for the other states increases. This can be understood in terms of the broadening of the oscillator levels caused by the interaction, which mixes the ground state with the excited states, thus depleting its probability with respect to the Boltzmann distribution value.

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APPENDIX A

In order to obtain an equation for $W(p, q, t)$, we will first derive an equation for $R(\xi, \eta, t)$. According to the definition Eq. (16), we have

$$R(\xi, \eta, t) = \langle \exp i(\xi Q + \eta \dot{Q}) \rangle ,$$

and consequently

$$\left(\frac{\partial}{\partial t} + \bar{\omega}^2 \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} + 2\Gamma\eta \frac{\partial}{\partial \eta}\right) R$$
$$= \tfrac{1}{2}\langle K(t) \exp i(\xi Q + \eta \dot{Q}) + \text{h.c.}\rangle$$
$$= \tfrac{1}{2}\langle K_1 \exp i(\xi Q_1 + \eta \dot{Q}_1) + \text{h.c.}\rangle$$
$$+ \tfrac{1}{2}\langle K_2 \exp i(\xi Q_2 + \eta \dot{Q}_2) + \text{h.c.}\rangle \quad . \tag{A1}$$

The last step is a consequence of the initial condition (8).

Next we note the following identity, which is valid whenever the distribution of Q and $\dot{Q}$ is Gaussian:

$$g = \langle (Ma + Na^+) \exp(\mu a + \lambda a^+)\rangle$$
$$= \langle (Ma + Na^+)(\mu a + \lambda a^+)\rangle \langle \exp(\mu a + \lambda a^+)\rangle \quad . \tag{A2}$$

In order to prove (A2), we start from the auxiliary quantity

$$f = \langle \exp(\mu a + \lambda a^+)\rangle = \exp \tfrac{1}{2}\lambda\mu \langle aa^+ + a^+a\rangle \quad ,$$

where the last equality follows from the Bloch theorem.[24] Deriving f with respect to λ and μ, we can establish the following two equalities:

$$\frac{\partial f}{\partial \lambda} = \tfrac{1}{2}\mu f + \langle a^+ \exp(\mu a + \lambda a^+)\rangle = \tfrac{1}{2}\mu \langle aa^+ + a^+a\rangle f \quad ,$$

$$\frac{\partial f}{\partial \mu} = -\tfrac{1}{2}\lambda f + \langle a \exp(\mu a + \lambda a^+)\rangle = \tfrac{1}{2}\lambda \langle aa^+ + a^+a\rangle f \quad .$$

Consequently, we have

$$g = \left(\frac{\partial f}{\partial \mu} + \tfrac{1}{2}\lambda f\right) M + \left(\frac{\partial f}{\partial \lambda} - \tfrac{1}{2}\mu f\right) N = (\lambda \langle aa^+\rangle M + \mu \langle a^+a\rangle N) f.$$

Applying this result to (A1), with the initial condition (8), we obtain, for $t \gg (1/M)$,

$$\left(\frac{\partial}{\partial t} + \bar{\omega}^2 \eta \frac{\partial}{\partial \xi} - \xi \frac{\partial}{\partial \eta} + 2\Gamma\eta \frac{\partial}{\partial \eta}\right) R(\xi, \eta, t)$$
$$= -[a'(t)\eta^2 + b'(t)\xi\eta] R(\xi, \eta, t) \quad , \tag{A3}$$

where $a' = \tfrac{1}{2}\langle KQ + QK\rangle, \quad b' = \tfrac{1}{2}\langle K\dot{Q} + \dot{Q}K\rangle$.

Equation (20) follows directly from (A3) by Fourier transformation.

APPENDIX B

Equation (A3) can be written

$$\dot{R} = -iLR \quad . \tag{B1}$$

Defining the operator D through

$$DR = (1/2\pi)\int_0^{2\pi} d\varphi\, R \ , \tag{B2}$$

we can separate R in the form

$$R = R_{\text{d.}} + R_{\text{o.d.}} \quad , \tag{B3}$$

where $R_{\text{d.}} = DR, \quad R_{\text{o.d.}} = (1 - D)R$. (B4)

From Eq. (B1), we obtain the two equations

$$\dot{R}_{\text{d.}} = -iDLR_{\text{d.}} - iDLR_{\text{o.d.}} \quad , \tag{B5a}$$

$$\dot{R}_{\text{o.d.}} = -i(1-D)LR_{\text{d.}} - i(1-D)LR_{\text{o.d.}} \quad , \tag{B5b}$$

which couple the diagonal and off-diagonal parts of

R. Equations (B5a) and (B5b) can now be used to derive an equation for the matrix elements of the RDO $P_{mn}(t)$. We will show in this Appendix how this can be done for the diagonal elements P_{nn}. The generalization to the off-diagonal elements is straightforward.

