On the applicability of the theory of quantum Markov processes to Brownian motion

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The stationary function of the momentum and the mean square of the displacement of a quantum Brownian particle are calculated using the theory of quantum Markov processes and, alternatively, the fluctuation dissipation theorem. The results are presented graphically. Comparison shows that the theory of quantum Markov processes is not applicable to the selected example of a system interacting with a heat bath.

1. INTRODUCTION

In a number of studies,[1–6] a theory of quantum Markov processes has been developed based on the quantum master equation

$$\dot{\rho}=\hat{L}\rho. \tag{1.1}$$

Here ρ is the system density of states in Schrödinger's representation and $\hat{L}$ is an operator acting in operator space. As is known, the ordinary *nonquantum* theory of Markov processes is perfectly adequate to describe the behavior of physical systems interacting with a heat bath. It is not at all obvious that the quantum version of this theory based on Eq. (1.1) gives a correct description of quantum systems interacting with a heat bath. Reference 7 expresses some doubt about this. One would expect that the application of theory of quantum Markov processes will lead to results inconsistent with the fluctuation dissipation theorem, or equivalently with the quantum Nyquist formula. The inapplicability of theory of quantum Markov processes to systems in interaction with a heat bath is rather a general rule than an exception. The reason for this is that the theory of quantum Markov processes yields correlation functions similar to those for the classical case, whereas the fluctuation dissipation theorem leads to more complex forms.

In the present paper we address the question of the applicability the theory of quantum Markov processes to a quantum Brownian particle described by the linear equation

$$m\ddot{\mathbf{r}}=-\gamma m\dot{\mathbf{r}}+\mathbf{F}(t), \tag{1.2}$$

where $\mathbf{r}$ is the radius vector operator of the particle and $\mathbf{F}$, the force on the particle. The medium is assumed to be isotropic. Reference 6 suggests the following equation to describe such a particle:

$$i\hbar\dot{\rho}=[H+A,\rho]+\frac{i\gamma_0}{\hbar}\{2\mathbf{C}\rho\mathbf{C}^+-[\mathbf{C}^+\mathbf{C},\rho]_+\}, \tag{1.3}$$

where

$$A=\frac{1}{4}\gamma_0(kTm)^{-1}[\mathbf{p},\mathbf{r}]_+,\quad \gamma_0=kT\gamma m,$$
$$\mathbf{C}=\mathbf{r}+\frac{i\hbar}{4kTm}\mathbf{p}, \tag{1.4}$$

and $H=p^2/2m$ is the Hamiltonian of the particle. It is shown in that paper that the above equation is a generalization of the familiar Fokker–Planck equation for a nonquantum particle, that is, in the limit $\hbar\to 0$ we obtain the equation for a nonquantum particle.

In the following, an equation of a more general nature than (1.3)–(1.4) will be employed. From that, equations for the relevant mean values and correlation functions are derived.

The stationary correlation function and the derivative of the mean square of displacement, as obtained by this method and from the quantum Nyquist formula, are presented graphically for various values of the dimensionless parameter $y=\hbar\gamma/kT$. In the quantum region, when this parameter is comparable to unity, one observes an appreciable discrepancy between the results of the two theories, which does not speak in favor of the theory of quantum Markov processes.

2. QUANTUM MARKOV THEORY OF BROWNIAN MOTION

The mean value of any operator B of a chosen system (a Brownian particle in the present case) at time t is

$$\langle B\rangle_t=\mathrm{Tr}[B\rho(t)]. \tag{2.1}$$

Differentiating both sides of this relation with respect to time and using (1.1) we obtain

$$d\langle B\rangle_t/dt=\mathrm{Tr}\{B[\hat{L}\rho(t)]\}.$$

On the right, the operator $\hat{L}$ may be transferred to B giving

$$d\langle B\rangle_t/dt=\mathrm{Tr}\{[\hat{L}^TB]\rho(t)\}$$

or, in view of (2.1),

$$d\langle B\rangle_t/dt=\langle\hat{L}^TB\rangle_t. \tag{2.2}$$

Here the transposed operator $\hat{L}^T$ is defined by the equation

$$\mathrm{Tr}[M(\hat{L}\rho)]=\mathrm{Tr}[(\hat{L}^TM)\rho]$$

valid for any M and ρ. Equation (2.2) will be used below.

