Aging effects in the quantum dynamics of a dissipative free particle: non-ohmic case

Alain Mauger\textsuperscript{1} and Noëlle Pottier\textsuperscript{2}

\textsuperscript{1} Laboratoire des Milieux Désordonnés et Hétérogènes, CNRS UMR 7603, Université Paris 6, 4, place Jussieu, 75252 Paris Cedex 05, France

\textsuperscript{2} Groupe de Physique des Solides, CNRS UMR 7588, Universités Paris 6 et Paris 7, 2, place Jussieu, 75251 Paris Cedex 05, France

We report new 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 $t_w/\tau$ of the waiting time to the observation time, as characterized by an exponent directly linked to $\delta$.

PACS numbers: 05.30.-d, 05.40.+j, 02.50.Ey

In complex out-of-equilibrium systems such as structural glasses and spin glasses, the trend towards equilibrium is accompanied by aging effects: for instance the two-time correlation functions of certain 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, which is valid for dynamic variables at equilibrium, is not verified in this case. Actually the study of aging effects and of the related violation of the fluctuation-dissipation theorem (FDT) is a fundamental problem of the physics of dissipative out-of-equilibrium systems \cite{1}. Several aspects of this problem still stand as largely open questions, especially in the case of quantum dissipative systems.

In order to be able to discuss these questions at any temperature, 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 also encountered, not only in complex systems, but also in simpler systems, nor disordered nor frustrated \cite{2}, it is very natural, to begin with, to carry out the study of quantum aging in this latter type of systems.

One archetype of a simple quantum dissipative system displaying aging effects is a particle coupled to a thermal bath but otherwise free, that is evolving in the absence of potential. Aging effects on the displacement correlation function and the corresponding violation of the quantum FDT have recently been discussed \cite{3} for a specific model of dissipation, namely the so-called ohmic model. It corresponds to a particle undergoing standard quantum Brownian motion \cite{4,5}. The damped ohmic equation of motion can be given a non retarded form in the classical limit, in which diffusion is normal. However, the ohmic model does not allow to handle all the physical situations of interest, for instance those in which the 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.

In this Letter, we examine aging effects in this simple system using 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 thermal bath having a continuous distribution of modes of bandwidth $\omega_{c}$. (Caldeira and Leggett model \cite{6,7}). The central ingredient of the model is the product of the density of modes of the bath $g(\omega)$ times the squared coupling constant $|\lambda(\omega)|^2$, a product assumed to vary as $\omega^\delta$ at frequencies $\omega \ll \omega_{c}$. In the ohmic model, the dissipative exponent $\delta$ is equal to 1. The algebraic cases $0 < \delta < 1$ and $\delta > 1$ are known, respectively, as the subohmic or superohmic dissipation models \cite{8,9,10}.

In the following we first show that for $0 < \delta < 2$ the particle velocity equilibrates at large times and does not age. Then, turning to the study of the particle coordinate, we discuss the domain of $(\delta, T)$ parameters for which aging is taking place, or not. Actually the question is a non-trivial one. Indeed the two following properties have been demonstrated \cite{11,12,13}. 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 $1 \leq \delta < 2$, 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 a result, we find clear-cut behaviors: as far as the coordinate is concerned, the localized particle does not age, while the diffusing one ages.

In the Caldeira and Leggett model, the particle is coupled linearly to a set of harmonic oscillators in thermal equilibrium at temperature $T$. The Hamiltonian of the
particle-plus-bath system reads, in obvious notations,
\[ H = \frac{p^2}{2m} - x \sum_\nu \lambda_\nu (b_\nu + b_\nu^\dagger) + \sum_\nu \hbar \omega_\nu b_\nu b_\nu^\dagger + x^2 \sum_\nu \frac{\lambda_\nu^2}{\hbar \omega_\nu}, \]
where \( \lambda_\nu \) 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
\[ K(\omega) = 2\gamma (\frac{\omega}{\gamma})^{\delta - 1} f_c(\frac{\omega}{\omega_c}), \]
where \( \gamma \) is a coupling frequency and \( f_c \) a high-frequency cut-off function of typical width \( \omega_c \). The definition of \( K(\omega) \) is extended to \( \omega < 0 \) by imposing that it must be an even function of \( \omega \). The particle position operator obeys the retarded equation of motion
\[ \ddot{x}(t) + \int_{t_i}^t dt' k(t-t')\dot{x}(t') = -x(t_i)k(t-t_i) + \frac{1}{m} F(t), \]
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
\[ C_{FF}(t) = m \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Re \tilde{K}(\omega) \hbar \omega \coth \frac{\beta \hbar \omega}{2} e^{-i\omega t} \]
with \( \Re \tilde{K}(\omega) = \frac{1}{2} K(\omega) \) and \( \beta = (k_B T)^{-1} \).