Applying the projection rules Eq. (22), we have on the left-hand side simply $\dot{P}_{nn}(t)$. On the right-hand side we will consider separately the contribution of the two terms. From the first term, we have

$$-i\int_0^\infty dr\, l_n(r) DLR_{\text{d.}} = -(1/\pi)\int_0^\infty dr \int_0^{2\pi} d\varphi\, l_n(r) \times\left(2\Gamma \sin^2\varphi\, r\frac{\partial}{\partial r} + r(a' \sin^2\varphi + b' \sin\varphi\cos\varphi)\right) \times \sum_{m=0}^{\infty} l_m(r) P_m(t) \ , \tag{B6}$$

where $l_n(x) = e^{-x/2}L_n(x)$ is the Laguerre function of order n. Using simple properties of the Laguerre[25] functions, we can reduce (B6) to the form

$$-i\int_0^\infty dr\, l_n(r) DLR_{\text{d.}} = (a' - \Gamma)nP_{n-1} + (a' + \Gamma) \times (n+1)P_{n+1} + [\Gamma - (2n+1)a']P_n \ .$$

The contribution of the second term can be written

$$-i\int_0^\infty dr\, l_n(r) DLR_{\text{n.d.}} = -\int_0^\infty dr\, l_n(r) \times \sum_{N=2}^{\infty}\left(\frac{\frac{1}{2}(N-2)!}{\frac{1}{2}(N+2)!}\right)^{1/2}\left[\Gamma(P_N^{(2)} + P_N^{(-2)})\left(1 + r\frac{\partial}{\partial r}\right) \times r l^{(2)}_{(N-2)/2}(r) + r^2 l^{(2)}_{(N-2)/2}[\tfrac{1}{2}(a' + ib')P_N^{(-2)} + \tfrac{1}{2}(a' - ib')P_N^{(2)}]\right]. \tag{B7}$$

We have the following two types of integrals which can be evaluated by elementary methods[25]:

$$\int_0^\infty dr\, r^2 l_n^{(2)} l_m(r) = (m+1)(m+2)\delta_{n,m} - m(m+1)\,\delta_{n+1,m} + m(m-1)\delta_{n+2,m} \ , \tag{B8}$$

$$\int_0^\infty dr\, l_m(r)\left(1 + r\frac{\partial}{\partial r}\right) r l_n^{(2)} = \tfrac{1}{2}(m+1)(m+2)\delta_{n,m} - \tfrac{1}{2}m(m-1)\delta_{n+2,m} \ .$$

Replacing the results for the integrals Eqs. (B8) in Eq. (B7), and collecting all terms together, we arrive at the final form of the equation for the diagonal part of $P_{mn}(t)$:

$$\dot{P}_n(t) = (a' - \Gamma)nP_{n-1} + (a' + \Gamma)(n+1)P_{n+1} + [\Gamma - (2n+1)a']P_n - \tfrac{1}{2}[(n+1)(n+2)]^{1/2}[(a' + ib' - \Gamma) \times P_{n+2,n} + (a' - ib' + \Gamma)P_{n,n+2}] - \tfrac{1}{2}[n(n-1)]^{1/2} \times[(a' - ib' - \Gamma)P_{n-2,n} + (a' + ib' - \Gamma)P_{n,n-2}] + [n(n+1)]^{1/2}[(a' - ib')P_{n-1,n+1} + (a' + ib')P_{n+1,n-1}],$$

where $P_n \equiv P_{nn}$; we see here explicitly a coupling of the diagonal to the nondiagonal parts.

