Non-Markovian dynamics of quantum systems. I. Formalism and transport coefficients

Z. Kanokov,[1,2] Yu. V. Palchikov,[1] G. G. Adamian,[1,3] N. V. Antonenko,[1] and W. Scheid[4]
[1]*Joint Institute for Nuclear Research, 141980 Dubna, Russia*
[2]*National University, 700174 Tashkent, Uzbekistan*
[3]*Institute of Nuclear Physics, 702132 Tashkent, Uzbekistan*
[4]*Institut für Theoretische Physik der Justus-Liebig-Universität, D-35392 Giessen, Germany*
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Generalized Langevin equations and fluctuation-dissipation relations are derived for the case of a nonlinear non-Markovian noise. The explicit expressions for the time-dependent friction and diffusion coefficients are presented for the case of general and linear couplings in the coordinate and momentum between the collective harmonic oscillator and heat bath. The long-time tails of correlation functions are investigated in the low- and high-temperature regimes of dissipation for different couplings. The Onsager's regression hypothesis is discussed for the non-Markovian dynamics. The Lindblad theory is justified on the basis of the microscopical model.

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I. INTRODUCTION

Different methods have been used to derive the equations of motion for a damped quantum oscillator in a quantum-mechanical heat bath on the basis of a microscopical description [1–8]. The thermal relaxation of a system was mainly restricted by the Markovian limit (instantenious dissipation, Gaussian δ-time-correlated fluctuations) and by the weak-coupling limit between the oscillator and heat bath, and by high temperatures. If the dynamics of the system is very fast, a colored noise and nonlocal dissipation should be assumed. There are many systems that cannot be described by a Markovian process: for example, the case of a low bath temperature, particularly if the dynamics involves tunneling transitions through the potential barrier. In many new devices needed for the emerging fields of nanotechnology and quantum computing the non-Markovian effects are very important. The question of the behavior of the dissipative quantum system beyond the weak-coupling and high-temperature limits has raised interest in simple exactly solvable models [7,9–15]. In these models the heat bath is assumed to be a set of harmonic oscillators interacting linearly in coordinates with the collective harmonic oscillator subsystem. The density and coupling constants of the environmental modes are chosen in such a way that the equations of motion take the familiar classical forms. Important progress beyond the limitations mentioned above was made in Refs. [7,12,13,15] using the path integral technique. For instance, the nonexponential decay of correlation functions was found in the low-temperature range. However, the complicated structure of the path integral scheme makes even a numerical evaluation in many cases very cumbersome [7]. There is still a need for simpler, although approximate, equations of motion. The present paper is an effort in this direction.

We use the Langevin approach which is widely applied to finding the effects of fluctuations and dissipations in macroscopical systems. The Langevin method in the kinetic theory significantly simplifies the calculation of nonequilibrium quantum and thermal fluctuations and provides a clear picture of the dynamics of the process [1,3]. In Sec. II A we present a fully quantum-mechanical derivation of generalized non-Markovian Langevin equations. These equations fulfill the quantum fluctuation-dissipation theorem as shown in Sec. II B. The time-dependent transport coefficients which take the memory effects into consideration are obtained for the general and linear couplings in coordinate and momentum between the collective harmonic oscillator and bath subsystems in Secs. II C and IV. The microscopic justification of the Lindblad axiomatic theory is provided in Sec. III. In Sec. V we discuss the dynamics of the fully coupled (FC) normal and inverted oscillators, and free motion. The analysis of the harmonic oscillator in the rotating-wave approximation (RWA) is done in Sec. VI. The results of illustrative numerical calculations of diffusion and friction coefficients and variances for FC oscillator are presented in Sec. VII.

A second paper follows this paper which is devoted to the treatment of the escape rate from the metastable potential as well as the capture probability into the metastable well with the time-dependent transport coefficients obtained for the FC oscillator.

II. COUPLING OF GENERAL FORM

A. Generalized non-Markovian Langevin equations

In order to derive the quantum non-Markovian Langevin equations and the time-dependent transport coefficients for a collective subsystem, a suitable microscopic Hamiltonian of the whole system (the heat bath plus collective subsystem) has first to be formulated. In Refs. [16–18] the following Hamiltonian was suggested:

$$H = H_c + H_b + H_{cb},$$

$$H_c = p\frac{1}{2\mu(q)}p + U(q),$$

$$H_b = \sum_{\nu} \hbar\omega_{\nu} b_{\nu}^{\dagger} b_{\nu},$$

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$$H_{cb} = \sum_\nu V_\nu(q)(b_\nu^\dagger + b_\nu) + i\sum_\nu G_\nu(q,p)(b_\nu^\dagger - b_\nu), \quad (1)$$

which explicitly depends on the collective coordinate q, canonically conjugated momentum p, and intrinsic heat bath degrees of freedom expressed through the bath phonon operators of creation $b_\nu^\dagger$ and annihilation b_ν. Under the condition $G_\nu(q,p)=\{\widetilde{G}_\nu(q),p\}_+=\widetilde{G}_\nu(q)p+p\widetilde{G}_\nu(q)$ the Hamiltonian H is time reversible. The terms H_c, H_b, and H_{cb} are the Hamiltonians of the collective subsystem depending on mass parameter $\mu(q)$ and potential $U(q)$, of the bath subsystem, and of the collective-bath interaction, respectively. The model of heat bath is an assembly of harmonic oscillators with frequencies ω_ν. The coupling to the heat bath is linear in the bath operators and corresponds to the energy being transferred to and from the bath by the absorption or emission of bath quanta. The coupling term can have important consequences on the dynamics of the collective subsystem by altering the effective collective potential and by allowing energy to be exchanged with the thermal reservoir, thereby allowing the subsystem to attain the thermal equilibrium with the heat bath. For simplicity we consider here the two-dimensional collective reduced phase space.

The system of Heisenberg equations of motion for the variables q and p and the bath phonon operators b_ν and $b_\nu^\dagger$ is obtained by commuting them with H:

$$\dot{q} = \frac{i}{\hbar}[H,q] = \frac{1}{2}\{\mu^{-1}(q),p\}_+ + i\sum_\nu G'_{\nu,p}(q,p)(b_\nu^\dagger - b_\nu),$$

$$\dot{p} = \frac{i}{\hbar}[H,p] = -H'_{c,q}(q,p) - \sum_\nu V'_{\nu,q}(q)(b_\nu^\dagger + b_\nu) - i\sum_\nu G'_{\nu,q}(q,p)(b_\nu^\dagger - b_\nu), \quad (2)$$

$$\dot{b}_\nu^\dagger = \frac{i}{\hbar}[H,b_\nu^\dagger] = i\omega_\nu b_\nu^\dagger + \frac{1}{\hbar}[iV_\nu(q) + G_\nu(q,p)],$$

$$\dot{b}_\nu = \frac{i}{\hbar}[H,b_\nu] = -i\omega_\nu b_\nu + \frac{1}{\hbar}[-iV_\nu(q) + G_\nu(q,p)]. \quad (3)$$

Here, we use the following notation: $\widetilde{H}'_{c,q}(q,p) = \partial\widetilde{H}_c(q,p)/\partial q$, $V'_{\nu,q}(t)=\partial V_\nu(q(t))/\partial q$, and $G'_{\nu,p}(t) = \partial G_\nu(q(t),p(t))/\partial p$. The solutions of Eqs. (3) are

$$b_\nu^\dagger(t) + b_\nu(t) = f_\nu^\dagger(t) + f_\nu(t) - \frac{2V_\nu(q)}{\hbar\omega_\nu} - \frac{i}{\omega_\nu}\int_0^t d\tau[\dot{\Phi}^\dagger(\tau)e^{i\omega_\nu(t-\tau)} - \dot{\Phi}(\tau)e^{-i\omega_\nu(t-\tau)}],$$

$$b_\nu^\dagger(t) - b_\nu(t) = f_\nu^\dagger(t) - f_\nu(t) + \frac{2iG_\nu(q,p)}{\hbar\omega_\nu} - \frac{i}{\omega_\nu}\int_0^t d\tau[\dot{\Phi}^\dagger(\tau)e^{i\omega_\nu(t-\tau)} + \dot{\Phi}(\tau)e^{-i\omega_\nu(t-\tau)}], \quad (4)$$

where

$$f_\nu(t) = \left[b_\nu(0) + \frac{i}{\omega_\nu}\Phi(0)\right]e^{-i\omega_\nu t},$$

$$\Phi(t) = \frac{1}{\hbar}[-iV_\nu(q(t)) + G_\nu(q(t),p(t))].$$

If we substitute Eqs. (4) into Eqs. (2) and, respectively, eliminate the bath variables from the equations of motion of the collective subsystem, we obtain a set of nonlinear integro-differential stochastic dissipative equations

$$\dot{q} = \frac{1}{2}\{\widetilde{\mu}^{-1}(q),p\}_+ - \frac{1}{2}\int_0^t d\tau\{K_{GV}(t,\tau),\dot{q}(\tau)\}_+ + \frac{1}{2}\int_0^t d\tau\{K_{GG}(t,\tau),\dot{p}(\tau)\}_+ + F_q(t),$$

$$\dot{p} = -\widetilde{H}'_{c,q}(q,p) - \frac{1}{2}\int_0^t d\tau\{K_{VV}(t,\tau),\dot{q}(\tau)\}_+ + \frac{1}{2}\int_0^t d\tau\{K_{VG}(t,\tau),\dot{p}(\tau)\}_+ + F_p(t). \quad (5)$$

To obtain Eqs. (5), we disregard the terms of the second order in $\hbar$: $[[G'_{\nu,p}(t),\dot{q}(t')],V'_{\nu,q}(t')]$, $[[G'_{\nu,q}(t),\dot{q}(t')],V'_{\nu,q}(t')]$, $[[G'_{\nu,q}(t),\dot{q}(t')],G'_{\nu,q}(t')]$, $[[G'_{\nu,p}(t),\dot{q}(t')],G'_{\nu,q}(t')]$, $[[G'_{\nu,p}(t),\dot{p}(t')],G'_{\nu,p}(t')]$, and $[[G'_{\nu,q}(t),\dot{p}(t')],G'_{\nu,p}(t')]$. This assumption, which is equivalent to the trancation of the cumulant expansion after the second order, allows us to consider only the dissipations which are propotional to dq/dt (linear dissipation) and dp/dt. In the literature the linear dissipation is mainly discussed [1–8]. In the case of linear coupling in the momentum (G_ν are linear functions of p) and arbitrary coupling in the coordinate (V_ν are complicated functions of q), Eqs. (5) would be exact.

The collective Hamiltonian for the variables q and p in Eqs. (5) is

$$\widetilde{H}_c(q,p) = p\frac{1}{2\widetilde{\mu}(q)}p + \widetilde{U}(q,p),$$

with the renormalized mass parameter

$$\widetilde{\mu}^{-1}(q(t)) = \mu^{-1}(q(t)) - 2\sum_\nu \frac{[G'_{\nu,p}(t)]^2}{\hbar\omega_\nu}$$

and the potential energy

$$\tilde{U}(q(t)) = U(q(t)) - \sum_\nu \frac{[V_\nu(q(t))]^2}{\hbar\omega_\nu}.$$

The dissipative coefficients in Eqs. (5) are recognized as the terms which are proportional to the operators $\dot{q}$ and $\dot{p}$ [9]. Thus, the dissipative kernels are

$$K_{GV}(t,\tau) = \sum_\nu \frac{1}{\hbar\omega_\nu}(\{G'_{\nu,p}(t),V'_{\nu,q}(\tau)\}_+\sin(\omega_\nu[t-\tau]) - \{G'_{\nu,p}(t),G'_{\nu,q}(\tau)\}_+\cos(\omega_\nu[t-\tau])),$$

$$K_{VG}(t,\tau) = -\sum_\nu \frac{1}{\hbar\omega_\nu}(\{G'_{\nu,q}(t),G'_{\nu,p}(\tau)\}_+\cos(\omega_\nu[t-\tau]) + \{V'_{\nu,q}(t),G'_{\nu,p}(\tau)\}_+\sin(\omega_\nu[t-\tau])),$$

$$K_{VV}(t,\tau) = \sum_\nu \frac{1}{\hbar\omega_\nu}([\{V'_{\nu,q}(t),V'_{\nu,q}(\tau)\}_+ + \{G'_{\nu,q}(t),G'_{\nu,q}(\tau)\}_+] \times \cos(\omega_\nu[t-\tau]) + [\{V'_{\nu,q}(t),G'_{\nu,q}(\tau)\}_+ - \{G'_{\nu,q}(t),V'_{\nu,q}(\tau)\}_+]\sin(\omega_\nu[t-\tau])),$$

$$K_{GG}(t,\tau) = \sum_\nu \frac{1}{\hbar\omega_\nu}\{G'_{\nu,p}(t),G'_{\nu,p}(\tau)\}_+\cos(\omega_\nu[t-\tau]). \quad (6)$$

Since these kernels do not contain the phonon occupation numbers, they are independent of the temperature T of the heat bath. The temperature and fluctuations enter in the analysis through the specification of the distribution of the initial conditions. In Eqs. (5) the operators of random forces in the coordinate and momentum,

$$F_q(t) = \sum_\nu F_q^\nu(t) = i\sum_\nu G'_{\nu,p}(t)[f_\nu^\dagger(t) - f_\nu(t)],$$

$$F_p(t) = \sum_\nu F_p^\nu(t) = -\sum_\nu V'_{\nu,q}(t)[f_\nu^\dagger(t) + f_\nu(t)] - i\sum_\nu G'_{\nu,q}(t) \times[f_\nu^\dagger(t) - f_\nu(t)], \quad (7)$$

play the role of random forces in the coordinate and momentum and depend on $q(t)$ and $p(t)$ and on the initial conditions for the operators. Following the usual procedure of statistical mechanics, we identify the operators $F_q^\nu(t)$ and $F_p^\nu(t)$ as fluctuations because of the uncertainty in the initial conditions for the bath operators. To specify the statistical properties of the fluctuations, we consider an ensemble of initial states in which the operators of the collective subsystem are fixed at values $q(0)$ and $p(0)$ and the initial bath operators are drawn from an ensemble which is canonical with respect to the collective subsystem [9]. The initial distribution is then the conditional density matrix $\rho_0(\{b_\nu^\dagger, b_\nu\}|q(0),p(0)) = \exp[-\sum_\nu \hbar\omega_\nu(b_\nu^\dagger - i\Phi^*/\omega_\nu)(b_\nu + i\Phi/\omega_\nu)/T]/Z(T)$, where $Z(T)$ is conditional partition function. In this ensemble the fluctuations $F_q^\nu(t)$ and $F_p^\nu(t)$ are distributed as Gaussians and have zero average values

$$\langle\langle F_q^\nu(t)\rangle\rangle = \langle\langle F_p^\nu(t)\rangle\rangle = 0, \quad (8)$$

and nonzero second moments. Here, the symbol $\langle\langle\cdots\rangle\rangle$ denotes the average over the bath. The Gaussian nature of the random forces is endorsed in the case when the bath is treated as a set of harmonic oscillators or when the interaction is the cumulative effect of a large number of weak interactions where a central-limit theorem can be applied [1,3,7]. In order to calculate the correlation functions of the fluctuations, we use the Bose-Einstein statistics of the bath:

$$\langle\langle f_\nu^\dagger(t) f_{\nu'}^\dagger(t')\rangle\rangle = \langle\langle f_\nu(t) f_{\nu'}(t')\rangle\rangle = 0,$$

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

$$\langle\langle f_\nu(t) f_{\nu'}^\dagger(t')\rangle\rangle = \delta_{\nu,\nu'}(n_\nu+1)e^{-i\omega_\nu(t-t')}, \quad (9)$$

with occupation numbers for phonons depending on temperature T: $n_\nu = [\exp(\hbar\omega_\nu/T)-1]^{-1}$.

Thus, we have obtained a set of generalized nonlinear quantum Langevin equations (5). The presence of the integral parts in these equations indicates the non-Markovian character of the system. As one can see, the dissipative kernels have the form of a memory functions, since they make the equations of motion at time t dependent on the values of $\dot{q}$ and $\dot{p}$ for previous times. If kernels are rapidly decaying functions, Eqs. (5) have a short memory. It should be noted also that for the reduced system the velocity is not necessary to be proportional to the momentum. Equations (5) can be solved numerically in the general case.

