Statistical properties of quantum systems: The linear oscillator

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Statistical fluctuations in linear quantum-mechanical systems are shown to result from a projection of the total quantum system onto a restricted subspace. The resulting equations of motion are of the generalized Langevin form, with fluctuating and dissipative terms. These terms are related by a quantum-mechanical fluctuation-dissipation relation that ensures thermal equilibration. We analyze the dynamical behavior of the subsystem and elucidate the meaning and interrelation of several ubiquitous concepts in the following context: weak-coupling limit, Markovian limit, rotating-wave approximation (RWA), and low-temperature behavior. The three most salient consequences of our analysis are as follows: (1) The time scale for the correlation of fluctuations and the dissipation can be quite distinct, (2) the traditional implementation of the RWA only gives valid results in the strict weak-coupling limit, and (3) a reformulation of the RWA valid at arbitrary coupling strengths, and hence at arbitrarily low temperatures, is possible.

I. INTRODUCTION

The description of the thermal relaxation of systems interacting with a heat bath has long been of central interest in statistical mechanics.[1–18] Particularly elusive has been the proper description of the relaxation of a quantum system in a heat bath that must also be described quantum mechanically.[5–9,11–24] The proper quantum description is, of course, necessary for any system at sufficiently low temperatures. We note that even room temperatures may be "low" in some cases.[22]

There has been a recent resurgence of interest in the problem of the relaxation of quantum systems.[20–24] The resurgence of interest is due in part to the recognition that experiments in such diverse areas as the vibrational relaxation of polyatomic molecules[16–19] and exciton transport at low temperatures[22] can only be completely understood in terms of fully quantum-mechanical treatments of the fluctuations caused by the interactions of the system with the surrounding heat bath.

The simplest situation that one can consider in this context is that of the Brownian motion of a quantum oscillator in a quantum-mechanical heat bath. There exist several treatments of this problem going back over a period of more than 20 years.[5–9,11–20] The original work of Schwinger[6] and of Senitzky[7] concerned itself with a theory applicable to dissipative effects on the electromagnetic radiation field in a resonant cavity. It was restricted to the *Markovian limit* (instantaneous dissipation, delta-correlated fluctuations) and to the *weak-coupling limit* (weak coupling between the oscillator and the heat bath). Lax[8] in a series of classic papers on quantum noise also discussed the problem of quantum Brownian motion. He was particularly concerned with conditions that would permit a Markovian description of the problem. In this context he argued that a Markovian description is only possible if one makes the "*rotating-wave approximation*" (RWA). (This approximation is implicit in the work of Senitzky.) The RWA is based on ignoring rapidly oscillating terms in the oscillator–heat-bath coupling. In their seminal work Ford, Kac, and Mazur[5] constructed a detailed microscopic model leading to Brownian motion (classical and quantum). They were the first to establish rigorous conditions that lead to instantaneous dissipation. Agarwal[9] treated the problem of the Brownian motion of a quantum oscillator using the coherent-state representation. He discussed some aspects of the relation between the weak-coupling limit and the RWA. Quantum oscillators have been used extensively as models for the laser[11–15] and for vibrational relaxation.[16–19] An extensive literature exists in each of these areas, but we mention only a few papers that contain the aspects of interest to the present general discussion. The evolution of the field in a laser coupled to a thermal bath is discussed by Haken.[15] In his discussion (and in others in this field) all three approximations mentioned above are made: Markovian limit, weak-coupling limit, and RWA. With few exceptions the problem of vibrational relaxation is also treated using the same three approximations.[16–19] Most recently activity in the development of descriptions of the statistical mechanics of quantum oscillators continues unabated. Benguria and Kac[20] and Grabert and Talkner[21] have discussed various aspects of the approach of the quantum oscillator to thermal equilibrium. Ruggiero and Zannetti[24] discuss the interplay of purely quantum ($T=0$) and thermal fluctuations, an area of growing interest in quantum electrodynamics.

The behavior of the quantum oscillator can be characterized by four energy parameters.

(1) The natural frequency $E/\hbar$ of the isolated oscillator.

(2) The coupling strength λE between the oscillator and the heat bath.

(3) The memory time $\tau_c \equiv \gamma^{-1}$ of the dissipation of oscillator energy by the heat bath.

(4) The temperature T of the heat bath.

The various above-mentioned approximations involve choosing limiting values for these parameters. Thus, for instance, instantaneous dissipation corresponds to taking $\gamma \to \infty$ while the weak-coupling limit implies $\lambda \to 0$. In the past these various parameter variations have been done independently, i.e., the results have been assumed to be independent of the order in which the limits are taken. It is one of the major purposes of this paper to explore the interdependence of the various approximations and, in particular, of the special role played by the temperature in the quantum oscillator system. Towards this end we present a fully quantum-mechanical derivation of a generalized Langevin equation. We obtain a quantum fluctuation-dissipation relation which is different from the classical one and reduces to it only in the high-temperature limit. The main consequence of this relation is that *spontaneous fluctuations in the quantum system can only be taken as Markovian under special circumstances.* Thus, even if the dissipative kernel is a delta function in time ($\gamma \to \infty$), the fluctuations necessarily remain correlated over a *finite* time that depends on the temperature. This in turn induces macroscopic effects whose origin is quantum mechanical and which are absent in the classical limit.

The second major (related) issue that we address is the way in which the RWA has been implemented in the past. The analysis in Sec. IV shows that the subsequent approximations so often made on systems described by a RWA Hamiltonian lead to divergences in the system dynamics. These divergences disappear only in the weak-coupling limit and therefore the formalism is only applicable strictly in the limit $\lambda \to 0$. We present a reformulation of the RWA that overcomes this limitation.

In Sec. II we derive equations of motion for the oscillator based on a fully quantum-mechanical Hamiltonian for the oscillator coupled to the heat bath. The heat-bath degrees of freedom are explicitly eliminated leaving a generalized quantum Langevin equation for the oscillator. We do this for the oscillator in the RWA ("RWA oscillator") as well as for the case in which the RWA approximation is not made ["fully coupled (FC) oscillator"]. In Sec. III we discuss the dynamics of the FC oscillator. We consider the interdependency of the various parameters by analyzing the appropriate approximations to the exact solutions. In Sec. IV we redo the analysis for the RWA oscillator. We review the traditional implementation and contrast this with our modified procedure. The results for the FC oscillator and the RWA oscillator are compared and contrasted in Sec. V. Also in Sec. V we discuss some general implications of the present findings.

II. EQUATIONS OF MOTION

Consider a quantum oscillator with creation and annihilation operator $a^\dagger$ and a, respectively, and with natural frequency $E/\hbar$. The oscillator is in contact with a heat bath of bosons labeled by index ν, created and annihilated by $b_\nu^\dagger$ and b_ν, respectively. The analysis is restricted to a bath of harmonic bosons of frequency ω_ν. The coupling between the oscillator and the heat bath is assumed to be bilinear. The Hamiltonian for the composite system is

$$H = H_S + H_B + H_{SB} \ . \tag{2.1}$$

Here H_S is the Hamiltonian of the isolated system

$$H_S = E a^\dagger a \ . \tag{2.2}$$

The Hamiltonian of the isolated bath is

$$H_B = \sum_\nu \hbar \omega_\nu b_\nu^\dagger b_\nu \ . \tag{2.3}$$

The system-bath interaction distinguishes the FC oscillator from the RWA oscillator. We discuss the two cases separately.

A. FC oscillator

For the FC oscillator the coupling Hamiltonian is[8,19]

$$H_{SB} = \lambda^{1/2} \sum_\nu \Gamma_\nu (a^\dagger + a)(b_\nu^\dagger + b_\nu) \ . \tag{2.4}$$

The Γ_ν's are real coupling constants and λ is a parameter that measures the average strength of the interaction. For the analysis that follows it is convenient to rewrite the Hamiltonian (2.1) as

$$H = H_S^{(m)} + H_B + H_{SB}^{(m)} \ , \tag{2.5}$$

where $H_S^{(m)}$ is the "modified" system Hamiltonian

$$H_S^{(m)} = E a^\dagger a - \sum_\nu \hbar \omega_\nu G_\nu^2 \tag{2.6}$$

and where

$$H_B + H_{SB}^{(m)} = \sum_\nu \hbar \omega_\nu (b_\nu^\dagger + G_\nu)(b_\nu + G_\nu) \ , \tag{2.7}$$

with

$$G_\nu \equiv \lambda^{1/2} \frac{\Gamma_\nu}{\hbar \omega_\nu} (a^\dagger + a) \ . \tag{2.8}$$

The dynamical equations for the system operators are given by

$$\dot{a} = \frac{i}{\hbar} [H_S^{(m)}, a] - \frac{i}{\hbar} \lambda^{1/2} \sum_\nu \Gamma_\nu (b_\nu^\dagger + b_\nu + 2G_\nu) \tag{2.9}$$

and its Hermitian conjugate. To eliminate the bath operators from (2.9) we similarly write their dynamical equations $\dot{b}_\nu = \hbar^{-1} i [H, b_\nu]$ and its Hermitian conjugate for each ν. It is more convenient instead to consider the dynamical equations for the contributions $(b_\nu^\dagger + G_\nu)$ and $(b_\nu + G_\nu)$ that actually appear in (2.9), i.e.,

$$\frac{d}{dt}(b_\nu^\dagger + G_\nu) = i \omega_\nu (b_\nu^\dagger + G_\nu) + \dot{G}_\nu \tag{2.10}$$

and its conjugate. Since the bath equations are formally linear, they can be reduced to quadrature

$$b_\nu^\dagger(t)+G_\nu(t)=[b_\nu^\dagger(0)+G_\nu(0)]e^{i\omega_\nu t} + \int_0^t d\tau e^{i\omega_\nu(t-\tau)}\dot{G}_\nu(\tau) . \tag{2.11}$$

Substitution of (2.11) and its conjugate into (2.9) gives the dynamical equation

$$\dot{a}=\frac{i}{\hbar}[H_S^{(m)},\, a]-\frac{i}{\hbar}\lambda^{1/2}\sum_\nu \Gamma_\nu[F_\nu^\dagger(t)+F_\nu(t)] -2i\frac{\lambda}{\hbar}\sum_\nu \frac{\Gamma_\nu^2}{\hbar\omega_\nu}\int_0^t d\tau[\dot{a}(\tau)+\dot{a}^\dagger(\tau)]\cos[\omega_\nu(t-\tau)] , \tag{2.12}$$

where

$$F_\nu^\dagger(t)\equiv[b_\nu^\dagger(0)+G_\nu(0)]e^{i\omega_\nu t} \tag{2.13}$$

depends only on initial operator values.