APPENDIX C

We show here how we can transform Eq. (40) for the probability of occupation of the renormalized state $|n\rangle$ into a finite sum involving the functions $\alpha, \beta, \gamma, u, v, w$. To this end, we first transform the integral in Eq. (40) to an integral over polar variables defined by

$$x^2 = r\cos^2\varphi, \quad y^2 = r\sin^2\varphi \ .$$

Thus, we have

$$P_n(t) = (1/2\pi)\int_0^{2\pi} d\varphi \int_0^\infty dr\, L_n(r) L_N(rH(t)) e^{-rI(t)}, \tag{C1}$$

where

$$H(t) = u\cos^2\varphi + v\sin^2\varphi + 2w\sin\varphi\cos\varphi \ ,$$
$$I(t) = \alpha\cos^2\varphi + \beta\sin^2\varphi + 2\gamma\sin\varphi\cos\varphi \ . \tag{C2}$$

The integral over r in (C1) can be readily evaluated,[26] and we obtain

$$P_n(t) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi \frac{[I(t) - 1]^n [I(t) - H(t)]^N}{I(t)^{N+n+1}} \times {}_2F_1\left(-n, -N; 1; \frac{H(t)}{[I(t) - 1][I(t) - H(t)]}\right) , \tag{C3}$$

where ${}_2F_1$ is the hypergeometric function. Introducing the change of variable $z = e^{2i\varphi}$, this last integral can be transformed into an integral along the unit circle in the complex z plane; thus,

$$P_n(t) = 4\{[F(t) - G(t)]^N / F(t)^{N+1}\}(1/2\pi i) \times \int_c dz \frac{(z - A_1)^n (z - A_2)^n (z - B_1)^N (z - B_2)^N}{(z - z_1)^{N+n+1}(z + z_2)^{N+n+1}} \times {}_2F_1\left(-n, -N; 1; 4z \times \frac{G(t)(z - M_1)(z - M_2)}{F(t)[F(t) - G(t)](z - A_1)(z - A_2)(z - B_1)(z - B_2)}\right) \tag{C4}$$

The quantities $F, G, A_{1,2}, B_{1,2}, M_{1,2}$, and $z_{1,2}$ have been defined in the text.

Since ${}_2F_1$ is a polynomial of order equal to the smaller of (n, N), the integrand in (C4) has only one pole inside the unit circle, at z_1; thus, the integral is simply the residue at this pole, and by evaluating it by elementary methods we arrive at Eq. (48).

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Ion Motion in Plasma Line Broadening*

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A recently developed method to study ion-motion effects on plasma line broadening in the dipole approximation is extended to the general interaction. Coupling-constant and binary-collision expansions are obtained for the "width and shift" operator. This operator is investigated for a model system to show the limits of the static-ion approximation.

I. INTRODUCTION

The spectral line shapes for atoms emitting radiation in a plasma are determined by the interaction of the atom with all the components of the plasma.[1] For a large portion of the line profile, the relatively heavy ions may be treated as static and their effects accounted for by the introduction of an ion microfield.[1,2] It was shown recently[3] that the ion microfield function can be introduced formally exactly, thus explicitly accounting for the large static-field contributions without the usual static-ion assumptions. The dynamics of the perturbers in interaction with the atom was treated in a collisional approximation by second-order perturbation theory. The resulting expression for the line shape is formally similar to earlier work,[2,4] with generalization to include ion motion. Another important advantage is that ion-electron interactions need not be treated in an indirect manner.[5]

Here, this method of investigating the role of ion dynamics will be continued and extended. Reference 3 was limited to the case of dipole interaction between the atom and perturber. This is extended in Sec. II to the general case in which all charges interact through a Coulomb potential. The width and shift operator is determined to second order in the plasma-atom interaction. Since the Coulomb interaction is large for small distances this result cannot be correct for close, or strong collisions. To account for these, a binary-collision expansion[6] of the width and shift operator is given in Sec. III. The first term in the expansion is essentially the impact approximation[1,7] including ion-motion effects. In the last section, a random-phase approximation is used to determine how close to the line center a static-ion theory should be used. The region in which ion motion is important is found to be an order of magnitude larger than usually estimated. However, it is indicated that this result is not realistic due to an unjustified extension of the electron strong-collision cutoff procedure to the ions. The cutoff for the electrons has been studied by Shen and Cooper[8] by an evaluation of the atom-electron t matrix. The starting point for a corresponding study of the ions is provided by the results of