It is quite natural that $\langle B\rangle_t$ is exactly the mean of the operator $B(t)$ in Heisenberg's representation. Let us present here a proof of the corresponding equality

$$\langle B\rangle_t=\langle B(t)\rangle. \tag{2.3}$$

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The Schrödinger density matrix $\rho(t)$ of the chosen system relates to the matrix density $\rho_{tot}(t)$ of the total system (the chosen system plus the heat bath) by the relation

$$\rho(t)=\mathrm{Tr}_T\rho_{tot}(t), \qquad (2.4)$$

where Tr_T is the trace over the heat bath (in our case, medium) variables. Recall that the trace over the variables of the chosen system is denoted by Tr. The mean value of any observable can be written in two ways: in Heisenberg's representation we have

$$\langle B(t)\rangle=\mathrm{Tr}\,\mathrm{Tr}_T[B(t)\rho_{tot}(0)],$$

whereas in the Schrödinger picture

$$\langle B(t)\rangle=\mathrm{Tr}\,\mathrm{Tr}_T[B\rho_{tot}(t)]. \qquad (2.5)$$

If B is an operator of the chosen system, then the right-hand side of the last equation may be written as $\mathrm{Tr}\{B[\mathrm{Tr}_T\rho_{tot}(t)]\}$ or, in view of (2.4), as $\mathrm{Tr}\{B\rho(t)\}$. Therefore (2.5) gives (2.3). The index t on the average $\langle ...\rangle$ is henceforth dropped.

The behavior of the Brownian particle will be described by the equation

$$\dot{\rho}=\frac{1}{i\hbar}[H+A,\rho]+\frac{\gamma}{\hbar}\sum_{j=1}^{r}\{2\mathbf{C}_j\rho\mathbf{C}_j^+-[\mathbf{C}_j^+\mathbf{C}_j,\rho]_+\} \qquad (2.6)$$

of a more general form than (1.3). Here

$$\mathbf{C}_j=\lambda u_j\mathbf{r}+\lambda^{-1}v_j p,\quad A=\tfrac{1}{2}z[\mathbf{r},\mathbf{p}]_+, \qquad (2.7)$$

where $u_j=u_{1j}+iu_{2j}$ and $v_j=v_{1j}+iv_{2j}$ are complex numbers; z, u_{1j}, u_{2j}, v_{1j}, and v_{2j} are real numbers; and $\lambda=(\gamma m)^{1/2}$ is introduced to render u_j, v_j dimensionless. It is easy to verify that Eq. (2.6) ensures the conservation, in time, of the normalization, hermiticity, and nonnegative definiteness of the density matrix. Operators (2.7) are chosen such as to yield a solution in the class of Gaussian matrices $\rho(t)$.

Knowing the operator $\hat{L}$, i.e., the form of the right-hand side of (2.6), it is easily found that

$$\hat{L}^T B=\frac{1}{i\hbar}[B,H+A]+\frac{\gamma}{\hbar}\sum_{j=1}^{r}\{2\mathbf{C}_j^+B\mathbf{C}_j-[\mathbf{C}_j^+\mathbf{C}_j,B]_+\}. \qquad (2.8)$$

The expression in the curly brackets may also be written as

$$\mathbf{C}_j^+[B,\mathbf{C}_j]+[\mathbf{C}_j^+,B]\mathbf{C}_j.$$

In Eq. (2.2) we first put $B=r_\alpha$ and then $B=p_\alpha$. Using (2.8) in the case $H=p^2/2m$ we have

$$\frac{d\langle\mathbf{r}\rangle_t}{dt}=\frac{\langle\mathbf{p}\rangle}{m}-\gamma\Big[z-2\sum_j(u_{1j}v_{2j}-u_{2j}v_{1j})\Big]\langle\mathbf{r}\rangle,$$
$$\frac{d\langle\mathbf{p}\rangle_t}{dt}=-\gamma\Big[z+2\sum_j(u_{1j}v_{2j}-u_{2j}v_{1j})\Big]\langle\mathbf{p}\rangle. \qquad (2.9)$$