Following the usual statistical-mechanical viewpoint, we identify the operators $F_\nu(t)$ as fluctuations because of the uncertainty in the initial values of the bath operators. To specify the statistical properties of the fluctuations we consider an ensemble of initial states in which the system operators are fixed at the values $(a^\dagger(0),\, a(0))$ and the initial bath operators are drawn from an ensemble that is canonical relative to the system.[1,25] The initial distribution is then the conditional density matrix

$$\rho_0\equiv\rho(\{b^\dagger(0),\, b(0)\}\,|\,a^\dagger(0),\, a(0)) =\frac{1}{Z(\beta)}\exp[-\beta(H_B+H_{SB}^{(m)})] \tag{2.14}$$

in terms of the portion of the Hamiltonian given in Eq. (7). Here $Z(\beta)$ is the conditional partition function

$$Z(\beta)=\mathrm{Tr}\exp[-\beta(H_B+H_{SB}^{(m)})] \tag{2.15}$$

and $\beta=(kT)^{-1}$. In this ensemble the fluctuations $F_\nu(t)$ are Gaussian and zero centered, i.e.,

$$\langle F_\nu(t)\rangle=0 , \tag{2.16}$$

where $\langle\theta\rangle\equiv\mathrm{Tr}(\rho_0\theta)$. The correlation functions of the fluctuations are

$$\langle F_\nu(t)F_{\nu'}(t')\rangle=0 , \tag{2.17a}$$

$$\langle F_\nu^\dagger(t)F_{\nu'}(t')\rangle=n_\nu e^{i\omega_\nu(t-t')}\delta_{\nu\nu'} , \tag{2.17b}$$

$$\langle F_\nu(t)F_{\nu'}^\dagger(t')\rangle=(n_\nu+1)e^{-i\omega_\nu(t-t')}\delta_{\nu\nu'} , \tag{2.17c}$$

where we have used the Bose statistics of the bath to set

$$\langle[b_\nu^\dagger(0)+G_\nu(0)][b_{\nu'}(0)+G_{\nu'}(0)]\rangle=n_\nu\delta_{\nu\nu'} , \tag{2.18}$$

with

$$n_\nu=\frac{1}{e^{\beta\hbar\omega_\nu}-1} . \tag{2.19}$$

Equation (2.12) is the stochastic differential equation on which we base the remaining analysis. We can rewrite (2.12) in the more familiar form of a generalized Langevin equation

$$\dot{a}(t)=-\frac{i}{\hbar}\epsilon a(t)+i\Delta a^\dagger(t)-if_{\mathrm{FC}}(t) -i\hbar\int_0^t d\tau K_{\mathrm{FC}}(t-\tau)[\dot{a}(\tau)+\dot{a}^\dagger(\tau)] \tag{2.20}$$

and its Hermitian conjugate. Here

$$\Delta\equiv\frac{2\lambda}{\hbar}\sum_\nu\frac{\Gamma_\nu^2}{\hbar\omega_\nu} \tag{2.21}$$

and ϵ is the shifted energy

$$\epsilon=E-\hbar\Delta . \tag{2.22}$$

The fluctuations are given by

$$f_{\mathrm{FC}}(t)=\frac{\lambda^{1/2}}{\hbar}\sum_\nu\Gamma_\nu[F_\nu^\dagger(t)+F_\nu(t)]\equiv\lambda^{1/2}\sum_\nu f_\nu^{\mathrm{FC}}(t) \tag{2.23}$$

and the kernel is

$$K_{\mathrm{FC}}(t-\tau)=\frac{2\lambda}{\hbar^2}\sum_\nu\frac{\Gamma_\nu^2}{\hbar\omega_\nu}\cos[\omega_\nu(t-\tau)] \tag{2.24}$$

so that $\Delta=\hbar K_{\mathrm{FC}}(0)$.

B. RWA oscillator

The coupling Hamiltonian for the RWA oscillator is[6–9,11–19]

$$H_{SB}=\lambda^{1/2}\sum_\nu(\Gamma_\nu^* a^\dagger b_\nu+\Gamma_\nu a b_\nu^\dagger) \tag{2.25}$$

(we have followed convention here and taken Γ_ν complex). The FC and RWA couplings thus differ by the exclusion of the $a^\dagger b_\nu^\dagger$ and ab_ν terms from the latter. We again rewrite the Hamiltonian (2.1) in the form (2.5), but now with

$$H_S^{(m)}=\epsilon a^\dagger a , \tag{2.26}$$

where[26]

$$\epsilon=E-\hbar\Delta,\quad \Delta=\frac{\lambda}{\hbar}\sum_\nu\frac{|\Gamma_\nu|^2}{\hbar\omega_\nu} , \tag{2.27}$$

and consequently

$$H_B+H_{SB}^{(m)}=\sum_\nu\hbar\omega_\nu\left[b_\nu^\dagger+\lambda^{1/2}\frac{\Gamma_\nu^* a^\dagger}{\hbar\omega_\nu}\right]\left[b_\nu+\lambda^{1/2}\frac{\Gamma_\nu a}{\hbar\omega_\nu}\right] . \tag{2.28}$$

For the oscillator operator we now obtain the dynamical equation

$$\dot{a}=-\frac{i\epsilon}{\hbar}a-\frac{i\lambda^{1/2}}{\hbar}\sum_\nu\Gamma_\nu^*\left[b_\nu+\lambda^{1/2}\frac{\Gamma_\nu}{\hbar\omega_\nu}a\right] . \tag{2.29}$$

The solution of the bath-operator equation of motion proceeds as in the FC case and is given by

$$b_\nu(t)+\lambda^{1/2}\frac{\Gamma_\nu}{\hbar\omega_\nu}a(t)=\left[b_\nu(0)+\lambda^{1/2}\frac{\Gamma_\nu}{\hbar\omega_\nu}a(0)\right]e^{-i\omega_\nu t}+\lambda^{1/2}\frac{\Gamma_\nu}{\hbar\omega_\nu}\int_0^t d\tau e^{-i\omega_\nu(t-\tau)}\dot{a}(\tau)\ . \tag{2.30}$$

Substituting (2.30) into (2.29) yields

$$\dot{a}=-\frac{i\epsilon}{\hbar}a-if_{\rm RWA}(t)-i\hbar\int_0^t d\tau K_{\rm RWA}(t-\tau)\dot{a}(\tau)\ , \tag{2.31}$$

where

$$f_{\rm RWA}(t)=\frac{\lambda^{1/2}}{\hbar}\sum_\nu\Gamma_\nu^*\left[b_\nu(0)+\lambda^{1/2}\frac{\Gamma_\nu}{\hbar\omega_\nu}a(0)\right]e^{-i\omega_\nu t}\equiv\lambda^{1/2}\sum_\nu f_\nu^{\rm RWA}(t) \tag{2.32}$$

and

$$K_{\rm RWA}(t-\tau)=\frac{\lambda}{\hbar^2}\sum_\nu\frac{|\Gamma_\nu|^2}{\hbar\omega_\nu}e^{-i\omega_\nu(t-\tau)}\ . \tag{2.33}$$

The distribution to be used in calculating averages over the fluctuations $f_{\rm RWA}(t)$ is (2.14) with $H_B+H_{SB}^{(m)}$ given by (2.28). Equations (2.20)—(2.24) for the FC oscillator and the corresponding equations (2.31)—(2.33) for the RWA oscillator are the equations on which the subsequent analysis is based.

III. FULLY COUPLED (FC) OSCILLATOR

Let us begin with Eq. (2.20). We recall that the oscillator displacement operator is $q(t)=(\hbar^2/E)^{1/2}[a^\dagger(t)+a(t)]$, and we note that the last term in (2.20) is proportional to the velocity operator $\dot{q}(t)$. Thus the last term is recognized as a *dissipation*. Equation (2.20) can be more simply rewritten as

$$\dot{a}(t)=-\frac{i\epsilon}{\hbar}a(t)+i\,\Delta a^\dagger(t)-if_{\rm FC}(t)-E\int_0^t d\tau K_{\rm FC}(t-\tau)[a(\tau)-a^\dagger(\tau)]\ . \tag{3.1}$$

Equation (3.1) is obtained by noting that (2.20) leads to

$$i[\dot{a}(t)+\dot{a}^\dagger(t)]=\frac{E}{\hbar}[a(t)-a^\dagger(t)]\ , \tag{3.2}$$

which is simply the operator version of the Newtonian relation $\dot{q}=p$.

The temporal properties of the dissipative kernel $(E/\hbar)K_{\rm FC}(t-\tau)$ are determined by the bath frequencies ω_ν and by the coupling constants $\lambda^{1/2}\Gamma_\nu$ [cf. (2.24)]. Ford, Kac, and Mazur[5] gave the conditions under which (2.24) reduces to a delta function (instantaneous dissipation), e.g.,

$$K_{\rm FC}(t-\tau)=\frac{2\lambda}{\hbar}\delta(t-\tau)\ . \tag{3.3a}$$

A somewhat less restrictive kernel is given by the exponential form

$$K_{\rm FC}(t-\tau)=\frac{\lambda}{\hbar}\gamma e^{-\gamma|t-\tau|}\ , \tag{3.3b}$$

where γ^{-1}, the memory time of the dissipation, is essentially the inverse of the phonon bandwidth of the heat-bath excitations that couple to the oscillator. Equation (3.3b) reduces to (3.3a) in the limit $\gamma\to\infty$, a limit to be analyzed later.

A. Fluctuation-dissipation relation

The fluctuations $f_{\rm FC}(t)$ and the dissipation are related manifestations of the interaction of the oscillator with the heat bath. In classical systems the fluctuation-dissipation relation is the general principle that ensures eventual thermal equilibration.[1–5,10,25] From the correspondence principle one would expect an analogous relation to hold for quantum systems. Such a relation is usually *assumed* to hold in quantum systems; we show here that the actual quantum relation is not of the same form as the classical one and reduces to it only in the high-temperature limit.

