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Quantum dynamics of a damped free particle

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Résumé. — Nous étudions la dynamique exacte d'une particule libre quantique amortie par son interaction avec un bain harmonique, dans le cas où le couplage effectif se comporte comme ω^δ à basse fréquence. Nous trouvons divers régimes selon les valeurs de δ et de la température. Aux grands temps, l'écart quadratique moyen du déplacement ou bien diverge comme t^ν , l'exposant ν étant inférieur ou égal à 2 ou bien tend vers une valeur finie, ce qui est la caractéristique d'un confinement au sens large. De surcroît, pour $\delta > 1$, une oscillation (absente dans le système non couplé) apparaît dans la dynamique : à cause de la friction sur les modes de basse fréquence dominants et des effets de mémoire, la particule est contrainte à relaxer en moyenne vers sa position initiale, l'effet dynamique global du bain étant analogue à celui d'un potentiel appliqué. Dans la limite $\delta \rightarrow 0$, la particule est bloquée.

Abstract. — We investigate the exact quantum dynamics of a free particle damped through its interaction with an harmonic bath, when the effective coupling strength behaves as ω^δ at low frequency. We find that various regimes can occur depending on the value of δ and of the temperature. At large times, the mean square displacement is shown either to diverge as t^ν , the exponent ν being never greater than 2 or to tend towards a finite value, indicating a confinement in the broad sense. In addition, for $\delta < 1$, an oscillation (absent in the uncoupled system) is found : due to the friction on the dominant low-frequency modes and to the existence of retardation effects, the particle is forced to relax in the mean towards its initial location, the net dynamical effect of the bath being similar to that of an applied potential. In the limit $\delta \rightarrow 0$, the particle is frozen.

1. Introduction.

We here give an account of some results about the motion of a free particle of bare mass m subjected to friction as a consequence of its interaction with an infinite number of harmonic modes (bath). As proposed by Caldeira and Leggett [1], one can set up the friction through a coupling which is bilinear with respect to both the coordinate of the particle and the coordinates of the oscillators. Otherwise stated, the friction is realized by attaching masses and springs to the particle [2]. As contrasted to more complex situations resulting from the effect of an external

non-linear static force, the free particle [2, 3] shares with the harmonic oscillator [5-9], for this kind of coupling, the property of being an exactly solvable model. Furthermore, the solutions can be found in a standard and elementary way ; however the dynamics of the harmonic oscillator is in a way less rich, due to the existence of a finite frequency in the problem.

The central ingredient in such a model is the product of the density of modes of the bath times the squared coupling strength which, in the continuum limit, produces a smooth function of the frequency, $\Lambda(\omega)$ [1]. As far as long-time behaviours are concerned, and except maybe for pathological cases, it is enough to know the behaviour of $\Lambda(\omega)$ at low frequencies, it being understood that, for physical reasons, $\Lambda(\omega) \rightarrow 0$ when $\omega \rightarrow +\infty$ as pictured by some cut-off function f_c .

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For SQUID's problems, it has been argued [1] that $\Lambda \sim \omega$ for $\omega \rightarrow 0$ (ohmic model) but this is clearly a very particular situation. Generally speaking and depending of the dimensionality of the surrounding medium, one rather expects $\Lambda \sim \omega^\delta$ where δ is a small integer ; one can even conceive the case where δ is not an integer, for example in disordered media [10]. Anyway, it is important for the dissipation to occur, that modes of arbitrarily small frequency be present.

In a recent paper [11], we studied the Brownian motion of an ohmic particle in a periodic potential. It was shown that, when 2nd-order perturbation treatment is valid, the influence of the potential can be described by a modification of the noise and of the friction. Actually, when the friction is high enough, the particle behaves like an equivalent non-ohmic free particle, the exponent δ being simply related to the dimensionless coupling constant with the bath and taking any value between 0 and 1. In that case, a trend towards localization was observed and this motivated our study of the free damped non-ohmic particle *per se*.

It can be anticipated, on purely physical grounds, that the dynamics will be strongly dependent on δ . For δ small, the low-frequency modes are dominant and act as a quasi-static disorder on the particle ; the coupling with such soft modes tends to slow down the motion. Indeed, for $\delta < 1$, the particle goes back in the average to its initial location, whereas for $1 < \delta < 2$, its motion at large times follows a $t^{\delta-1}$ law, displaying a slowing down as compared to a free undamped particle. Moreover, it turns out that the proper relaxation time at $T = 0$ does indeed go to infinity when $\delta \rightarrow 0$. In that limit, the final mean square displacement of the particle vanishes, indicating a localization in the broad sense. On the contrary, when δ is large, the low frequency modes are strongly depressed and therefore the dynamics can become dependent upon the high frequency part of the spectrum.

Thus, it is worthy to study the dynamics when δ is any given real positive number and this is done in the following in a straightforward manner, by a direct calculation of the correlation functions of interest. Grabert *et al.* have recently treated this problem [12] by an alternative approach using the Feynman-Vernon formalism, a method which, although powerful, is not always necessary and leads more often to tedious calculations. Among other things, it is shown by these authors that, at zero temperature, anomalous diffusion occurs and confinement of the particle is obtained for $\delta < 1$. In addition, they find, at finite T and for $\delta > 2$, that the dynamics is governed at large times by a kinematical term involving a renormalized mass and depending on the initial velocity of the particle. In other words, for $\delta > 2$, the system is not ergodic in the sense that the initial conditions are

relevant at any time. Our results are in agreement with those of these authors.

