

Short-time behavior of the correlation functions for the quantum Langevin equation

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We analyze the quantum Langevin equation obtained for the Ford-Kac-Mazur and related models. We study an explicit expression for the correlation function of the noise, obtained by making use of the normal-ordered product of operators. Such an expression is divergence-free, does not require any frequency cutoff, and yields the classical (Markoffian) case in the limit of vanishing \hbar . We also bring to light and discuss two different regimes for the momentum autocorrelation. The high-temperature and weak-coupling limits are considered, and the latter is shown to be related to van Hove's " $\lambda^2 T$ " limit.

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The derivation of a dissipative equation from an underlying Hamiltonian dynamics is a long-standing problem. Many important contributions on this subject have been given during the last decades. Even though we still lack a thorough comprehension of dissipative and irreversible phenomena, the essential features of a self-consistent physical framework are now becoming more clear.

The analysis of solvable models provides very useful insights into the above-mentioned issues. One of such models was originally proposed by Ford, Kac, and Mazur (FKM) in a pioneering paper [1]. This model consists of an ensemble of coupled oscillators interacting via a quadratic Hamiltonian. The reduced dynamics of one of these oscillators yields, in an appropriate macroscopic limit, a Langevin equation [2,3].

Several other examples of this sort have been proposed. Among others, the "independent oscillator" model [4-7] and a whole class of related models [8-10] have played an important role in clarifying several aspects related to dissipative phenomena [9-11]. The similarities and differences among them have been discussed and clarified in Refs. [5,7]. In all the above-mentioned examples, the influence of a "heat bath," composed of harmonic oscillators, on the equation of motion of the "Brownian particle" is described by a phenomenological equation: The reduced description of the system always turns out to be of the Langevin type.

The aim of the present paper is to discuss some features of the Langevin equation in the quantum case. We shall consider an explicit expression for the correlation function of the noise in the quantum case. This expression, which was first derived by Gardiner [12], is divergence-free and therefore does not require any frequency cutoff. Moreover, by making use of this result, it is possible to discuss some interesting general features of the momentum autocorrelation, and bring to light the presence of two temporal regimes in the evolution of the quantum system. The deviations of the momentum autocorrelation function from a purely exponential behavior were considered by Lee [13], and are very significant in the context of dissipation in quantum mechanics. In the light of a recent remark by Leggett [14], this issue may have interesting spinoffs on the quantum measurement problem [15,16]. Finally, we shall put forward a curious analogy between the short-time behavior of the noise correlation, the

momentum autocorrelation and the "survival probability" of quantum-mechanical states (quantum Zeno effect) [17-19].

It should be emphasized that it is possible to adhere to a different standpoint and postulate (rather than derive) an equation of the Langevin type for some quantum-mechanical operators, involving operator-valued random terms [20]. In such a case, the Langevin equation is viewed as a phenomenological starting point. In the white-noise case, this approach can be put on a sound mathematical basis [21] and brings to light other interesting aspects of dissipation, related to van Hove's " $\lambda^2 T$ " limit [22]. Interestingly, we shall see that the above limit is related to one of the temporal regimes to be considered in this paper.

In the FKM model [1] an ensemble of $2N+1$ coupled oscillators is described via the Hamiltonian

$$H = \frac{1}{2} \sum_{j=-N}^N \frac{p_j^2}{m} + \frac{1}{2} \sum_{j,k=-N}^N q_j A_{jk} q_k + V(q_0), \quad (1)$$

where q_j and p_j are the coordinates and momenta of the oscillators, m their (common) mass, V a potential acting on the zeroth oscillator and the $(2N+1) \times (2N+1)$ interaction matrix A_{ij} is assumed to be symmetric, cyclic, and with non-vanishing eigenvalues (the last condition is eventually relaxed in order to meet the requirement of Markoffianity). The oscillators are taken to be identical (with the only exception that the zeroth one is acted upon by an external force), and one looks for an interaction matrix A_{ij} such that the zeroth oscillator ("Brownian particle"), follows a Langevin equation.

Ford, Lewis, and O'Connell [7] pointed out that the FKM model is related, via a canonical coordinate transformation, to the "independent-oscillator" model

$$H = \frac{P^2}{2m} + V(X) + \frac{1}{2} \sum_j \left[\frac{p_j^2}{m_j} + \omega_j^2 (q_j - \gamma_j X)^2 \right], \quad (2)$$

where X and P are the coordinate and momentum of the (Brownian) particle and q_j, p_j the coordinates and momenta of the (bath) oscillators. (The constants γ_j can either be taken equal to one or alternatively proportional to ω_j^{-2} .) For this reason, the conclusions we shall draw in the present

paper hold true also for the Hamiltonian (2). The independent oscillator model frequently appears in the literature, although in somewhat different forms [4–7]. Notice also [5] that a class of similar models [8–10] can be brought into the form (2).