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 \[ [11] \]. For \( 0 < \delta < 2 \) (\( \delta \neq 1 \)), the average particle velocity \( \langle v(t) \rangle \) relaxes towards zero at large \( t-t_i \) like \( (t-t_i)^{\delta-2} \) (the average is taken over the variables of the initial state of the particle and over the bath variables). For \( \delta = 1 \), the relaxation is exponential. The initial value \( \langle v(t_i) \rangle \) being forgotten for \( 0 < \delta < 2 \), this situation may in this sense be qualified of ergodic. For \( \delta > 2 \), the dynamics is governed at large times by a kinematical term involving the renormalized mass and \( \langle v(t_i) \rangle \) is never forgotten \[ [11] \].

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 \[ [5] \], thus generalizes to non-ohmic models with \( 0 < \delta < 2 \). The two-time velocity correlation function depends only on the time difference and can be computed via Fourier analysis and the Wiener-Khintchine theorem:
\[ C_{vv}(t) = \frac{1}{m} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \Re \tilde{K}(\omega \hbar \omega \coth \frac{\beta \hbar \omega}{2} e^{-i\omega t}. \]
With the modelization (2) for \( K(\omega) \) and a lorentzian cut-off function \( f_c = \omega_c^\delta/(\omega_c^\delta + \omega^2) \), one has:
\[ \Im \tilde{K}(\omega) = \omega (\frac{\omega}{\gamma})^{\delta-2} f_c(\frac{\omega}{\omega_c}) \times \left[ \cot \frac{\delta \pi}{2} + (\frac{\omega}{\gamma})^{\delta-2} \frac{1}{\sin \frac{\delta \pi}{2}} \right]. \]

Then, setting
\[ C_{vv}(\omega) = \frac{1}{m} \frac{\Re \tilde{K}(\omega) \hbar \omega \coth \frac{\beta \hbar \omega}{2},}{|K(\omega) - i\omega|^2} \]
one may attempt to define the coordinate 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 which must be independent of \( t \). Checking the small-\( \omega \) behavior of the integrand with the chosen modelization for the memory kernel, 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 \( x(t) = \int_{-\infty}^{t} v(t') dt' \). The two-time position correlation function
\[ C_{xx}(t, t') = \frac{1}{2} \{ \langle x(t), x(t') \rangle \} + , \]
where the symbol \( \{ \ldots \} + \) stands for the anticommutator, only depends on \( t-t' \) and does not age. In particular one has
\[ \Delta x^2(t) = 2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} C_{xx}(\omega) (1 - \cos \omega t), \]
that is, in terms of the integrated velocity correlation function \( D(t) = \int_0^t du C_{vv}(u) \),
\[ \Delta x^2(t) = \Delta x^2(\infty) - 2 \int_t^{\infty} D(t') dt'. \]
The asymptotic behavior at large times of \( D(t) \) allows to characterize the relaxation of the mean square displacement towards \( \Delta x^2(\infty) \).

