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Correlation in the Langevin theory of Brownian motion

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In a paper with the same title as the above, Manoliu and Kittel calculated the high temperature ensemble average of the nonequal time product of the displacement and random force in the classical Brownian motion problem. Here, using a generalized quantum Langevin equation (GLE), we generalize these considerations to the quantum case and to the case of an arbitrary heat bath (such as, e.g., the blackbody radiation heat bath). Also, we consider an arbitrary temperature and we generalize beyond Brownian motion to the case of a harmonically bound particle in a heat bath. In addition, we point out that correlations of the type considered are widely used in many applications in a variety of different areas of physics and we review some recent applications of the GLE.

I. INTRODUCTION

The motion of a "Brownian particle" [1] (an otherwise free particle in a dissipative environment) is described most elegantly by Langevin's stochastic classical differential equation[2]

$$m\ddot{x}+m\gamma\dot{x}=F(t), \tag{1}$$

where m and x denote the mass and coordinate of the particle, respectively, and the dot denotes differentiation with respect to time. The force on the particle consists of the frictional (dissipative) term-$m\gamma\dot{x}$ and the random (fluctuation or noise) term $F(t)$.

Since the past motion does not appear in Eq. (1), one says there is no memory. In addition, the autocorrelation of the random force is a δ function and is also proportional to γ. The latter result is a manifestation of the fluctuation–dissipation relation.

The question of the ensemble average of the product of the displacement and the random force was examined by Manoliu and Kittel in a paper in this journal.[3] In particular, they verified an assertion of Langevin that, for the case of Eq. (1),

$$\langle x(t)F(t)\rangle=0. \tag{2}$$

Equation (1) describes what is often referred to as the Ohmic (or Drude) model (no memory terms) of a classical heat bath. The question arises as to the correctness or otherwise of Eq. (2), when one considers more realistic models, since Eq. (1) is essentially a phenomenological model which has not been derived from microscopic considerations. Further, the calculations of Ref. 3 are confined to the case of high temperature. Thus, we wish to consider the possible effect of extending the calculations of Ref. 3 to the quantum, arbitrary temperature domain with inclusion of possible memory effects. In addition, we wish to go beyond Brownian motion by considering the effect of an external potential. The machinery required to do this is the generalized quantum Langevin equation (GLE). This equation will be discussed at length in the next section. We will then go on to apply our results to various situations and we show how the results of Manoliu and Kittel[3] get modified in the more general case. In particular, we also demonstrate that the results of Ref. 3 follow simply and elegantly from our general formalism. Finally, we present a discussion of our results.

However, before moving on to our specific problem, we would like to discuss its relevance to a broad range of investigations which incorporate dissipation and fluctuations as an essential element.

The study of fluctuation phenomena in science began in essence in 1827 with the observations of the Scottish botanist, Robert Brown.[1] It is interesting to note that these early observations are still a source of great interest and controversy.[4] An explanation of these results was first provided by Einstein[5] using a discrete time assumption. An entirely new approach was later presented by Langevin[2] in the form of a stochastic differential equation. For a survey of this early work we refer to the treatise by Gardiner,[6] but we would be remiss if we did not refer to the major contributions and extensions of the theory described in Refs. 7–9. It soon became apparent that a Langevin-type equation provides the framework for discussing fluctuation and dissipative phenomena over a wide spectrum of physical phenomena.

In general, there is an intimate connection between fluctuations and dissipation which is referred to as the fluctuation-dissipation (FD) theorem. For example, Nyquist[10] showed that the random fluctuations in voltage across a resistor measured by Johnson[11] are determined by its impedance. A general quantum formulation of the FD theorem appears in the celebrated paper of Callen and Welton.[12] This theorem is a key ingredient of the pioneering work of Kubo[13,14] on linear response theory in nonequilibrium statistical mechanics. Correlations of the type discussed in the present paper are widely used in the work of Kubo and others. Another major advance is contained in the work of Mori,[15] who showed that a microscopic equation of motion can generally be transformed into the form of a GLE.