In Refs. [7,9] the quantum Langevin equations were derived for a linear-in-q system-bath coupling. In Ref. [9] the collective potential was a harmonic oscillator. The equations of motion (5) were obtained for more general collective Hamiltonian (arbitrary coordinate-dependent mass parameter and more complicated potential) and coupling between collective system and thermal bath. The consequences of this fact is that the Eqs. (5) contain additional random forces F_q and dissipative kernels K_{VG}, K_{GV}, and K_{GG}. As will be shown, these terms are responsible for the appearance of additional friction and diffusion coefficients λ_q and D_{qq}. In contrast to Refs. [7,9], the dissipation and random forces are functions of the coordinate and momentum in our case. The interaction between the bath and collective system renormalizes the potential energy as well as the mass parameter. Equations (5) can be applied to the systems coupled linearly in p and arbitrary in q with the bath.

B. Fluctuation-dissipation relations for general coupling

The fluctuation-dissipation relations are the relations between the dissipation of a collective subsystem and the fluctuations of random forces. Those relations express the nonequilibrium behavior of the system in terms of equilibrium or quasiequilibrium characteristics. They ensure that the system approaches the state of equilibrium. Using the properties (8) and (9) of random forces (7) and neglecting terms of $O(\hbar)$ [this is consistent with the fact that the double commutator terms in Eqs. (5) are disregarded], we get the following symmetrized correlation functions $(k,k'=q,p)\,\phi^{\nu}_{kk'}(t,t')=\langle\langle F^{\nu}_{k}(t)F^{\nu}_{k'}(t')+F^{\nu}_{k'}(t')F^{\nu}_{k}(t)\rangle\rangle$:

$$\phi^{\nu}_{qp}(t,t')=[2n_\nu+1](-\{G'_{\nu,p}(t),G'_{\nu,q}(t')\}_{+}\cos(\omega_\nu[t-t'])+\{G'_{\nu,p}(t),V'_{\nu,q}(t')\}_{+}\sin(\omega_\nu[t-t'])),$$

$$\phi^{\nu}_{pq}(t,t')=-[2n_\nu+1](\{G'_{\nu,q}(t),G'_{\nu,p}(t')\}_{+}\cos(\omega_\nu[t-t'])+\{V'_{\nu,q}(t),G'_{\nu,p}(t')\}_{+}\sin(\omega_\nu[t-t'])),$$

$$\phi^{\nu}_{pp}(t,t')=[2n_\nu+1]([\{V'_{\nu,q}(t),V'_{\nu,q}(t')\}_{+}+\{G'_{\nu,q}(t),G'_{\nu,q}(t')\}_{+}]\cos(\omega_\nu[t-t'])+[\{V'_{\nu,q}(t),G'_{\nu,q}(t')\}_{+}-\{G'_{\nu,q}(t),V'_{\nu,q}(t')\}_{+}]\times\sin(\omega_\nu[t-t'])),$$

$$\phi^{\nu}_{qq}(t,t')=[2n_\nu+1]\{G'_{\nu,p}(t),G'_{\nu,p}(t')\}_{+}\cos(\omega_\nu[t-t']). \tag{10}$$

The disregarded terms would lead to relations between them in addition to Eqs. (10). Using Eqs. (6) and (10) and taking into consideration that $2n_\nu+1=\coth[\hbar\omega_\nu/(2T)]$, we obtain the quantum fluctuation-dissipation relations

$$\sum_\nu \phi^{\nu}_{qp}(t,t')\frac{\tanh[\hbar\omega_\nu/(2T)]}{\hbar\omega_\nu}=K_{GV}(t,t'), \tag{11}$$

$$\sum_\nu \phi^{\nu}_{pq}(t,t')\frac{\tanh[\hbar\omega_\nu/(2T)]}{\hbar\omega_\nu}=K_{VG}(t,t'). \tag{12}$$

$$\sum_\nu \phi^{\nu}_{pp}(t,t')\frac{\tanh[\hbar\omega_\nu/(2T)]}{\hbar\omega_\nu}=K_{VV}(t,t'), \tag{13}$$

$$\sum_\nu \phi^{\nu}_{qq}(t,t')\frac{\tanh[\hbar\omega_\nu/(2T)]}{\hbar\omega_\nu}=K_{GG}(t,t'). \tag{14}$$

The validity of the fluctuation-dissipation relations means that we have properly identified the dissipative terms in the non-Markovian dynamical equations of motion. Quantum fluctuation-dissipations relations of a similar form have been obtained before in Ref. [9] and references therein for the simple cases of FC and RWA oscillators. We generalized the quantum fluctuation-dissipation theorem for the case of a more general form of H_{cb}. The quantum fluctuation-dissipation relations differ from the classical ones and are reduced to them in the limit of high temperature T (or $\hbar\to 0$):

$$\sum_\nu \phi^{\nu}_{qp}(t,t')=2TK_{GV}(t,t'),$$

$$\sum_\nu \phi^{\nu}_{pq}(t,t')=2TK_{VG}(t,t'),$$

$$\sum_\nu \phi^{\nu}_{pp}(t,t')=2TK_{VV}(t,t'),$$

$$\sum_\nu \phi^{\nu}_{qq}(t,t')=2TK_{GG}(t,t'). \tag{15}$$

These classical realations contain only the thermal fluctuations. Our formalism naturally leads to the generalization of classical fluctuation-dissipation relation by including the quantum fluctuations in addition to the thermal fluctuations. Since Eqs. (5) and, following from them, the equations of motion for the collective coordinate and momentum are consistent with the fluctuation-dissipation relations, our formalism provides a basis for describing the quantum statistical effects of collective motion.

C. Derivation of nonstationary transport coefficients for the harmonic oscillator

Assuming in Eqs. (5) the functionals $\tilde{\mu}$, $V'_{\nu,q}$, $G'_{\nu,q}$, and $G'_{\nu,p}$ weakly dependent on p and q in the considered interval of t and replacing them by their average values, we can obtain a set of generalized non-Markovian equations which can be solved analytically. Approximating locally the renormalized potential by a harmonic oscillator, $\tilde{U}=\tilde{\delta}q^2/2$, and applying the Laplace transformation $\mathcal{L}$ to Eqs. (5), we obtain the following set of linear equations for the transforms:

$$q(s)\{s[1+K_{GV}(s)]\}-p(s)[1/\tilde{\mu}+sK_{GG}(s)]=q(0)[1+K_{GV}(s)]-p(0)K_{GG}(s)+F_q(s),$$

$$q(s)[\tilde{\delta}+sK_{VV}(s)]+p(s)s[1-K_{VG}(s)]=q(0)K_{VV}(s)+p(0)[1-K_{VG}(s)]+F_p(s). \tag{16}$$

For the solution of this system of equations, one should find the roots s_i of its determinant:

$$d(s)\equiv s^2[1+K_{GV}(s)][1-K_{VG}(s)]+[\tilde{\delta}+sK_{VV}(s)]\times[1/\tilde{\mu}+sK_{GG}(s)]=0. \tag{17}$$

The explicit solutions for the originals are

$$q(t)=A_tq(0)+B_tp(0)+\int_0^t d\tau[C_\tau F_q(t-\tau)+\tilde{C}_\tau F_p(t-\tau)],$$

$$p(t)=M_tq(0)+N_tp(0)+\int_0^t d\tau[L_\tau F_p(t-\tau)+\tilde{L}_\tau F_q(t-\tau)], \tag{18}$$

where the time-dependent coefficients are denoted as follows:

$$A_t = \mathcal{L}^{-1}\left[\frac{s[1+K_{GV}(s)][1-K_{VG}(s)]+[1/\tilde{\mu}+sK_{GG}(s)]K_{VV}(s)}{d(s)}\right],$$

$$N_t = \mathcal{L}^{-1}\left[\frac{s[1-K_{VG}(s)][1+K_{GV}(s)]+[\tilde{\delta}+sK_{VV}(s)]K_{GG}(s)}{d(s)}\right],$$

$$B_t = \mathcal{L}^{-1}\left[\frac{\tilde{\mu}^{-1}[1-K_{VG}(s)]}{d(s)}\right], \quad M_t = -\mathcal{L}^{-1}\left[\frac{\tilde{\delta}[1+K_{GV}(s)]}{d(s)}\right], \quad C_t = \mathcal{L}^{-1}\left[\frac{s[1-K_{VG}(s)]}{d(s)}\right],$$

$$L_t = \mathcal{L}^{-1}\left[\frac{s[1+K_{GV}(s)]}{d(s)}\right], \quad \tilde{C}_t = \mathcal{L}^{-1}\left[\frac{1/\tilde{\mu}+sK_{GG}(s)}{d(s)}\right], \quad \tilde{L}_t = -\mathcal{L}^{-1}\left[\frac{\tilde{\delta}+sK_{VV}(s)}{d(s)}\right].$$

Here, $\mathcal{L}^{-1}$ denotes the inverse Laplace transformation and $K_{VV}(s)$, $K_{GG}(s)$, $K_{GV}(s)$, and $K_{VG}(s)$ are the Laplace transforms of the dissipative kernels. The subscripts t and τ denote the time dependence. The exact solutions $q(t)$ and $p(t)$ in terms of roots s_i can be given by the residue theorem.

Using the time dependence of q and p, we obtain the values $\langle q(t)\rangle$ and $\langle p(t)\rangle$ averaged over the whole system,

$$\langle q(t)\rangle = A_t\langle q(0)\rangle + B_t\langle p(0)\rangle,$$

$$\langle p(t)\rangle = M_t\langle q(0)\rangle + N_t\langle p(0)\rangle, \tag{19}$$

and correlation functions $\sigma_{q_tq_{t'}}=\langle q(t)q(t')\rangle$, $\sigma_{p_tp_{t'}}=\langle p(t)p(t')\rangle$, $\sigma_{q_tp_{t'}}=\langle q(t)p(t')\rangle$, and $\sigma_{p_tq_{t'}}=\langle p(t)q(t')\rangle$:

$$\sigma_{q_tq_{t'}} = A_tA_{t'}\sigma_{q_0q_0} + B_tB_{t'}\sigma_{p_0p_0} + A_tB_{t'}\sigma_{q_0p_0} + B_tA_{t'}\sigma_{p_0q_0} + J_{q_tq_{t'}},$$

$$\sigma_{p_tp_{t'}} = M_tM_{t'}\sigma_{q_0q_0} + N_tN_{t'}\sigma_{p_0p_0} + M_tN_{t'}\sigma_{q_0p_0} + N_tM_{t'}\sigma_{p_0q_0} + J_{p_tp_{t'}},$$

$$\sigma_{q_tp_{t'}} = A_tM_{t'}\sigma_{q_0q_0} + B_tN_{t'}\sigma_{p_0p_0} + A_tN_{t'}\sigma_{q_0p_0} + B_tM_{t'}\sigma_{p_0q_0} + J_{q_tp_{t'}},$$

$$\sigma_{p_tq_{t'}} = M_tA_{t'}\sigma_{q_0q_0} + N_tB_{t'}\sigma_{p_0p_0} + N_tA_{t'}\sigma_{p_0q_0} + M_tB_{t'}\sigma_{q_0p_0} + J_{p_tq_{t'}}, \tag{20}$$

where

$$J_{q_tq_{t'}} = \int_0^t\int_0^{t'} d\tau d\tau'[C_\tau C_{\tau'}I_{qq}(t-\tau,t'-\tau') + C_\tau\tilde{C}_{\tau'}I_{qp}(t-\tau,t'-\tau') + \tilde{C}_\tau C_{\tau'}I_{pq}(t-\tau,t'-\tau') + \tilde{C}_\tau\tilde{C}_{\tau'}I_{pp}(t-\tau,t'-\tau')],$$

$$J_{p_tp_{t'}} = \int_0^t\int_0^{t'} d\tau d\tau'[L_\tau L_{\tau'}I_{pp}(t-\tau,t'-\tau') + L_\tau\tilde{L}_{\tau'}I_{pq}(t-\tau,t'-\tau') + \tilde{L}_\tau L_{\tau'}I_{qp}(t-\tau,t'-\tau') + \tilde{L}_\tau\tilde{L}_{\tau'}I_{qq}(t-\tau,t'-\tau')],$$

$$J_{q_tp_{t'}} = \int_0^t\int_0^{t'} d\tau d\tau'[C_\tau L_{\tau'}I_{qp}(t-\tau,t'-\tau') + \tilde{C}_\tau L_{\tau'}I_{pp}(t-\tau,t'-\tau') + \tilde{C}_\tau\tilde{L}_{\tau'}I_{pq}(t-\tau,t'-\tau') + C_\tau\tilde{L}_{\tau'}I_{qq}(t-\tau,t'-\tau')],$$

$$J_{p_tq_{t'}} = \int_0^t\int_0^{t'} d\tau d\tau'[L_\tau C_{\tau'}I_{pq}(t-\tau,t'-\tau') + \tilde{L}_\tau C_{\tau'}I_{qq}(t-\tau,t'-\tau') + \tilde{L}_\tau\tilde{C}_{\tau'}I_{qp}(t-\tau,t'-\tau') + L_\tau\tilde{C}_{\tau'}I_{pp}(t-\tau,t'-\tau')]. \tag{21}$$

The symbol $\langle\cdots\rangle$ in $I_{qq}(t,\tau)=\langle F_q(t)F_q(\tau)\rangle$, $I_{pp}(t,\tau)=\langle F_p(t)F_p(\tau)\rangle$, $I_{pq}(t,\tau)=\langle F_p(t)F_q(\tau)\rangle$, and $I_{qp}(t,\tau)=\langle F_q(t)F_p(\tau)\rangle$ means an average over the whole system.

In order to determine the friction and diffusion coefficients, we consider the equations for the first and second moments, and correlation functions. Making derivative in t

of Eqs. (19) and (20) and simple but tedious algebra, we obtain the following equations:

$$\frac{d}{dt}\langle q(t)\rangle = -\lambda_q(t)\langle q(t)\rangle + \frac{1}{m(t)}\langle p(t)\rangle,$$

$$\frac{d}{dt}\langle p(t)\rangle = -\xi(t)\langle q(t)\rangle - \lambda_p(t)\langle p(t)\rangle \quad (22)$$

and

$$\frac{d}{dt}\sigma_{q_tq_{t'}} = -\lambda_q(t)\sigma_{q_tq_{t'}} + \frac{1}{m(t)}\sigma_{p_tq_{t'}} + D_{q_tq_{t'}},$$

$$\frac{d}{dt}\sigma_{p_tp_{t'}} = -\lambda_p(t)\sigma_{p_tp_{t'}} - \xi(t)\sigma_{q_tp_{t'}} + D_{p_tp_{t'}},$$

$$\frac{d}{dt}\sigma_{q_tp_{t'}} = -\lambda_q(t)\sigma_{q_tp_{t'}} + \frac{1}{m(t)}\sigma_{p_tp_{t'}} + D_{q_tp_{t'}},$$

$$\frac{d}{dt}\sigma_{p_tq_{t'}} = -\lambda_p(t)\sigma_{p_tq_{t'}} - \xi(t)\sigma_{q_tq_{t'}} + D_{p_tq_{t'}}, \quad (23)$$

where

$$\lambda_q(t) = \frac{\dot{A}_tN_t - \dot{B}_tM_t}{B_tM_t - A_tN_t}, \quad (24)$$

$$\lambda_p(t) = \frac{A_t\dot{N}_t - B_t\dot{M}_t}{B_tM_t - A_tN_t}, \quad (25)$$

$$1/m(t) = \frac{\dot{A}_tB_t - \dot{B}_tA_t}{B_tM_t - A_tN_t}, \quad (26)$$

$$\xi(t) = \frac{\dot{M}_tN_t - \dot{N}_tM_t}{B_tM_t - A_tN_t}, \quad (27)$$

$$D_{q_tq_{t'}} = \lambda_q(t)J_{q_tq_{t'}} - \frac{1}{m(t)}J_{p_tq_{t'}} + \frac{dJ_{q_tq_{t'}}}{dt}, \quad (28)$$

$$D_{p_tp_{t'}} = \lambda_p(t)J_{p_tp_{t'}} + \xi(t)J_{q_tp_{t'}} + \frac{dJ_{p_tp_{t'}}}{dt}, \quad (29)$$

$$D_{q_tp_{t'}} = \lambda_q(t)J_{q_tp_{t'}} - \frac{1}{m(t)}J_{p_tp_{t'}} + \frac{dJ_{q_tp_{t'}}}{dt}, \quad (30)$$

$$D_{p_tq_{t'}} = \lambda_p(t)J_{p_tq_{t'}} + \xi(t)J_{q_tq_{t'}} + \frac{dJ_{p_tq_{t'}}}{dt}. \quad (31)$$

Here, $m(t)$ depends on $\tilde{\mu}$ through Eq. (26) and an overdot means time derivative.