In other cases, that is at \( T = 0 \) for \( 1 \leq \delta < 2 \) and at finite \( T \) for \( 0 < \delta < 2 \), the integral \( \int_0^\infty (d\omega/2\pi) C_{xx}(\omega) \) diverges and \( \langle x^2(t) \rangle \) and \( C_{xx}(t, t') \) are infinite. The particle diffuses. Since it is then no more possible to define an absolute position, we focus the interest on the displacement \( x(t) - x(t_0) \) \( (t \geq t_0) \). This quantity does not equilibrate with the bath, even at large times: it ages. The mean square displacement \( \Delta x^2(t) \) diverges at infinite time and \( D(t) \) 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 \( 1 < \delta < 2 \)).
bandwidth limit $\omega_c \to \infty$ in which case calculations are more simple. One has:

$$D(t) = \frac{\hbar}{m\pi} \gamma^{\delta - 2} \int_0^\infty d\omega \coth \frac{\beta h \omega}{2} \sin \omega t \times$$

$$\left[ \omega^{\delta - 1} + \omega^{\delta - 2} (|\omega|^{\delta - 2} \cot \frac{\delta \pi}{2} - \gamma^{\delta - 2})^2 \right]^{-1}. \quad (11)$$

At finite $T$, it is interesting to discuss on the same footing the classical counterpart of $D(t)$, namely $D^{cl}(t)$ deduced from $D(t)$ by replacing $\coth(\beta h \omega/2)$ by $2/\beta h \omega$ in formula (11). Several important features of $D(t)$ and $D^{cl}(t)$ can be obtained by contour integration.

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

$$D(t)_{\text{pole}} \sim \frac{\hbar}{m} \frac{1}{2 - \delta} e^{-\lambda t} \sin \Omega t,$$

(12)

where $\Omega$ and $\Lambda$ are known functions of $\delta$ and $\gamma$, and of a cut contribution behaving at large times as a power-law,

$$D(t)_{\text{cut}} \sim \frac{\hbar}{m \pi} (\gamma t)^{\delta - 2} \sin^2 \frac{\delta \pi}{2} \Gamma(2 - \delta), \quad (13)$$

where $\Gamma$ denotes the Euler Gamma function.

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

$$D^{cl}(t)_{\text{pole}} \sim \frac{kT}{m \gamma} \frac{2}{2 - \delta} \left( \sin \frac{\delta \pi}{2} - e^{-\lambda t} \sin(\Omega t - \phi) \right) \quad (14)$$

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

$$D^{cl}(t)_{\text{cut}} \sim \frac{kT}{m \gamma} \frac{(\gamma t)^{\delta - 1} \sin \frac{\delta \pi}{2}}{\Gamma(\delta)}. \quad (15)$$

The behaviors of $D(t)$ and $D^{cl}(t)$ at several different temperatures are illustrated on Fig. 1 for $\delta = 0.5$ and on Fig. 2 for $\delta = 1.5$. Interestingly enough, for any given $\delta$, the curves corresponding to different bath temperatures do not intersect. Actually, it can be shown that, at any fixed time $t$, $D(t)$, like $D^{cl}(t)$, is a monotonously increasing function of $T$.

For times $t \ll t_{\text{th}}$ ($t_{\text{th}} = \hbar/2\pi k_B T$) and for any value of $\delta$, 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 $D^{cl}(t)$ but with a smaller amplitude). For certain values of $\delta$ and $T$, this oscillation may even result in negative values of $D(t)$ during a finite time interval.

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

FIG. 1. In full lines, $D(t)$ plotted as a function of $\gamma t$ 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 limit value). In dashed lines, the corresponding $D^{cl}(t)$.

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

These features of $D(t)$, especially the large times ones, are essential for describing the aging properties of the displacement correlation function, as defined by

$$C_{xx}(t, t'; t_0) = \frac{1}{2} \langle [x(t) - x(t_0)] [x(t') - x(t_0)] \rangle_+. \quad (16)$$

In the classical case, a modified FDT can be written
as

\[ \chi_{xx}(t, t') = \beta \Theta(t - t') X^{cl}(t, t'; t_0) \frac{\partial C_{xx}(t, t'; t_0)}{\partial t'}, \]  

(17)

where \( \chi_{xx}(t, t') \) is the displacement response function. For a diffusing particle, the fluctuation-dissipation ratio \( X^{cl}(t, t'; t_0) \) can be obtained from \( D^{cl}(\tau) \) and \( D^{cl}(t_w) \) \(^{[8]}\), where \( \tau = t - t' \) denotes the observation time and \( t_w = t' - t_0 \) the waiting time:

\[ X^{cl}(\tau, t_w) = \frac{D^{cl}(\tau)}{D^{cl}(\tau) + D^{cl}(t_w)}. \]  