Over the past 10 yr, two of us (G.W.F. and R.F.O.) have collaborated extensively with Lewis on problems involving the GLE. In Ref. 16 we gave a detailed discussion of this equation and we discussed various models of a heat bath which have appeared in the literature. The particular case of a blackbody radiation heat bath was discussed at length[16,17] for the purpose of calculating atomic energy shifts due to blackbody radiation.[18] Transport theory was also discussed[19] and, in fact, Hu and O'Connell have shown that a many-body Hamiltonian problem may be reformulated in terms of a GLE for the center-of-mass of the electrons,[20,21] which led them to an expression for the conductivity which is actually simpler than that obtained using the Kubo approach. In addition, we note that G.W.F. and R.F.O. returned to the problem of a blackbody radiation heat bath to obtain an improved equation for the radiating election;[22] this equation, in contrast to the Abraham–Lorentz equation, is second order, it does not display runaway solutions and it leads to a modification of the familiar Larmor formula.[23]

Modern lithographic methods have led to a burgeoning of interest in mesoscopic systems which, by their nature, are more sensitive to the dissipative effects caused by their environment. In particular, quantum tunneling in a variety of systems is affected by dissipation, a subject which was discussed in the pioneering paper of Caldeira and Leggett.[24] The starting point of the latter authors and most others[25] is a Lagrangian which permits use of path integral, instanton, and functional integral methods. By contrast, our starting point is a Hamiltonian which is used to derive a GLE. In particular, this enabled us to develop a GLE approach to dissipative quantum tunneling.[26] The Langevin approach has also been used by Cleland *et al.*[27] and by Hu and O'Connell[28] to calculate the effect of charge fluctuations, arising from the environment, on current-voltage curves for small-capacitance tunnel junctions.

Finally, we note that Brownian motion is being interpreted in a new light by investigators in the relatively new field of fractals; the path of the microscopic particles observed by Brown is referred to as a Brownian fractal curve.[29,30]

II. GENERALIZED QUANTUM LANGEVIN EQUATION

In recent years, there has been widespread interest in dissipative problems arising in a variety of areas in physics. As it turns out, solutions to many of these problems are encompassed by a generalization of Eq. (1) to encompass quantum, memory, and non-Markovian effects, as well as arbitrary temperature and the presence of an external potential $V(x)$. We refer to this as the GLE

$$m\ddot{x}+\int_{-\infty}^{t} dt'\,\mu(t-t')\dot{x}(t')+V'(x)=F(t), \tag{3}$$

where $V'(x)=dV(x)/dx$ is the negative of the time-independent external force and $\mu(t)$ is the so-called memory function.

A detailed discussion of Eq. (3) appears in Ref. 16. In particular, it was pointed out the GLE corresponds to a macroscopic description of a quantum system interacting with a quantum-mechanical heat bath and that this description can be precisely formulated, using such general principles as causality and the second law of thermodynamics. We also stressed that this is a model-independent description. However, the GLE can be realized with a simple and convenient model, viz. the independent-oscillator (IO) model. The Hamiltonian of the IO system is

$$H=\frac{p^2}{2m}+V(x)+\sum_j\left(\frac{p_j^2}{2m_j}+\frac{1}{2}m_j\omega_j^2(q_j-x)^2\right). \tag{4}$$

Here m is the mass of the quantum particle while m_j and ω_j refer to the mass and frequency of heat-bath oscillator j. In addition, x and p are the coordinate and momentum operators for the quantum particle and q_j and p_j are the corresponding quantities for the heat-bath oscillators. Use of the Heisenberg equations of motion lead to the GLE, Eq. (3), describing the time development of the particle motion, with

$$\mu(t)=\sum_j m_j\omega_j^2\cos(\omega_j t)\theta(t), \tag{5}$$

where $\theta(t)$ is the Heaviside step function. Also

$$F(t)=\sum_j m_j\omega_j^2 q_j^h(t), \tag{6}$$

where $q_j^h(t)$ denotes the general solution of the homogeneous equation for the heat-bath oscillators (corresponding to no interaction). These results were used to obtain the (model-independent) result for the (symmetric) autocorrelation of $F(t)$ viz.