In accordance with (1.2) it is assumed that the coefficient of liquid friction is γm, that is,

$$\frac{d\langle\mathbf{p}\rangle}{dt}=-\gamma\langle\mathbf{p}\rangle,\quad \frac{d\langle\mathbf{r}\rangle}{dt}=\frac{\langle\mathbf{p}\rangle}{m}. \qquad (2.10)$$

Comparing these equations with (2.9) we find that

$$z=1/2,\quad \sum_j(u_{1j}v_{2j}-u_{2j}v_{1j})=1/4. \qquad (2.11)$$

Next, by specifying B in (2.2) as r^2, p^2, and $[\mathbf{r},\mathbf{p}]_+$ successively, we obtain

$$\frac{d\langle r^2\rangle}{dt}=\frac{1}{m}\langle[\mathbf{r},\mathbf{p}]_+\rangle+\frac{6\hbar}{m}|\mathbf{V}|^2, \qquad (2.12)$$

$$\frac{d\langle p^2\rangle}{dt}=-2\gamma\langle p^2\rangle+6\hbar\gamma^2m|\mathbf{U}|^2, \qquad (2.13)$$

$$\frac{d\langle[\mathbf{r},\mathbf{p}]_+\rangle}{dt}=\frac{2}{m}\langle p^2\rangle-\gamma\langle[\mathbf{r},\mathbf{p}]_+\rangle-12\hbar\gamma\mathbf{U}\mathbf{V}. \qquad (2.14)$$

Here we have used expressions (2.11) and introduced $2r$-dimensional vectors

$$\mathbf{U}=(u_{11},u_{21},...,u_{1r},u_{2r}),\quad \mathbf{V}=(v_{11},v_{21},...,v_{1r},v_{2r}).$$

In addition to $\mathbf{U}$ and $\mathbf{V}$, we can also introduce a vector $\mathbf{U}'=(-u_{21},u_{11},...,-u_{2r},u_{1r})$ which, as can be readily verified, is orthogonal to $\mathbf{U}$ and is of the same magnitude, $|\mathbf{U}'|=|\mathbf{U}|$. Then the second equation of (2.11) can be written as

$$\mathbf{U}'\mathbf{V}=\frac{1}{4}. \qquad (2.15)$$

Let us consider the case when the momentum $\mathbf{p}(t)$ represents a stationary quantum process. Applying the quantum regression theorem (see, e.g., Refs. 1 and 5), and using the first equation of (2.10), one easily finds

$$\partial\langle p_\alpha(t+\tau)p_\beta(t)\rangle/\partial t=-\gamma\langle p_\alpha(t+\tau)p_\beta(t)\rangle,\quad \tau>0,$$

which enables one to obtain the stationary correlation function

$$\langle p_\alpha(t+\tau)p_\beta(t)\rangle=\tfrac{1}{3}\langle p^2\rangle_{st}\exp(-\gamma|\tau|)\delta_{\alpha\beta}. \qquad (2.16)$$

Here $\langle p^2\rangle_{st}$ is the stationary dispersion. Also, from Eq. (2.13) in the stationary case we find

$$|\mathbf{U}|^2=(3\hbar\gamma m)^{-1}\langle p^2\rangle_{st}, \qquad (2.17)$$

because the quantity $\langle p^2\rangle=\langle p^2\rangle_{st}$ is then a constant.

It is not difficult to find the solution to equations (2.12) and (2.14) if one knows the initial values $\langle r^2\rangle_0$ and $\langle[\mathbf{r},\mathbf{p}]_+\rangle_0$. We will proceed in a somewhat different way, however: introduce $\Delta\mathbf{r}(t)=\mathbf{r}(t)-\mathbf{r}(0)$, the displacement of the Brownian particle in a time t, and consider its mean square value. We have

$$\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle}{dt}=\frac{d\langle r^2(t)\rangle}{dt}-\frac{d\langle[\mathbf{r}(t),\mathbf{r}(0)]_+\rangle}{dt}. \qquad (2.18)$$

Applying again the quantum regression theorem discussed above, with the aid of the second of Eqs. (2.10) we find

$$\frac{d\langle[\mathbf{r}(t),\mathbf{r}(0)]_+\rangle}{dt}=\frac{1}{m}\langle[\mathbf{p}(t),\mathbf{r}(0)]_+\rangle. \qquad (2.18')$$