The Onsager's regression hypothesis states that the regression of fluctuations is governed by macroscopical equations describing the approach to equilibrium [3,6]. One can derive from Eqs. (22) and (23) the equations

$$\frac{d^2}{dt^2}\langle q(t)\rangle + \left[\lambda_p(t) + \lambda_q(t) + \frac{\dot{m}(t)}{m(t)}\right]\frac{d}{dt}\langle q(t)\rangle + \left[\frac{\xi(t)}{m(t)} + \lambda_p(t)\lambda_q(t) + \dot{\lambda}_q(t) + \lambda_q(t)\frac{\dot{m}(t)}{m(t)}\right]\langle q(t)\rangle = 0,$$

$$\frac{d^2}{dt^2}\sigma_{q_tq_{t'}} + \left[\lambda_p(t) + \lambda_q(t) + \frac{\dot{m}(t)}{m(t)}\right]\frac{d}{dt}\sigma_{q_tq_{t'}} + \left[\frac{\xi(t)}{m(t)} + \lambda_p(t)\lambda_q(t) + \dot{\lambda}_q(t) + \lambda_q(t)\frac{\dot{m}(t)}{m(t)}\right]\sigma_{q_tq_{t'}} - \left[\frac{\dot{m}(t)}{m(t)} + \lambda_p(t)\right]D_{q_tq_{t'}} - \frac{1}{m(t)}D_{p_tq_{t'}} - \frac{d}{dt}D_{q_tq_{t'}} = 0.$$

The last equation can be rewritten as

$$\frac{d^2}{dt^2}\tilde{\sigma}_{q_tq_{t'}} + \left[\lambda_p(t) + \lambda_q(t) + \frac{\dot{m}(t)}{m(t)}\right]\frac{d}{dt}\tilde{\sigma}_{q_tq_{t'}} + \left[\frac{\xi(t)}{m(t)} + \lambda_p(t)\lambda_q(t) + \dot{\lambda}_q(t) + \lambda_q(t)\frac{\dot{m}(t)}{m(t)}\right]\tilde{\sigma}_{q_tq_{t'}} = 0,$$

where $\tilde{\sigma}_{q_tq_{t'}} = \sigma_{q_tq_{t'}} - J_{q_tq_{t'}}$. Due to the nonzero coefficients $D_{k_tl_{t'}}$ ($k,l=q$ and p) (or $J_{q_tq_{t'}}$), the equations for the correlations are not identical to the equations for the average values and the Onsager's regression hypothesis does not hold exactly for the non-Markovian dynamics of the damped harmonic oscillator. In particular case of $t'=0$ from Eqs. (21) and (28)–(31) we obtain $D_{k_tl_{t'}}=0$ and $J_{q_tq_{t'}}=0$, which means that the Onsager principle is valid the whole time, $t>0$. In Ref. [19] the validity of the Onsager principle was demonstrated at the same condition, $t'=0$.

When we set $t=t'$ in Eqs. (23), we obtain the equations for the variances in the coordinate $\sigma_{qq}(t)=\langle q^2(t)\rangle-\langle q(t)\rangle^2 =\sigma_{q_tq_t}-\langle q(t)\rangle^2$ and in the momentum $\sigma_{pp}(t)=\langle p^2(t)\rangle -\langle p(t)\rangle^2=\sigma_{p_tp_t}-\langle p(t)\rangle^2$, and the one for the mixed variance $\sigma_{qp}(t)=\frac{1}{2}\langle p(t)q(t)+q(t)p(t)\rangle-\langle p(t)\rangle\langle q(t)\rangle=\frac{1}{2}(\sigma_{q_tp_t} +\sigma_{p_tq_t})-\langle p(t)\rangle\langle q(t)\rangle$:

$$\dot{\sigma}_{qq}(t) = -2\lambda_q(t)\sigma_{qq}(t) + \frac{2}{m(t)}\sigma_{qp}(t) + 2D_{qq}(t),$$

$$\dot{\sigma}_{pp}(t) = -2\lambda_p(t)\sigma_{pp}(t) - 2\xi(t)\sigma_{qp}(t) + 2D_{pp}(t),$$

$$\dot{\sigma}_{qp}(t) = -[\lambda_p(t) + \lambda_q(t)]\sigma_{qp}(t) - \xi(t)\sigma_{qq}(t) + \frac{1}{m(t)}\sigma_{pp}(t) + 2D_{qp}(t). \quad (32)$$

From the structure of Eqs. (22) and (32) it is seen that the dynamics of system is determined by the nonstationary friction coefficients $\lambda_q(t)$ in the coordinate and $\lambda_p(t)$ in the momentum, inverse mass parameter $1/m(t)$, stiffness coefficient $\xi(t)$, and diffusion coefficients in the coordinate,

$$D_{qq}(t) = \lambda_q(t)J_{q_tq_t} - \frac{1}{2m(t)}(J_{q_tp_t} + J_{p_tq_t}) + \frac{1}{2}\dot{J}_{q_tq_t}, \quad (33)$$

and in the momentum,

$$D_{pp}(t) = \lambda_p(t)J_{p_tp_t} + \frac{\xi(t)}{2}(J_{q_tp_t} + J_{p_tq_t}) + \frac{1}{2}\dot{J}_{p_tp_t}, \quad (34)$$

and the mixed diffusion coefficient:

$$D_{qp}(t) = \frac{1}{2}\left[\frac{\lambda_p(t) + \lambda_p(t)}{2}(J_{q_tp_t} + J_{p_tq_t}) + \xi(t)J_{q_tq_t} - \frac{1}{m(t)}J_{p_tp_t} + \frac{1}{2}(\dot{J}_{q_tp_t} + \dot{J}_{p_tq_t})\right]. \quad (35)$$

Therefore, we have obtained the Markovian-type (local in time) equations for the first and second moments, but with a general form of transport coefficients which explicitly depend on time. It can be shown that the appropriate microcanonical equilibrium distribution is achieved in the course of the time evolution. At $t\to\infty$ the system reaches the equilibrium state ($\dot{\sigma}_{pp}=\dot{\sigma}_{qq}=\dot{\sigma}_{qp}=0$) and the asymptotic diffusion coefficients can be derived from Eq. (32):

$$D_{qq}(\infty) = \lambda_q(\infty)\sigma_{qq}(\infty) - \frac{1}{m(\infty)}\sigma_{qp}(\infty),$$

$$D_{pp}(\infty) = \lambda_p(\infty)\sigma_{pp}(\infty) + \xi(\infty)\sigma_{qp}(\infty),$$

$$D_{qp}(\infty) = \frac{1}{2}\left[[\lambda_p(\infty) + \lambda_q(\infty)]\sigma_{qp}(\infty) + \xi(\infty)\sigma_{qq}(\infty) - \frac{1}{m(\infty)}\sigma_{pp}(\infty)\right]. \quad (36)$$

Comparing Eqs. (33)–(36), we obtain that $\sigma_{qq}(\infty)=J_{q_\infty q_\infty}$, $\sigma_{pp}(\infty)=J_{p_\infty p_\infty}$, and $\sigma_{qp}(\infty)=\frac{1}{2}(J_{q_\infty p_\infty}+J_{p_\infty q_\infty})$. If $\sigma_{qp}(\infty)=0$ in Eqs. (36), then the asymptotic diffusion and friction coefficients are connected by the well-known fluctuation-dissipation relations

$$D_{qq}(\infty) = \lambda_q(\infty)\sigma_{qq}(\infty),$$

$$D_{pp}(\infty) = \lambda_p(\infty)\sigma_{pp}(\infty),$$

connecting diffusion and damping constants.

It is strightforward to show that the energy of the system,

$$E(t) = \langle\tilde{H}_c(t)\rangle = \frac{\sigma_{pp}(t) + \langle p(t)\rangle^2}{2m(t)} + \xi(t)\frac{\sigma_{qq}(t) + \langle q(t)\rangle^2}{2},$$

is changed in accordance with the equation

$$\dot{E}(t) = -\left[2\lambda_p(t) + \frac{\dot{m}(t)}{m(t)}\right]\frac{\sigma_{pp}(t) + \langle p(t)\rangle^2}{2m(t)} - [2\lambda_q(t)\xi(t) + \dot{\xi}(t)]\frac{\sigma_{qq}(t) + \langle q(t)\rangle^2}{2} + \frac{D_{pp}(t)}{m(t)} + \xi(t)D_{qq}(t).$$

One can see from these equations that for the harmonic oscillator dissipation rate increases with $\lambda_q(t)$ and $\lambda_p(t)$ but decreases with increasing $D_{pp}(t)$ and $D_{qq}(t)$. For the case of inverted oscillators, $\xi<0$, the friction in coordinate $\lambda_q(t)$ increases E but diffusion coefficient in coordinate $D_{qq}(t)$ decreases it.

Only the diffusion coefficient D_{pp} in momentum is often used in applications. The other diffusion coefficients D_{qq} and D_{pq} in the coordinate and mixed in the coordinate and momentum are assumed to be zero. It was shown in Refs. [20,21] that the tunneling through a potential barrier, decay of a metastable state, and decoherence depends crucially on the transport coefficients. With the diffusion coefficient in the coordinate the decoherence increases slower than in the case with $D_{qq}=0$. The penetrability of a barrier is larger in the case of $D_{qq}\neq 0$ due to a stronger coherence between different states.

D. Relationship with the Lindblad theory

The equations of motion (22) and (32) for the expectation values and variances of the collective coordinate and momentum can be also obtained from the following master equation for the reduced density matrix $\rho(t)$:

$$\dot{\rho} = -\frac{i}{\hbar}[\tilde{H}_c,\rho] + \frac{i\lambda_q(t)}{2\hbar}[p,\{q,\rho\}_+] - \frac{i\lambda_p(t)}{2\hbar}[q,\{p,\rho\}_+] - \frac{D_{qq}(t)}{\hbar^2}[p,[p,\rho]] - \frac{D_{pp}(t)}{\hbar^2}[q,[q,\rho]] + \frac{D_{qp}(t)}{\hbar^2}([p,[q,\rho]] + [q,[p,\rho]]) \quad (37)$$

or from the following Fokker-Planck-type equation for the Wigner reduced phase-space distribution function $W(q,p,t)$:

$$\dot{W} = -\frac{p}{m(t)}\frac{\partial W}{\partial q} + \xi(t)q\frac{\partial W}{\partial p} + \lambda_p(t)\frac{\partial(pW)}{\partial p} + \lambda_q(t)\frac{\partial(qW)}{\partial q} + D_{qq}(t)\frac{\partial^2 W}{\partial q^2} + D_{pp}(t)\frac{\partial^2 W}{\partial p^2} + 2D_{qp}(t)\frac{\partial^2 W}{\partial q\partial p}. \quad (38)$$

Here, for the general coupling we assume again that the friction and diffusion coefficients depend on t and on the moments but not on p and q. In the case of linear coupling they depend only on t and this assumption is not necessary. Despite the generally non-Markovian nature of the dynamics of the open system defined by Eqs. (5), the evolution of $\hat{\rho}$ and W is governed by differential equations local in time. The memory effects are encoded in the time-dependent transport coefficients. The general coupling with the environment results in the friction and diffusion coefficients in the coordinate and momentum. This is the consequence of the existence of random forces in the momentum as well as in the coordinate. It is easily seen that Eqs. (37) and (38) are similar in structure to the corresponding Lindbland equations with constant transport coefficients [20–25]. The Lindblad theory describes the Markovian dynamics after the decay of fast transients and establishes the most general form of the generators $\mathcal{L}''$ of dissipative quantum dynamics $\dot{\rho}=\mathcal{L}''\rho$ preserving the positivity of the density operator under certain conditions of the friction and diffusion coefficients. Our Eqs. (37) and (38) are shown to be a generalization of Lindblad-type equations in the case of nonstationary non-Markovian transport coefficients. So our model can be seen as a microscopical justification of the Lindblad theory for open quantum systems.

E. Overdamped limit

If friction in the momentum becomes very large $[\lambda_p(t) \gg \sqrt{\xi(t)/m(t)}]$, the motion becomes overdamped. This motion is marked by equilibrium values for $\langle p(t)\rangle$, $\sigma_{pp}(t)$, and $\sigma_{qp}(t)$—i.e., $(d/dt)\langle p(t)\rangle = \dot{\sigma}_{pp}(t) = \dot{\sigma}_{qp}(t) = 0$. Then, the equations for $\langle q(t)\rangle$ and $\sigma_{qq}(t)$ in Eqs. (22) and (23) are reduced to

$$\frac{d}{dt}\langle q(t)\rangle = v(t) = -\frac{\xi(t) + m(t)\lambda_q(t)\lambda_p(t)}{m(t)\lambda_p(t)}\langle q(t)\rangle,$$

$$\dot{\sigma}_{qq}(t) = -2\frac{\xi(t) + m(t)\lambda_q(t)\lambda_p(t)}{m(t)\lambda_p(t)}\sigma_{qq}(t) + D^{ov}_{qq}(t), \quad (39)$$

where $v(t)$ is the drift coefficient and the diffusion coefficient in the coordinate is

$$D^{ov}_{qq}(t) = 2\left[D_{qq}(t) + \frac{D_{pp}(t) + 2m(t)\lambda_p(t)D_{qp}(t)}{m^2(t)\lambda_p(t)[\lambda_p(t) + \lambda_q(t)]}\right]. \quad (40)$$

In the limit of $\lambda_q(\infty) = D_{qp}(\infty) = D_{qq}(\infty) = 0$ we obtain the well-known relation

$$D^{ov}_{qq}(\infty) = 2D_{pp}(\infty)/[m(\infty)\lambda_p(\infty)]^2.$$

The asymptotic value of the variance is obtained from Eq. (41) as follows:

$$\sigma_{qq}(\infty) = \frac{D_{pp}(\infty) + 2m(\infty)\lambda_p(\infty)D_{qp}(\infty)}{m(\infty)[\lambda_p(\infty) + \lambda_q(\infty)][\xi(\infty) + m(\infty)\lambda_q(\infty)\lambda_p(\infty)]} + \frac{m(\infty)\lambda_p(\infty)D_{qq}(\infty)}{\xi(\infty) + m(\infty)\lambda_q(\infty)\lambda_p(\infty)}. \quad (41)$$

The quantum variance (41) can significantly deviate from the classical one $\sigma^{cl}_{qq}(\infty) = T/\tilde{\delta}$, especially in the case of small T.

Equations (39) are the same as ones obtained from the equation for the position distribution function $P(q,t)$ (here, q is the c number):

$$\dot{P} = -\frac{\partial}{\partial q}[v(t)P] + \frac{1}{2}D^{ov}_{qq}(t)\frac{\partial^2}{\partial q^2}P. \quad (42)$$

This equation is a quantum version of the classical Smoluchowsky equation for the coupling of general form. The quantum Smoluchowsky-type equation was obtained in Ref. [26] by another method for the anharmonic potential and linear coupling in coordinate.

If the transient times of $D^{ov}_{qq}(t)$ and $v(t)$ are equal or smaller than the characteristic time $1/\lambda_p(\infty)$ of equilibrium of the momentum distribution, then it is a good approximation to use the asymptotic quantum diffusion and drift coefficients, $D^{ov}_{qq}(\infty)$ and $v(\infty)$, respectively, in the equations of motion.

