Aging effects in the quantum dynamics of a dissipative free particle: Non-Ohmic case

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We report the results related to the two-time dynamics of the coordinate of a quantum free particle, damped through its interaction with a fractal thermal bath (non-Ohmic coupling $\sim\omega^{\delta}$ with $0<\delta<1$ or $1<\delta<2$). When the particle is localized, its position does not age. When it undergoes anomalous diffusion, only its displacement may be defined. It is shown to be an aging variable. The finite temperature aging regime is self-similar. It is described by a scaling function of the ratio t_w/τ of the waiting time to the observation time, as characterized by an exponent directly linked to δ.

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In a broad range of out-of-equilibrium systems, the dynamics displays aging effects. For instance, the two-time correlation functions of some out-of-equilibrium dynamic variables may not be invariant by time translation, even in the limit of a large waiting time (or age). The fluctuation-dissipation theorem (FDT), which is valid for dynamic variables at equilibrium, is then not verified. The study of aging effects and of the related violation of the FDT is a fundamental problem of the physics of dissipative out-of-equilibrium systems. In order to discuss these questions at any temperature T, one has to work within a quantum framework, the time scale $\hbar/kT$ playing a crucial role in the low-temperature dynamics. Since aging effects are encountered, not only in complex systems such as spin glasses [1], but also in simpler systems neither disordered nor frustrated [2], it is very natural, to begin with, to carry out the study of quantum aging in this latter type of system.

One archetype of a simple quantum dissipative system displaying aging is a particle coupled to a thermal bath but otherwise free. Aging effects on the displacement correlation function and the corresponding violation of the quantum FDT have recently been discussed [3] for a specific model of dissipation, namely, the so-called Ohmic model. The fluctuation-dissipation ratio allowing us to write a modified FDT at finite temperature admits in this case a nontrivial limit value 1/2. Yet the Ohmic model, which corresponds to a particle undergoing standard quantum Brownian motion [4,5], does not allow us to handle all the dissipative situations of interest.

In this paper we extend the study of the two-time dynamics to the situations in which the particle damped motion is described by a truly retarded equation even in the classical limit and in which either localization or anomalous diffusion phenomena are taking place. Such situations are encountered in various problems of condensed matter physics [6]. We use for the dissipation a versatile model able to generate various damped equations of motion, either instantaneous or retarded in the classical limit. The dissipation is introduced via a linear coupling of the particle to a set of harmonic oscillators in thermal equilibrium, this bath having a continuous distribution of modes of bandwidth ω_c (Caldeira and Leggett model [7,8]). A central ingredient is the product of the bath density of modes times the squared coupling constant $|\lambda(\omega)|^2$, a product assumed to vary as ω^{δ} at frequencies $\omega\ll\omega_c$. In the Ohmic model the dissipative exponent δ is equal to 1. The algebraic cases $0<\delta<1$ and $\delta>1$ are known, respectively, as the sub-Ohmic or super-Ohmic models [6,9–11].

Studying a dissipative free particle, one is faced with two dynamical variables, namely, the particle velocity and the particle coordinate, which are of a very different character as far as equilibration properties (and therefore aging) are concerned. In the following we first show that for $0<\delta<2$ the velocity equilibrates at large times and does not age. Then, turning to the study of the coordinate, we discuss the domain of (δ,T) parameters for which aging is taking place. This question is nontrivial. Indeed the two following properties have been demonstrated [6,9–11]. First, at $T=0$ for $0<\delta<1$, the particle is localized, in the sense that the mean square displacement $\Delta x^2(t)=\langle[x(t)-x(0)]^2\rangle$ tends towards a constant at infinite time. Second, at $T=0$ for $1\leqslant\delta<2$, and also at finite T for $0<\delta<2$, $\Delta x^2(t)$ diverges at infinite time, the diffusion being anomalous except at finite T for $\delta=1$. As for the two-time dynamics, which is the subject of the present paper, we find clear-cut behaviors: as far as the coordinate is concerned, the localized particle does not age, while the diffusing one ages. In this latter case we provide analytic expressions for the effective temperature and the fluctuation-dissipation ratio. We show in particular that the finite temperature aging regime is self-similar.