Using this and (2.12), we have from (2.18)

$$\frac{d\langle|\Delta\mathbf{r}|^2\rangle}{dt}=\frac{1}{m}\langle[\Delta\mathbf{r},\mathbf{p}]_+\rangle+\frac{6\hbar}{m}|\mathbf{V}|^2. \tag{2.19}$$

Similarly, from (2.14) we can deduce

$$\frac{d\langle[\Delta\mathbf{r},\mathbf{p}]_+\rangle}{dt}=-\gamma\langle[\Delta\mathbf{r},\mathbf{p}]_+\rangle+\frac{2}{m}\langle p^2\rangle-12\hbar\gamma\mathbf{UV}. \tag{2.20}$$

Needless to say, Eqs. (2.19) and (2.20) must be solved for the trivial boundary conditions

$$\langle|\Delta\mathbf{r}|^2\rangle_0=0,\quad \langle[\Delta\mathbf{r},\mathbf{p}]_+\rangle_0=0.$$

For a stationary $\mathbf{p}(t)$ process, when $\langle p^2\rangle=\langle p^2\rangle_{\rm st}$, the solution to Eq. (2.20) is trivial:

$$\langle[\Delta\mathbf{r},\mathbf{p}]_+\rangle=6\hbar(|\mathbf{U}|^2-2\mathbf{UV})(1-e^{-\gamma t})$$

[using (2.17)]. Hence (2.19) takes the form

$$\frac{d\langle|\Delta\mathbf{r}|^2\rangle}{dt}=\frac{6\hbar}{m}|\mathbf{U}-\mathbf{V}|^2(1-e^{-\gamma t})+\frac{6\hbar}{m}|\mathbf{V}|^2e^{-\gamma t}. \tag{2.21}$$

From this,

$$\frac{\langle|\Delta\mathbf{r}|^2\rangle}{dt}=\frac{6\hbar}{m}|\mathbf{U}-\mathbf{V}|^2t-\frac{6\hbar}{m\gamma}(|\mathbf{U}|^2-2\mathbf{UV})(1-e^{-\gamma t}). \tag{2.22}$$

We see that for large times $t\gg\gamma^{-1}$, the motion is virtually pure diffusive, i.e.,

$$\langle|\Delta\mathbf{r}|^2\rangle=6Dt,$$

where

$$D=\hbar m^{-1}|\mathbf{U}-\mathbf{V}|^2 \tag{2.23}$$

is the diffusion coefficient. Therefore the first term on the right-hand side of (2.22) may be viewed as being determined by the quantity D. As for the second term on the right-hand side of (2.21), for this we have derived in the Appendix the inequality

$$|\mathbf{V}|^2\geqslant D_0+|\mathbf{U}|^2-2(|\mathbf{U}|^2D_0-1/16)^{1/2}, \tag{2.24}$$

where $D_0=\hbar^{-1}mD$ and $|\mathbf{U}|^2=\langle p^2\rangle_{\rm st}/(3\hbar\gamma m)$. It is assumed that $|\mathbf{U}|^2D_0\geqslant 1/16$.

In the special case (1.3), (1.4) we have

$$r=1,\quad \mathbf{U}=\left(\frac{kT}{\hbar\gamma}\right)^{1/2}(1,0),\quad \mathbf{V}=\frac{1}{4}\left(\frac{\hbar\gamma}{kT}\right)^{1/2}(0,1),$$
$$\langle p^2\rangle_{\rm st}=3kTm,\quad D=D_{\rm cl}+\frac{\gamma\hbar^2}{16kTm}, \tag{2.25}$$

where $D_{\rm cl}=kT/(m\gamma)$ is the classical diffusion coefficient. In this case (2.24) and (A5) hold with the equality sign.