III. APPLICATION TO LINEAR COUPLING IN THE COORDINATE AND MOMENTUM WITH A SPECIFIC BATH

For a system with linear coupling, the term H_{cb} of the Hamiltonian H (1) can be written as

$$H_{cb} = q\sum_\nu \alpha_\nu(b^\dagger_\nu + b_\nu) + ip\sum_\nu g_\nu(b^\dagger_\nu - b_\nu), \quad (43)$$

where α_ν and g_ν are real coupling constants. In this case we get a set of Langevin equations (5) where the renormalized collective Hamiltonian $\tilde{H}_c(q,p)$ contains

$$\tilde{\mu}^{-1} = \mu^{-1} - 2\sum_\nu \frac{g^2_\nu}{\hbar\omega_\nu}$$

and

$$\tilde{U}(q) = U(q) - q^2\sum_\nu \frac{\alpha^2_\nu}{\hbar\omega_\nu}.$$

Here, we take μ independent of q. The operators of random forces and dissipative kernels in the equations for $\dot{q}(t)$ and for $\dot{p}(t)$ are

$$F_q(t) = = i\sum_\nu g_\nu[f^\dagger_\nu(t) - f_\nu(t)],$$

$$F_p(t) = = -\sum_\nu \alpha_\nu[f^\dagger_\nu(t) + f_\nu(t)] \quad (44)$$

and

$$K_{GV}(t,\tau) = -K_{VG}(t,\tau) = 2\sum_\nu \frac{\alpha_\nu g_\nu}{\hbar\omega_\nu}\sin(\omega_\nu[t-\tau]),$$

$$K_{GG}(t,\tau) = 2\sum_\nu \frac{g^2_\nu}{\hbar\omega_\nu}\cos(\omega_\nu[t-\tau]),$$

$$K_{VV}(t,\tau) = 2\sum_\nu \frac{\alpha^2_\nu}{\hbar\omega_\nu}\cos(\omega_\nu[t-\tau]). \quad (45)$$

It is convenient to introduce the spectral density $D(\omega_0)$ of the heat bath excitations, which allows us to replace the sum over different oscillators ν by an integral over the frequency: $\sum_\nu \cdots \to \int_0^\infty d\omega_0 D(\omega_0)\cdots$. Let us consider the following spectral functions [9]:

$$D(\omega_0)\frac{|\alpha_\nu|^2}{\hbar\omega_\nu} = \frac{\alpha^2}{\pi}\frac{\gamma^2}{\gamma^2 + \omega_0^2},$$

$$D(\omega_0)\frac{|g_\nu|^2}{\hbar\omega_\nu} = \frac{g^2}{\pi}\frac{\gamma^2}{\gamma^2 + \omega_0^2},$$

$$D(\omega_0)\frac{\alpha_\nu g_\nu}{\hbar\omega_\nu} = \frac{\alpha g}{\pi}\frac{\gamma^2}{\gamma^2 + \omega_0^2}, \quad (46)$$

where the memory time γ^{-1} of the dissipation is inverse to the phonon bandwidth of the heat bath excitations which are coupled with the collective oscillator. This is the Ohmic dissipation with a Lorenzian cutoff (Drude dissipation) [1,3,7]. The relaxation time of the heat bath should be much less than the period of the collective oscillator—i.e., $\gamma \gg \omega$.

Using Eqs. (45) we obtain the dissipative kernels and their Laplace transforms in forms convenient for the further calculations:

$$K_{GV}(t,\tau) = -K_{VG}(t,\tau) = \frac{2\alpha g\gamma^2}{\pi}\int_0^\infty d\omega_0 \frac{\sin(\omega_0[t-\tau])}{\gamma^2+\omega_0^2},$$

$$K_{GV}(s) = -K_{VG}(s) = \frac{\alpha g\gamma^2 \ln(s^2/\gamma^2)}{\pi(s^2-\gamma^2)},$$

$$K_{GG}(t,\tau) = g^2\gamma e^{-\gamma|t-\tau|},$$

$$K_{GG}(s) = \frac{g^2\gamma}{s+\gamma},$$

$$K_{VV}(t,\tau) = \alpha^2\gamma e^{-\gamma|t-\tau|},$$

$$K_{VV}(s) = \frac{\alpha^2\gamma}{s+\gamma}. \quad (47)$$

In the limit of large bandwidth, $\gamma\to\infty$, Eqs. (47) are reduced to

$$K_{GV}(t,\tau) = -K_{VG}(t,\tau) = \frac{2\alpha g}{\pi}\mathrm{P}\left(\frac{1}{t-\tau}\right),$$

$$K_{GG}(t,\tau) = 2g^2\delta(t-\tau),$$

$$K_{VV}(t,\tau) = 2\alpha^2\delta(t-\tau), \quad (48)$$

where P denotes the principal value. The δ-function kernels mean an instantaneous Markovian dissipation.

A. Harmonic oscillator

In the case of a damped quantum oscillator $U(q) = \mu\omega^2q^2/2$ $[\tilde{U}(q)=\tilde{\delta}q^2/2]$ we obtain the solutions (18) for the collective variables where

$$A_t = \sum_{i=1}^4 \beta_i\left\{s_i\left[s_i+\gamma+\frac{g\alpha\gamma^2}{\pi(s_i-\gamma)}\ln\left(\frac{s_i^2}{\gamma^2}\right)\right]^2 + \gamma\alpha^2\left(\frac{s_i+\gamma}{\tilde{\mu}}+g^2\gamma s_i\right)\right\}e^{s_it},$$

$$B_t = \frac{1}{\tilde{\mu}}\sum_{i=1}^4 \beta_i[s_i+\gamma]\left[s_i+\gamma+\frac{g\alpha\gamma^2}{\pi(s_i-\gamma)}\ln\left(\frac{s_i^2}{\gamma^2}\right)\right]e^{s_it},$$

$$M_t = -\tilde{\delta}\tilde{\mu}B_t,$$

$$N_t = \sum_{i=1}^4 \beta_i\left[s_i\left[s_i+\gamma+\frac{g\alpha\gamma^2}{\pi(s_i-\gamma)}\ln\left(\frac{s_i^2}{\gamma^2}\right)\right]^2 + g^2\gamma[\tilde{\delta}(s_i+\gamma) + \alpha^2\gamma s_i]\right]e^{s_it},$$

$$C_t = \sum_{i=1}^4 C_t^i = L_t = \sum_{i=1}^4 L_t^i = \sum_{i=1}^4 \beta_i s_i[s_i+\gamma]\left[s_i+\gamma + \frac{g\alpha\gamma^2}{\pi(s_i-\gamma)}\ln\left(\frac{s_i^2}{\gamma^2}\right)\right]e^{s_it},$$

$$\tilde{C}_t = \sum_{i=1}^4 \tilde{C}_t^i = \sum_{i=1}^4 \beta_i[s_i+\gamma]\left[\frac{s_i+\gamma}{\tilde{\mu}}+g^2\gamma s_i\right]e^{s_it},$$

$$\tilde{L}_t = \sum_{i=1}^4 \tilde{L}_t^i = -\sum_{i=1}^4 \beta_i[s_i+\gamma][\tilde{\delta}(s_i+\gamma)+\alpha^2\gamma s_i]e^{s_it}. \quad (49)$$

Here, $\tilde{\delta}=\mu\omega^2-\alpha^2\gamma$ and the constants

$$\beta_1 = \frac{1}{(s_1-s_2)(s_1-s_3)(s_1-s_4)},$$

$$\beta_2 = \frac{1}{(s_2-s_1)(s_2-s_3)(s_2-s_4)},$$

$$\beta_3 = \frac{1}{(s_3-s_1)(s_3-s_2)(s_3-s_4)},$$

$$\beta_4 = \frac{1}{(s_4-s_1)(s_4-s_2)(s_4-s_3)}$$

are expressed in terms of roots s_i (i=1, 2, 3, and 4) of the determinant [see Eq. (17)]

$$(s+\gamma)^2d(s) = s^2\left[s+\gamma+\frac{g\alpha\gamma^2}{\pi(s-\gamma)}\ln\left(\frac{s^2}{\gamma^2}\right)\right]^2 + \left[\frac{s+\gamma}{\tilde{\mu}} + g^2\gamma s\right][\tilde{\delta}(s+\gamma)+\alpha^2\gamma s] = 0, \quad (50)$$

in which the term $g\alpha\gamma^2\ln(s^2/\gamma^2)/\pi(s-\gamma)$ was disregarded.

The expressions for time-dependent transport coefficients follow from Eqs. (24)–(27) and (33)–(35) in which we should set

$$J_{q_tq_t} = \frac{\hbar\gamma^2}{\pi}\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0[2n_{\omega_0}+1]}{\gamma^2+\omega_0^2}[G_{ij}(t) - G_{ij}^c(t)\cos(\omega_0t) - G_{ij}^s(t)\sin(\omega_0t)], \quad (51)$$

$$G_{ij}(t) = a_{ij}[g^2(C_t^iC_t^j + C_0^iC_0^j) + \alpha^2(\tilde{C}_t^i\tilde{C}_t^j + \tilde{C}_0^i\tilde{C}_0^j)] + 2b_{ij}g\alpha[C_t^i\tilde{C}_t^j + C_0^i\tilde{C}_0^j],$$

$$G_{ij}^c(t) = a_{ij}[g^2(C_t^iC_0^j + C_0^iC_t^j) + \alpha^2(\tilde{C}_t^i\tilde{C}_0^j + \tilde{C}_0^i\tilde{C}_t^j)] + 2b_{ij}g\alpha[C_t^i\tilde{C}_0^j + C_0^i\tilde{C}_t^j],$$

$$G_{ij}^s(t) = b_{ij}[g^2(C_t^iC_0^j - C_0^iC_t^j) + \alpha^2(\tilde{C}_t^i\tilde{C}_0^j - \tilde{C}_0^i\tilde{C}_t^j)] - 2a_{ij}g\alpha[C_t^i\tilde{C}_0^j - C_0^i\tilde{C}_t^j],$$

$$J_{q_tp_t} + J_{p_tq_t} = \frac{2\hbar\gamma^2}{\pi}\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0[2n_{\omega_0}+1]}{\gamma^2+\omega_0^2}[P_{ij}(t) - P_{ij}^c(t)\cos(\omega_0t) - P_{ij}^s(t)\sin(\omega_0t)], \quad (52)$$

$$P_{ij}(t) = a_{ij}[g^2(C_t^i\tilde{L}_t^j + C_0^i\tilde{L}_0^j) + \alpha^2(\tilde{C}_t^iL_t^j + \tilde{C}_0^iL_0^j)] + b_{ij}g\alpha[C_t^iL_t^j + C_0^iL_0^j + \tilde{C}_t^j\tilde{L}_t^i + \tilde{C}_0^j\tilde{L}_0^i],$$

$$P_{ij}^c(t) = a_{ij}[g^2(C_t^i\tilde{L}_0^j + C_0^i\tilde{L}_t^j) + \alpha^2(\tilde{C}_t^iL_0^j + \tilde{C}_0^iL_t^j)] + b_{ij}g\alpha[C_t^iL_0^j + C_0^iL_t^j + \tilde{C}_0^j\tilde{L}_t^i + \tilde{C}_t^j\tilde{L}_0^i],$$

$$P_{ij}^s(t) = b_{ij}[g^2(C_t^i\tilde{L}_0^j - C_0^i\tilde{L}_t^j) + \alpha^2(\tilde{C}_t^iL_0^j - \tilde{C}_0^iL_t^j)] - a_{ij}g\alpha[C_t^iL_0^j - C_0^iL_t^j + \tilde{C}_0^j\tilde{L}_t^i - \tilde{C}_t^j\tilde{L}_0^i].$$

Here,

$$a_{ij} = \frac{s_is_j + \omega_0^2}{(s_i^2+\omega_0^2)(s_j^2+\omega_0^2)},$$

$$b_{ij} = \frac{(s_j - s_i)\omega_0}{(s_i^2+\omega_0^2)(s_j^2+\omega_0^2)}.$$

The expression for the $J_{p_tp_t}$ can be obtained from expression for the $J_{q_tq_t}$ by the following replacements: $C_t^i \to L_t^i$ and $\tilde{C}_t^i \to \tilde{L}_t^i$. As in the case of the general coupling Hamiltonian, the linear coupling in the coordinate and momentum gives us also nonzero diffusion and friction coefficients in the coordinate and momentum. The random forces are incorporated in the equations for $\dot{p}(t)$ as well as for $\dot{q}(t)$. So the equation for the reduced density matrix has Lindblad-type structure. For the given coupling, the fluctuation-dissipation relations are exactly satisfied in the forms (11)–(14).

B. Inverted harmonic oscillator

For the potential $U(q) = -\mu\omega^2q^2/2$, we can apply all the above formulas for A_t, B_t, M_t, N_t, C_t, $\tilde{C}_t$, $\tilde{L}_t$ (Sec. III A), $J_{q_tq_t}$, $J_{p_tp_t}$, and $J_{q_tp_t}+J_{p_tq_t}$ of the harmonic oscillator and obtain the transport coefficients by using Eqs. (24)–(27) and (33)–(35). The only differences are that another $\tilde{\delta} = -(\mu\omega^2 + \alpha^2\gamma)$ and the roots s_i of the equation

$$s^2\left[s + \gamma + \frac{g\alpha\gamma^2}{\pi(s-\gamma)}\ln\left(\frac{s^2}{\gamma^2}\right)\right]^2 - \left[\frac{s+\gamma}{\tilde{\mu}} + g^2\gamma s\right] \times [-\tilde{\delta}\gamma + \mu\omega^2 s] = 0$$

should be used.

C. Free motion

If $U(q)=0$, then $\tilde{\delta} = -\alpha^2\gamma$ and s_i are the roots of the equation

$$s^2\left[s + \gamma + \frac{g\alpha\gamma^2}{\pi(s-\gamma)}\ln\left(\frac{s^2}{\gamma^2}\right)\right]^2 - \left[\frac{s+\gamma}{\tilde{\mu}} + g^2\gamma s\right]\alpha^2\gamma^2 = 0.$$

We can apply all above results of Sec. III A to obtain the transport coefficients.