$$\frac{1}{2}\langle F(t)F(t')+F(t')F(t)\rangle$$
$$=\frac{1}{\pi}\int_0^\infty d\omega\,\mathrm{Re}[\tilde{\mu}(\omega+i0^+)]\hbar\omega \times\coth(\hbar\omega/2kT)\cos[\omega(t-t')], \tag{7}$$

where $\tilde{\mu}(\omega)$ is the Fourier transform of the memory function $\mu(t)$. This type of equation is referred to by Kubo[13] as the second fluctuation-dissipation theorem and we note that it can be written down explicitly once the GLE is obtained. On the other hand, the first fluctuation-dissipation theorem is an equation involving the autocorrelation of $x(t)$ and its explicit evaluation requires a knowledge of the generalized susceptibility $\alpha(\omega)$ (to be defined below) which is equivalent to knowing the solution to the GLE. This solution is readily obtained when $V(x)=0$, corresponding to the original Brownian motion problem. As shown by Ford, Lewis, and O'Connell,[17,19] a solution is also possible in the case of an oscillator. Taking $V(x)=1/2m\omega_0^2x^2$, these authors obtained [see Eqs. (1)–(3) of Ref. 17]

$$\tilde{x}(\omega)=\alpha(\omega)\tilde{F}(\omega), \tag{8}$$

where

$$\alpha(\omega)=[-m\omega^2+m\omega_0^2-i\omega\tilde{\mu}(\omega)]^{-1} \tag{9}$$

and the superposed tilde is used to denote the Fourier transform. Thus, $\tilde{x}(\omega)$ is the Fourier transform of the operator $x(t)$

$$\tilde{x}(\omega)=\int_{-\infty}^{\infty} dt\,x(t)e^{i\omega t}. \tag{10}$$

Also, since Eq. (5) implies that $\mu(t)$ is 0 for negative t, we have

$$\tilde{\mu}(\omega)=\int_0^\infty dt\mu(t)e^{i\omega t},\quad \mathrm{Im}\,\omega>0. \tag{11}$$

Thus $\tilde{\mu}(\omega)$ is analytic in the upper half-plane, $\mathrm{Im}\,\omega>0$.

We have now all the tools we need to calculate various correlation functions. Before doing so, it is convenient to rewrite Eq. (7) in the form

$$C_{FF}(\tau)\equiv\frac{1}{2}\langle F(t)F(t')+F(t')F(t)\rangle =\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\tilde{C}_{FF}(\omega)e^{-i\omega\tau}, \tag{12}$$

where $\tau=t-t'$ and where

$$\tilde{C}_{FF}(\omega)=\mathrm{Re}[\tilde{\mu}(\omega+i0^+)]\hbar\omega\coth(\hbar\omega/2kT). \tag{13}$$

In deriving this result we have used the fact that the integrand on the right side of Eq. (7) is an even function of ω. Next, using Eqs. (8) and (12), it is straightforward to prove that

$$C_{xx}(\tau)\equiv\frac{1}{2}\langle x(t)x(t')+x(t')x(t)\rangle =\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\tilde{C}_{xx}(\omega)e^{-i\omega\tau}, \tag{14}$$

where

$$\tilde{C}_{xx}(\omega)=|\alpha(\omega)|^2\tilde{C}_{FF}(\omega)=\hbar\,\mathrm{Im}\,\alpha(\omega)\coth(\hbar\omega/2kT), \tag{15}$$

where the second equality in Eq. (15) follows from use of the relation

$$\mathrm{Im}\,\alpha(\omega)=\omega|\alpha(\omega)|^2\,\mathrm{Re}\,\tilde{\mu}(\omega), \tag{16}$$

which, in turn, follows directly from Eq. (9). We note that Eqs. (14) and (15) are nothing more than the fluctuation-dissipation theorem of the first kind.[13]

In a similar manner, we obtain, for the ensemble average of the product of the displacement and random force, the quantity of interest to Manoliu and Kittel,[3] the result

$$C_{XF}(\tau)=\frac{1}{2}\langle x(t)F(t')+F(t')x(t)\rangle =\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\,\tilde{C}_{XF}(\omega)e^{-i\omega\tau}, \tag{17}$$

where

$$\tilde{C}_{XF}(\omega)=\alpha(\omega)\tilde{C}_{FF}(\omega) =\alpha(\omega)\mathrm{Re}\,\tilde{\mu}(\omega)\hbar\omega\coth(\hbar\omega/2kT). \tag{18}$$