The quantum fluctuation-dissipation relation can be constructed using the statistical properties (2.17) and is given by [cf. (2.23)][27]

$$\sum_\nu\Phi_\nu^{\rm FC}(t-\tau)(\hbar\omega_\nu)^{-1}\tanh\left[\frac{\beta\hbar\omega_\nu}{2}\right]=K_{\rm FC}(t-\tau)\ , \tag{3.4}$$

where $\Phi_\nu^{\rm FC}$ is the symmetrized correlation function[20]

$$\Phi_\nu^{\rm FC}(t-\tau)=\lambda\langle f_\nu^{\rm FC}(t)f_\nu^{\rm FC}(\tau)+f_\nu^{\rm FC}(\tau)f_\nu^{\rm FC}(t)\rangle\ . \tag{3.5}$$

The consequences of relation (3.4) can be seen more clearly if we also state here the corresponding classical relation[1–5,10,16,25]

$$\Phi_{\rm FC}(t-\tau)=2kTK_{\rm FC}(t-\tau)\ , \tag{3.6}$$

where

$$\Phi_{\rm FC}(t-\tau)=\sum_\nu\Phi_\nu^{\rm FC}(t-\tau)\ . \tag{3.7}$$

We note that (3.6) can be obtained from (3.4) by taking the limit $\hbar\to0$. The relation (3.4) is an important result in this paper. This result has been obtained before by many authors in a variety of forms,[5,8,22,28] but we have seen no detailed discussion of its consequences prior to our recent work.[22]

To understand the implications of (3.4) let us consider the particular dissipative kernel (3.3b). We rewrite (2.24) as an integral over bath frequencies with a density of states $D(\omega)$:

$$K_{\rm FC}(t-\tau)=\frac{2\lambda}{\hbar^2}\int_0^\infty d\omega\,D(\omega)\frac{\Gamma^2(\omega)}{\hbar\omega}\cos[\omega(t-\tau)]\ . \tag{3.8}$$

Choosing

$$D(\omega)\frac{\Gamma^2(\omega)}{\hbar^2\omega}=\frac{1}{\pi}\frac{\gamma^2}{\gamma^2+\omega^2} \tag{3.9}$$

leads to (3.3b). The associated correlation function (3.7) with $n_\omega\equiv(e^{\beta\hbar\omega}-1)^{-1}$ is

$$\Phi_{\rm FC}(t-\tau)=\frac{\lambda\gamma^2}{\pi}\int_0^\infty d\omega\frac{\omega}{\gamma^2+\omega^2}(2n_\omega+1)\cos[\omega(t-\tau)]\ . \tag{3.10}$$

We note that the choice (3.9) is sensible only if $\gamma\gg E/\hbar$. At high temperatures or in the classical limit ($kT\gg\gamma$ or $\hbar\to 0$) (3.10) reduces to (3.6) with (3.8) and hence $\Phi_{\rm FC}$ decays on a time scale γ^{-1}. At lower temperatures ($kT\ll\hbar\gamma$) an analysis of (3.10) reveals that *the correlation function decays on a time scale* $(\hbar/kT)$ *rather than* γ^{-1}. The interpretation of this result is based on an idea that seems not to have been previously invoked:[22] whereas the bath can *dissipate* excitations whose energies lie in the range $(0,\hbar\gamma)$, the *spontaneous fluctuations* occur only in the range $(0,kT)$ if $kT<\hbar\gamma$. The correlation time of the fluctuations is therefore the longer of $(\hbar/kT)$ and γ^{-1}. As the temperature is lowered, the correlations in the fluctuations become increasingly long lived even for an infinitely broad bath spectrum. *The idea, then, is that fluctuations and dissipation can have quite distinct time scales.* The usual assumption is that their characteristic time scales are the same. Some consequences of this new idea will become apparent in the discussion of the moment properties of the FC oscillator later in this section.

B. Solution of rate equations

The physical properties of the FC oscillator are implicit in the solution of (3.2) and its Hermitian conjugate. Since the equations are linear, they can be solved explicitly. The convolution on the right-hand side suggests that we Laplace transform (3.2) according to

$$\hat a(s)\equiv\int_0^\infty dt\, e^{-st}a(t)\ . \tag{3.11}$$

We define the matrices

$$\hat{\underline{A}}(s)\equiv\begin{bmatrix}\hat a\\ \hat a^\dagger\end{bmatrix},$$

$$\hat{\underline{B}}(s)=\begin{bmatrix}s+\frac{i\epsilon}{\hbar}+E\hat K_{\rm FC}(s) & -i\Delta-E\hat K_{\rm FC}(s)\\ i\Delta-E\hat K_{\rm FC}(s) & s-\frac{i\epsilon}{\hbar}+E\hat K_{\rm FC}(s)\end{bmatrix}, \tag{3.12}$$

$$\hat{\underline{f}}(s)=\begin{bmatrix}a(0)-i\hat f_{\rm FC}(s)\\ a^\dagger(0)+i\hat f_{\rm FC}(s)\end{bmatrix}$$

and write the solution of the transformed equation as

$$\hat{\underline{A}}(s)=\hat{\underline{B}}^{-1}(s)\hat{\underline{f}}(s)\ . \tag{3.13}$$

In Appendix A we Laplace invert (3.13) to obtain

$$a(t)=\sum_{j=1}^3 e^{s_jt}\left[A_j+T_j\int_0^t d\tau f_{\rm FC}(\tau)e^{-s_j\tau}\right] \tag{3.14}$$

and its Hermitian conjugate, where

$$A_j\equiv a(0)R_j+a^\dagger(0)Q_j \tag{3.15}$$

and where the s_j, R_j, Q_j, and T_j can be read off Eqs. (A5) and (A6) in Appendix A.

C. Relaxation to equilibrium population

We denote the time- and temperature-dependent population of the FC oscillator by[27]

$$n_{\rm FC}(T,t)=\langle a^\dagger(t)a(t)\rangle\ . \tag{3.16}$$

From (3.14) we obtain

$$n_{\rm FC}(T,t)=\sum_{j=1}^3\sum_{l=1}^3 e^{(s_j^*+s_l)t}\left[A_j^*A_l+T_j^*T_l\int_0^t d\tau_1\int_0^t d\tau_2\phi_{\rm FC}(\tau_1-\tau_2)e^{-(s_j^*\tau_1+s_l\tau_2)}\right], \tag{3.17}$$

where

$$\phi_{\rm FC}(\tau_1-\tau_2)=\langle f_{\rm FC}(\tau_1)f_{\rm FC}(\tau_2)\rangle$$
$$=\frac{\lambda\gamma^2}{\pi}\int_0^\infty d\omega\frac{\omega}{\gamma^2+\omega^2}[(n_\omega+1)e^{-i\omega(\tau_1-\tau_2)}+n_\omega e^{i\omega(\tau_1-\tau_2)}]\ . \tag{3.18}$$

In (3.18) we have used the continuum form for the sum in (2.23) with the form (3.9) for the coupling and the density of bath states. Explicitly carrying out the time integrations in (3.17) and retaining terms to leading order in λ gives

$$n_{\rm FC}(T,t)=n_{\rm FC}(T,0)e^{-2\lambda(E/\hbar)t}+n_{\rm FC}(T,\infty)(1+e^{-2\lambda(E/\hbar)t})$$
$$-2\frac{\lambda\gamma^2\hbar}{\pi}e^{-\lambda(E/\hbar)t}\int_0^\infty d\omega\frac{\hbar\omega}{\gamma^2+\omega^2}\left[\frac{(n_\omega+1)\cos[(E+\hbar\omega)t/\hbar]}{\lambda^2E^2+(E+\hbar\omega)^2}+\frac{n_\omega\cos[(E-\hbar\omega)t/\hbar]}{\lambda^2E^2+(E-\hbar\omega)^2}\right], \tag{3.19}$$

where the equilibrium population $n_{\rm FC}(T,\infty)$ is analyzed below. We see that the population relaxes to its equilibrium level on a time scale determined by $\lambda E/\hbar$. The result (3.19) differs from that of the usual RWA (cf. Sec. IV A). We note that to $O(\lambda)$ the only contribution to (3.17) comes from the term $j=l=2$, i.e., from the pole $s_2\approx-(\lambda E+iE)/\hbar$. The pole $s_1\approx-\gamma$ damps out very rapidly, contributing to $O(\lambda e^{-\gamma t})$. It is therefore neglected. The pole $s_3\simeq-(\lambda E-iE)/\hbar$ gives contributions of higher order in λ $[O(\lambda^2)]$.

The equilibrium population of the FC oscillator is obtained by taking the $t\to\infty$ limit of (3.17):

$$n_{\mathrm{FC}}(T,\infty)=\frac{\lambda\gamma^2\hbar}{\pi}\int_0^\infty d\omega\frac{\hbar\omega}{\gamma^2+\omega^2}\times\left[\frac{n_\omega}{\lambda^2E^2+(\hbar\omega-E)^2}+\frac{n_\omega+1}{\lambda^2E^2+(\hbar\omega+E)^2}\right]\times[1+O(\lambda)]\ . \tag{3.20}$$

At zero temperature the leading contribution to the equilibrium population obtained from (3.20) is

$$n_{\mathrm{FC}}(0,\infty)=\frac{\lambda}{\pi}\ln\frac{\hbar\gamma}{E}-\frac{\lambda}{2}+O\left[\frac{\lambda E}{\hbar\gamma}\right]\ , \tag{3.21}$$

where we have retained terms to lowest order in λ and highest order in $\hbar\gamma/E$. This residual population is small under the condition $\lambda\gamma\ll E/\hbar$ used to arrive at (3.20) from the eigenvalue analysis in Appendix A. Equation (3.21) seems to be the first quantitative estimate of the residual equilibrium population for weak but finite coupling.

At finite temperatures (3.20) cannot be evaluated in closed form except at high and at low temperatures. At high temperatures ($kT\gg E$) the peak in the neighborhood of $\hbar\omega=E$ of the Lorentzian in the integrand of (3.20) dominates and (for $\hbar\gamma\gg kT$) yields the usual Bose population

$$n_{\mathrm{FC}}(T,\infty)-n_{\mathrm{FC}}(0,\infty)=\frac{1}{e^{\beta E}-1}[1+O(\lambda)]\ . \tag{3.22}$$

At low temperatures ($kT\ll E$) for $\gamma\to\infty$ there are two positive frequency peaks in the integrand of (3.20), one in the neighborhood of $\hbar\omega=E$ and another at $\omega=0$. The relative importance of the contributions of these peaks depends on the relative values of λ and (kT/E). The peak around $\omega=0$ dominates if $\lambda\gg(E/kT)^2\exp(-E/kT)$ or, conversely, if $kT\ll E/\ln(1/\lambda)$. When this condition is satisfied we obtain the series expansion

$$n_{\mathrm{FC}}(T,\infty)-n_{\mathrm{FC}}(0,\infty)=\frac{4\lambda}{\pi}\left[\frac{kT}{E}\right]^2\left[\xi(2)-30\xi(4)\left[\frac{kT}{E}\right]^2+\cdots\right]\ , \tag{3.23}$$

where ξ is the zeta function and (3.23) is correct to $O((kT/E)^6)$. Thus there is a marked deviation from the usual anticipated behavior (3.22) at low temperatures.

We emphasize that in the above analysis we took λ to be small, a condition often called the "weak-coupling limit." However, from this analysis it is clear that true weak coupling is only achieved at high temperatures in addition to λ being small. At sufficiently low temperatures the effect of the coupling is macroscopically observable as a deviation from the Bose population (3.22).