Note that the result (2.22) seems somewhat strange because the limit

$$\lim_{t\to 0}\frac{1}{t^2}\langle|\Delta\mathbf{r}(t)|^2\rangle=\lim_{t\to 0}\frac{6\hbar}{mt}|\mathbf{V}|^2=\infty \tag{2.26}$$

turns out to differ from the mean of the absolute velocity squared

$$\langle v^2\rangle_{\rm st}=\langle p^2\rangle_{\rm st}/m^2.$$

Moreover, the limit (2.26) cannot be made finite because one cannot equate $|\mathbf{V}|$ to zero in view of (2.15). If on the other hand we put $\langle p^2\rangle_{\rm st}=\infty$, then, by (2.24), we have $|\mathbf{V}|^2=\infty$ and hence $\langle|\Delta\mathbf{r}|^2\rangle=\infty$, which is absurd.

In concluding this section we consider the case of non-stationary momentum fluctuations by assuming, namely, that at time $t=0$ the temperature jumps from T_1 to T_2 while remaining constant both before and after this. Then the calculation of the derivative (2.21) requires Eq. (2.20), but to determine $\langle p^2(t)\rangle$ one needs to solve the nontrivial equation (2.13). For the values given in (2.25), it has the form

$$d\langle p^2\rangle/dt+2\gamma\langle p^2\rangle=6\gamma kT_2m$$

for $t>0$. Solving the last equation for the initial condition $\langle p^2(0)\rangle=3kT_1m$, and (2.20) for the above-mentioned zero initial condition, (2.19) yields

$$\frac{d\langle|\Delta\mathbf{r}|^2\rangle}{dt}=\frac{6k}{\gamma m}(1-e^{-\gamma t})[(1-e^{-\gamma t})T_2+e^{-\gamma t}T_1]+\frac{3\hbar^2\gamma}{8kT_2m}. \tag{2.27}$$

In the following, the above results are compared with those from a non-Markovian theory.

3. BROWNIAN MOTION CALCULATION USING THE QUANTUM NYQUIST FORMULA

A different behavior of a quantum Brownian particle results from the fluctuation dissipation theorem, or equivalently from the quantum Nyquist formula. Introducing the velocity vector $\mathbf{v}=\dot{\mathbf{r}}$ reduces (1.2) to

$$m\dot{\mathbf{v}}+\gamma m\mathbf{v}=\mathbf{f},$$

with $\mathbf{f}$ the external force. It is expedient at this point to go over to spectra. The impedance $Z_{\alpha\beta}(\omega)$ is defined by the relation

$$f_\alpha(\omega)=\sum_\beta Z_{\alpha\beta}(\omega)V_\beta(\omega).$$

Using the above equations we find

$$Z_{\alpha\beta}(\omega)=m(i\omega+\gamma)\delta_{\alpha\beta}. \tag{3.1}$$

The quantum Nyquist formula is (see, e.g., Ref. 7)

$$[S_{\alpha\beta}(\omega)]_F=\hbar\omega\coth\left(\frac{\hbar\omega}{2kT}\right)\mathrm{Re}\,Z_{\alpha\beta}(\omega), \tag{3.2}$$

provided $Z_{\alpha\beta}(\omega)=Z_{\beta\alpha}(\omega)$ as is the case here. The formula determines the spectral density of a random force $\mathbf{F}(t)$ of mean zero. Substituting (3.1) into (3.2) we obtain

$$[S_{\alpha\beta}(\omega)]_F=\hbar\omega\gamma m\coth\left(\frac{\hbar\omega}{2kT}\right)\delta_{\alpha\beta}. \tag{3.3}$$

Taking account of the random force $\mathbf{F}$ and assuming that the external force $\mathbf{f}$ is zero we obtain instead of (1.2) the equation $\dot{\mathbf{p}}+\gamma\mathbf{p}=\mathbf{F}$, or in spectral form,

$$(i\omega+\gamma)p(\omega)=F(\omega).$$

Here $\mathbf{p}=m\mathbf{v}$ is the particle momentum. Using this along with (3.3) we obtain the momentum spectral density

$$[S_{\alpha\beta}(\omega)]_p=\frac{\hbar\omega\gamma m}{\omega^2+\gamma^2}\coth\left(\frac{\hbar\omega}{2kT}\right)\delta_{\alpha\beta}. \tag{3.4}$$