Equations (17) and (18) provide a general expression for the desired ensemble average of the product of the displacement and the random force. Since it is generally convenient to evaluate the integral appearing in Eq. (17) by use of contour integration, it is useful to recall that ω has a positive imaginary part. Thus in carrying out contour integrations, it should be noted that the contour will be an amount 0^+ above the real axis or, in other words, it will go from $-\infty+i\epsilon$ to $\infty+i\epsilon$ where $\epsilon=0^+$. In this context, we note that $\alpha(\omega)$ is an analytic function in the upper half-plane (UHP). Finally, $\coth(\hbar\omega/2kT)$ has simple poles at $\omega=i\omega_n$ (with $n=0,\pm1,\pm2,\ldots$), where

$$\omega_n=(2\pi kT/\hbar)n, \tag{19}$$

are the Matsubara frequencies.[31,32] Also, the residue of each of these poles is $2kT/\hbar$.

III. RESULTS FOR THE POSITION-FORCE CORRELATION

A. Classical Brownian motion in an ohmic heat bath

The original Brownian motion problem is described by Eq. (1), corresponding to a free particle ($\omega_0=0$) in an ohmic heat bath [$\mathrm{Re}\,\tilde{\mu}(\omega)=m\gamma$ or $\mu(t)=m\delta(t)$, which implies no memory effects] and also $kT\gg\hbar\omega$ (absence of quantum effects). This corresponds to the case considered in Ref. 3. Then, using Eq. (18), we see that Eq. (17) reduces to

$$C_{XF}(\tau)=\frac{m\gamma}{2\pi}2kT\int_{-\infty}^{\infty} d\omega\,\alpha(\omega)e^{-i\omega\tau} =2m\gamma kTG(\tau), \tag{20}$$

where $G(\tau)$ is, by definition, the inverse Fourier transform of $\alpha(\omega)$. [This is the only exception to our convention of denoting the Fourier transform of any function, $A(t)$ say, by $\tilde{A}(\omega)$. The reason for this exception is to conform to commonly accepted practice in the literature]. In the above limits, we also see, from Eq. (9), that $\alpha(\omega)=[-m\omega(\omega+i\gamma)]^{-1}$.

We now turn to the evaluation of the integral in Eq. (20). For $\tau<0$, we complete the contour in the UHP. But, since $\alpha(\omega)$ is analytic in the UHP, it follows that

$$C_{XF}(\tau)=0 \quad \text{if } \tau<0. \tag{21}$$

In other words, the correlation between the position x at time t and the fluctuation F at a later time t' is zero. This is in conformity with our physical intuition that there is no effect before a cause (causality principle).

In the case where $\tau>0$, we complete the contour in the lower-half-plane (LHP). Since $\alpha(\omega)$ has poles at $\omega=0$ and $\omega=-i\gamma$, it follows from Eq. (20) that

$$C_{XF}(\tau)=2kT(1-e^{-\gamma\tau}) \quad \text{if } \tau>0. \tag{22}$$

In particular, we note that $C_{XF}(0)=0$ and also that $C_{XF}(\tau)\to 0$ as $\gamma\to 0$. Also, Eq. (22) corresponds to the result obtained in Ref. 3 [see their Eqs. (7) and (19)]. Thus, if the force is applied at a time t' there is a correlation between it and the position of the particle at a later time t. Another way of seeing this is to note that if we take the inverse Fourier transform of Eq. (8) then, by the Fourier convolution theorem,

$$x(t)=\int_{-\infty}^{t} dt'\, G(t-t')F(t'), \tag{23}$$

where $G(t)$, the retarded Green's function, is the inverse Fourier transform of $\alpha(\omega)$, i.e.,

$$G(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \alpha(\omega)e^{-i\omega t}, \tag{24}$$

and it is clear from Eq. (24), and the fact that $\alpha(\omega)$ has no poles in the UHP, that $G(t)$ is zero for $t<0$. We see from Eq. (23) that $x(t)$ is determined by the force at all previous times from $-\infty$ to t, which explains the correlation between $x(t)$ and $F(t')$ for the case $t>t'$ (i.e., $\tau>0$) since, in this case, $x(t)$ contains a contribution from $F(t')$. Thus, even in this simple case, there is a manifestation of "memory" in the relation between the displacement and the fluctuation force, as is made manifest in Eq. (23).