D. Correlation function

The energy absorption and emission properties of an oscillator are determined, respectively, by the two-time correlation functions

$$C_{\mathrm{FC}}^{\mathrm{abs}}(\tau)=\lim_{\tau\to\infty}\langle\mu(t)\mu(t+\tau)\rangle \tag{3.24}$$

and

$$C_{\mathrm{FC}}^{\mathrm{em}}(\tau)=\lim_{t\to\infty}\langle\mu(t+\tau)\mu(t)\rangle\ , \tag{3.25}$$

where μ is the dipole operator

$$\mu(t)=a^\dagger(t)+a(t)\ . \tag{3.26}$$

The absorption and emission spectra are the Fourier transforms of the corresponding correlation functions

$$S_{\mathrm{FC}}(\omega)=\int_{-\infty}^{\infty}d\tau e^{-i\omega\tau}C_{\mathrm{FC}}(\tau)\ . \tag{3.27}$$

Using (3.14) one can integrate (3.27) exactly to obtain to leading order in λ

$$S_{\mathrm{FC}}^{\mathrm{abs}}(\omega)=\frac{4\lambda\hbar^2\gamma^2\omega(n_\omega+1)}{\pi(\gamma^2+\omega^2)}\times\frac{(\lambda^2E^2+\hbar^2\omega^2)}{[\lambda^2E^2+(\hbar\omega+E)^2][\lambda^2E^2+(\hbar\omega-E)^2]} \tag{3.28}$$

and

$$S_{\mathrm{FC}}^{\mathrm{em}}(\omega)=\frac{4\lambda\hbar^2\gamma^2\omega n_\omega}{\pi(\gamma^2+\omega^2)}\times\frac{(\lambda^2E^2+\hbar^2\omega^2)}{[\lambda^2E^2+(\hbar\omega+E)^2][\lambda^2E^2+(\hbar\omega-E)^2]}\ . \tag{3.29}$$

We now discuss each of these spectra, restricting the analysis to positive frequencies.[29]

The absorption spectrum (3.28) is essentially a Lorentzian centered at $\hbar\omega=E$ and of width λE. In the weak-coupling limit absorption occurs exactly at $\hbar\omega=E$:

$$\lim_{\lambda\to0}S_{\mathrm{FC}}^{\mathrm{abs}}(\omega)=\frac{\hbar\gamma^2}{\gamma^2+E^2}(n_E+1)\delta(\hbar\omega-E)\ . \tag{3.30}$$

The overall intensity of absorption decreases with temperature and settles to a residual value of quantum-mechanical origin at zero temperature (i.e., $n_\omega+1\to1$ as $T\to0$). The absorption characteristics are thus determined mainly by the properties of the coupled oscillator, the heat bath essentially providing only a temperature that determines the overall level. The emission spectrum behaves quite differently as a function of temperature. At zero temperature there is no emission. At low temperatures the emission spectrum peaks at $\omega=0$ and decreases exponentially: its shape is dominated by the thermal factor $\hbar\omega n_\omega$. This is a macroscopic manifestation of the quantum nature of the composite system. At high temperatures ($kT\gg E$) the spectrum is again essentially a Lorentzian centered at E and of width λE. This behavior can be understood as follows. At high temperatures the heat bath can accommodate all excitation frequencies of the FC oscillator equally. The emission properties of the composite system are thus determined by those of the oscillator. At low temperatures, on the other hand, the bath

is only excited in the range $(0,kT)$ of energies. The composite system then emits energy primarily in this restricted range.

IV. ROTATING-WAVE APPROXIMATION (RWA)

The equation of motion (2.31) for the RWA oscillator is not the one usually found in the literature.[7,8,15] To convince oneself that (2.31) is in fact the appropriate equation of motion, the inconsistencies in the traditional description of the RWA oscillator must be uncovered. To do this we begin this section with a digression on the standard derivation.

A. Traditional RWA (Refs. 8 and 15)

We again begin with the Hamiltonian (2.1)–(2.3) with the RWA coupling (2.25). The equation of motion for the oscillator is given by

$$\dot{a}=-\frac{iEa}{\hbar}-\frac{i\lambda^{1/2}}{\hbar}\sum_\nu \Gamma_\nu^* b_\nu \tag{4.1}$$

and the integrated equation for each bath variable is

$$b_\nu(t)=b_\nu(0)e^{-i\omega_\nu t} -i\frac{\lambda^{1/2}\Gamma_\nu}{\hbar}\int_0^t d\tau e^{-i\omega_\nu(t-\tau)}a(\tau)\ . \tag{4.2}$$

Substituting (4.2) into (4.1) yields

$$\dot{a}=-\frac{iEa}{\hbar}-i\bar{f}_{\rm RWA}(t)-\int_0^t d\tau \bar{K}_{\rm RWA}(t-\tau)a(\tau)\ , \tag{4.3}$$

where

$$\bar{f}_{\rm RWA}(t)=\frac{\lambda^{1/2}}{\hbar}\sum_\nu \Gamma_\nu^* b_\nu(0)e^{-i\omega_\nu t} \tag{4.4}$$

and

$$\bar{K}_{\rm RWA}(t-\tau)=\frac{\lambda}{\hbar^2}\sum_\nu |\Gamma_\nu|^2 e^{-i\omega_\nu(t-\tau)}\ . \tag{4.5}$$

The operator $\bar{f}_{\rm RWA}$ is interpreted as fluctuating due to the uncertainty in the initial state of the bath. The distribution of initial states is taken to be the canonical distribution

$$\bar{\rho}_0=\frac{1}{\bar{Z}(\beta)}\exp(-\beta H_B)\ , \tag{4.6}$$

where

$$\bar{Z}(\beta)=\mathrm{Tr}\exp(-\beta H_B)\ . \tag{4.7}$$

The fluctuations are thus zero centered and Gaussian, with correlation functions

$$\langle \bar{f}_{\rm RWA}(t)\bar{f}_{\rm RWA}(t')\rangle=0\ , \tag{4.8a}$$

$$\langle \bar{f}^\dagger_{\rm RWA}(t)\bar{f}_{\rm RWA}(t')\rangle=\frac{\lambda}{\hbar^2}\sum_\nu |\Gamma_\nu|^2 n_\nu e^{i\omega_\nu(t-t')}\ , \tag{4.8b}$$

$$\langle \bar{f}_{\rm RWA}(t)\bar{f}^\dagger_{\rm RWA}(t')\rangle=\frac{\lambda}{\hbar^2}\sum_\nu |\Gamma_\nu|^2 (n_\nu+1)e^{-i\omega_\nu(t-t')}\ . \tag{4.8c}$$

The last term in (4.3) is usually interpreted as a dissipation and the corresponding $\bar{K}_{\rm RWA}(t-\tau)$ is taken to be a dissipative memory kernel.

The next step in the traditional procedure is to establish a fluctuation-dissipation relation between $\bar{K}_{\rm RWA}$ and $\bar{f}_{\rm RWA}$. Guided by the classical form of this relation, arguments are mustered to convince one of a direct proportionality between the correlation function (4.8b) or (4.8c) and the dissipative memory kernel (4.5). The usual arguments (which we will show to be fraught with difficulties) go as follows: The correlation functions (4.8) always occur as integrands multiplied by $\exp[\pm iE(t-t')/\hbar]$ in integrals over time. This procedure essentially filters the correlation function and selects only the $\hbar\omega_\nu=E$ component. This argument then leads one to replace (4.8) with the "equivalent" forms

$$\langle \bar{f}^\dagger_{\rm RWA}(t)\bar{f}_{\rm RWA}(t')\rangle=\frac{\lambda}{\hbar^2}n_E\sum_\nu |\Gamma_\nu|^2 e^{i\omega_\nu(t-t')}\ , \tag{4.9a}$$

$$\langle \bar{f}_{\rm RWA}(t)\bar{f}^\dagger_{\rm RWA}(t')\rangle=\frac{\lambda}{\hbar^2}(n_E+1)\sum_\nu |\Gamma_\nu|^2 e^{-i\omega_\nu(t-t')} \tag{4.9b}$$

so that the fluctuation-dissipation relation is

$$\langle \bar{f}^\dagger_{\rm RWA}(t')\bar{f}_{\rm RWA}(t)\rangle=n_E\bar{K}_{\rm RWA}(t-t')\ . \tag{4.10}$$

Finally, it is then customary to make the Markovian approximation, i.e., to assume that (4.5) can be approximated by a delta function (cf. discussion in Sec. IV B on this approximation)

$$\bar{K}_{\rm RWA}(t-\tau)=2\lambda E\delta(t-\tau)\ . \tag{4.11}$$

With these assumptions it can then easily be shown that the equilibrium population of the oscillator is

$$\bar{n}_{\rm RWA}(T,\infty)=\frac{1}{e^{\beta E}-1} \tag{4.12}$$

and that the relaxation towards this value is exponential:

$$\bar{n}_{\rm RWA}(T,t)=\bar{n}_{\rm RWA}(T,0)e^{-2\lambda(E/\hbar)t} +\bar{n}_{\rm RWA}(T,\infty)(1-e^{-2\lambda(E/\hbar)t})\ . \tag{4.13}$$

Although these results are physically reasonable *(provided kT is not too small,* cf. Sec. III), it is our contention that they have been obtained via a series of erroneous assumptions containing mutually correcting errors that disappear only in the strict limit $\lambda\to 0$. In particular, the errors persist at low temperatures and therefore (4.12) and (4.13) are not valid for these temperature values in spite of their use in this regime.[19] We end this subsection by listing and detailing these errors. A corrected version of the RWA oscillator will be presented in Sec. IV B, and the rationale for the corrections will then become clear.

(1) We show below that the last term in (4.3) cannot be interpreted as a dissipation and that $\bar{K}_{\rm RWA}(t-\tau)$ is therefore not a proper dissipative kernel.

(2) It then follows that the correlation functions (4.8) need not be related to $\bar{K}_{\rm RWA}(t-\tau)$.

(3) The fact that the correlation functions (4.8) and $\bar{K}_{\mathrm{RWA}}(t-\tau)$ cannot, in fact, be related by a fluctuation-dissipation relation follows from a brief inspection of their respective forms. Thus, for instance, if $\bar{K}_{\mathrm{RWA}}(t-\tau)$ is sharply peaked [i.e., $D(\omega)\,|\,\Gamma(\omega)\,|^2 \simeq$const independent of ω in the continuum limit], then the n_ν population factor appearing in the correlation functions (4.8) causes a logarithmic *divergence* at low frequencies [i.e., $D(\omega)\,|\,\Gamma(\omega)\,|^2 n_\omega \sim \mathrm{const}/\omega$ for small ω]. A sharply peaked $\bar{K}_{\mathrm{RWA}}$ thus leads to a divergent correlation function. Conversely, a sharply peaked correlation function corresponds to a $\bar{K}_{\mathrm{RWA}}$ that is not sharply peaked.