The inverse Fourier transform

$$\langle p_\alpha(t+\tau)p_\beta(t)\rangle\equiv[K_{\alpha\beta}(\tau)]_p$$
$$=\frac{1}{2\pi}\int_{\infty}^{\infty}e^{i\omega\tau}[S_{\alpha\beta}(\omega)]_p d\omega$$

determines the stationary correlation function of the momentum. Using (3.4) and performing the integral by means of residue theory,

$$[K_{\alpha\beta}(\tau)]_p=K_p(\tau)\delta_{\alpha\beta},$$
$$K_p(\tau)=\hbar\gamma m\left\{2\sigma^2\sum_{n=1}^{\infty}\frac{2\pi n\exp(-2\pi n\sigma|\tau|)}{(2\pi n\sigma)^2-\gamma^2}+\frac{1}{2}\exp(-\gamma|\tau|)\cot\left(\frac{y}{2}\right)\right\}, \tag{3.5}$$

where we have introduced the notation $\sigma=kT/\hbar=\gamma/y$.

The momentum correlation function tends to infinity as $|\tau|\to 0$, that is, the mean square of the momentum is infinite in the quantum case. This relates to the fact that the integral of (3.4) is logarithmically divergent for infinite limits of integration. This infinity can be related to the temperature-independent "background" part $K_p^0(\tau)$ by writing the correlation function as a sum

$$K_p(\tau)=K_p^{(1)}(\tau)+K_p^{(0)}(\tau),$$

where $K^{(1)}$ is the nonsingular part and $K^{(0)}$ describes the "background" (or "vacuum") momentum fluctuations. The latter part is separated out by taking the limit $T\to 0$. Calculation shows that

$$[S_{\alpha\beta}^{(0)}(\omega)]_p=\frac{\hbar|\omega|\gamma m}{\omega^2+\gamma^2}\delta_{\alpha\beta},$$
$$K_p^{(0)}(\tau)=-(2\pi)^{-1}\hbar\gamma m\{e^{-\gamma|\tau|}E_i(\gamma|\tau|)+e^{\gamma|\tau|}E_1(\gamma|\tau|)\}.$$

The right-hand side of this expression the exponential integral (see, e.g., Ref. 8).

The behavior of the correlation function (3.5) is more complex than that of the function (2.16), which has a classical form independent of the "quantization" parameter $y=\hbar\gamma/kT$. In Fig. 1 are shown the functions $K_p(\tau)/(kTm)$ (curves *1*) and $K_p^{(1)}(\tau)/(kTm)$ (curves *2*) plotted against the dimensionless time $x=\gamma\tau$ for two values of y ($y=0.5$: dashed lines; $y=1$: solid lines).

Now let us consider the particle displacement

$$\Delta\mathbf{r}(t)=\frac{1}{m}\int_0^t\mathbf{p}(t')dt'.$$

Using this equation we find

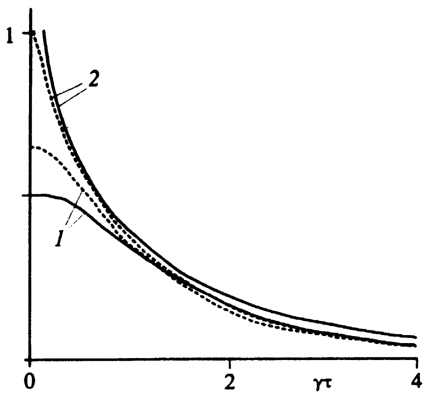

FIG. 1. Momentum correlation functions $K_p(\tau)$ (*1*) and $K_p^{(1)}(\tau)$ (*2*) calculated for quantization parameter values of $y=0.5$ (dashed lines) and $y=1$ (solid lines) using the fluctuation dissipation theorem.

$$\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle}{dt}=\frac{2}{m^2}\int_0^t\langle\mathbf{p}(t')\mathbf{p}(t)\rangle dt'$$
$$=\frac{2}{m^2}\int_0^t\langle\mathbf{p}(0)\mathbf{p}(t'')\rangle dt''.$$

Here we have put $t''=t-t'$ and used the stationarity of the momentum fluctuations. Substituting $[K_{\alpha\beta}(\tau)]_p=K(\tau)\delta_{\alpha\beta}$, we obtain

$$\frac{d\langle|\Delta\mathbf{r}|^2\rangle}{dt}=\frac{6}{m^2}\int_0^t K(\tau)d\tau.$$