In the Caldeira and Leggett model, the Hamiltonian of the particle-plus-bath system reads, in obvious notations,

$$H=\frac{p^2}{2m}-x\sum_{\nu}\lambda_{\nu}(b_{\nu}+b_{\nu}^{\dagger})+\sum_{\nu}\hbar\omega_{\nu}b_{\nu}^{\dagger}b_{\nu}+x^2\sum_{\nu}\frac{\lambda_{\nu}^2}{\hbar\omega_{\nu}},\tag{1}$$

where λ_{ν} is a real coupling constant. For $\omega>0$, the quantity $2\pi g(\omega)|\lambda(\omega)|^2=\frac{1}{2}m\hbar\omega K(\omega)$ is modeled as

$$K(\omega)=2\gamma\left(\frac{\omega}{\gamma}\right)^{\delta-1}f_c\left(\frac{\omega}{\omega_c}\right),\tag{2}$$

where γ is a coupling frequency and f_c a high-frequency cutoff function of typical width ω_c. The definition of $K(\omega)$ is then extended to $\omega<0$ by imposing that it must be an even function of ω. The particle position operator obeys the retarded equation of motion

$$\ddot{x}(t)+\int_{t_i}^{t}dt'k(t-t')\dot{x}(t')=-x(t_i)k(t-t_i)+\frac{1}{m}F(t), \tag{3}$$

where t_i denotes the initial time at which the coupling is switched on. In Eq. (3), the inverse Fourier transform $k(t)$ of $K(\omega)$ plays the role of a memory kernel, and $F(t)$ is a linear combination of bath operators, acting as a stationary random force of correlation function

$$C_{FF}(t)=m\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathrm{Re}\widetilde{K}(\omega)\hbar\omega\coth\frac{\beta\hbar\omega}{2}e^{-i\omega t}, \tag{4}$$

with $\mathrm{Re}\widetilde{K}(\omega)=\frac{1}{2}K(\omega)$ and $\beta=(k_BT)^{-1}$. As for $\mathrm{Im}\widetilde{K}(\omega)$, with the modelization (2) for $K(\omega)$ and a Lorentzian cutoff function $f_c=\omega_c^2/(\omega_c^2+\omega^2)$, one has:

$$\mathrm{Im}\widetilde{K}(\omega)=\omega\left(\frac{|\omega|}{\gamma}\right)^{\delta-2}f_c\left(\frac{\omega}{\omega_c}\right)\times\left[\cot\frac{\delta\pi}{2}+\left(\frac{\omega_c}{|\omega|}\right)^{\delta-2}\frac{1}{\sin\frac{\delta\pi}{2}}\right]. \tag{5}$$

Let us first consider the particle velocity. It has been demonstrated that, for $0<\delta<2$, the total mass of the particle and of the bath oscillators diverges, while for $\delta>2$ it remains finite and can be considered as a renormalized mass. For $0<\delta<2$ $(\delta\neq 1)$, the nonequilibrium expected value of the particle velocity relaxes towards zero at large $t-t_i$ like $(t-t_i)^{\delta-2}$. For $\delta=1$, the relaxation is exponential. The initial expected value of the velocity being forgotten for $0<\delta<2$, this situation may in this sense be qualified as ergodic. For $\delta>2$, the dynamics is governed at large times by a kinematical term involving the renormalized mass, and the initial expected value of the velocity is never forgotten [6,9–11].

In the following, we limit ourselves to the ergodic case $0<\delta<2$. Then the velocity equilibrates at large times and does not age. This property, already obtained in the Ohmic case [3], thus generalizes to non-Ohmic models with $0<\delta<2$. The two-time velocity correlation function $C_{vv}(t,t')$ only depends on the time difference and will be denoted as $C_{vv}(t-t')$. It can be computed via the Wiener-Khintchine theorem as the Fourier transform of

$$C_{vv}(\omega)=\frac{1}{m}\frac{\mathrm{Re}\widetilde{K}(\omega)}{|\widetilde{K}(\omega)-i\omega|^2}\hbar\omega\coth\frac{\beta\hbar\omega}{2}. \tag{6}$$