(4) The relation (4.10) is, in view of the remarks in point (3), invalid. It was obtained using the approximation (4.9), which in turn is based on a fallacious argument. The fact is that the correlation functions (4.8) do always occur as integrands, but *not* multiplied by $\exp[\pm iE(t-t')/\hbar]$ [cf. remarks preceding (4.9)]. Rather they occur multiplied by $\exp[(\pm iE-\lambda E)(t-t')/\hbar]$, and hence all frequency components of the correlation function, and not just the one at $\hbar\omega_\nu = E$, enter, including those low-frequency components that bring about a divergence when $\bar{K}_{\mathrm{RWA}}$ is assumed sharply peaked.

The above theory thus culminates in the following dilemma. If one insists on identifying $\bar{K}_{\mathrm{RWA}}(t-\tau)$ in (4.3) as a dissipative kernel, then one of two difficulties arise. If the kernel is sharply peaked ("Markovian approximation"), then the correlation function of the fluctuations diverges. The approximation (4.9) that avoids this divergence is simply incorrect (except in the *strict* limit $\lambda \to 0$). If, on the other hand, the correlation function is sharply peaked, then the kernel is not, and the system necessarily has a finite dissipative memory. This latter behavior is unphysical. We are therefore forced to conclude that the initial identification of $\bar{K}_{\mathrm{RWA}}$ as the dissipative kernel is incorrect and that the last term in (4.3) is not the correct dissipative contribution. The physical basis for this conclusion is presented in Sec. V A.

B. Modified RWA and fluctuation-dissipation relation

We now return to the equation of motion (2.31) and compare it with the traditional one, Eq. (4.3):

$$\dot{a} = -\frac{i\epsilon}{\hbar}a - if_{\mathrm{RWA}}(t) - i\hbar\int_0^t d\tau K_{\mathrm{RWA}}(t-\tau)\dot{a}(\tau)\ . \tag{2.31}$$

We observe that (2.31) can be obtained from Eq. (2.20) for the fully coupled oscillator by simply omitting the terms $i\Delta a^\dagger(t)$ and $\dot{a}^\dagger(\tau)$ in the right side of (2.20). The traditional RWA oscillator, Eq. (4.3), on the other hand, cannot be obtained simply from (2.20). *We interpret the last term in (2.31) as the dissipation.* Note that this interpretation of (2.31) associates the dissipation with the rate of change of the annihilation operator rather than with the operator itself [cf. (4.3)]. We emphasize that whenever one uses a creation-annihilation operator (quantum) or a normal mode (classical) representation, the proper dissipative term appears as the coefficient of a rate and not of an amplitude, customary usage notwithstanding (cf. Sec. V).

We further point out that K_{RWA} [cf. (2.33)] contains the same weighting factors $|\Gamma_\nu|^2/\hbar\omega_\nu$ as does K_{FC} [cf. (2.24)], whereas $\bar{K}_{\mathrm{RWA}}$ [cf. (4.5)] does not. It is then to be expected that one can here construct a fluctuation-dissipation relation that parallels that of the FC oscillator and that circumvents the divergences that arise in the traditional RWA.

The fluctuation-dissipation relation follows directly from (2.32) and (2.33) and is given in complete analogy to (3.4) as

$$\sum_\nu \Phi_\nu^{\mathrm{RWA}}(t-\tau)(\hbar\omega_\nu)^{-1}\tanh\left[\frac{\beta\hbar\omega_\nu}{2}\right] = K_{\mathrm{RWA}}(t-\tau)\ , \tag{4.14}$$

where Φ is again the symmetrized correlation function

$$\Phi_\nu^{\mathrm{RWA}}(t-\tau) = \lambda\langle f_\nu^{\mathrm{RWA}}(t) f_\nu^{\mathrm{RWA}\dagger}(\tau) + f_\nu^{\mathrm{RWA}\dagger}(\tau) f_\nu^{\mathrm{RWA}}(t)\rangle\ . \tag{4.15}$$

Equation (4.14) reduces to the usual classical form in the limit $\hbar \to 0$. The further discussion of this relation parallels that of the FC oscillator in Sec. III A. In particular, the decay time of the fluctuations can be quite different from that of the dissipative memory kernel.

Let us now turn to an analysis of the RWA dissipative kernel and to a comparison of its behavior with that of the FC kernel. The continuum form of K_{RWA} is given by [cf. (3.8)]

$$K_{\mathrm{RWA}}(t) = \frac{\lambda}{\hbar^2}\int_0^\infty d\omega \frac{D(\omega)}{\hbar\omega}\,|\,\Gamma(\omega)\,|^2 e^{-i\omega t} \tag{4.16}$$

$$= \tfrac{1}{2}K_{\mathrm{FC}}(t) - i\frac{\lambda}{\hbar^2}\int_0^\infty d\omega \frac{D(\omega)}{\hbar\omega}\,|\,\Gamma(\omega)\,|^2 \sin(\omega t)\ . \tag{4.17}$$

The particular choice (3.9) for the spectral strength leads to

$$K_{\mathrm{RWA}}(t) = \frac{\lambda\gamma}{2\hbar}e^{-\gamma|t|} - \frac{i\lambda\gamma^2}{\hbar\pi}\int_0^\infty d\omega \frac{\sin(\omega t)}{\gamma^2+\omega^2}\ . \tag{4.18}$$

In the limit of large phonon bandwidth γ, (4.18) reduces to the familiar form[7,8,15]

$$K_{\mathrm{RWA}}(t) = \frac{\lambda}{\hbar}\delta(t) - i\frac{\lambda}{\pi\hbar}\mathrm{P}\left[\frac{1}{t}\right]\ , \tag{4.19}$$

where P denotes the principal value. There is considerable discussion in the literature on the principal-value term, first introduced by Senitzky.[7] The discussion concerns the correctness of its presence and the importance of its contribution. Lax[8] eliminates it altogether by introducing negative as well as positive frequencies in (4.16). Haken[15] states (but does not show) that its contribution to the physical behavior of the system in the traditional RWA is small and that it does not matter whether it is included or excluded; he therefore chooses to exclude it.[30] In our analysis we shall retain it (since it seems to us that the restriction to positive frequencies is physically correct) and we shall determine its effect explicitly. We note that such a term does not occur in the FC oscillator, i.e., it arises

here because of the RWA. We furthermore note that such a term also appears in the kernel $\bar{K}_{\mathrm{RWA}}$ of the traditional method, Eq. (4.11), but we followed Lax[8] and Haken[15] in our outline of the usual procedure and hence omitted it in that discussion.[30] Our further analysis is thus based on the full form (4.18).

C. Solution of rate equations

To solve the equation of motion (2.31) we again use the Laplace transform technique to obtain

$$\hat{a}(s)=\frac{-i\hat{f}_{\mathrm{RWA}}(s)+[1+i\hbar\hat{K}_{\mathrm{RWA}}(s)]a(0)}{i\epsilon/\hbar+s[1+i\hbar\hat{K}_{\mathrm{RWA}}(s)]}, \tag{4.20}$$

where

$$\hat{K}_{\mathrm{RWA}}(s)=\frac{\lambda\gamma}{2\hbar(s+\gamma)}-\frac{i\lambda\gamma^2}{2\pi\hbar(s^2-\gamma^2)}\ln\frac{s^2}{\gamma^2}. \tag{4.21}$$

The Laplace inversion of (4.20) is given in Appendix B. For $\lambda\gamma \ll \epsilon/\hbar$ we obtain [cf. Eq. (B2)]

$$a(t)=\sum_{j=1}^{2} e^{s_j t}\left[a(0)B_j+C_j\int_0^t d\tau f_{\mathrm{RWA}}(\tau)e^{-s_j\tau}\right] \tag{4.22}$$

and its Hermitian conjugate, where the B_j, C_j, and s_j are read directly from (B2).

Let us compare the formal solution (4.22) with that of the FC oscillator, (3.14). Two differences are immediately apparent. First, there is one fewer root s_j in (4.22). The two that appear in (4.22) are, to leading orders in λ, $s_1=-\gamma$ and $s_2=-(\lambda\epsilon+i\epsilon)/\hbar$. These are, to the same order, equal to those in (3.14) [note that the difference between ϵ and E is of order λ, cf. (2.27)]. The third root in (3.14), $s_3=-(\lambda E+iE)/\hbar$, arises from the cross coupling that is neglected in the RWA and thus does not appear in (4.22). The second difference between the two solutions is that the latter is not dependent on $a^\dagger(0)$, again because of the decoupling approximation.

These differences notwithstanding, the solutions (4.22) and (3.14) are, in fact, identical in form to $O(\lambda)$. Again neglecting the contribution from s_1 we obtain

$$a(t)=a(0)e^{-\epsilon(\lambda+i)t/\hbar}-i\int_0^t d\tau e^{-\epsilon(\lambda+i)(t-\tau)/\hbar}f_{\mathrm{RWA}}(\tau) \tag{4.23}$$

and its Hermitian conjugate.

It is important to note that the same result (4.22) to $O(\lambda)$ would have been obtained if we had replaced (4.18) by $K_{\mathrm{RWA}}(t)=(\lambda\gamma/\hbar)\exp(-\gamma|t|)$ and made a corresponding adjustment in the fluctuations so that the fluctuation-dissipation relation (4.14) is maintained. This procedure is equivalent to the Lax presciption.[8,30]

D. Population and correlation functions

To calculate RWA oscillator populations and correlation functions we need the correlation function of the fluctuations. From (2.32), (2.28), and (2.14) we obtain

$$\phi_{\mathrm{RWA}}(\tau_1-\tau_2)=\langle f^\dagger_{\mathrm{RWA}}(\tau_1)f_{\mathrm{RWA}}(\tau_2)\rangle=\frac{\lambda\gamma^2}{\pi}\int_0^\infty d\omega\frac{\omega n_\omega}{\gamma^2+\omega^2}e^{i\omega(\tau_1-\tau_2)}. \tag{4.24}$$

With (4.24) we obtain for the population $n_{\mathrm{RWA}}(T,t)$ [cf. (3.16)] to leading order in λ

$$n_{\mathrm{RWA}}(T,t)=n_{\mathrm{RWA}}(T,0)e^{-2\lambda(\epsilon/\hbar)t}+n_{\mathrm{RWA}}(T,\infty)(1+e^{-2\lambda(\epsilon/\hbar)t})-2\frac{\lambda\gamma^2\hbar}{\pi}e^{-\lambda(\epsilon/\hbar)t}\int_0^\infty d\omega\frac{\hbar\omega n_\omega}{\gamma^2+\omega^2}\frac{\cos[(\epsilon-\hbar\omega)t/\hbar]}{\lambda^2\epsilon^2+(\epsilon-\hbar\omega)^2}[1+O(\lambda)]. \tag{4.25}$$

The relaxation to equilibrium occurs on the time scale $\lambda\epsilon/\hbar$ and is different from that of the traditional RWA oscillator [cf. (4.13)].