Using (3.5), we have after integration that

$$\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle}{dt}=\frac{6kT}{m\gamma}\left[1-2\gamma^2\sum_{n=1}^{\infty}\frac{\exp(-2\pi n\sigma t)}{(2\pi n\sigma)^2-\gamma^2}-\frac{y}{2}e^{-\gamma t}\cot\left(\frac{y}{2}\right)\right].$$

In Fig. 2 the resulting dependence—or more accurately the function $(6D_{cl})^{-1}d\langle|\Delta\mathbf{r}(t)|^2\rangle/dt$—is depicted by solid lines for several values of the parameter $y=\gamma\hbar/kT$. The dashed lines show the same dependence corresponding—for the same y's—to Eq. (2.21) with the parameters (2.25): the dependence, in other words, obtained from the quantum Markov theory. The dash-dot line corresponds to the classical limit.

In the temperature jump case discussed at the end of the preceding section, we shall assume that the nonstationary force correlation function is defined by a simple interpolation formula:

$$[K_{\alpha\beta}(t_1,t_2)]_F=\begin{cases}[K_{\alpha\beta}^{(1)}(t_1-t_2)]_F & \text{for} \quad t_1+t_2<0\\ [K_{\alpha\beta}^{(2)}(t_1-t_2)]_F & \text{for} \quad t_1+t_2>0.\end{cases} \tag{3.6}$$

Here $[K_{\alpha\beta}^{(i)}(\tau)]_F$ is the correlation function of stationary force fluctuations at constant temperature T_i, defined by a formula of the type (3.5). From $\dot{\mathbf{p}}+\gamma\mathbf{p}=\mathbf{F}$ we have

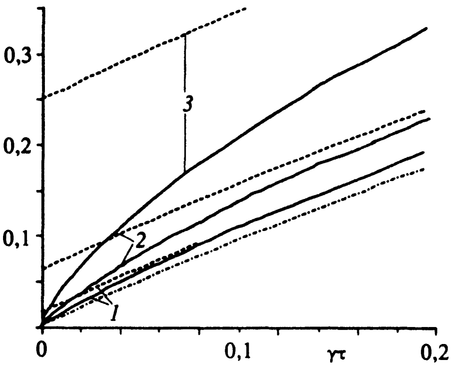

FIG. 2. Derivatives of the mean of the squared displacement, $d\langle|\Delta\mathbf{r}(t)|^2\rangle/dt$, calculated for different values of the quantization parameter using the fluctuation dissipation theorem (solid lines) and the quantum master equation (dashed lines): $y=0.5$ (curves *1*); $y=1$ (curves *2*); $y=2$ (curves *3*).

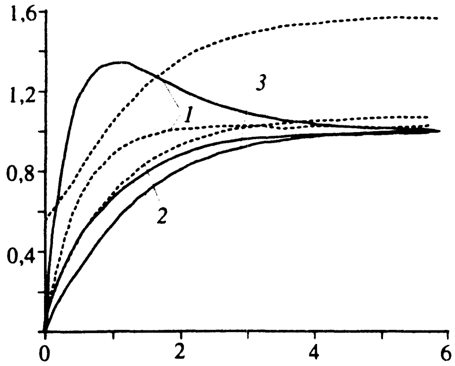

FIG. 3. The derivative of the mean of the squared displacement calculated in two ways for various values of the "quantization" parameter in the temperature jump case: $y=0.5$ (curves *1*); $y=1$ (curves *2*); $y=3$ (curves *3*).

$$\mathbf{p}(t)=\int_{-\infty}^{t}\exp[-\gamma(t-t')]_F(t')dt'.$$

Therefore

$$\langle p_\alpha(t_1)p_\beta(t_2)\rangle=\int_{-\infty}^{t_1}dt_1'\int_{-\infty}^{t_2}dt_2'\exp\int -\gamma(t_1+t_2)+\gamma(t_1'+t_2')]K_{\alpha\beta}(t_1't_2')_F.$$

Substituting (3.7) one finds the nonstationary momentum correlation function giving the derivative

$$\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle}{dt}=\frac{2}{m^2}\int_0^t\langle\mathbf{p}(t_1)\mathbf{p}(t)\rangle dt_1.$$