Let us now turn to the study of the particle coordinate. One may attempt to define its spectral density as $C_{xx}(\omega)=C_{vv}(\omega)/\omega^2$. If convergent, the integral $\int_{-\infty}^{\infty}(d\omega/2\pi)C_{xx}(\omega)$ represents $\langle x^2(t)\rangle$, a quantity that must be independent of t. Checking the small-ω behavior of the integrand with the chosen modelization for $\widetilde{K}(\omega)$, one sees that this is only possible at $T=0$ for $0<\delta<1$. In this case, the particle is localized and it makes sense to define its position in an absolute way as $x(t)=\int_{-\infty}^{t}dt'v(t')$. The two-time position correlation function

$$C_{xx}(t,t')=\frac{1}{2}\langle\{x(t),x(t')\}_+\rangle, \tag{7}$$

where the symbol $\{\cdot,\cdot\}_+$ stands for the anticommutator, only depends on $\tau=t-t'$ (observation time): it does not age.

In other cases, that is, at $T=0$ for $1\leqslant\delta<2$ and at finite T for $0<\delta<2$, the integral $\int_{-\infty}^{\infty}(d\omega/2\pi)C_{xx}(\omega)$ diverges. Then $\langle x^2(t)\rangle$ and $C_{xx}(t,t')$ as defined by Eq. (7) are infinite. The particle diffuses. The integrated velocity correlation function $D(t)=\int_0^t du C_{vv}(u)$ represents the time-dependent diffusion coefficient (in an extended sense when diffusion is anomalous, that is, at $T=0$ for $1<\delta<2$, and at finite T for $0<\delta<1$ and $1<\delta<2$). In this case, it is no longer possible to define an absolute position. We thus focus interest on the displacement $x(t)-x(t_0)$ $(t\geqslant t_0)$. This quantity does not equilibrate with the bath, even at large times. The displacement correlation function

$$C_{xx}(t,t';t_0)=\frac{1}{2}\langle\{[x(t)-x(t_0)],[x(t')-x(t_0)]\}_+\rangle \tag{8}$$

depends on both $\tau=t-t'$ and $t_w=t'-t_0$ (waiting time): it ages. As demonstrated in Ref. [3], the aging properties of $C_{xx}(t,t';t_0)$ can be described in terms of the time-dependent diffusion coefficients $D(\tau)$ and $D(t_w)$.

Therefore, before describing the violation of the equilibrium FDT, we need to study in detail the behavior of the time-dependent diffusion coefficient $D(t)$. Note, however, that the integrated velocity correlation function $\int_0^t du C_{vv}(u)$ takes the meaning of a time-dependent diffusion coefficient only when the mean-square displacement increases without bounds: when the particle is localized, this quantity characterizes the relaxation of the mean square displacement $\Delta x^2(t)$ towards its finite limit $\Delta x^2(\infty)$. Since $0<\delta<2$, one can restrict the study to the infinite bath bandwidth limit $\omega_c\to\infty$, in which case calculations are more simple. One has

$$D(t)=\frac{\hbar}{m\pi}\gamma^{\delta-2}\int_0^{\infty}d\omega\coth\frac{\beta\hbar\omega}{2}\sin\omega t\times\left[\omega^{\delta-1}+\omega^{3-\delta}\left(|\omega|^{\delta-2}\cot\frac{\delta\pi}{2}-\gamma^{\delta-2}\right)^2\right]^{-1}. \tag{9}$$

At finite T, it is interesting to discuss on the same footing the classical counterpart of $D(t)$, namely, $D^{\mathrm{cl}}(t)$ deduced from $D(t)$ by replacing $\coth(\beta\hbar\omega/2)$ by $2/\beta\hbar\omega$ in Eq. (9). Several important features of $D(t)$ and $D^{\mathrm{cl}}(t)$ can be obtained by contour integration.