The equilibrium population is

$$n_{\mathrm{RWA}}(T,\infty)=\frac{\lambda\gamma^2\hbar}{\pi}\int_0^\infty d\omega\frac{\hbar\omega n_\omega}{(\gamma^2+\omega^2)[\lambda^2\epsilon^2+(\epsilon-\hbar\omega)^2]}\times[1+O(\lambda)]. \tag{4.26}$$

At zero temperature (4.26) vanishes, as distinct from (3.21). The residual population of the RWA oscillator is thus, at most, of $O(\lambda^2)$. The physical source of this difference is discussed in Sec. V. At finite temperatures, for $kT\gg\epsilon$ and $\hbar\gamma\gg kT$, (4.26) again yields the usual Bose population

$$n_{\mathrm{RWA}}(T,\infty)=\frac{1}{e^{\beta\epsilon}-1}[1+O(\lambda)]. \tag{4.27}$$

At low temperatures ($kT\ll\epsilon$) for $\gamma\to\infty$, we obtain the series

$$n_{\mathrm{RWA}}(T,\infty)=\frac{2\lambda}{\pi}\left[\frac{kT}{\epsilon}\right]^2\left[\xi(2)+4\xi(3)\left[\frac{kT}{\epsilon}\right]-30\xi(4)\left[\frac{kT}{\epsilon}\right]^2+\cdots\right], \tag{4.28}$$

where ξ is the zeta function. As in the FC oscillator we conclude that the high-temperature behavior is of the usually expected Bose form. At low temperatures, on the other hand, there are marked deviations from that behavior even when the coupling parameter λ is small. Again, this effect should by physically observable.

The correlation functions for energy absorption and emission of the RWA oscillator are defined as in (3.24) and (3.25) and yield the spectra

$$S^{\mathrm{abs}}_{\mathrm{RWA}}(\omega)=\frac{\lambda\hbar^2\gamma^2\omega(n_\omega+1)}{\pi(\omega^2+\gamma^2)[\lambda^2\epsilon^2+(\hbar\omega-\epsilon)^2]} \tag{4.29}$$

and

$$S^{\rm em}_{\rm RWA}(\omega)=\frac{\lambda\hbar^2\gamma^2 n_\omega}{\pi(\omega^2+\gamma^2)[\gamma^2\epsilon^2+(\hbar\omega-\epsilon)^2]}\ . \tag{4.30}$$

The discussion of the shape and temperature dependence of these spectra parallels that of the spectra of the FC oscillator in Sec. III D. We note the absence in (4.29) and (4.30) of the peak that would occur in the FC spectra at $\hbar\omega=-E$ if we had included negative frequencies.

V. DISCUSSION

A number of general implications about quantum-mechanical dynamical systems are contained in the analysis in Secs. I–IV. For clarity, we have postponed their detailed discussion until the present section.

A. Dissipation, fluctuations, and their relationships

The utility of a Langevin description for the dynamics of a system lies in the relation one can construct between the fluctuations and the dissipation. This relation ensures that a thermodynamically closed system will equilibrate. Thus the proper identification of these terms in the equations of motion is crucial. When the dynamical equations (classical or quantum mechanical) are in a configuration representation (i.e., p,q), there is no ambiguity in the identification of the dissipation: It is the term in the force equation that is linear in the velocity [cf. paragraph preceding Eq. (3.1)]. In other representations, e.g., mode amplitudes in classical systems and creation-annihilation operators in quantum systems, there seems to be a great deal of confusion over the identification. The common folklore says that in a mode amplitude or creation-annihilation operator rate equation $\dot a=F(a,a^\dagger)$, the term of the form $-\int_0^t d\tau G(t-\tau)a(\tau)$ or its Markovian limit $-\eta a(t)$ with real G and η should be interpreted as the dissipation [e.g., Eq. (4.3)]. This interpretation is *incorrect* and, in particular, it is inconsistent with that made in configuration space. The difficulty becomes clear if we transform back to configuration space and obtain

$$\dot p=iE^{1/2}(\dot a^\dagger-\dot a)=-iE^{1/2}\eta(a^\dagger-a)+\cdots\ , \tag{5.1}$$

where $\cdots$ represents other terms. The "dissipative" term is proportional to the momentum rather than to the velocity $(\hbar/E)^{1/2}(\dot a^\dagger+\dot a)$. When momentum and velocity are proportional, this distinction is spurious. However, when they are not (as is the case, for instance, in the RWA, cf. Secs. V C and V D), the distinction becomes crucial.

The resolution of the difficulty lies in changing one's interpretation of dissipative terms from those given above to terms of the form $-i\hbar\int_0^t d\tau K(t-\tau)\dot a(\tau)$ or $-i\lambda E\dot a(t)$ [e.g., Eq. (2.31)]. These terms can be obtained from one of the form $-\int_0^t d\tau G(t-\tau)a(\tau)$ by an integration of the latter by parts. It follows that the incorrect form *contains* the dissipative contribution but also contains nondissipative contributions (cf. Sec. V D). With this association the force law becomes

$$\begin{aligned}\dot p&=-\lambda E(\hbar^2/E)^{1/2}(\dot a^\dagger+\dot a)+\cdots\\&=-\lambda E\dot q+\cdots\ ,\end{aligned} \tag{5.2}$$

where $\cdots$ represents other terms, thus yielding a dissipative force linear in the velocity.

Only with the proper identification of the dissipative terms in the dynamical equations (Markovian or non-Markovian) is one able to construct a generalized fluctuation-dissipation relation. This relation takes the form

$$K(t-\tau)=\sum_\nu \Phi_\nu(t-\tau)(\hbar\omega_\nu)^{-1}\tanh\left[\frac{\hbar\omega_\nu}{2kT}\right]\ , \tag{5.3}$$

where Φ_ν is the symmetrized correlation function of the fluctuations[20]

$$\Phi_\nu(t-\tau)=\lambda\langle f_\nu(t)f_\nu^\dagger(\tau)+f_\nu^\dagger(\tau)f_\nu(t)\rangle\ . \tag{5.4}$$

The index ν labels bath modes. Relation (5.3) arises from any model in which the bath consists of a collection of harmonic oscillators and the system-bath coupling is bilinear [e.g., Eqs. (3.4) and (4.14)].[31] At high temperatures (5.3) reduces to the classical relation

$$\sum_\nu \Phi_\nu(t-\tau)=2kTK(t-\tau) \tag{5.5}$$

so that the correlations of the fluctuations and the dissipative memory kernel regress on the same time scale. At arbitrary temperatures this is not the case, however. If γ^{-1} is the decay time of $K(t-\tau)$, then the correlations in the fluctuations relax on the *longer* of the two time scales $(kT/\hbar)^{-1},\gamma^{-1}$. Thus at low temperatures ($kT\ll\hbar\gamma$) the fluctuations have long persistence times even if the bath energy bandwidth γ is large. This is a macroscopic quantum-mechanical effect whose consequences should be readily observable in population measurements and in spectral measurements (cf. Secs. III C, III D, and IV D).

B. "Weak coupling," temperature, and initial conditions

The notions of a temperature and of statistical-mechanical fluctuations enter in the analysis through the specification of a distribution of initial conditions [cf. (2.14)]. One introduces such a distribution because in practice the degrees of freedom of the heat bath cannot be predetermined experimentally. There is a certain amount of latitude in the choice of the initial distribution. We have chosen (2.14) for a number of reasons.

(1) It is often physically reasonable that the bath at time $t=0$ should be thermally adjusted to the initial state of the oscillator. This is consistent with the notion of a time-scale separation between oscillator and bath, i.e., the bath relaxes rapidly to the state of the oscillator.

(2) *Regardless of the coupling strength* between the oscillator and the bath, with the choice (2.14) the oscillator relaxes to a canonical distribution proportional to $\exp(-\beta H_S)$ in the classical limit.

(3) Any other choice of initial distribution, e.g., a canonical distribution for the isolated heat bath [cf. (4.6)] does *not* lead to a canonical equilibrium of the oscillator in the classical limit except in the weak-coupling limit.

As an aside, we find it remarkable that the inclusion of the oscillator-bath interaction in the *initial* bath distribution is sufficient to ensure that the *final* oscillator distribution depend only on the isolated oscillator Hamiltonian

H_S and not on the interaction (in the classical limit). We note that this behavior is peculiar to systems with c-number commutation relations.[31] In general (e.g., for spin systems, in which the commutators are operators[31]), there is no choice of initial bath distribution in terms of H_B and H_{SB} that will lead to a final canonical distribution involving only H_S. The interaction H_{SB} necessarily enters the final distribution except in the weak-coupling limit.

We stress that in our analysis only the *initial* bath distribution has been fixed. After $t=0$, the bath is allowed to evolve as determined by the equations of motion. This evolution brings the bath out of equilibrium (to which it returns as $t\to\infty$). The effect of the system on the bath, fully included in the description [e.g., in Eq. (2.11) or Eq. (2.30)] is precisely the origin of the dissipation in the system equations of motion. When this effect is ignored (e.g., when the bath is assumed to be in equilibrium at all times, a frequent assumption[17]) then the dissipation must be reintroduced heuristically in an *ad hoc* fashion.

In most discussions of relaxation properties of quantum systems the weak-coupling limit plays a prominent role. By weak-coupling limit one is given to understand that the interaction strength vanishes, i.e., that $\lambda\to 0$ in (2.4) or (2.25). The context in which this limit is usually taken is characterized by two energy relationships: that the coupling energy λE be much smaller than the characteristic oscillator energy E and that λE be much smaller than the phonon bandwidth $\hbar\gamma$. The fourth important energy, kT, is never mentioned in relation to the other energies. Temperature dependences are then often considered *after* the weak-coupling limit has been implemented. This protocol can introduce grave errors. In particular, it is clearly improper to take the $T\to 0$ limit after implementing the weak-coupling limit. If the temperature $kT \ll E/\ln(1/\lambda)$, then the usual weak-coupling limit results are not valid and results such as (3.23) are the appropriate ones. The above discussion leads to the following physically satisfying interpretation. At high temperatures ($kT \gg E$) the equilibrium population of the oscillator is provided by the heat bath; the coupling mainly provides a mechanism for energy transfer between the bath and the oscillator and the equilibrium population therefore has a λ-independent level [cf. (3.22)]. At low temperatures [$kT \ll E/\ln(1/\lambda)$], on the other hand, the oscillator population is provided by the interaction energy itself since the bath excitations cannot populate the oscillator. In this regime, then, the oscillator population is proportional to λ and vanishes in the weak-coupling limit [cf. (3.23)]. This same mechanism may cause a residual population of the oscillator at zero temperature [cf. (3.21)].