Under certain conditions for the interaction matrix A_{ij} , the Hamiltonian (1) yields the following equation of motion in the $N \rightarrow \infty$ limit:

$$\dot{p}_0 + \xi \frac{p_0}{m} + V'(q_0) = \eta(t), \quad (3)$$

where ξ is an effective friction constant and $\eta(t)$ an effective “noise” term [2,3]. (For the independent oscillator model, p_0, q_0 are substituted by P, X in the above equation.) The friction constant ξ is closely related to the interaction, and is therefore representative of the coupling between the Brownian particle and the remaining oscillators. In some cases, it is even possible to obtain an explicit expression for ξ . For example, the independent oscillator model, with the ansatz $\gamma_j \equiv \gamma/\omega_j^2$ [4] and the Debye approximation, yields

$$\xi = \frac{9\pi N \gamma^2}{2\omega_T^3}, \quad (4)$$

where N is the total number of degrees of freedom of the system of oscillators and ω_T a frequency cutoff. (A misprint in Ref. [4] has been corrected.) The relation (4) is of more general validity than one might think at first sight, and its general features can also be derived within different schemes than Zwanzig’s [6].

The Langevin equation (3) is obtained in both the classical and quantum case. The expectation value of the noise, computed according to the canonical distribution, is zero in both cases. The only important difference concerns the correlation function of the noise. In the classical case

$$\langle \eta(t) \eta(t+\tau) \rangle_{\text{cl}} = \frac{2\xi}{\beta} \delta(\tau), \quad (5)$$

as we expect from the fluctuation-dissipation theorem [$\beta = (kT)^{-1}$ is the inverse temperature of the bath and $\langle \cdot \rangle_{\text{cl}}$ denotes a statistical (Boltzmann) average]. In the quantum case the result depends on whether one chooses the symmetric or the normal-ordered product of operators. The first case is the one usually considered in the literature: One gets

$$\begin{aligned} \langle \{ \eta(t) \eta(t+\tau) \} \rangle &\equiv \frac{1}{2} \langle \eta(t) \eta(t+\tau) + \eta(t+\tau) \eta(t) \rangle \\ &= \frac{\xi}{\pi} \int_0^\infty d\omega \hbar \omega \coth \frac{\beta \hbar \omega}{2} \cos \omega \tau, \end{aligned} \quad (6)$$

$\langle \cdot \rangle$ being the quantum-mechanical expectation value over the thermal state of the oscillators. On the other hand, in the second case one obtains

$$\langle : \eta(t) \eta(t+\tau) : \rangle = \frac{2\xi}{\pi} \int_0^\infty d\omega \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \cos \omega \tau. \quad (7)$$

Notice that the two definitions differ for the zero-point energy fluctuations of the heat bath. In the first case the energy of each oscillator is taken to be

$$E_\beta(\hbar \omega) = \frac{\hbar \omega}{2} + \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} = \frac{\hbar \omega}{2} \coth \frac{\beta \hbar \omega}{2}, \quad (8)$$

while in the second case

$$E_\beta^{(0)}(\hbar \omega) = E_\beta(\hbar \omega) - \frac{\hbar \omega}{2} = \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1}. \quad (9)$$

Both $E_\beta(\hbar \omega)$ and $E_\beta^{(0)}(\hbar \omega)$ yield the classical equipartition energy kT in the high-temperature limit.

As emphasized by FKM, there are many alternative definitions of correlation function, corresponding to different orderings and symmetrizations of the operators. Which of these possible definitions correspond to a real quantum fluctuation phenomenon must, in the last analysis, be determined by experiment [1]. See Gardiner’s lucid discussion on this point [12]. The usual definition of correlation function is taken to be (6). The purpose of this paper is to show that the physical results obtained by normal ordering of the operators are very appealing. Let us start by observing that the integral (6) is divergent and requires a frequency cutoff. The normal-ordered product (7) does not suffer from the same drawback. Moreover, the integral (7) is solvable, as first noted in Ref. [12]: By choosing the rectangle $[0, \infty, \infty + 2\pi i/\beta \hbar, 2\pi i/\beta \hbar]$ as integration contour, one gets after a straightforward, if lengthy, calculation

$$\begin{aligned} f_\hbar(\beta, \xi; \tau) &\equiv \langle : \eta(t) \eta(t+\tau) : \rangle \\ &= \frac{\xi \hbar}{\pi} \left[\frac{1}{\tau^2} - \frac{\pi^2}{\beta^2 \hbar^2 \sinh^2(\pi \tau / \beta \hbar)} \right]. \end{aligned} \quad (10)$$