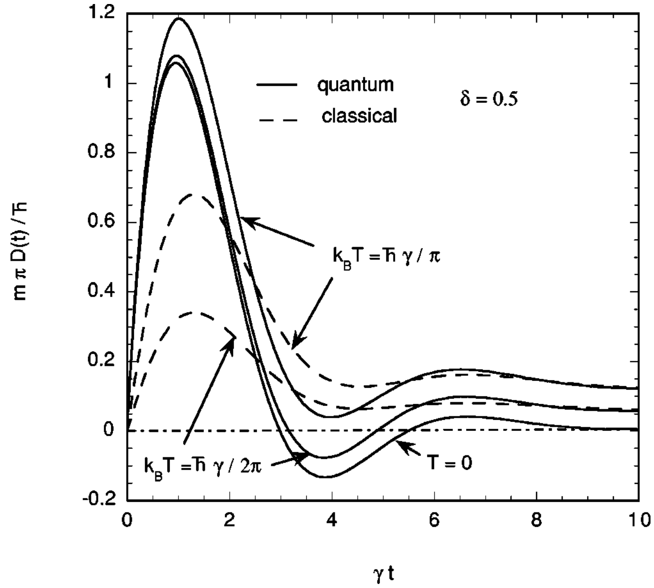

FIG. 1. The solid lines show the quantum diffusion coefficient $D(t)$ plotted as a function of γt for $\delta=0.5$ and for bath temperatures $T=0$, $k_BT=\hbar\gamma/2\pi$, $k_BT=\hbar\gamma/\pi$ [at $T=0$, $D(t)$ is not a diffusion coefficient, but characterizes the relaxation of $\Delta x^2(t)$ towards its finite limit value $\Delta x^2(\infty)$]. The dashed lines show the corresponding $D^{\rm cl}(t)$.

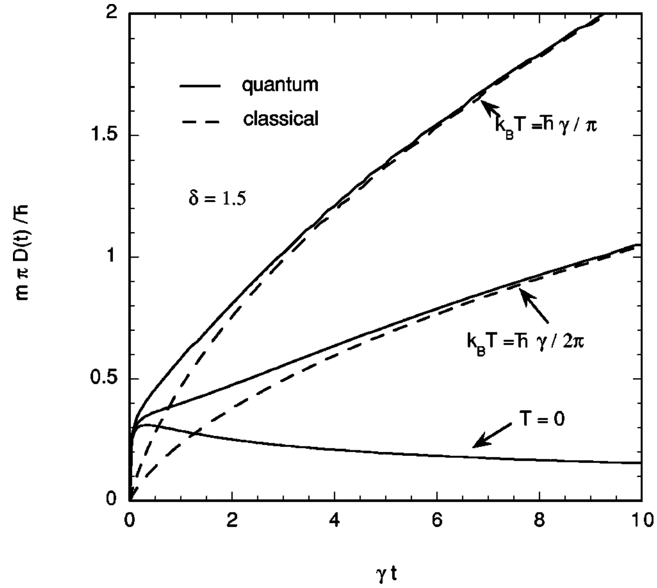

FIG. 2. The solid lines show the quantum diffusion coefficient $D(t)$ plotted as a function of γt for $\delta=1.5$ and for bath temperatures $T=0$, $k_BT=\hbar\gamma/2\pi$, $k_BT=\hbar\gamma/\pi$. The dashed lines show the corresponding $D^{\rm cl}(t)$.

At $T=0$, $D(t)$ is found to be the sum of a pole contribution, which exists only for $0<\delta<1$, given by the oscillating function

$$D(t)_{\rm pole}\sim\frac{\hbar}{m}\frac{1}{2-\delta}e^{-\Lambda t}\sin\Omega t, \qquad (10)$$

where Ω and Λ are known functions of δ and γ, and of a cut contribution behaving at large times as a power law,

$$D(t)_{\rm cut}\sim\frac{\hbar}{m\pi}(\gamma t)^{\delta-2}\sin^3\frac{\delta\pi}{2}\Gamma(2-\delta), \qquad (11)$$

where Γ denotes the Euler Gamma function.