C. Comparison of the FC oscillator and the modified RWA oscillator

In this subsection we compare and contrast the behavior of the fully coupled oscillator with that of the oscillator in the rotating-wave approximation. We stress that our modified RWA oscillator differs from the traditional one, not in the starting Hamiltonian [which is given by (2.1)–(2.3) and (2.25) for both], but rather in our choice of the initial bath distribution and in the subsequent interpretation of terms. In this subsection the comparison is between the FC oscillator and the *modified* RWA oscillator. The comparison of the modified and the traditional RWA oscillators is made in Sec. V D.

The motivation for the RWA is twofold: it decouples the equation of motion of the creation from that of the annihilation operator and it thereby presumably eliminates high-frequency deterministic components from the oscillator dynamics. The analysis in Secs. III and IV shows explicitly the effects of the RWA on the solution $a(t)$. The FC oscillator solution (3.14) [neglecting terms of $O(e^{-\gamma t})$] is

$$a_{\rm FC}(t)\approx a(0)e^{-(E/\hbar)(\lambda+i)t} -i\int_0^t d\tau\, e^{(-E/\hbar)(\lambda+i)(t-\tau)}f_{\rm FC}(\tau) +O(\lambda^2 e^{-(E/\hbar)(\lambda-i)t})\ ; \tag{5.6}$$

that of the RWA oscillator is [cf. (4.23)]

$$a_{\rm RWA}(t)\approx a(0)e^{-(\epsilon/\hbar)(\lambda+i)t} -i\int_0^t d\tau\, e^{-(\epsilon/\hbar)(\lambda+i)(t-\tau)}f_{\rm RWA}(\tau)\ . \tag{5.7}$$

There are two formal differences between the solutions. The first is in the eigenvalues $(E/\hbar)(\lambda+i)$ and $(\epsilon/\hbar)(\lambda+i)$, which differ by $O(\lambda)$. The second (more interesting) difference is in the appearance of the eigenvalue $(E/\hbar)(\lambda-i)$ in (5.6) but not in (5.7). It is precisely this eigenvalue that contributes high-frequency oscillations in the average quantities in the FC oscillator and whose sources are the very terms in H_{SB} eliminated in going to the RWA. We note that the magnitude of these contributions in (5.6) is second order in λ and therefore negligible in the weak-coupling limit.

Having established the formal equivalence of (5.6) and (5.7) for small λ, it remains to compare the statistical properties of $f_{\rm FC}(t)$ and $f_{\rm RWA}(t)$ to determine if (5.7) is an adequate approximation to (5.6). Since both are zero-centered Gaussian processes, we need only compare their correlation functions. For the FC oscillator we have [cf. (3.18)]

$$\phi_{\rm FC}(\tau-\tau')=\langle f^\dagger_{\rm FC}(\tau)f_{\rm FC}(\tau')\rangle =\lambda\sum_\nu \frac{|\Gamma_\nu|^2}{\hbar^2\omega_\nu}[(n_\nu+1)e^{-i\omega_\nu(\tau-\tau')} +n_\nu e^{i\omega_\nu(\tau-\tau')}]\ , \tag{5.8}$$

while in the modified RWA [cf. (4.24)]

$$\phi_{\rm RWA}(\tau-\tau')=\langle f^\dagger_{\rm RWA}(\tau)f_{\rm RWA}(\tau')\rangle =\lambda\sum_\nu \frac{|\Gamma_\nu|^2}{\hbar^2\omega_\nu}n_\nu e^{i\omega_\nu(\tau-\tau')}\ . \tag{5.9}$$

These correlation functions are clearly not equal and hence the behavior of the FC oscillator is not identical to that of the modified RWA oscillator even when the high-frequency contributions to the former are neglected. Our analysis in Secs. III and IV shows the following differences.

(1) The FC oscillator has a residual population at $T=0$ [cf. Eq. (3.21)], whereas the modified RWA oscillator does not. The FC residual population arises from the interaction terms of the form $a^\dagger b^\dagger$ in the Hamiltonian, terms that can create excitations even at $T=0$. The RWA interaction Hamiltonian only contains number-preserving terms ($a^\dagger b, b^\dagger a$) and hence produces no residual population.

(2) The symmetry of the temperature dependence of the equilibrium population of each of the two oscillators at low temperatures is quite different. Odd-order terms in (kT/E) appear in the modified RWA oscillator [cf. (4.28)] and not in the FC oscillator [cf. (3.23)]. The coefficients of the comparable terms in the two series are also different.

These differences are important at low temperatures and disappear at high temperatures ($kT \gg E$) where to $O(\lambda)$ the two oscillators behave identically. We therefore conclude that the *modified* RWA oscillator can be an adequate approximation to the FC oscillator if λ is small and the temperature is high, but it is certainly inadequate at low temperatures.

As a final comment we note that the way in which noise enters the equations of motion in the (p,q) representation is quite different for the FC and RWA oscillators. In the former case the fluctuations and dissipation enter only in the force law ($\dot{p}$); the other equation is $\dot{q}=p$, i.e., it is a defining equation for the momentum operator in terms of the velocity operator. In the RWA, fluctuations and dissipation enter in both equations, thus shrouding the relation between velocity and momentum.[23] It is precisely this obscurity that causes difficulties in the traditional RWA, as discussed below.

D. Traditional versus modified RWA

The traditional and modified RWA begin with the same Hamiltonian and consequently share the same equations of motion. The differences between them arise in the interpretation of the terms in the equations.

The major difference is the identification of the dissipative term. The physical implications of this difference have been discussed in Sec. V A: in the traditional RWA one supposes (incorrectly) the dissipation to be proportional to the momentum while the modified RWA assumes (correctly) proportionality to velocity. Since the momentum is not proportional to the velocity in the RWA, this is a substantial difference. As an added argument for the modified RWA we note that the dissipation in the modified RWA oscillator and in the FC oscillator are related by $2\,\mathrm{Re}K_{\mathrm{RWA}}(t)=K_{\mathrm{FC}}(t)$, whereas the dissipative kernel $\bar{K}_{\mathrm{RWA}}(t)$ in the traditional RWA and $K_{\mathrm{FC}}(t)$ are not simply related. In fact, we argued in Sec. IV that a sharply peaked K_{FC} implies a *divergent* $\bar{K}_{\mathrm{RWA}}$.

The second difference between the two versions of the RWA occurs in the fluctuations. The formal expressions (2.32) for $f_{\mathrm{RWA}}(t)$ (modified) and (4.4) for $\bar{f}_{\mathrm{RWA}}(t)$ (traditional) differ by the appearance of the oscillator initial values in the former. At this point two possibilities present themselves. One can choose the same distribution of initial conditions for both, with the result that f_{RWA} and $\bar{f}_{\mathrm{RWA}}$ have different statistical properties. This option is not particularly useful. The other possibility is to choose different initial distributions in such a way that the resulting statistics of f_{RWA} and $\bar{f}_{\mathrm{RWA}}$ are identical. This has been done in Sec. IV.

We thus arrive at two equations of motion with statistically equivalent fluctuations but with very different dissipative terms. In the traditional RWA there is no fluctuation-dissipation relation between $\bar{f}_{\mathrm{RWA}}(t)$ and the kernel $\bar{K}_{\mathrm{RWA}}(t)$ (except in the strict $\lambda\to 0$ limit, as discussed in Sec. IV A). The modified RWA, on the other hand, not only possesses a fluctuation-dissipation relation between $f_{\mathrm{RWA}}(t)$ and $K_{\mathrm{RWA}}(t)$ valid for arbitrary values of λ, but the relation has the same form as that for the FC oscillator.

E. Commutation relations

One way that has been used in the literature[8] to assess the validity of different heuristic equations of motion is to determine whether the correct commutation relations are satisfied on the average at all times if they are satisfied initially. These relations are $\langle [a, a^\dagger]\rangle = 1$, $\langle [a, a]\rangle = 0$ or their equivalent in the p,q representation, $\langle [q, p]\rangle = i\hbar$. In particular, this criterion has been invoked to choose between possible second-order properties of the fluctuations in the equation of motion. Lax[8] used this type of an argument as follows. Consider the equations of motion of the FC oscillator in the q,p representation and in the "Markovian limit" (i.e., for an infinite phonon bandwidth γ):

$$\dot{q}=p\ , \tag{5.10a}$$

$$\dot{p}=-\lambda\frac{E}{\hbar}p-\frac{E^2}{\hbar^2}q+F(t)\ . \tag{5.10b}$$

Senitzky[7] chooses the correlation function

$$\langle F(t)F(u)\rangle = 2\lambda\frac{E}{\hbar}\left[(n_E+\tfrac{1}{2})\delta(t-u) - \frac{i}{2\pi}\mathrm{P}\left[\frac{1}{t-u}\right]\right] \tag{5.11}$$

corresponding to the commutation rule

$$\langle [F(t), F(u)]\rangle = \frac{2i\lambda E^2}{\hbar\pi}\mathrm{P}\left[\frac{1}{t-u}\right]\ . \tag{5.12}$$

Lax shows that with this commutation rule one obtains

$$\langle [q, p]\rangle = i\hbar\left[1-\frac{\lambda}{\pi}\right]+O(\lambda^2)\ . \tag{5.13}$$

On this basis he concludes that the correct commutator for the Langevin force should rather be

$$\langle [F(t), F(u)]\rangle = 2i\lambda E\delta'(t-u) \tag{5.14}$$

since this leads *exactly* to the correct commutation relation

$$\langle [q, p]\rangle = i\hbar\ . \tag{5.15}$$

The choice (5.14) is also made by Benguria and Kac[20] and by us in the FC oscillator.