B. Brownian motion at arbitrary temperature in an ohmic heat bath

As in Sec. III A, we take $\text{Re}\,\tilde{\mu}(\omega)=m\gamma$ and $\omega_0=0$, so that Eq. (17) becomes

$$C_{XF}(\tau)=\frac{m\gamma}{2\pi}\int_{-\infty}^{\infty} d\omega\, \hbar\omega\alpha(\omega)\coth(\hbar\omega/2kT)e^{-i\omega\tau}$$
$$=-\frac{\gamma\hbar}{2\pi}\int_{-\infty}^{\infty} d\omega\, \frac{1}{\omega+i\gamma}\coth(\hbar\omega/2kT)e^{-i\omega\tau}. \tag{25}$$

For $\tau<0$, in contrast to Sec. III A, this quantity is no longer zero because of the poles of $\coth(\hbar\omega/2kT)$ in the UHP at $\omega=i\omega_n$ $(n=1,2,...)$. Thus

$$C_{XF}(\tau)=-2kT\gamma\sum_{n=1}^{\infty}\frac{1}{\omega_n+\gamma}e^{-\omega_n|\tau|} \quad \text{if } \tau<0, \tag{26}$$

where ω_n is given by Eq. (19). It is clear that $C_{XF}(\tau)\to 0$ in the high temperature limit and also in the limit $\gamma\to 0$.

The question now arises as to why, in the case $\tau<0$, we get a nonzero result here, as distinct from Sec. III A. The answer is that in the latter case, it is clear, using Eqs. (12) and (13), that $C_{FF}(\tau)$, the autocorrelation of the random force is equal to $2m\gamma kT\delta(\tau)$, i.e., we are dealing with "white noise." On the other hand, $C_{FF}(\tau)$ is not proportional to a δ function in this section. [See the discussion after Eq. (2.11) in Ref. 16 where, in particular, we point out that "··· although there is no memory, the quantum-mechanical process is not Markovian in the customary sense of the term"]. As a result, for $t<t'$, we deduce that $x(t)$ [which according to Eq. (23) contains contributions from $F(t'')$ for all values of $t''<t$] can be correlated with $F(t')$, the random force at a later time.

Considering now the case $\tau>0$, our contour integral is in the LHP and encloses poles at $\omega=-i\omega_n$ $(n=0,1,2,...)$ and at $\omega=-i\gamma$. Thus, from Eq. (25) and the fact that $\coth(ix)=-i\cot x$, we obtain

$$C_{XF}(\tau)=-\hbar\gamma\cot\left(\frac{\hbar\gamma}{2kT}\right)e^{-\gamma\tau}$$
$$+2kT\left(1-\gamma\sum_{n=1}^{\infty}\frac{1}{\omega_n-\gamma}e^{-\omega_n\tau}\right)$$
$$=2kT\gamma\left(\sum_{n=0}^{\infty}\frac{1}{\omega_n-\gamma}(e^{-\gamma\tau}-e^{-\omega_n\tau})\right.$$
$$\left.-\sum_{n=1}^{\infty}\frac{1}{\omega_n+\gamma}e^{-\gamma\tau}\right) \quad \text{if } \tau>0, \tag{27}$$

where ω_n is given by Eq. (19). In the high-temperature limit, it is clear that Eq. (27) reduces to Eq. (22). Finally, we note, from the $\tau\to 0$ limits of Eqs. (26) and (27), that $C_{XF}(\tau)$ approaches the same logarithmic divergence from both sides of $\tau=0$.

C. Brownian motion of a charged particle in a blackbody radiation heat bath

The motion of a charged oscillator (with charge e and natural frequency ω_0) in a blackbody radiation heat bath was discussed extensively in Refs. 16, 17, and 19. We take the limit $\omega_0=0$ of these results for the Brownian motion problem (which also implies that the corresponding "γ" is zero since $\gamma=\omega_0^2\tau_e$ in this case)[16,17] to get, in the large cutoff limit,

$$\alpha(\omega)=-(1-i\omega\tau_e)/M\omega^2, \tag{28}$$

and

$$\text{Re}\,\tilde{\mu}(\omega)=M\tau_e^{-1}\omega^2/(\omega^2+\tau_e^{-2}), \tag{29}$$

where M is the renormalized mass of the charged particle and $\tau_e=2e^2/3MC^3=6.2\times 10^{-24}$ s, for the electron. Thus

$$\alpha(\omega)\text{Re}\,\tilde{\mu}(\omega)=i/(\omega-i\tau_e^{-1}). \tag{30}$$