IV. FC OSCILLATOR

For the FC oscillator $U(q) = \mu\omega^2q^2/2$, the coupling Hamiltonian is

$$H_{cb} = \lambda^{1/2}\sum_\nu \Gamma_\nu(a^\dagger + a)(b_\nu^\dagger + b_\nu) = \sqrt{\frac{2\lambda\mu\omega}{\hbar}}q\sum_\nu \Gamma_\nu(b_\nu^\dagger + b_\nu).$$

Here, $a^\dagger$ and a are the annihilation and creation operators of the quantum oscillator, respectively, Γ_ν's real coupling constants, and λ a parameter that measures the average strength of the interaction. Inserting $g_\nu = 0$ and $\alpha_\nu = (2\mu\omega\lambda/\hbar)^{1/2}\Gamma_\nu = (\kappa/\hbar)\lambda^{1/2}\Gamma_\nu$ in Eq. (43) with $\kappa = (2\mu\omega\hbar)^2$, we obtain a set of Langevin equations for the damped quantum FC oscillator:

$$\dot{q}(t) = \frac{p(t)}{\mu},$$

$$\dot{p}(t) = -\tilde{\delta}q(t) - \kappa^2\int_0^t d\tau K(t-\tau)\dot{q}(\tau) + \kappa F(t), \quad (53)$$

where

$$F(t) = F_p(t)/\kappa = -\frac{\lambda^{1/2}}{\hbar}\sum_\nu \Gamma_\nu[f_\nu^\dagger(t) + f_\nu(t)],$$

$$f_\nu(t) = \left(b_\nu(0) + \frac{\kappa\lambda^{1/2}\Gamma_\nu}{\hbar^2\omega_\nu}q(0)\right)e^{-i\omega_\nu t},$$

$$\tilde{\delta} = \mu\omega^2 - \frac{2\lambda\kappa^2}{\hbar^2}\sum_\nu \frac{\Gamma_\nu^2}{\hbar\omega_\nu},$$

$$K(t-\tau) = K_{VV}(t,\tau)/\kappa^2 = \frac{2\lambda}{\hbar^2}\sum_\nu \frac{\Gamma_\nu^2}{\hbar\omega_\nu}\cos(\omega_\nu[t-\tau]).$$

The set of equations (53) has the following solutions [see Eqs. (18)]:

$$q(t) = A_tq(0) + B_tp(0) + \kappa\int_0^t d\tau\tilde{C}_\tau F(t-\tau),$$

$$p(t) = M_tq(0) + N_tp(0) + \kappa\int_0^t d\tau L_\tau F(t-\tau), \quad (54)$$

where

$$B_t = \tilde{C}_t = \frac{1}{\mu}\mathcal{L}^{-1}\left[\frac{1}{s^2 + 2\hbar\omega sK(s) + \tilde{\delta}/\mu}\right],$$

$$A_t = \mu\dot{B}_t + \kappa^2\int_0^t d\tau B_\tau K(t-\tau) = \mathcal{L}^{-1}\left[\frac{s + 2\hbar\omega K(s)}{s^2 + 2\hbar\omega sK(s) + \tilde{\delta}/\mu}\right],$$

$$M_t = -\mu\tilde{\delta}B_t,$$

$$N_t = L_t = \mu\dot{B}_t. \quad (55)$$

Here, $K(s)$ is the Laplace transformation of $K(t)$. If we rewrite the sum Σ_ν as an integral over bath frequencies with a density of states $D(\omega_0)$ $[D(\omega_0)|\Gamma(\omega_0)|^2/\hbar^2\omega_0 = \gamma^2/\pi(\gamma^2 + \omega_0^2)]$, then

$$K(t) = \frac{\lambda\gamma}{\hbar}e^{-\gamma|t|},$$

$$K(s) = \frac{\lambda\gamma}{\hbar(s+\gamma)},$$

$$\tilde{\delta} = \mu(\omega^2 - 2\lambda\gamma\omega),$$

$$B_t = \sum_{i=1}^{3} B_t^i = \frac{1}{\mu}\sum_{i=1}^{3}\beta_i(s_i+\gamma)e^{s_i t},$$

$$A_t = \sum_{i=1}^{3}\beta_i[s_i(s_i+\gamma) + 2\omega\lambda\gamma]e^{s_i t},$$

$$\beta_1 = \frac{1}{(s_1-s_2)(s_1-s_3)},$$

$$\beta_2 = \frac{1}{(s_2-s_1)(s_2-s_3)},$$

$$\beta_3 = \frac{1}{(s_3-s_1)(s_3-s_2)},$$

and $s_i(i=1,2,3)$ are the roots of the cubic equation following Eq. (17):

$$d(s) = s^2 + 2\hbar\omega sK(s) + \tilde{\delta}/\mu = [(s+\gamma)(s^2+\omega^2) - 2\omega\lambda\gamma^2]/(s+\gamma) = 0. \quad (56)$$

At $\gamma\to\infty$ we have the instantaneous dissipation with the kernel $\kappa^2K(t)=(2\lambda\kappa^2/\hbar)\delta(t)$. From Eq. (13) it is easily to show that the fluctuation-dissipation relation holds for the quantum FC oscillator.

For a damped quantum FC oscillator, the expressions for transport coefficients follow from Eqs. (24)–(27), (33)–(35), (51), and (52), and we obtain

$$\lambda_q(t) = D_{qq}(t) = 0,$$

$$m(t) = \mu,$$

$$D_{pp}(t) = \lambda_p(t)J_{p_tp_t} + \frac{1}{2}[\dot{J}_{p_tp_t} + \mu\xi(t)\dot{J}_{q_tq_t}],$$

$$D_{qp}(t) = \frac{1}{2}\left[\xi(t)J_{q_tq_t} - \frac{1}{\mu}J_{p_tp_t} + \frac{\mu}{2}[\lambda_p(t)\dot{J}_{q_tq_t} + \ddot{J}_{q_tq_t}]\right] \quad (57)$$

and

$$J_{q_tq_t} = \frac{2\hbar\omega\mu\lambda\gamma^2}{\pi}\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0[2n_{\omega_0}+1]}{\gamma^2+\omega_0^2}(a_{ij}\{[B_t^iB_t^j + B_0^iB_0^j] - [B_t^iB_0^j + B_0^iB_t^j]\cos(\omega_0t)\} - b_{ij}[B_t^iB_0^j - B_0^iB_t^j]\sin(\omega_0t)),$$

$$J_{p_tp_t} = \frac{2\hbar\omega\mu^3\lambda\gamma^2}{\pi}\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0[2n_{\omega_0}+1]}{\gamma^2+\omega_0^2}(a_{ij}\{[\dot{B}_t^i\dot{B}_t^j + \dot{B}_0^i\dot{B}_0^j] - [\dot{B}_t^i\dot{B}_0^j + \dot{B}_0^i\dot{B}_t^j]\cos(\omega_0t)\} - b_{ij}[\dot{B}_t^i\dot{B}_0^j - \dot{B}_0^i\dot{B}_t^j]\sin(\omega_0t)),$$

$$J_{q_tp_t} + J_{p_tq_t} = \frac{4\hbar\omega\mu^2\lambda\gamma^2}{\pi}\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0[2n_{\omega_0}+1]}{\gamma^2+\omega_0^2}(a_{ij}\{\dot{B}_t^iB_t^j - [\dot{B}_t^iB_0^j + \dot{B}_0^iB_t^j]\cos(\omega_0t)\} - b_{ij}[\dot{B}_t^iB_0^j - \dot{B}_0^iB_t^j]\sin(\omega_0t)), \quad (58)$$

where a_{ij} and b_{ij} are the same as in Sec. III A.

For the quantum FC oscillator, the equation for the reduced density matrix (or the Wigner distribution function) has no the Lindblad structure because it does not contain the terms $[i\lambda_q(t)/2\hbar][p,\{q,\hat{\rho}\}_+]$ and $-[D_{qq}(t)/\hbar^2][p,[p,\hat{\rho}]]$. This is the consequence of the absence of random forces in the equation for $\dot{q}(t)$. However, the positivity of the density matrix is guaranteed through the time dependence of friction, diffusion coefficients in the momentum and of the mixed diffusion coefficient, and by the special ratio between D_{pp} and λ_p. Indeed, the self-consistently obtained friction and diffusion coefficients should not violate the uncertainty principle for the momentum and coordinate. The non stationary transport coefficients for the quantum FC oscillator were derived before in Refs. [10,12,14,15] using the microscopic dynamics and the path integral representation, but with another spectral density of the internal heat bath excitations than used by us. In the classical limit the time-dependent friction and diffusion coefficients were obtained in Ref. [27].

In accordance with Eqs. (36) the diffusion coefficients have the following form at $t\to\infty$:

$$D_{pp}(\infty) = \lambda_p(\infty)\sigma_{pp}(\infty),$$

$$D_{qp}(\infty) = \frac{1}{2}\left[\xi(\infty)\sigma_{qq}(\infty) - \frac{1}{\mu}\sigma_{pp}(\infty)\right]. \quad (59)$$

If $0>\mathrm{Re}(s_2)=\mathrm{Re}(s_3)>\mathrm{Re}(s_1)$, then using the relationship between the roots of Eq. (56), $s_1+s_2+s_3=-\gamma$, $s_1s_2+s_1s_3+s_2s_3=\omega^2$, and $s_1s_2s_3=\gamma(2\lambda\gamma\omega-\omega^2)$, we obtain

$$\lambda_p(\infty) = -(s_2+s_2^*),$$

$$\xi(\infty) = \tilde{\delta}\frac{|s_2+\gamma|^2}{|s_2+\gamma|^2 - 2\lambda\gamma\omega}.$$

The asymptotic variances are

$$\sigma_{qq}(\infty)=J_{q_\infty q_\infty}=\frac{2\hbar\omega\lambda\gamma^2}{\pi\mu}\int_0^\infty d\omega_0\frac{\omega_0\coth[\hbar\omega_0/(2T)]}{(s_1^2+\omega_0^2)(s_2^2+\omega_0^2)(s_3^2+\omega_0^2)}=\frac{2T\omega\lambda\gamma^2}{\mu}\sum_{n=0}^{\infty}\frac{(\delta_{n,0}-2)(x_n+s_1+s_2+s_3)}{(x_n+s_1)(x_n+s_2)(x_n+s_3)(s_1+s_2)(s_1+s_3)(s_2+s_3)}$$

$$=\frac{T}{\mu}\sum_{n=0}^{\infty}\frac{(2-\delta_{n,0})(x_n-\gamma)}{x_n^3-\gamma x_n^2+\omega^2x_n+(2\lambda\gamma\omega-\omega^2)\gamma},$$

$$\sigma_{pp}(\infty)=J_{p_\infty p_\infty}=\frac{2\hbar\omega\mu\lambda\gamma^2}{\pi}\int_0^\infty d\omega_0\frac{\omega_0^3\coth[\hbar\omega_0/(2T)]}{(s_1^2+\omega_0^2)(s_2^2+\omega_0^2)(s_3^2+\omega_0^2)}$$

$$=2T\omega\lambda\gamma^2\mu\sum_{n=0}^{\infty}\frac{(\delta_{n,0}-2)(x_n(s_1s_2+s_1s_3+s_2s_3)+s_1s_2s_3)}{(x_n+s_1)(x_n+s_2)(x_n+s_2)(s_1+s_2)(s_1+s_3)(s_2+s_3)}=T\mu\sum_{n=0}^{\infty}\frac{(2-\delta_{n,0})[x_n\omega^2+(2\lambda\omega\gamma-\omega^2)\gamma]}{x_n^3-\gamma x_n^2+\omega^2x_n+(2\lambda\gamma\omega-\omega^2)\gamma},$$

$$\sigma_{qp}(\infty)=\frac{1}{2}(J_{q_\infty p_\infty}+J_{p_\infty q_\infty})=0, \tag{60}$$

where $x_n=2\pi Tn/\hbar$. To evaluate the integrals in Eqs. (60), one commonly expands the hyperbolic cotangent into a uniformly convergent series.

At the high-temperature (the classical) limit and weak-coupling limit (small λ), Eqs. (59), are transformed into

$$D_{pp}(\infty)=\lambda_p(\infty)\mu T,\quad D_{qp}(\infty)=0, \tag{61}$$

because

$$\xi(\infty)=\tilde{\delta},$$

$$\sigma_{qq}(\infty)=-\frac{2T\omega\lambda\gamma^2(s_1+s_2+s_3)}{\mu s_1s_2s_3(s_1+s_2)(s_1+s_3)(s_2+s_3)}=\frac{T}{\mu(\omega^2-2\lambda\gamma\omega)}$$

$$=\frac{T}{\tilde{\delta}},$$

$$\sigma_{pp}(\infty)=-\frac{2T\omega\lambda\gamma^2\mu}{(s_1+s_2)(s_1+s_3)(s_2+s_3)}=\mu T.$$

Here, we again use the relationships between the roots of the cubic equation (56). Thus, at the limits of high temperature and of small damping the classical equipartition theorem holds true.

At the low-temperature limit ($T\to 0$) we obtain from Eqs. (60) the following asymptotic variances:

$$\sigma_{qq}(\infty)=\frac{\hbar\omega\lambda\gamma^2}{\pi\mu}\frac{s_1^2\ln\left(\frac{s_2^2}{s_3^2}\right)+s_2^2\ln\left(\frac{s_3^2}{s_1^2}\right)+s_3^2\ln\left(\frac{s_1^2}{s_2^2}\right)}{(s_1^2-s_2^2)(s_1^2-s_3^2)(s_2^2-s_3^2)},$$

$$\sigma_{pp}(\infty)=\frac{2\hbar\omega\lambda\gamma^2\mu}{\pi}\frac{s_2^2s_3^2\ln\left(\frac{s_2^2}{s_3^2}\right)+s_1^2s_2^2\ln\left(\frac{s_1^2}{s_2^2}\right)+s_1^2s_3^2\ln\left(\frac{s_3^2}{s_1^2}\right)}{(s_1^2-s_2^2)(s_1^2-s_3^2)(s_2^2-s_3^2)}. \tag{62}$$

At the weak-coupling limit we have $\sigma_{pp}(\infty)=\hbar\mu\omega/2$ and $\sigma_{qq}(\infty)=\hbar/2\mu\omega$.

The asymptotics ($t\gg t'>0$) of the symmetric correlation functions,

$$\sigma_{q_tq_{t'}}^{as}=\frac{2\hbar\omega\lambda\gamma^2}{\pi\mu}\int_0^\infty d\omega_0\frac{\omega_0\coth[\hbar\omega_0/(2T)]\cos[\omega_0(t-t')]}{(s_1^2+\omega_0^2)(s_2^2+\omega_0^2)(s_3^2+\omega_0^2)},$$

$$\sigma_{p_tp_{t'}}^{as}=\frac{2\hbar\omega\mu\lambda\gamma^2}{\pi}\int_0^\infty d\omega_0\frac{\omega_0^3\coth[\hbar\omega_0/(2T)]\cos[\omega_0(t-t')]}{(s_1^2+\omega_0^2)(s_2^2+\omega_0^2)(s_3^2+\omega_0^2)}, \tag{63}$$

have different decay behavior at the low- and high-temperature regimes:

$$\sigma_{q_tq_{t'}}^{as}(T\to 0)\to\frac{-2\hbar\omega\lambda\gamma^2}{\pi\mu s_1^2s_2^2s_3^2}\frac{1}{(t-t')^2}=\frac{-2\hbar\lambda}{\pi\mu\omega^3}\frac{1}{(t-t')^2},$$

$$\sigma_{q_tq_{t'}}^{as}(T\to\infty)\to\frac{-T}{2\mu\omega^2\gamma}\left[\frac{s_2s_3(s_2+s_3)e^{s_1(t-t')}}{(s_2-s_1)(s_3-s_1)}+\frac{s_1s_3(s_1+s_3)e^{s_2(t-t')}}{(s_1-s_2)(s_3-s_2)}+\frac{s_1s_2(s_1+s_2)e^{s_3(t-t')}}{(s_1-s_3)(s_2-s_3)}\right],$$

$$\sigma_{p_tp_{t'}}^{as}(T\to 0)\to-\frac{i\hbar\mu}{2}\left[\frac{s_1^2(s_2+s_3)e^{s_1(t-t')}}{(s_2-s_1)(s_3-s_1)}+\frac{s_2^2(s_1+s_3)e^{s_2(t-t')}}{(s_1-s_2)(s_3-s_2)}+\frac{s_3^2(s_1+s_2)e^{s_3(t-t')}}{(s_1-s_3)(s_2-s_3)}\right],$$

$$\sigma_{p_tp_{t'}}^{as}(T\to\infty)\to-\frac{\mu T}{2}\left[\frac{s_1(s_2+s_3)e^{s_1(t-t')}}{(s_2-s_1)(s_3-s_1)}+\frac{s_2(s_1+s_3)e^{s_2(t-t')}}{(s_1-s_2)(s_3-s_2)}+\frac{s_3(s_1+s_2)e^{s_2(t-t')}}{(s_1-s_3)(s_2-s_3)}\right]. \tag{64}$$

So at low temperature the FC oscillator exhibits powerlike decay of the correlation function in the coordinate in the long-time limit. This effect is not manifested in the classical limit where we have an exponential decay.

A. FC inverted oscillator

We can also apply the formulas obtained for the FC oscillator to the inverted oscillator with $U(q)=-\mu\omega^2 q^2/2$. In these formulas we should use $\tilde{\delta}=-\mu[2\omega\lambda\gamma+\omega^2]$ and the roots s_i of the equation

$$(s+\gamma)(s^2-\omega^2)-2\omega\lambda\gamma^2=0.$$

Since for the inverted oscillator we have no equilibrium regime for large times in comparison to the harmonic oscillator, the direct use of asymptotic formulas leads to unphysical results like the negative diffusion coefficient in the momentum at low temperature.