This function is shown in Fig. 1. It must be stressed that the result (10) diverges *only* for $\beta = \tau = 0$. Notice that

$$f_\hbar(0^+, \xi; \tau) \sim \frac{\xi \hbar}{\pi \tau^2}, \quad f_\hbar(\beta, \xi; 0^\pm) \sim \frac{\xi \pi}{3\beta^2 \hbar}. \quad (11)$$

It is also worth emphasizing that (for $\beta \neq 0$) the correlation function f_\hbar has a vanishing derivative for $\tau = 0$. This is an important point to which we shall come back later. It is interesting to look at the very shape of f_\hbar in Fig. 1. Incidentally, observe also that the integrand in Eq. (7) is not analytic in $\beta = 0$, so that the naive high-temperature expansion

$$E_\beta(\hbar \omega) \simeq \frac{1}{\beta} + \beta \frac{(\hbar \omega)^2}{12} \quad (12)$$

in (9) and in the integral (7) leads to a different (wrong) result, after integration.

On the other hand, the classical correlation function (5) is obtained by (10) in the $\hbar \rightarrow 0$ limit: To this end, observe that

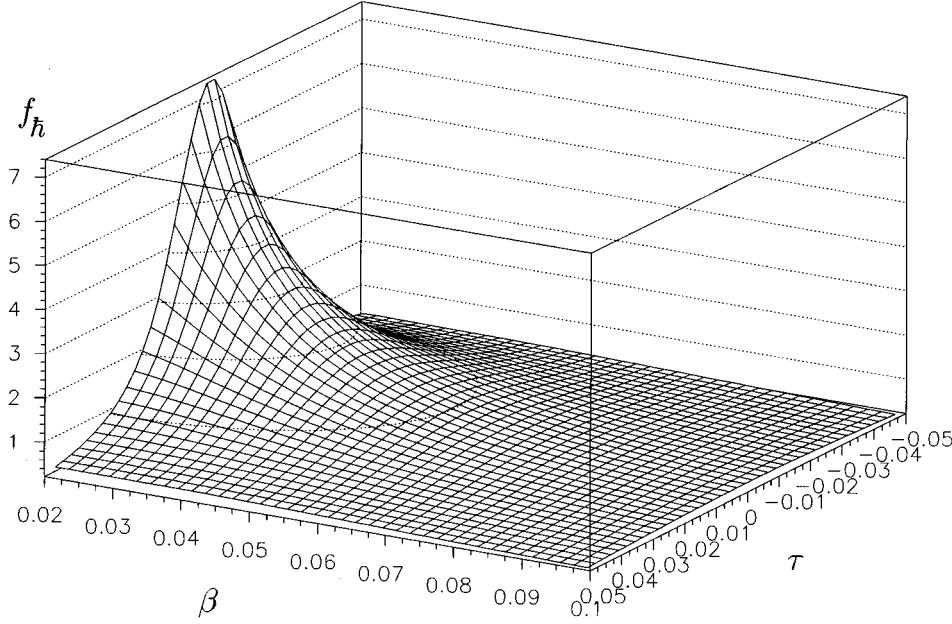


FIG. 1. Normal-ordered correlation function f_h vs τ and β (arbitrary units).

$$\int_{-\infty}^{\infty} d\tau f_h(\beta, \xi; \tau) = \frac{2\xi}{\beta} \quad (\beta \neq 0), \quad (13)$$

a result that is independent of \hbar . [Since the function f_h in (10) is continuous for $\beta \neq 0$, the integral (13) is computed in Riemann's sense *without* making use of Cauchy's principal value.] Equation (13) allows us to infer that

$$f_h(\beta, \xi; \tau) \xrightarrow{\hbar \rightarrow 0} \frac{2\xi}{\beta} \delta(\tau) = \langle \eta(t) \eta(t+\tau) \rangle_{\text{cl}}, \quad (14)$$

in agreement with (5). This has interesting spinoffs: The somewhat disturbing divergence of f_h in $\beta = \tau = 0$ [see Eq. (11)] turns out to be of classical, rather than of quantum-mechanical origin.