(18)

For any \( \tau \) and \( t_w \), one can define an effective inverse temperature as \( \beta_{\text{eff}}(\tau, t_w) = \beta X^{cl}(\tau, t_w) \). Since \( X^{cl} \) does not depend on \( T \), the bath temperature is rescaled by a factor \( 1/X^{cl} \) larger than 1, due to those fluctuations of the particle displacement which take place during the waiting time. At large times \( (\tau, t_w \gg \gamma^{-1}, t_{th}) \), one can use in formula \(^{[18]}\) the asymptotic expressions of \( D^{cl}(\tau) \) and \( D^{cl}(t_w) \) as given by Eq. \(^{[15]}\). Eq. \(^{[15]}\) then displays the fact that, in a subohmic or superohmic model of exponent \( \delta \) (\( 0 < \delta < 1 \) or \( 1 < \delta < 2 \)), a self-similar aging regime takes place at large times, as pictured by

\[ X^{cl,ag}(\tau, t_w) = \frac{1}{1 + \left( \frac{t_w}{\tau} \right)^{\delta-1}}. \]  

(19)

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

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

\[ DT_{\text{eff}}(\tau) = D(\tau) + D(t_w). \]  

(20)

Eq. \(^{[20]}\) also allows to define \( T_{\text{eff}} \) at \( T = 0 \) for \( 1 \leq \delta < 2 \). Since \( D(t) \) is a monotonously increasing function of \( T \), Eq. \(^{[20]}\) yields for \( T_{\text{eff}}(\tau, t_w) \) a uniquely defined value.

The curves representing \( \beta_{\text{eff}}(\tau, t_w) \) as a function of \( \tau \) for \( \delta = 0.5 \) and \( \delta = 1.5 \) at a given finite temperature and for a given \( t_w \gg \gamma^{-1}, t_{th} \), are plotted on Fig. 3. Quantum effects do not persist beyond times \( \tau \approx t_{th} \). Thus, for times \( \tau \gg \gamma^{-1}, t_{th} \), \( X^{cl,ag}(\tau, t_w) \) as given by formula \(^{[14]}\) allows for a proper description of aging effects.

In conclusion, we have shown that the two-time dynamics of the coordinate of a quantum dissipative free particle coupled to a thermal bath (coupling \( \sim \omega_c \) with \( 0 < \delta < 2 \)) displays extremely rich behaviors. According to the values of \( T \) and \( \delta \), one may find 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 (\( T = 0, 1 \leq \delta < 2 \), or \( T \) finite, \( 0 < \delta < 2 \)). The aging regime at finite \( T \) is properly described by the large times expression of the classical fluctuation-dissipation ratio, which for \( \delta \neq 1 \) is a self-similar function of \( t_w/\tau \), solely parametrized by \( \delta \).

---

1. J.-P. Bouchaud, L.F. Cugliandolo, J. Kurchan and M. Mézard, in *Spin glasses and random fields*, edited by A.P. Young editor (World Scientific, Singapore, 1997).
2. L.F. Cugliandolo, J. Kurchan and G. Parisi, J. Phys. A. 4, 1641 (1994).
3. N. Pottier and A. Mauger, Physica A 282, 77 (2000).
4. V. Hakim and V. Ambegaokar, Phys. Rev. A 32, 423 (1985).
5. C. Aslangul, N. Pottier and D. Saint-James, J. Stat. Phys. 40, 167 (1985).
6. A. Caldeira and A.J. Leggett, Ann. Phys. 149, 374 (1983).
7. A.J. Leggett, S. Chakravarty, A.T. Dorsey, M.P.A. Fisher, A. Garg and W. Zwerger, Rev. Mod. Phys. 59, 1 (1987).
8. P. Schramm and H. Grabert, J. Stat. Phys. 49, 767 (1987).
9. H. Grabert, P. Schramm and G.-L. Ingold, Phys. Rep. 168, 115 (1988).
10. C. Aslangul, N. Pottier and D. Saint-James, J. Physique 48, 1871 (1987).
11. U. Weiss, *Quantum dissipative systems*, Second Edition, World Scientific, Singapore, 1999.