We will now combine this result with Eqs. (17) and (18). We will also consider only the high-temperature limit in order to separate quantum effects from memory effects which clearly arise from the frequency-dependence of $\text{Re}\,\tilde{\mu}(\omega)$. Thus

$$C_{XF}(\tau)=\frac{i}{2\pi}2kT\int_{-\infty}^{\infty} d\omega\,\frac{e^{-i\omega\tau}}{\omega-i\tau_e^{-1}}. \tag{31}$$

Since the integrand has only one pole at $\omega=i\tau_e$ it follows that

$$C_{XF}(\tau) = -2kTe^{-|\tau|/\tau_e} \quad \text{if } \tau < 0. \tag{32}$$

In addition, it would appear from Eq. (31) that $C_{XF}=0$ if $\tau>0$. However, this is not so. The reason is that our expression for $\alpha(\omega)$ given in Eq. (28) incorporates the large cutoff limit of quantum electrodynamics (see the discussion in Refs. 17 and 19). For most applications (such as the $\tau<0$ calculation which we have just carried out) this is permissible. However, there are other situations (such as the $\tau>0$ calculation) for which the large cutoff limit should not be taken until the end of the calculation. Thus, more generally, when reduced to its essentials, the expression for $\alpha(\omega)$ given in Eq. (28) should be multiplied by the factor $i\Omega'/(\omega+i\Omega')$ and then one lets $\Omega'\to\infty$ at the end of the calculation. [The denominator factor $(\omega+i\Omega')$ first appears in Eq. (19) of Ref. 17 and we refer to the discussion following this equation, and also to Ref. 19, for further details]. This factor does not affect the calculation for $\tau<0$ where we are only concerned with poles in the UHP. However, for $\tau>0$, we have now got a pole at $\omega=-i\Omega'$ in the LHP so, as a consequence,

$$C_{XF}(\tau) = -2kTe^{-\Omega'\tau} \quad \text{if } \tau>0. \tag{33}$$

For all nonzero positive values of τ this expression gives 0 in the limit $\Omega'\to\infty$ but if we let $\tau\to 0$ prior to letting $\Omega'\to\infty$ then we get $C_{XF}(0)=-2kT$, in agreement with Eq. (32). In other words, the correlation function is also continuous at $\tau=0$ provided that we go to the large cutoff limit by letting Ω' be very large but not infinite. The nonzero result here should be contrasted with the zero result given by Eqs. (21) and (22) in the limit $\gamma\to 0$. This is a manifestation of memory effects. It is surprisingly large and it reflects the fact that the random force autocorrelation function is no longer a δ function.

D. Classical oscillator in an ohmic heat bath

Here, we are going beyond Brownian motion to consider the effect of a harmonic confining potential. The equation of motion in this case is

$$m\ddot{x}+m\gamma\dot{x}+m\omega_0^2 x = F(t). \tag{34}$$

Thus $\mathrm{Re}\,\tilde{\mu}(\omega)=m\gamma$, as in case A but now,

$$\alpha(\omega) = (-m(\omega^2+i\omega\gamma-\omega_0^2))^{-1}. \tag{35}$$

It follows that $C_{XF}(\tau)$ is still given by Eq. (20) but now

$$G(\tau) = -\frac{1}{2\pi m}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega\tau}}{(\omega-\omega_a)(\omega-\omega_b)}, \tag{36}$$

where

$$\omega_{a,b} = \mp\omega_1 - i(\gamma/2) \tag{37}$$

and

$$\omega_1 = \{\omega_0^2-(\gamma/2)^2\}^{1/2}. \tag{38}$$

Also, we are assuming $\omega_0>(\gamma/2)$ but we will consider the reverse case below. Thus, since both poles of the integrand lie in the LHP, it follows immediately that

$$C_{XF}(\tau)=0 \quad \text{if } \tau<0. \tag{39}$$

For $\tau>0$, we obtain

$$G(\tau) = \frac{i}{m}\left(\frac{e^{-i\omega_a\tau}}{\omega_a-\omega_b}+\frac{e^{-i\omega_b\tau}}{\omega_b-\omega_a}\right) = \frac{1}{m\omega_1}\sin(\omega_1\tau)e^{-(\gamma/2)\tau} \quad \text{if } \tau>0. \tag{40}$$