Calculation leads to the result

$$\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle}{dt}=\frac{d\langle|\Delta\mathbf{r}(t)|^2\rangle_{T_2}}{dt}+\frac{6kT}{m\gamma}\left\{\left(1-\frac{y_1}{y_2}\right)(e^{-\gamma t}-e^{-2\gamma t})-\sum_{i=1}^{2}\sum_{n=1}^{\infty}\frac{(-1)^i\exp[-(2\pi n\sigma_i+\gamma)2t]\sigma_i}{2\pi n\sigma_i+\gamma}\times\left[e^{\gamma t}-1+\frac{\gamma[\exp((4\pi\sigma_i n+\gamma)t)-1]}{4\pi n\sigma_i+\gamma}\right]\right\}.$$

The dependence thus obtained is represented in Fig. 3. The curves *1*, *2*, and 3 correspond to the values $y=0.5$, 1, and 3, respectively. The dashed lines show the behavior of the function (2.27) as calculated by Markov theory for the same values of the parameters.

One can see a considerable difference between the results of the two theories as shown in the figures. There exist no regions of simultaneous applicability of the two theories (except, of course, for the nonquantum limit $\hbar\gamma\ll kT$). This is indicative of the invalidity of Markov theory in the essentially quantum case.

APPENDIX. DERIVATION OF THE AUXILIARY INEQUALITY

Denoting $D_0=\hbar^{-1}mD$ and using (2.23) we have

$$D_0=|\mathbf{U}-\mathbf{V}|^2. \tag{A1}$$

Introduce orthogonal unit vectors $\mathbf{n}=\mathbf{U}/|\mathbf{U}|$ and $\mathbf{n}'=\mathbf{U}'/|\mathbf{U}|$ and define a vector

$$\mathbf{V}_\perp=\mathbf{V}-(\mathbf{Vn})\mathbf{n}-(\mathbf{Vn}')\mathbf{n}'$$

orthogonal to them. It is obvious that, in view of this orthogonality, the absolute square of the vectors

$$\mathbf{V}=(\mathbf{Vn})\mathbf{n}+(\mathbf{Vn}')\mathbf{n}'+\mathbf{V}_\perp$$

and

$$\mathbf{V}-\mathbf{U}=(\mathbf{Vn}-|\mathbf{U}|)\mathbf{n}+(\mathbf{Vn}')\mathbf{n}'+\mathbf{V}_\perp$$

can be written as

$$|\mathbf{V}|^2=(\mathbf{Vn})^2+(\mathbf{Vn}')^2+|\mathbf{V}_\perp|^2,$$
$$D_0=(\mathbf{Vn}-|\mathbf{U}|)^2+(\mathbf{Vn}')^2+|\mathbf{V}_\perp|^2 \tag{A2}$$

[using (A1)]. Solving the second of these equations for $\mathbf{Vn}$ we find

$$\mathbf{Vn}=|\mathbf{U}|\pm[D_0-(\mathbf{Vn}')^2-|\mathbf{V}_\perp|^2]^{1/2}. \tag{A3}$$

Substitution of (A3) into the first of Eqs. (A2) gives

$$|\mathbf{V}|^2=|\mathbf{U}|^2+D_0\pm2|\mathbf{U}|[D_0-(\mathbf{Vn}')^2-|\mathbf{V}_\perp|^2]^{1/2}. \tag{A4}$$

Now suppose

$$D_0\geqslant(\mathbf{Vn})^2=(\mathbf{UV})^2/|\mathbf{U}|^2.$$

Since

$$[D_0-(\mathbf{Vn}')^2-|\mathbf{V}_\perp|^2]^{1/2}\leqslant[D_0-(\mathbf{Vn}')^2]^{1/2},$$

we obtain from (A4) the inequalities

$$|\mathbf{V}|^2\geqslant D_0+|\mathbf{U}|^2-2[D_0|\mathbf{U}|^2-(\mathbf{U}'\mathbf{V})^2]^{1/2},$$
$$|\mathbf{V}|^2\leqslant D_0+|\mathbf{U}|^2+2[D_0|\mathbf{U}|^2-(\mathbf{U}'\mathbf{V})^2]^{1/2}. \tag{A5}$$

In view of (2.15), we can write here 1/16 instead of $(U'V)^2$.

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Translated by E. Strelchenko

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