At finite T, $D^{\rm cl}(t)$ is also found to be the sum of an oscillating function, which exists only for $0<\delta<1$,

$$D^{\rm cl}(t)_{\rm pole}\sim\frac{kT}{m\gamma}\frac{2}{2-\delta}\left(\sin\frac{\delta\pi}{2}\right)^{1/(2-\delta)}e^{-\Lambda t}\sin(\Omega t-\phi), \qquad (12)$$

with $\phi=\pi\delta/2(2-\delta)$, and of a cut contribution behaving at large times as a power law,

$$D^{\rm cl}(t)_{\rm cut}\sim\frac{kT}{m\gamma}(\gamma t)^{\delta-1}\frac{\sin\left(\frac{\delta\pi}{2}\right)}{\Gamma(\delta)}. \qquad (13)$$

The behaviors of $D(t)$ and $D^{\rm cl}(t)$ at several different temperatures are illustrated in Fig. 1 for $\delta=0.5$ and in Fig. 2 for $\delta=1.5$. Interestingly enough, for any given δ, the curves corresponding to different bath temperatures do not intersect. Actually, it can be shown that, at any fixed time t, $D(t)$, like $D^{\rm cl}(t)$, is a monotonously increasing function of T. For times $t\ll t_{\rm th}$ ($t_{\rm th}=\hbar/2\pi k_BT$) and for any value of δ, the curves for $D(t)$ at finite T nearly coincide with those at $T=0$, as it should.

At intermediate times, and for $0<\delta<1$, an oscillation due to the pole contribution takes place in $D(t)$ [and also in $D^{\rm cl}(t)$ but with a smaller amplitude]. For certain values of δ and T, this oscillation may even result in negative values of $D(t)$ during a finite time interval.

At large times $t\gg\gamma^{-1},t_{\rm th}$ and for any finite T, the curves of $D(t)$ and $D^{\rm cl}(t)$ join together: $D(t)$ describes a subdiffusive regime when $0<\delta<1$, and a superdiffusive one when $\delta>1$. At $T=0$, $D(t)$ describes the relaxation of $\Delta x^2(t)$ towards $\Delta x^2(\infty)$ for $0<\delta<1$, and a subdiffusive regime for $1<\delta<2$.

In the classical case, a modified FDT can be written as [1,2]

$$\chi_{xx}(t,t')=\beta\Theta(t-t')X^{\rm cl}(t,t';t_0)\frac{\partial C_{xx}(t,t';t_0)}{\partial t'}, \qquad (14)$$

where $\chi_{xx}(t,t')$ is the displacement response function. For a diffusing particle, the fluctuation-dissipation ratio $X^{\rm cl}(t,t';t_0)$ can be obtained from $D^{\rm cl}(\tau)$ and $D^{\rm cl}(t_w)$ [3]:

$$X^{\rm cl}(\tau,t_w)=\frac{D^{\rm cl}(\tau)}{D^{\rm cl}(\tau)+D^{\rm cl}(t_w)}. \qquad (15)$$

For any τ and t_w, one can define an effective inverse temperature as $\beta^{\rm cl}_{\rm eff}(\tau,t_w)=\beta X^{\rm cl}(\tau,t_w)$. Since $X^{\rm cl}$ does not depend on T, the bath temperature is rescaled by a factor $1/X^{\rm cl}$ larger than 1, due to those fluctuations of the particle displacement, which take place during the waiting time. At

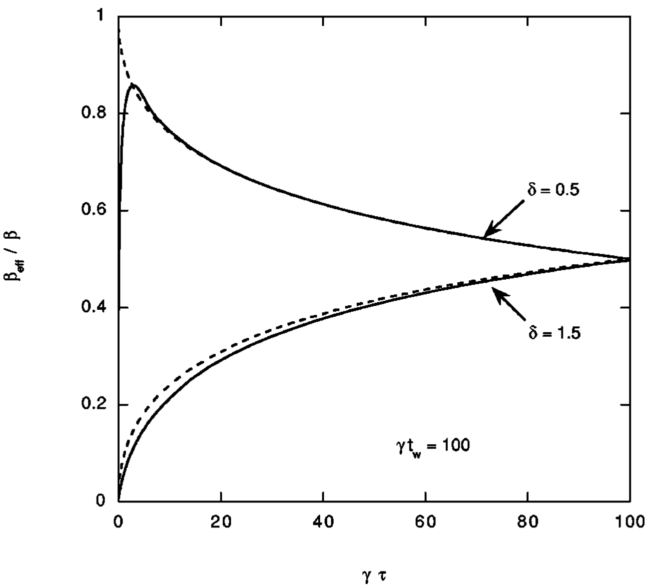

FIG. 3. The solid lines show the effective inverse temperature $\beta_{\rm eff}$, as computed from Eq. (17), plotted as a function of $\gamma\tau$ for a bath temperature $k_BT=\hbar\gamma/2\pi$ and two different values of δ. The dashed lines show the corresponding classical effective inverse temperature $\beta_{\rm eff}^{\rm cl,ag}$, as deduced from Eq. (16).