Thus, using Eq. (20), we obtain

$$C_{XF}(\tau) = (2\gamma kT/\omega_1)\sin(\omega_1\tau)e^{-(\gamma/2)\tau} \quad \text{if } \tau>0 \text{ and } \omega_0>(\gamma/2). \tag{41}$$

It is clear that $C_{XF}(\tau)\to 0$ as $\gamma\to 0$ and also $C_{XF}(0)=0$.

In the case where $(\gamma/2)>\omega_0$, we can still use Eq. (36) except that now

$$\omega_{a,b} = -i[(\gamma/2)\pm\omega_2], \tag{42}$$

where

$$\omega_2 = [(\gamma/2)^2-\omega_0^2]^{1/2}. \tag{43}$$

As before, both poles lie in the LHP. Thus Eq. (39) again holds but now Eq. (41) is replaced by

$$C_{XF}(\tau) = \frac{\gamma}{\omega_2}kTe^{-(\gamma/2)\tau}[e^{\omega_2\tau}-e^{-\omega_2\tau}] \quad \text{if } \tau>0 \text{ and } (\gamma/2)>\omega_0. \tag{44}$$

In the limit $(\gamma/2)\gg\omega_0$, we now see that $\omega_2=(\gamma/2)\,[1-2(\omega_0/\gamma)^2+\cdots]$ and hence

$$C_{XF}(\tau)\simeq 2kT(1-e^{-\gamma\tau})\{1+(\omega_0/\gamma)^2[2-\gamma\tau(1+e^{-\gamma\tau})/(1-e^{-\gamma\tau})]\} \quad \text{if } \tau>0. \tag{45}$$

In the limit $\omega_0\to 0$, we see that this result reduces to that given in Eq. (22). Further, it shows that the effect of the harmonic potential is to decrease the correlation between the displacement and the random force.

IV. CONCLUSIONS

We have considered Brownian motion in a very general heat bath by means of a GLE. We also presented a solution to this equation (and also to the more general equation describing the case of a harmonically bound particle in a heat bath). Next, these results are used to calculate the correlation between the displacement $x(t)$ and the random force $F(t)$ and it is shown that the classical limit of these results reproduce, in a simple and elegant manner, the results of Ref. 3. Particular emphasis was placed on "memory effects", as exemplified by consideration of the black-body radiation heat bath.

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Heisenberg's uncertainty relation and thermal vibrations in crystals

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It is shown how results obtained from crystal structure analysis may provide a practical illustration of Heisenberg's uncertainty relation. To this end lower limits for the vibrational amplitudes of atoms in crystals are derived and compared with experimental values.

I. INTRODUCTION

Heisenberg's uncertainty relation for position q and linear momentum p in one spatial dimension asserts that the product of the respective standard deviations[1] is limited by Planck's constant h,

$$\sigma(q_x)\sigma(p_x) \geqslant \frac{h}{4\pi}. \qquad (1)$$

The standard deviations here measure the width of the position and momentum distributions associated with a given state of a quantum mechanical system.

The purpose of the present note is to illustrate how experimental results from crystal structure analysis may give rise to a practical demonstration of the uncertainty relation. Such an examination based on empirical data appears to be a particularly instructive way of illuminating the operational significance of Eq. (1).

Occasionally, the quantum uncertainties that enter Eq. (1) are equated with experimental uncertainties, i.e., with measures of observational precision. However, in the rigorous derivation of Eq. (1) within the formalism of quantum mechanics no explicit reference is made to measurements, and the meaning of Eq. (1) is unambiguous: The uncertainty relation limits the statistical homogeneity within an ensemble of many identically prepared systems, but bears no relation to the precision of measurements.[2]

Contemporary crystal structure analysis allows the determination of atomic coordinates with an accuracy of up to 10^{-4} Å. In this context, it may be asked whether an ultimate limit to this accuracy is imposed by the uncer-