B. FC free motion

For the free motion $[U(q)=0]$, the formulas of the FC oscillator can be used with $\tilde{\delta}=-2\mu\omega\lambda\gamma$ and the roots s_i of the equation

$$(s+\gamma)s^2-2\omega\lambda\gamma^2=0.$$

V. RWA OSCILLATOR

In quantum optics and other fields the rotating-wave approximation is widely used [1,3,4]. The coupling Hamiltonian for the RWA oscillator is

$$H_{cb}=\lambda^{1/2}\sum_\nu(\Gamma_\nu^* a^\dagger b_\nu+\Gamma_\nu a b_\nu^\dagger)$$
$$=\sqrt{\frac{\lambda\mu\omega}{2\hbar}}q\sum_\nu(\Gamma_\nu^* b_\nu+\Gamma_\nu b_\nu^\dagger)+i\sqrt{\frac{\lambda}{2\hbar\mu\omega}}p\sum_\nu(\Gamma_\nu b_\nu^\dagger-\Gamma_\nu^* b_\nu).$$

Here, the coupling constants Γ_ν are taken as complex. The RWA coupling excludes the nonresonant $a^\dagger b_\nu^\dagger$ and ab_ν terms $a^\dagger b_\nu^\dagger$ and ab_ν. With this exclusion we disregard the rapidly oscillating terms. As in the case of the FC oscillator, the fluctuation-dissipation relation is satisfied for the RWA oscillator.

For the RWA oscillator with $U(q)=\mu\omega^2 q^2/2$ the solutions of the equations of motion are written as

$$q(t)=A_t q(0)+B_t p(0)+i\sqrt{\frac{\hbar}{2\mu\omega}}\int_0^t d\tau[C_\tau^* f^\dagger(t-\tau)-C_\tau f(t-\tau)],$$

$$p(t)=-\mu^2\omega^2 B_t q(0)+A_t p(0)-\sqrt{\frac{\hbar\mu\omega}{2}}\int_0^t d\tau[C_\tau^* f^\dagger(t-\tau)+C_\tau f(t-\tau)], \tag{65}$$

where

$$f(t)=\frac{\lambda^{1/2}}{\hbar}\sum_\nu\Gamma_\nu^*\left(b_\nu(0)+\frac{\Gamma_\nu}{\hbar\omega_\nu}\left[\sqrt{\frac{\lambda\mu\omega}{2\hbar}}q(0)+i\sqrt{\frac{\lambda}{2\hbar\mu\omega}}p(0)\right]\right)e^{-i\omega_\nu t},$$

$$A_t=\frac{1}{2}\left[C_t+C_t^*+i\hbar\int_0^t d\tau[C_\tau K(t-\tau)-C_\tau^* K^*(t-\tau)]\right],$$

$$B_t=\frac{i}{2\mu\omega}\left[C_t-C_t^*+i\hbar\int_0^t d\tau[C_\tau K(t-\tau)+C_\tau^* K^*(t-\tau)]\right],$$

$$K(t-\tau)=\frac{\lambda}{\hbar^2}\sum_\nu\frac{|\Gamma_\nu|^2}{\hbar\omega_\nu}e^{-i\omega_\nu(t-\tau)},$$

$$C_t=\mathcal{L}^{-1}\left[\frac{1}{s+i\hbar sK(s)+i\epsilon/\hbar}\right],$$

$$\epsilon=\hbar\omega-\lambda\sum_\nu\frac{|\Gamma_\nu|^2}{\hbar\omega_\nu}.$$

If we replace the sums above by the integral over the bath frequencies with a density $D(\omega_0)$ of states as in the previous section, then we obtain

$$K(t)=\frac{\lambda\gamma}{2\hbar}e^{-\gamma|t|}-\frac{i\lambda\gamma^2}{\hbar\pi}\int_0^\infty d\omega_0\frac{\sin(\omega_0 t)}{\omega_0^2+\gamma^2},$$

$$K(s)=\frac{\lambda\gamma}{2\hbar(s+\gamma)}-\frac{i\lambda\gamma^2\ln(s^2/\gamma^2)}{2\pi\hbar(s^2-\gamma^2)},$$

$$\epsilon=\hbar(\omega-\lambda\gamma),$$

$$A_t=\frac{1}{2}\sum_{j=1}^2[\beta_j\eta_j e^{s_j t}+\beta_j^*\eta_j^* e^{s_j^* t}],$$

$$B_t=\frac{i}{2\mu\omega}\sum_{j=1}^2[\beta_j\eta_j e^{s_j t}-\beta_j^*\eta_j^* e^{s_j^* t}],$$

$$C_t=\sum_{j=1}^2 C_t^j=\sum_{j=1}^2\beta_j(s_j+\gamma)e^{s_j t},$$

$$\eta_j=s_j+\gamma+\frac{i\lambda\gamma}{2}+\frac{\lambda\gamma^2\ln(s_j^2/\gamma^2)}{2\pi(s_j-\gamma)}.$$

Here, $\beta_1=-\beta_2=(s_1-s_2)^{-1}$, and s_1 and s_2 are two simple roots of the equation

$$s+i\hbar sK(s)+i\epsilon/\hbar=0,$$

in which the term proportional to $\ln(s^2/\gamma^2)$ is disregarded. This term does not introduce a singularity at $s=0$ because $s\ln(s)\to 0$ as $s\to 0$. This term leads to corrections of the next order in λ which are assumed to be small. In the limit of a large phonon bandwidth γ, the dissipative kernel is reduced to the familiar form [9] $K(t)=(\lambda/\hbar)\delta(t)-(i\lambda/\hbar\pi)P(1/t)$. It was stated in Ref. [28] that the effect of the principal-value term on the physical behavior of the system is small.

For the RWA oscillator, the time-dependent transport coefficients result as follows: friction coefficients in the coordinate and in momentum,

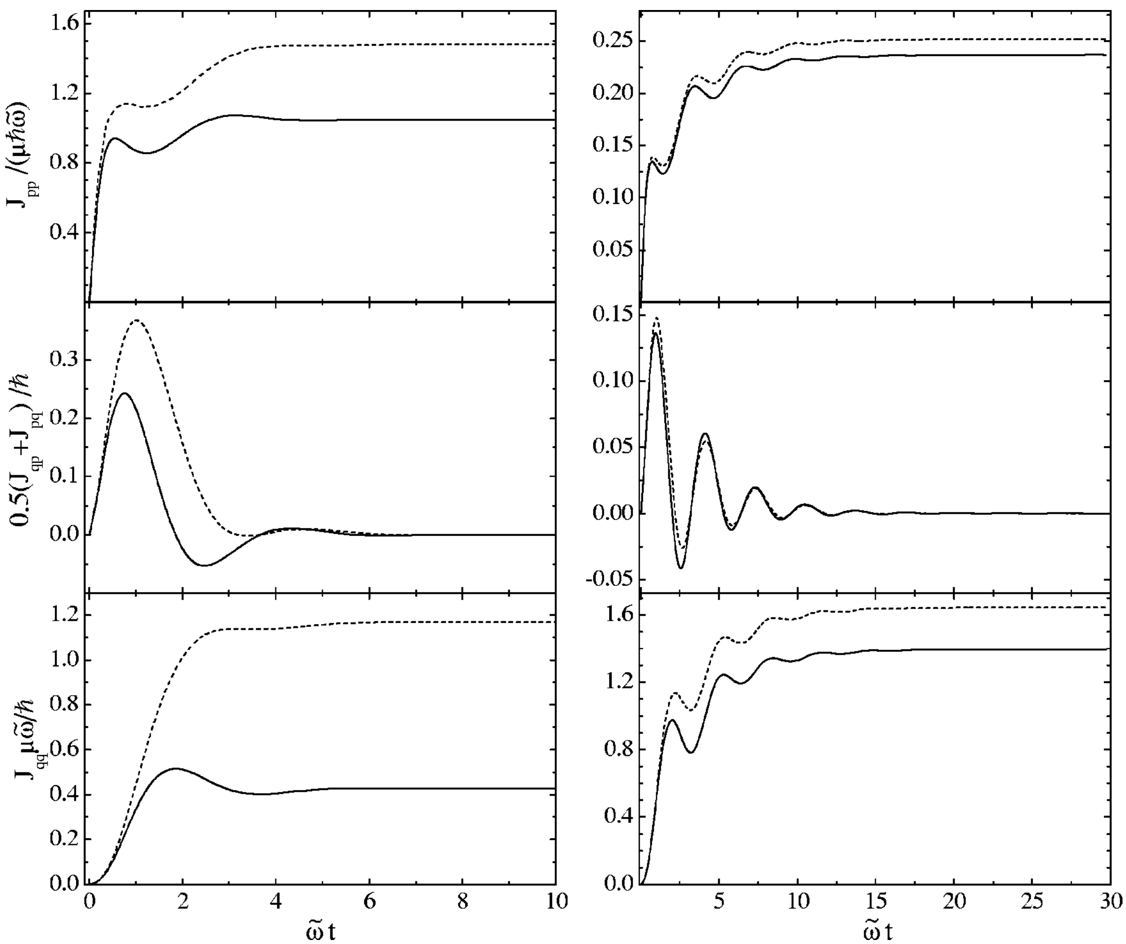

FIG. 1. Calculated time dependence of J_{pp}, J_{qp}, and J_{qq} for $\hbar\tilde{\omega}=1$ MeV and $\mu=448m_0$ (left side) and for $\hbar\tilde{\omega}=3$ MeV and $\mu=50m_0$ (right side). We set $\lambda_p/\tilde{\omega}=1/(\hbar\tilde{\omega})$. The results for $T/(\hbar\tilde{\omega})=0.1/(\hbar\tilde{\omega})$ and $1/(\hbar\tilde{\omega})$ are presented by solid and dashed lines, respectively.

$$\lambda_q(t) = \lambda_p(t) = -\frac{\dot{A}_t A_t + (\mu\omega)^2 \dot{B}_t B_t}{A_t^2 + (\mu\omega)^2 B_t^2}, \tag{66}$$

inverse mass parameter

$$1/m(t) = \frac{\dot{B}_t A_t - \dot{A}_t B_t}{A_t^2 + (\mu\omega)^2 B_t^2}, \tag{67}$$

stiffness coefficient

$$\xi(t) = (\mu\omega)^2 \frac{\dot{B}_t A_t - \dot{A}_t B_t}{A_t^2 + (\mu\omega)^2 B_t^2}, \tag{68}$$

and diffusion coefficients in the coordinate,

$$D_{qq}(t) = \lambda_q(t) J_{q_t q_t} + \frac{1}{2}\dot{J}_{q_t q_t}, \tag{69}$$

in the momentum,

$$D_{pp}(t) = (\mu\omega)^2 D_{qq}(t), \tag{70}$$

and mixed diffusion coefficients in the coordinate and momentum:

$$D_{qp}(t) = 0. \tag{71}$$

In expression (69),

$$J_{q_t q_t} = \frac{\hbar\lambda\gamma^2}{2\pi\mu\omega}\sum_{ij}\int_0^\infty d\omega_0 \frac{\omega_0 \coth[\hbar\omega_0/(2T)]\psi_{ij}(t)}{(\gamma^2+\omega_0^2)(s_i+i\omega_0)(s_j^*-i\omega_0)},$$

where

$$\psi_{ij}(t) = C_t^i C_t^{j*} + C_0^i C_0^{j*} - C_t^i C_0^{j*} e^{i\omega_\nu t} - C_0^i C_t^{j*} e^{-i\omega_\nu t}.$$

At the limit of $t\to\infty$,

$$D_{qq}(\infty) = \frac{1}{(\mu\omega)^2} D_{pp}(\infty) = \lambda_q(\infty)\sigma_{qq}(\infty). \tag{72}$$

This set of diffusion coefficients can be obtained from Eq. (37) assuming that the asymptotic state is a Gibbs $\hat{\rho}=\exp[-\tilde{H}_c/T]/\mathrm{Tr}(\exp[-\tilde{H}_c/T])$ [25]. If $\mathrm{Re}(s_1)>\mathrm{Re}(s_2)$, then

$$\lambda_q(\infty) = -\frac{1}{2}(s_2+s_2^*),$$

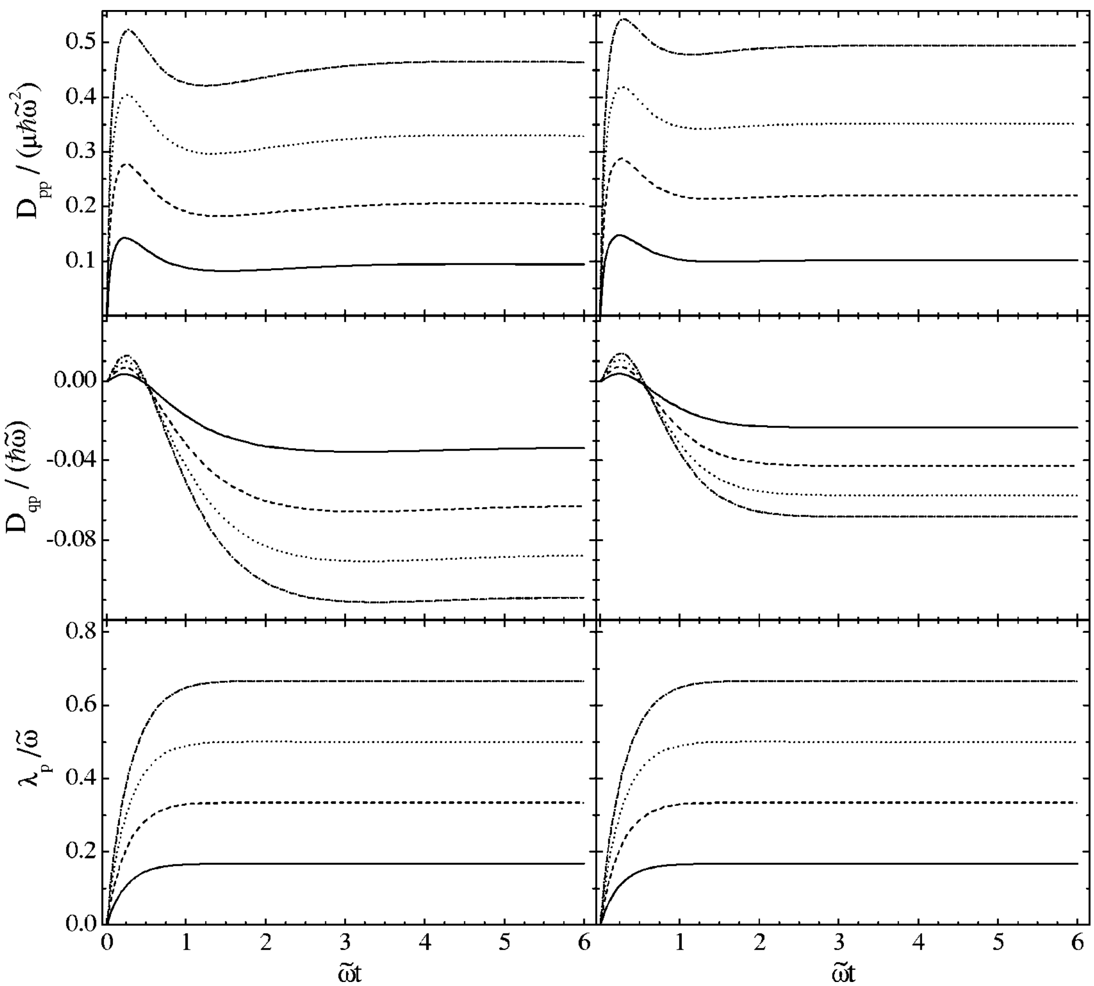

FIG. 2. Calculated time dependence of diffusion and friction coefficients for $\mu=50m_0$ and $\hbar\tilde{\omega}=3$ MeV at $T/(\hbar\tilde{\omega})=0.033$ (left side) and $T/(\hbar\tilde{\omega})=0.33$ (right side). The results leading to the friction coefficients $\lambda_p/\tilde{\omega}=0.17$, 0.33, 0.50, and 0.66 are presented by solid, dashed, dotted, and dash-dotted lines, respectively.

$$1/m(\infty) = \xi(\infty)/(\mu\omega)^2 = \frac{|\mathrm{Im}(s_2)|}{\mu\omega}. \tag{73}$$

The asymptotic variance in the coordinate can be easily derived:

$$\begin{aligned}\sigma_{qq}(\infty) = J_{q_\infty q_\infty} &= \frac{\lambda\hbar\gamma^2}{2\pi\omega\mu}\int_0^\infty d\omega_0 \frac{\omega_0 \coth[\hbar\omega_0/(2T)]}{|s_1+i\omega_0|^2|s_2+i\omega_0|^2} \\ &= \frac{\lambda\gamma^2 T}{\omega\mu}\left[\sum_{n=1}^{\infty}\left(\frac{s_1}{(s_1-x_n)(s_1+s_1^*)(s_1-s_2)(s_1+s_2^*)}\right.\right. \\ &\quad \left. - \frac{s_2}{(s_2-x_n)(s_2+s_2^*)(s_2-s_1)(s_2+s_1^*)} + \mathrm{H.c.}\right) \\ &\quad \left. - \frac{s_1+s_1^*+s_2+s_2^*}{(s_1+s_1^*)(s_2+s_2^*)(s_1^*+s_2)(s_2^*+s_1)}\right], \end{aligned} \tag{74}$$

where again $x_n=2\pi nT/\hbar$. At high temperature ($T\to\infty$) we have

$$\sigma_{qq}(\infty) = J_{q_\infty q_\infty} = -\frac{\lambda\gamma^2 T}{\omega\mu}\frac{s_1+s_1^*+s_2+s_2^*}{(s_1+s_1^*)(s_2+s_2^*)(s_1^*+s_2)(s_2^*+s_1)}, \tag{75}$$

which is positive because $\mathrm{Re}(s_1)<0$ and $\mathrm{Re}(s_2)<0$.