One can also compute the power spectrum of the noise, by observing that (7) is nothing but a Fourier cosine transform. The final result is

$$F(\omega) \equiv \int_{-\infty}^{\infty} d\tau f_h(\beta, \xi; \tau) e^{-i\omega\tau} = \frac{2\xi\hbar|\omega|}{e^{\beta\hbar|\omega|} - 1} \quad (15)$$

and vanishes in the $T \rightarrow 0$ limit. In this context, it is worth noting that FKM stressed that the normal-ordered product is "physically appropriate because it leads to a noise spectrum that vanishes at absolute zero" [1].

It should be emphasized that also the correlation function (6) yields the classical result (5) in the limit of vanishing \hbar . The advantage of (7), however, lies in the explicit expression of all the quantities considered. Moreover, as we shall see, the above analysis will enable us to draw some other general conclusions.

Let us now look at the momentum autocorrelation function. If we normal-order the operators, we obtain (let $\xi' = \xi/m$ and call it ξ again)

$$\begin{aligned} g_h(\beta, \xi; \tau) &\equiv \langle :p_0(t)p_0(t+\tau): \rangle \\ &= \frac{2m}{\pi\beta} \int_0^{\infty} d\omega \frac{\beta\hbar\omega}{e^{\beta\hbar\omega} - 1} \frac{\xi}{\omega^2 + \xi^2} \cos\omega\tau \\ &\equiv \frac{2m}{\pi\beta} \int_0^{\infty} d\omega A(\omega)B(\omega) \cos\omega\tau, \end{aligned} \quad (16)$$

A and B being the first and second factors in the integral, respectively. Let us first observe that, for all nonvanishing (i.e., physical) values of the parameters \hbar, β, ξ , a short-time expansion of the cosine yields

$$g_h \approx a - b\tau^2, \quad (17)$$

where a and b are nonvanishing positive constants that depend on the parameters \hbar, β, ξ . This result is of *general validity* [13], and shows that g_h [like f_h in Eq. (10)] always has a vanishing derivative for $\tau = 0$.

The functions A and B are bell shaped, with their maxima at the origin $\omega = 0$. Moreover, $A(\omega)$ has poles in $\omega_A = 2\pi ni/\beta\hbar$ (integer n), while $B(\omega)$ has poles in $\omega_B = \pm i\xi$. This suggests the presence of two different regimes, according to the value of the parameter $\xi\beta\hbar/2\pi$: Let us introduce the two relaxation times

$$\tau_{\text{cl}} \equiv \xi^{-1}, \quad \tau_q \equiv \beta\hbar/2\pi, \quad (18)$$

which characterize, respectively, a classical and a quantum regime. As previously emphasized, τ_{cl} is representative of the bath-particle interaction. If

$$\xi\beta\hbar \ll 2\pi \Leftrightarrow \tau_q \ll \tau_{\text{cl}}, \quad (19)$$

then the integral (16) can be approximated by the expression

$$g_{\hbar} \sim \tilde{B}(\tau) = m\beta^{-1} e^{-\xi|\tau|} = m\beta^{-1} e^{-|\tau|/\tau_{cl}} \quad (\tau \gg \tau_q), \quad (20)$$

where the tilde denotes the Fourier transform. Notice that the above expression is only valid for $\tau \gg \tau_q$. This is the *classical* regime [1], in which quantum effects are negligible and the process is Markoffian: FKM remarked how this result, together with (14), could be obtained in the limit of vanishing \hbar . Notice that, according to Eq. (19), the exponential behavior (20) can also be obtained in the limits of high temperature ($\beta \rightarrow 0$) and/or weak coupling ($\xi \rightarrow 0$). However, the latter limits must be considered with great care: For example, the naive high-temperature limit does not yield the correct noise correlation function [see (12)], which can be obtained by letting $\hbar \rightarrow 0$ [see (13) and (14)]. On the other hand, if

$$\xi\beta\hbar \gg 2\pi \Leftrightarrow \tau_q \gg \tau_{cl}, \quad (21)$$

then

$$g_{\hbar} \sim \tilde{A}(\tau) = \frac{\hbar m}{\xi\pi} \left[\frac{1}{\tau^2} - \frac{\pi^2}{\beta^2 \hbar^2 \sinh^2(\pi\tau/\beta\hbar)} \right] \\ = \frac{\hbar m}{\xi\pi} \left[\frac{1}{\tau^2} - \frac{1}{(2\tau_q)^2 \sinh^2(\tau/2\tau_q)} \right] \quad (\tau \gg \tau_{cl}). \quad (22)$$

In this regime, *quantum coherence effects* are not negligible and the process is not Markoffian. According to Eq. (21), this behavior is obtained in the low-temperature and/or strong-coupling limit.