Our analysis in Secs. III and IV shows precisely what the difficulty is with the choice (5.11) in (5.10). To understand the problem it must first be stressed that *all* of our equations of motion lead to the correct commutation relations: (3.2) with (3.18) for the FC oscillator, (2.31) with (4.24) for the modified RWA oscillator [and even (4.3) with (4.8) for the traditional RWA]. The reason is that all of our equations are, in fact, merely *transcriptions* of the exact dynamics into a Langevin form that contains the complete dynamics. What, then, is the problem with (5.11)? It is this: the correct fluctuation-dissipation relation is not satisfied. The correct relation is that for the FC oscillator and for our modified RWA oscillator [cf. (3.5) and (4.14)], i.e.,

$$\sum_\nu \Phi_\nu(t-\tau)(\hbar\omega_\nu)^{-1}\tanh\left[\frac{\beta\hbar\omega_\nu}{2}\right]=K(t-\tau)\ , \quad (5.16)$$

where

$$\Phi_\nu(t-\tau)=\lambda\langle f(t)f^\dagger(\tau)+f^\dagger(\tau)f(t)\rangle\ . \quad (5.17)$$

It is indeed appropriate for Φ_ν to contain a principal-value contribution *provided the corresponding dissipation contains the same contribution* [cf. Eq. (4.19)]. In (5.10) the dissipation *does not* contain such a term and hence neither should the fluctuations. One resolution of the problem is equivalent to that argued by Lax: omit the principal-value portion from the fluctuations *and* from the dissipation.[30] Another is to keep (5.12) but to replace (5.10b) with the formal expression

$$\dot p(t)=-\frac{\lambda E}{\hbar}p(t)+\frac{i\lambda E}{\pi\hbar}\mathrm{P}\left[\frac{1}{t-u}p(u)\right]-\frac{E^2}{\hbar^2}q(t)+F(t)\ . \quad (5.18)$$

The latter choice parallels that which appears in our modified RWA. Equation (5.18) together with (5.12) also provides the correct commutation relations for p and q.

We should emphasize that the apparent freedom in the choice of the commutation relations for the fluctuations is illusory. It arises only in phenomenological or heuristic discussions of the equations of motion. When the equations are derived from a Hamiltonian and the full Hamiltonian dynamics are preserved at all stages of the analysis, the commutation relations are predetermined. Thus the choices (5.10b) together with (5.14) and (5.18) together with (5.11) simply represent systems with different Hamiltonians.

F. Non-Markovian behavior

A question about Langevin systems that is often asked is whether they admit of a Markovian limit.[8,15] The usual first step towards an answer is to assume instantaneous dissipation (i.e., to take an infinite phonon bandwidth γ). In the classical limit instantaneous dissipation automatically implies that the correlations between fluctuations are also instantaneous, i.e., the spectrum of the fluctuations is frequency independent (white). The system is then Markovian.

In quantum systems the fluctuation-dissipation relation is more complicated. Instantaneous dissipation does not necessarily imply that the time scale of correlations between fluctuations vanishes. For the FC oscillator from (3.18) we obtain for the Fourier transform of the commutator

$$\langle[f^\dagger_{\mathrm{FC}}(\omega),\, f_{\mathrm{FC}}(\omega)]\rangle=2\omega\lambda(\omega)\ , \quad (5.19)$$

where [cf. (3.9)]

$$\lambda(\omega)\equiv\lambda\pi\frac{\Gamma^2(\omega)D(\omega)}{\hbar^2\omega}\ . \quad (5.20)$$

Instantaneous dissipation occurs in the limit in which $\lambda(\omega)$ approaches the coupling constant λ. Even in this limit (5.19) is clearly frequency dependent and the fluctuations can therefore not be white. This discussion was first presented by Lax.[8]

The modified RWA leads to the commutator

$$\langle[f^\dagger_{\mathrm{RWA}}(\omega),\, f_{\mathrm{RWA}}(\omega)]\rangle=2\omega n_\omega\lambda(\omega)\ , \quad (5.21)$$

thus giving a temperature-dependent spectrum. In the limit $\lambda(\omega)\to\lambda$ we are left with a spectrum that, in general, is frequency dependent but that at high temperatures ($kT\gg\hbar\gamma$) and/or in the classical limit ($\hbar\to0$) becomes white. Thus the modified RWA oscillator can admit of a Markovian description in these limits. We finally note that (5.21) is also obtained from the correlation functions (4.8) in the traditional RWA. The approximations discussed in Sec. IV A correspond to setting $\omega\lambda(\omega)=\mathrm{const}=\lambda E/\hbar$ and $n_\omega=n_E$, and calling the resulting spectrum white for all temperatures.

Note added in proof. We thank Dr. J. Roerdink for calling to our attention the earlier work of P. Ullersma on the quantum-mechanical fluctuation-dissipation relation [cf. Physica (Utrecht) 32, 27 (1966)].

APPENDIX A: EIGENVALUE ANALYSIS OF FC OSCILLATOR EQUATIONS ($\lambda\ll1$)

The inverse matrix appearing in Eq. (3.13) is given by

$$\hat{\underline{B}}^{-1}(s)=\frac{1}{s^2+E^2/\hbar^2+2E[s\hat K_{\mathrm{FC}}(s)-\Delta/\hbar]}\begin{bmatrix} s-i\epsilon/\hbar+E\hat K_{\mathrm{FC}}(s) & E\hat K_{\mathrm{FC}}(s)+i\Delta \\ E\hat K_{\mathrm{FC}}(s)-i\Delta & s+i\epsilon/\hbar+E\hat K_{\mathrm{FC}}(s)\end{bmatrix}\ . \quad (A1)$$

With the particular choice (3.9) we have

$$\hat K_{\mathrm{FC}}(s)=\frac{\lambda\gamma}{s+\gamma},\quad \Delta=\lambda\gamma\ , \quad (A2)$$

so that

$$\underline{\hat{B}}^{-1}(s)=\frac{1}{(s^2+E^2/\hbar^2)(s+\gamma)-2(E\lambda/\hbar)\gamma^2}\begin{bmatrix}(s-i\epsilon/\hbar)(s+\gamma)+E\lambda\gamma/\hbar & (E\lambda/\hbar)\gamma+i\lambda\gamma(s+\gamma)\\ (E\lambda/\hbar)\gamma-i\lambda\gamma(s+\gamma) & (s+i\epsilon/\hbar)(s+\gamma)+(E\lambda/\hbar)\gamma\end{bmatrix}. \tag{A3}$$

The Laplace inversion of (3.13) thus requires the solution of the cubic equation

$$\left[s^2+\frac{E^2}{\hbar^2}\right](s+\gamma)-2\frac{E\lambda}{\hbar}\gamma^2=0\,. \tag{A4}$$

The exact solution $a(t)$ in terms of the three roots s_1, s_2, and s_3 of (A4) is given by the residue theorem as

$$\begin{aligned}a(t)=&\frac{1}{(s_1-s_2)(s_1-s_3)}\left\{a(0)\left[\left[s_1-\frac{i\epsilon}{\hbar}\right](s_1+\gamma)+\frac{E\lambda}{\hbar}\gamma\right]e^{s_1t}+a^\dagger(0)\left[\frac{E\lambda}{\hbar}\gamma+i\lambda\gamma(s_1+\gamma)\right]e^{s_1t}\right.\\&\left.-i\left[s_1-\frac{iE}{\hbar}\right](s_1+\gamma)\int_0^t d\tau e^{s_1\tau}f_{\rm FC}(t-\tau)\right\}\\&+\frac{1}{(s_2-s_1)(s_2-s_3)}\left\{a(0)\left[\left[s_2-\frac{i\epsilon}{\hbar}\right](s_2+\gamma)+\frac{E\lambda}{\hbar}\gamma\right]e^{s_2t}+a^\dagger(0)\left[\frac{E\lambda}{\hbar}\gamma+i\lambda\gamma(s_2+\gamma)\right]e^{s_2t}\right.\\&\left.-i\left[s_2-\frac{iE}{\hbar}\right](s_2+\gamma)\int_0^t d\tau e^{s_2\tau}f_{\rm FC}(t-\tau)\right\}\\&+\frac{1}{(s_3-s_1)(s_3-s_2)}\left\{a(0)\left[\left[s_3-\frac{i\epsilon}{\hbar}\right](s_3+\gamma)+\frac{E\lambda}{\hbar}\gamma\right]e^{s_3t}+a^\dagger(0)\left[\frac{E\lambda}{\hbar}\gamma+i\lambda\gamma(s_3+\gamma)\right]e^{s_3t}\right.\\&\left.-i\left[s_3-\frac{iE}{\hbar}\right](s_3+\gamma)\int_0^t d\tau e^{s_3\tau}f_{\rm FC}(t-\tau)\right\}.\end{aligned} \tag{A5}$$

Although one could in principle (and with sufficient motivation) proceed with an exact calculation, for our present purposes we find it adequate to consider λ sufficiently small so that $\lambda\gamma\ll E/\hbar$. To first order in λ the three roots of (A4) are

$$s_1=-\gamma+\frac{2\lambda E\gamma^2\hbar}{\hbar^2\gamma^2+E^2},\quad s_{2,3}=-\frac{\lambda\gamma^2E\hbar}{\hbar^2\gamma^2+E^2}\mp i\left[\frac{E}{\hbar}-\frac{\lambda\gamma^3\hbar^2}{\hbar^2\gamma^2+E^2}\right]. \tag{A6}$$

APPENDIX B: EIGENVALUE ANALYSIS OF RWA OSCILLATOR EQUATIONS ($\lambda\ll1$)

The Laplace inversion of (4.20) requires us to find the zeros of its denominator, i.e., the roots of

$$\frac{i\epsilon}{\hbar}(s+\gamma)+s\left[(s+\gamma)+i\frac{\lambda\gamma}{2}+\frac{1}{2}\frac{\lambda\gamma^2}{\pi(s-\gamma)}\ln\frac{s^2}{\gamma^2}\right]=0\,, \tag{B1}$$

where we have used (4.21). We note that the logarithmic term does not introduce a singularity at $s=0$ because $s\ln s\to0$ as $s\to0$. Equation (B1) has two simple (i.e., first-order) roots s_0 and s_1, so that $a(t)$ is given by the residue theorem as

$$\begin{aligned}a(t)=&\frac{1}{(s_1-s_2)}\left\{a(0)\left[\left[s_1+\gamma+i\frac{\lambda\gamma}{2}+\frac{1}{2}\frac{\lambda\gamma^2}{\pi(s_1-\gamma)}\ln\frac{s_1^2}{\gamma^2}\right]e^{s_1t}-\left[s_2+\gamma+i\frac{\lambda\gamma}{2}+\frac{1}{2}\frac{\lambda\gamma^2}{\pi(s_2-\gamma)}\ln\frac{s_2^2}{\gamma^2}\right]e^{s_2t}\right]\right.\\&\left.-i(s_1+\gamma)\int_0^t d\tau e^{s_1\tau}f_{\rm RWA}(t-\tau)+i(s_2+\gamma)\int_0^t d\tau e^{s_2\tau}f_{\rm RWA}(t-\tau)\right\}.\end{aligned} \tag{B2}$$

To leading order in λ the roots of (B1) are given by

$$s_1=-\gamma+i\frac{\lambda\gamma}{2} \tag{B3a}$$

and

$$s_2=-i\frac{\epsilon}{\hbar}-\frac{\lambda}{\hbar}\,. \tag{B3b}$$

The contributions from s_1 decay rapidly and the residue at s_1 is of $O(\lambda)$. We neglect these contributions. The residue at s_2 is of order unity and is retained to $O(1)$ to give (4.23). We note that the logarithms in (B2) are given by their principal values.

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