At low temperature ($T\to 0$) the following expression is obtained:

$$\sigma_{qq}(\infty) = J_{q_\infty q_\infty} = \frac{\lambda\hbar\gamma^2}{2\omega\mu}\frac{i(s_1^*s_2^*-s_1s_2)}{(s_1+s_1^*)(s_2+s_2^*)(s_1^*+s_2)(s_2^*+s_1)}, \tag{76}$$

which is positive since $\mathrm{Im}(s_1s_2)>0$ up to the leading order of λ. In the weak-coupling limit $\lambda\ll 1$, Eqs. (75) and (76) are reduced to the known formulas

$$\sigma_{qq}(\infty) = \frac{T}{\mu\omega^2}$$

and

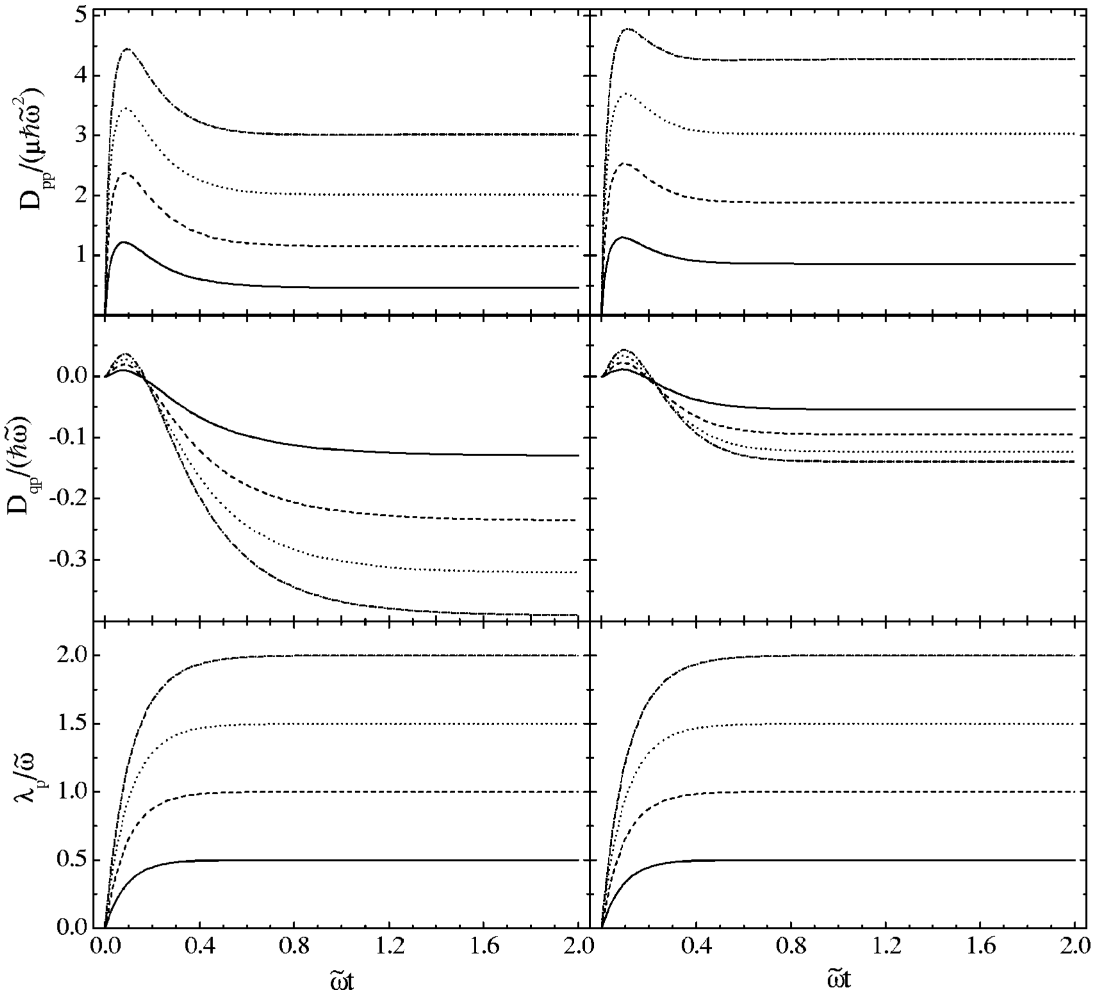

FIG. 3. Calculated time dependence of diffusion and friction coefficients for $\mu=448m_0$ and $\hbar\tilde{\omega}=1$ MeV at $T/(\hbar\tilde{\omega})=0.5$ (left side) and $T/(\hbar\tilde{\omega})=1.5$ (right side). The results leading to the friction coefficients $\lambda_p/\tilde{\omega}=0.5$, 1.0, 1.5, and 2.0 are presented by solid, dashed, dotted, and dash-dotted lines, respectively.

$$\sigma_{qq}(\infty)=\frac{\hbar}{2\mu\omega},$$

respectively.

Due to $\lambda_q\neq 0$ and $D_{qq}\neq 0$, the equation for the reduced density matrix (or the Wigner probability distribution function) has the Lindblad structure. The positivity of the density matrix holds for any initial states even if the asymptotic friction and diffusion coefficients in the coordinate and momentum are used in the master equation (35) under the condition that the density matrix be initially positive.

The symmetric correlation function in coordinate has the following structure:

$$\sigma_{q_tq_{t'}}=A_tA_{t'}\sigma_{q_0q_0}+B_tB_{t'}\sigma_{p_0p_0}+\frac{\hbar\lambda\gamma^2}{4\pi\mu\omega}\times\sum_{ij}\int_0^\infty d\omega_0\frac{\omega_0\coth[\hbar\omega_0/(2T)][\psi_{ij}(t,t')+\psi_{ji}^*(t,t')]}{[\gamma^2+\omega_0^2][s_i+i\omega_0][s_j^*-i\omega_0]}, \tag{77}$$

where

$$\psi_{ij}(t,t')=C_t^iC_{t'}^{j*}+C_0^iC_0^{j*}e^{i\omega_\nu(t-t')}-C_t^iC_0^{j*}e^{i\omega_\nu t'}-C_0^iC_{t'}^{j*}e^{-i\omega_\nu t}.$$

The asymptotic $(t\gg t'>0)$ symmetric correlation function

$$\sigma_{q_tq_{t'}}^{as}=\frac{\lambda\hbar\gamma^2}{2\pi\omega\mu}\int_0^\infty d\omega_0\frac{\omega_0\coth[\hbar\omega_0/(2T)]\cos(\omega_0[t-t'])}{|s_1+i\omega_0|^2|s_2+i\omega_0|^2} \tag{78}$$

has a nonexponential powerlike decay behavior at the zero- and high-temperature limits:

$$\sigma_{q_tq_{t'}}^{as}(T\to 0)\to\frac{-\lambda\hbar\gamma^2}{2\pi\omega\mu|s_1|^2|s_2|^2(t-t')^2}\approx\frac{-\lambda\hbar}{2\pi\omega^3\mu}\frac{1}{(t-t')^2}, \tag{79}$$

$$\sigma_{q_tq_{t'}}^{as}(T\to\infty)\to\frac{i\lambda\gamma^2T(s_1^*s_2^*[s_1+s_2]-s_1s_2[s_1^*+s_2^*])}{\pi\omega\mu|s_1|^4|s_2|^4(t-t')^2}\approx\frac{-2\lambda T}{\pi\mu\omega^4}\frac{1}{(t-t')^2}. \tag{80}$$

This is related to the pure quantum nature of the interaction

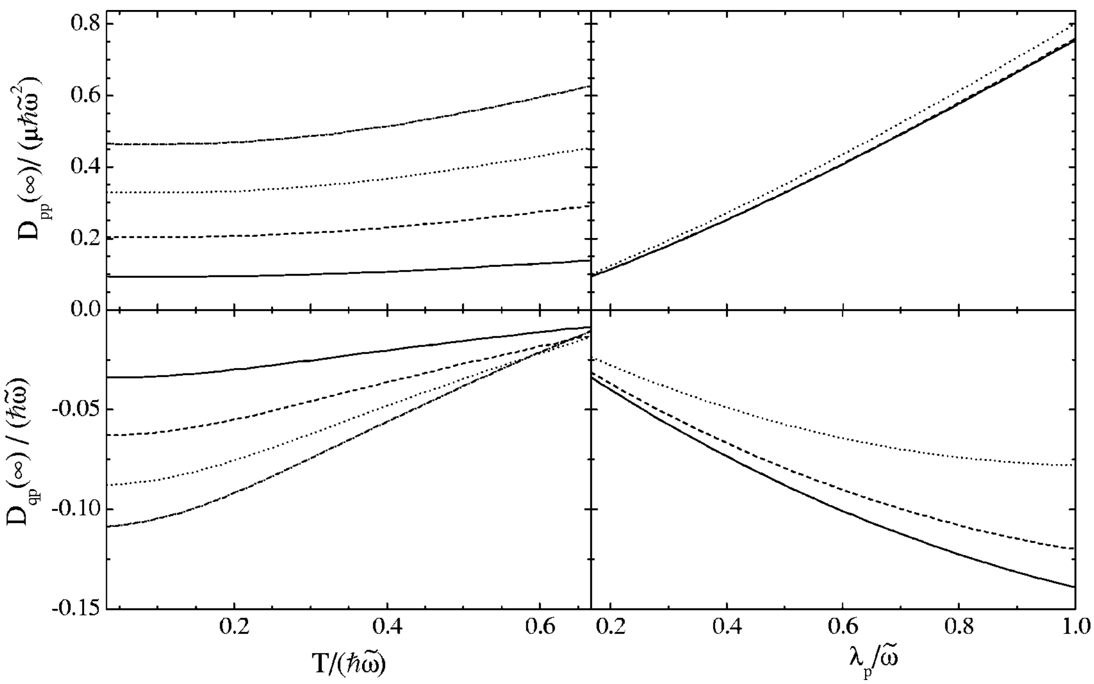

FIG. 4. The calculated asymptotic diffusion coefficients as functions of $T/(\hbar\tilde{\omega})$ (left side) and $\lambda_p/\tilde{\omega}$ (right side) for $\mu=50m_0$ and $\hbar\tilde{\omega}=3$ MeV. The dependence on temperature is presented for $\lambda_p/\tilde{\omega}=0.17$ (solid lines), 0.33 (dashed lines), 0.50 (dotted lines), and 0.66 (dash-dotted lines). The dependence on λ_p is presented for $T/(\hbar\tilde{\omega})=0.033$ (solid lines), 0.17 (dashed lines), and 0.33 (dotted lines).

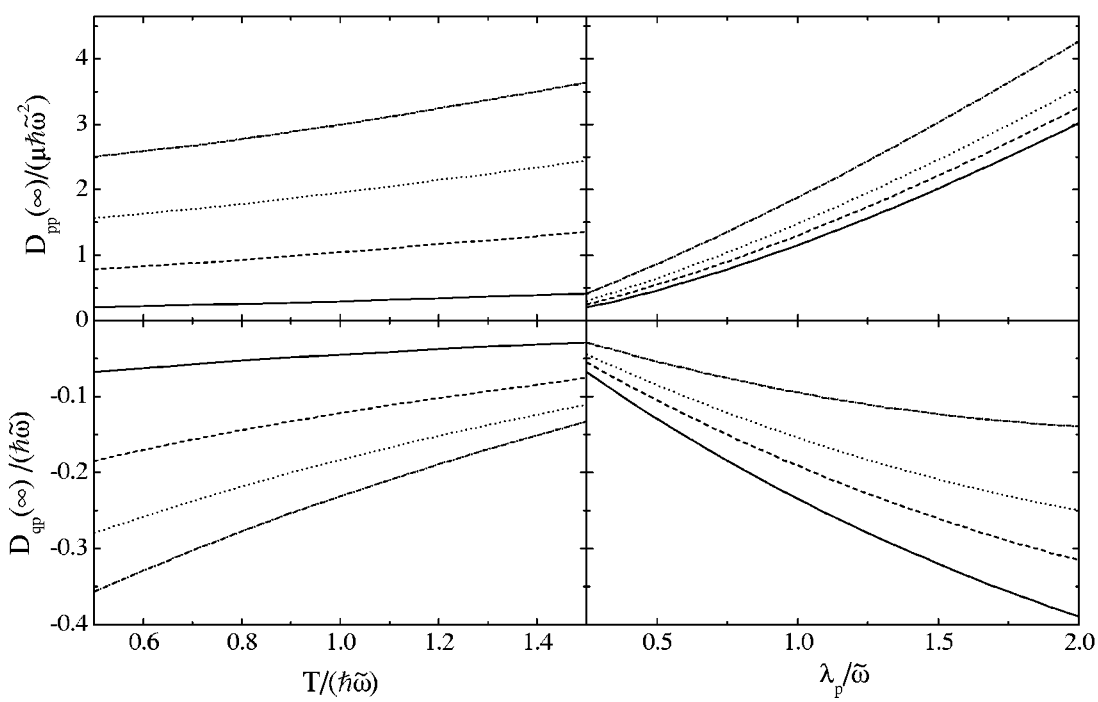

FIG. 5. The same as in Fig. 4, but for $\mu=448m_0$ and $\hbar\tilde{\omega}=1$ MeV. The dependence on temperature is presented for $\lambda_p/\tilde{\omega}=0.25$ (solid lines), 0.75 (dashed lines), 1.25 (dotted lines), and 1.75 (dash-dotted lines). The dependence on $\lambda_p/\tilde{\omega}$ is presented for $T/(\hbar\tilde{\omega})=0.5$ (solid lines), 0.75 (dashed lines), 1 (dotted lines), and 1.5 (dash-dotted lines).

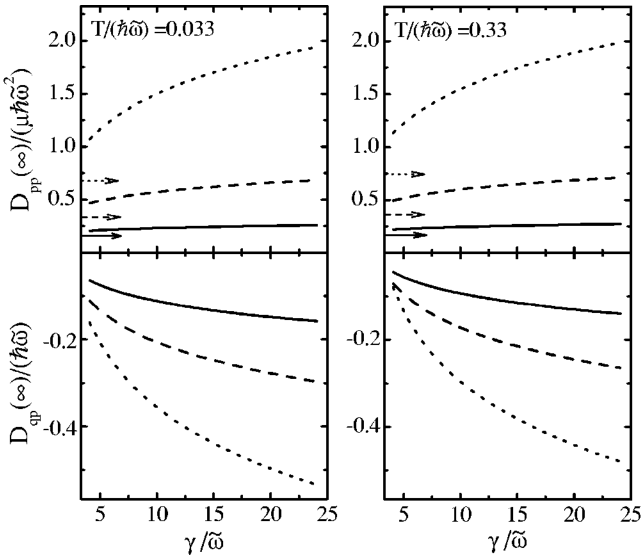

FIG. 6. For $\mu=50m_0$, $\hbar\tilde{\omega}=3$ MeV and the indicated temperatures, the calculated asymptotic diffusion coefficients are shown as functions of $\gamma/\tilde{\omega}$ at $\lambda_p/\tilde{\omega}=0.33$ (solid lines), 0.66 (dashed lines), and 1.33 (dotted lines). The values of "classic" diffusion coefficients $D^c_{pp}/(\mu\hbar\tilde{\omega}^2)$ are presented by the corresponding arrows.

between the collective and heat bath subsystems: each act of interaction must consist in the annihilation of a quantum in one subsystem and its creation in another subsystem. Note that the results (79) and (80) do not depend on γ.