large times ($\tau,t_w \gg \gamma^{-1},t_{\rm th}$), one can use in Eq. (15) the asymptotic expressions of $D^{\rm cl}(\tau)$ and $D^{\rm cl}(t_w)$ as given by Eq. (13). Equation (15) then displays the fact that, in a sub-Ohmic or super-Ohmic model of exponent δ ($0<\delta<1$ or $1<\delta<2$), a self-similar aging regime takes place at large times, as pictured by

$$X^{\rm cl,ag}(\tau,t_w)=\frac{1}{1+(t_w/\tau)^{\delta-1}}. \tag{16}$$

Interestingly enough, $X^{\rm cl,ag}$ and $T_{\rm eff}^{\rm cl,ag}=(k_B\beta_{\rm eff}^{\rm cl,ag})^{-1}$ are functions of t_w/τ, solely parametrized by δ. They do not depend on the other parameters of the model (i.e., γ or ω_c). For $\delta=1$, one retrieves the results $X^{\rm cl,ag}=1/2$ and $T_{\rm eff}^{\rm cl,ag}=2T$ [2,3]. For any other value of δ, $X^{\rm cl,ag}$ and $T_{\rm eff}^{\rm cl,ag}$ are algebraic functions of t_w/τ. The limits $\tau\to\infty$ and $t_w\to\infty$ do not commute.

In the quantum case, the effective temperature $T_{\rm eff}=(k\beta_{\rm eff})^{-1}$ can be obtained from the following equation [3]:

$$D_{T_{\rm eff}}(\tau)=D(\tau)+D(t_w). \tag{17}$$

Equation (17) also allows us to define $T_{\rm eff}$ at $T=0$ for $1\leqslant\delta<2$. Since $D(t)$ is a monotonously increasing function of T, Eq. (17) yields for $T_{\rm eff}(\tau,t_w)$ a uniquely defined value.

The curves representing $\beta_{\rm eff}(\tau,t_w)$ as a function of τ for $\delta=0.5$ and $\delta=1.5$ at a given finite temperature and for a given $t_w\gg\gamma^{-1},t_{\rm th}$ are plotted in Fig. 3. Quantum effects do not persist beyond times $\tau\sim t_{\rm th}$. Thus, for times $\tau\gg\gamma^{-1},t_{\rm th}$, $X^{\rm cl,ag}(\tau,t_w)$ [Eq. (16)] allows for a proper description of finite temperature aging.

In summary, we have shown that the two-time dynamics of a quantum dissipative free particle displays extremely rich behaviors. In particular, one finds either a localized regime in which the position can be defined in an absolute way and does not age ($T=0$, $0<\delta<1$), or (possibly anomalously) diffusing ones in which it only makes sense to consider the displacement, which displays aging ($T=0$, $1\leqslant\delta<2$, or T finite, $0<\delta<2$). We have demonstrated that (i) the aging regime at a finite temperature is properly described by the classical fluctuation-dissipation ratio, which for $\delta\neq1$ is a self-similar function of t_w/τ, parametrized by δ, (ii) the limit value of the fluctuation-dissipation ratio is conditioned by δ, the limit value 1/2 being specific of the Ohmic dissipation ($\delta=1$).

Let us add that this model, interesting *per se* [2], is not devoid of phenomenological interest. For instance, in the domain of single-charge tunneling, the phase in a junction treated as a capacitor coupled to a dissipative environment behaves as a sub-Ohmic dissipative free particle [6]. Our study suggests that aging should be displayed by the phase, while the conjugate variable, i.e., the charge on the capacitor, should not age.

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