Remember that the short-time behavior of the function g_{\hbar} is *always* given by Eq. (17): This yields a vanishing derivative for $t \rightarrow 0$, in agreement with (22), but not with (20). As a matter of fact, the exponential behavior is always the result of approximations or limiting procedures of some sort.

This difference in the short-time domain is, in our opinion, of general significance. Indeed, it is well known that the temporal evolution of the so-called “survival probability” of a quantum system, under general conditions, is roughly characterized by three distinct regions [17]: A Gaussian-like behavior at very short times, an (approximately) exponential decay at intermediate times, and a power law at long times. The asymptotic dominance of the exponential behavior is representative of a purely stochastic evolution, in which all quantum-mechanical phase correlations are lost, and this suggests a close connection between dissipation, quantum measurements, and exponential decay [14,18]. On the other hand, the Gaussian short-time behavior [17] is essentially ascribable to the persistence of quantum-mechanical phase correlations, leading to the so-called quantum Zeno effect [19]. The above conclusions are valid under very general conditions for the “survival” probability of any quantum-mechanical system (not necessarily unstable) [23].

Even though the above-mentioned issue and the analysis of the present paper reflect somewhat different aspects of the problem of dissipation, it is peculiar, in our opinion, that in both cases the quantum properties of the system be reflected in a *vanishing* derivative at very short times. This is true both for the quantum Zeno effect and in Eqs. (10), (16), (17), and (22). The contrast with the classical regime (20) is striking,

and reminds one of other macroscopic, weak-coupling limits yielding exponential laws [22,18]. It is indeed possible to put forward a curious link between the conditions of approximate validity of the exponential behavior (20) and van Hove’s limit. In the latter case [22], one considers the weak-coupling, macroscopic limit by keeping

$$\lambda^2 T = \text{finite}, \quad (23)$$

where T is time and λ the coupling constant, and shows that the temporal evolution of quantum-mechanical systems satisfies a master equation for time scales of order λ^{-2} . Consider now Eq. (4). In the macroscopic limit $N, \omega_T \rightarrow \infty$, with $N/\omega_T^3 = \text{finite}$, ξ is simply proportional to the square of the coupling constant

$$\xi \propto \gamma^2. \quad (24)$$

On the other hand, the approximate exponential law (20) is valid in the weak-coupling limit for times of order $\tau \sim \tau_{cl} = \xi^{-1} (\gg \tau_q)$, which, by virtue of (24), implies

$$\gamma^2 \tau = \text{finite}. \quad (25)$$

Equations (23) and (25) reflect the *same physical approximations*. Even though the latter equation is not derived in full generality, we cannot escape the feeling that this result is of broader significance. Incidentally, it is worth stressing that van Hove’s limit (23) provokes also the disappearance of the long-time power tail in quantum-mechanical temporal evolutions [17,23]. Such a powerlike long-time behavior appears also in the context of the momentum autocorrelation functions [13,24].

One may wonder whether these curious features of the quantum-mechanical case are of general significance or are rather a “fluke of the special FKM model” [25]. This problem is a very subtle one. The results derived in the present paper are obtained for a specific model of the system-environment interaction, and the (approximate) validity of a quantum Langevin equation in more general cases than a simple array of harmonic oscillators is a very open problem. Observe, for instance, that the product $\xi\beta\hbar$, which plays such an important role in our analysis, is the only dimensionless constant that can be constructed by starting from models leading to Eqs. (3) and (7). Nevertheless, it is difficult to believe that the above-mentioned essential features of the quantum temporal behavior be just casual. Rather, we feel that the vanishing derivative at short times of some quantum-mechanical expectation values reflects a deep, yet unclear, property of “persistence” of the quantum-mechanical phase correlation. Only when such a phase correlation is completely destroyed, for instance, by interacting, in an appropriate limit, with a dissipative environment (a “heat bath”) can the quantum system relax towards a classical (Markoffian) behavior, characterized by approximately exponential laws.

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