VI. ILLUSTRATIVE CALCULATIONS OF TRANSPORT COEFFICIENTS FOR THE FC OSCILLATOR

The diffusion and friction coefficients depend on the parameters ω, λ, and γ. The value of γ should be taken to hold the condition $\gamma \gg \omega$. We set $\hbar\gamma=12$ MeV. The values of ω and λ are fixed by given certain asymptotic values of $\xi(\infty)$ and $\lambda_p(\infty)$:

$$\xi = \xi(\infty) = \mu\tilde{\omega}^2, \quad \lambda_p(\infty) = \lambda_p.$$

We consider the case of a small mass $\mu=50m_0$ (m_0 is the nucleon mass) and a large value $\hbar\tilde{\omega}=3$ MeV and the case of a large mass $\mu=448m_0$ and a small $\hbar\tilde{\omega}=1$ MeV. As shown in Fig. 1, J_{pp}, J_{qq}, and J_{qp} start from zero at $t=0$ and in some time reach the asymptotic values which coincide with the asymptotic values of the variances as follows from Eqs. (60). The time dependences of the friction and diffusion coeffi-

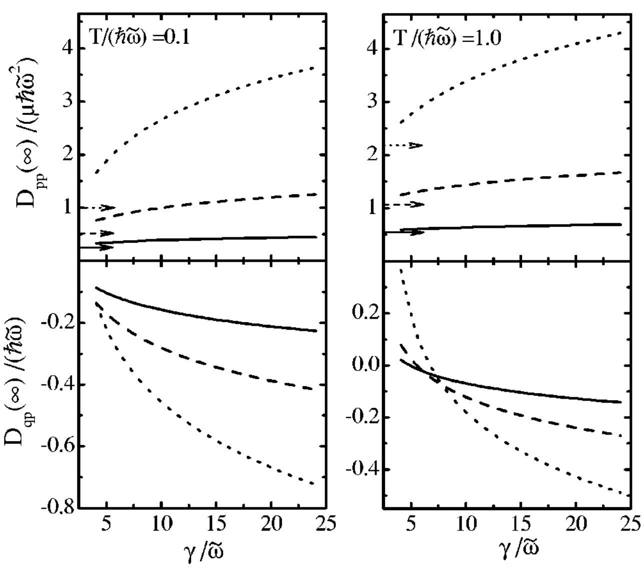

FIG. 7. The same as in Fig. 6, but for $\mu=448m_0$ ($\hbar\omega=1$ MeV) and $\lambda_p/\tilde{\omega}=0.5$ (solid lines), 1 (dashed lines), and 2 (dotted lines).

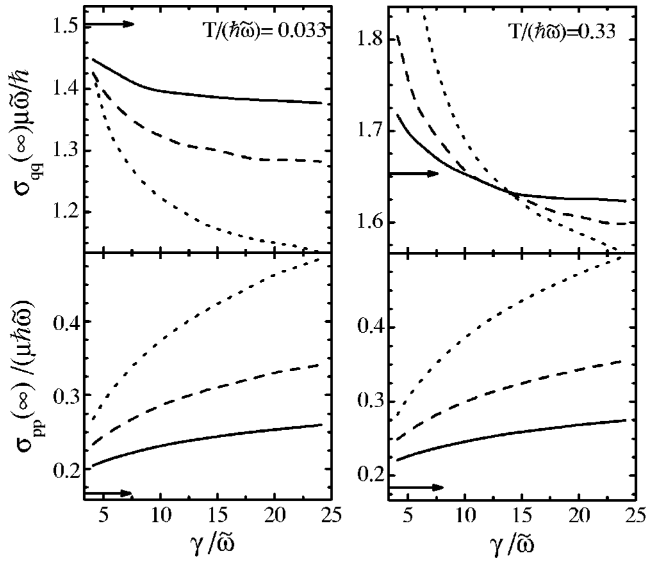

FIG. 8. For $\mu=50m_0$, $\hbar\tilde{\omega}=3$ MeV, and the indicated temperatures, the calculated asymptotic variances are shown as functions of $\gamma/\tilde{\omega}$ at $\lambda_p/\tilde{\omega}=0.33$ (solid lines), 0.66 (dashed lines), and 1.33 (dotted lines). The values of variances calculated with the "classic" diffusion coefficients D^c_{pp} are presented by arrows.

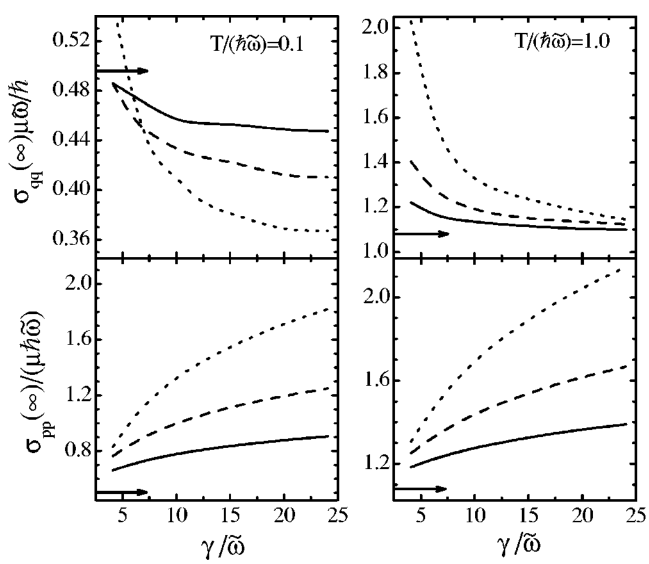

FIG. 9. The same as in Fig. 8, but for $\mu=448m_0$ and $\hbar\tilde{\omega}=1$ MeV. The calculations are performed for $\lambda_p/\tilde{\omega}=0.5$ (solid lines), 1 (dashed lines), and 2 (dotted lines).

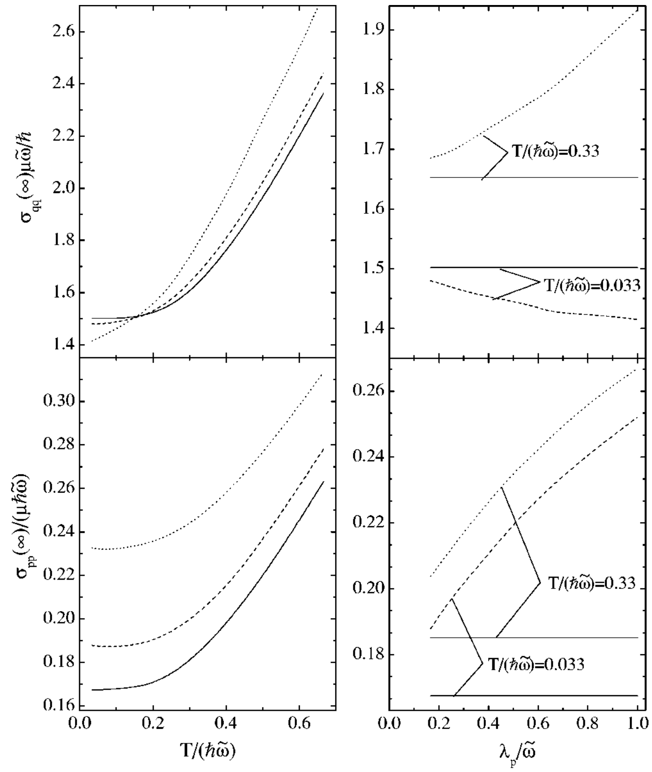

FIG. 10. For $\mu=50m_0$ and $\hbar\tilde{\omega}=3$ MeV, the calculated asymptotic variances $\sigma_{pp}(\infty)$ and $\sigma_{qq}(\infty)$ as functions of $T/(\hbar\tilde{\omega})$ (left side) and $\lambda_p/\tilde{\omega}$ (right side) are compared with the asymptotic variances obtained with the "classic" diffusion coefficients D_{pp}^c (solid lines). The temperature dependence is presented for $\lambda_p/\tilde{\omega}=0.17$ (dashed lines) and 0.66 (dotted lines). The dependence on λ_p is presented for $T/(\hbar\tilde{\omega})=0.033$ (dashed lines) and 0.33 (dotted lines).

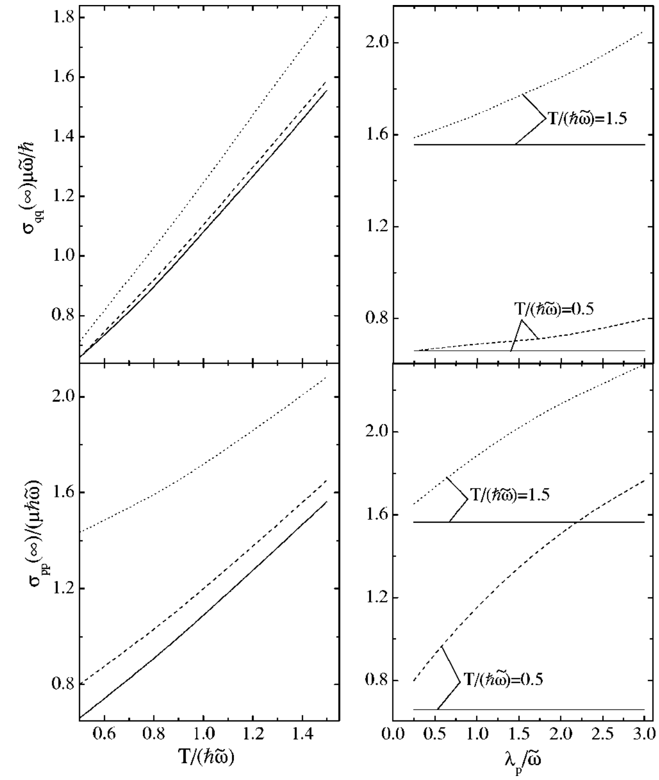

FIG. 11. The same as in Fig. 10, but for $\mu=448m_0$ and $\hbar\tilde{\omega}=1$ MeV. The temperature dependence is presented for $\lambda_p/\tilde{\omega}=0.5$ (dashed lines) and 2.0 (dotted lines). The dependence on $\lambda_p/\tilde{\omega}$ is presented for $T/(\hbar\tilde{\omega})=0.5$ (dashed lines) and 1.5 (dotted lines).

cients are shown in Figs. 2 and 3 for these cases. The diffusion and friction λ_p coefficients D_{pp}, D_{pq}, and λ_p, respectively, are equal to zero at initial time. After some transient time the coefficients take asymptotic values. The transient time increases with μ and λ_p. The values of D_{pp} and λ_p are positive at $t>0$. During a short initial time interval the value of D_{pq} is positive and becomes negative later on.

The dependences of asymptotic values of the coefficients D_{pp} and D_{pq} on T and λ_p are shown in Figs. 4 and 5. D_{pp} depends nearly linear on λ_p and T in the intervals considered. For larger $\tilde{\omega}$ in Fig. 4, the dependence of D_{pp} on T is rather weak because of the importance of quantum effects. With increasing temperature the absolute value of D_{pq} decreases approaching to zero in the limit $T\to\infty$.

The dependences of the calculated asymptotic values of D_{pp} and D_{pq} on the parameter γ are shown in Figs. 6 and 7 for various λ_p and two different T. The dependence on γ becomes steeper with increasing resulting λ_p. For $\hbar\gamma>7$ MeV, the value of D_{pq} is expected to be negative. For comparison, we show the "classic" values

$$D_{pp}^c = 0.5\hbar\lambda_p\mu\tilde{\omega}\coth[\hbar\tilde{\omega}/(2T)]$$

to demonstrate the resonability of the calculations with the chosen parameters. D_{pp}^c is smaller than the corresponding calculated D_{pp}. This difference increases with λ_p and $\tilde{\omega}$, but decreases with increasing T.

The dependence of the diffusion coefficients on γ leads to the dependence of the asymptotic variances σ_{qq} and σ_{pp} on γ (Figs. 8 and 9). As in the case of the diffusion coefficients, the dependence of σ_{qq} on γ becomes steeper with increasing λ_p. The asymptotic variances σ_{qq}^c and σ_{pp}^c obtained with the classic set of diffusion coefficients, $D_{pp}=D_{pp}^c$ and $D_{pq}=D_{qq}=0$, are shown in Figs. 8 and 9 as well. While, for $T=0.1$ MeV, $\sigma_{qq}<\sigma_{qq}^c$ for $\hbar\gamma>5$ MeV, we find, for large temperature $T=1$ MeV, $\sigma_{qq}>\sigma_{qq}^c$ for $\hbar\gamma<25$ MeV. The choice of $\hbar\gamma=12$ MeV looks reasonable for further applications in the case of $\hbar\tilde{\omega}<5$ MeV. In spite of a larger D_{pp} than the classic value, the difference between σ_{qq} and σ_{qq}^c is quite small due to the negativity of D_{pq}. Calculations of many observables like the penetrability of a barrier and the localization of a distribution in coordinate use often only σ_{qq}. Hence one cannot expect a large deviation of these calculated observables from the ones calculated with the classic D_{pp}^c. Therefore, the wide use of the classic diffusion coefficients is justified.

The calculated asymptotic variances as functions of T and λ_p are compared in Figs. 10 and 11 with the asymptotic variances σ_{qq}^c and σ_{pp}^c. The deviation of σ_{qq} and σ_{pp} from σ_{qq}^c and σ_{pp}^c, respectively, increases with λ_p. While the difference $\sigma_{qq}-\sigma_{qq}^c$ increases with T, the difference $\sigma_{pp}-\sigma_{pp}^c$ decreases weakly. In the purely quantum regime $\hbar\omega\gg T$, the value of σ_{qq} is smaller than σ_{qq}^c. With increasing T or decreasing $\hbar\omega$

the classic variance σ_{qq}^{c} underestimates σ_{qq}. However, the difference between σ_{qq} and σ_{qq}^{c} does not exceed 15% at $\hbar\lambda_p \leqslant 2$ MeV. Therefore, observables related to the asymptotic σ_{qq} can be obtained quite similarly with the present and classic diffusion coefficients. The corresponding comparison of the decay rate will be presented in paper II.

VII. SUMMARY

The generalized Linbland equations with nonstationary transport coefficients are derived from the Langevin equations for the case of nonlinear non-Markovian noise. The equations of motion for the collective coordinates are consistent with the generalized quantum fluctuation dissipation relations. Explicit expressions for the time-dependent transport coefficients are presented for the case of FC and RWA oscillators and a general linear coupling in the coordinate and momentum between the collective harmonic oscillator and heat bath.

The explicit equations for the correlation functions show that the Onsanger's regression hypothesis does not hold exactly for the non-Markovian equations of motion. However, under some conditions the regression of fluctuations goes to zero in the same manner as the average values.

In the low- and high-temperature regimes we found that the dissipation leads to long-time tails in correlation functions in the RWA oscillator. In the case of the FC oscillator a nonexponential powerlike decay of the correlation function in the coordinate is obtained only at the low-temperature limit.

The calculated results depend rather weakly on the parameter γ in many applications. The value of D_{pp}^{c} underestimates the asymptotic value of D_{pp}, but the asymptotic values of σ_{qq}^{c} and σ_{qq} are close due to the negativity of D_{qp}. The found transient times for $D_{pp}(t)$, $D_{qp}(t)$, and $D_{qq}(t)$ are quite short.

We plan to apply the elaborated formalism to the analysis of experiments on nuclear subbarrier fusion, fission, and binary reaction processes. For example, the lifetime of a dinuclear system with respect to the decay can be calculated in this approach. Also transient times in different nuclear dissipative non-Markovian processes can be investigated. In paper II we will study memory effects in the collective dynamics of a quantum system, in the escape through a potential barrier, in the capture into the potential well, and in the loss of quantum coherence.

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