2. General remarks and basic equations

In obvious notations, the translationally-invariant Hamiltonian of the Caldeira-Leggett model reads :

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

where the last counterterm insures the translational symmetry [2]. As shown in this latter work, the Hamiltonian can be rewritten as :

$$H = (p^2/2m) + \sum_\nu [(P_\nu^2/2m_\nu) + (1/2)m_\nu \omega_\nu^2 (X_\nu - x)^2] \quad (2)$$

displaying the fact that the friction is obtained by attaching masses and springs to the particle. The correspondance between the parameters is the following :

$$\lambda_\nu = (\hbar m_\nu \omega_\nu^3 / 2)^{1/2}. \quad (3)$$

From this Hamiltonian, the equations of motion for all the degrees of freedom can be readily written down and, after the elimination of the bath variables, the Heisenberg representation of the particle coordinate is seen to obey the exact following dynamical equation (see [3] for further details and [4]) :

$$d^2x/dt^2 + \int_{t_0}^{+\infty} dt' k(t-t') dx/dt' = -xk(t-t_0) + a(t-t_0) \quad (4)$$

where $a(t)$ is a random force per unit mass and $k(t)$ a retarded memory kernel related to $a(t)$ by a fluctuation-dissipation relation. These quantities have the explicit expressions :

$$k(t) = \sum_\nu (2 \lambda_\nu^2 / m \hbar \omega_\nu) \cos \omega_\nu t \quad (5)$$

$$a(t) = m^{-1} \sum_\nu \lambda_\nu (b_\nu e^{-i\omega_\nu t} + b_\nu^\dagger e^{i\omega_\nu t}) \quad (6)$$

t_0 denotes the time at which the interaction between the particle and the bath is switched on. The dynamics is completely determined by equation (4), implemented by the data of an initial state ; although this is by no means necessary, we will assume that, at $t = t_0$, the total density operator is factorized and is of the form $\rho_{\text{part}} \otimes \rho_{\text{bath}}$, with $\rho_{\text{bath}} = Z^{-1} e^{-\beta H}$. It is clear that *any* other initial state can be treated in the same framework.

The $\Lambda(\omega)$ function quoted in the introduction is the continuum limit of $\sum_\nu |\lambda_\nu|^2 \delta(\omega - \omega_\nu)$ and is assumed to behave as ω^δ at low frequencies ; the

ohmic case is recovered by setting $\delta = 1$. The precise form of $k(t)$ can now be written as :

$$k(t) = (2/\pi) \gamma^2 (\gamma \tau)^{\delta-2} \Theta(t) \int_0^{+\infty} dz z^{\delta-1} f_c(z) \times \cos(\gamma tz). \quad (7)$$

In this latter equation, $\Theta(t)$ is the unit step function, vanishing for $t < 0$; τ is a time to be identified later on (which coincides with the time τ_R in [3] when $\delta = 1$) and γ denotes the width of the cut-off function f_c . In other words, this phenomenological model depends upon three parameters : γ , τ and δ (or equivalently $g = \gamma \tau$, τ and δ) which could be calculated from first principles for a given physical situation ; we will come back on this point later on.

The cut-off function need not being fully precised (at least for δ not too large as compared to unity) and is only assumed to be an even, meromorphic function, devoid of any singularity on the real axis and having finite moments $M_\mu = \int_0^{+\infty} dz z^\mu f_c(z)$

for any real $\mu > -1$; this freedom is due to the fact that for long-time properties, only the low-frequency behaviour is relevant. It is interesting to note that the frequently used exponential cut-off $e^{-|z|}$ must be treated with some care since this function does have a singularity at $z = 0$.

In equation (7), one sees that, in order to have a well-defined physical model, δ is *a priori* only required to be strictly positive ; this insures that $k(t)$ is finite at all positive times including $t = 0_+$.

In the most commonly discussed problems, δ is an odd integer so that exponential decay of the memory is expected (see the Appendix A for details). This is for instance the case for the ohmic ($\delta = 1$) free damped particle studied in [3]. However, this turns out to be a rather special situation ; it may be said that the final occurrence of long-tails in the memory is in fact an ubiquitous phenomenon.

The above equations are exact and thus contain no approximation ; they allow to explicitly analyse the dynamics at any time, including transient effects resulting from any given initial non-equilibrium state, and to display the approach to the final permanent regime.

It is interesting to precise how the undamped limit can be recovered. For $\delta > 2$, the effective coupling constant is $G = g^{\delta-2} / \sin(\pi \delta / 2)$ (see Eqs. (A.2) and (A.4)) ; so the weak coupling limit ($G \ll 1$) is equivalent to $\delta \gg \delta_1(g) = (2/\pi) \sin^{-1} g^{\delta-2}$. This means that, for any given finite g greater than 1, the weak coupling limit can never be reached when $\delta \rightarrow 0$; this can be understood by the fact that when δ is very small, the number of modes of low frequency is relatively large, thus always yielding a

strong effective coupling. For any fixed $\delta < 2$, the free undamped particle is recovered by setting $g = +\infty$. On the contrary, for $\delta > 2$, the weak coupling condition is simply $g \ll 1$ and the undamped case is reached by taking $g = 0$. In what follows, we shall derive results valid for any coupling unless otherwise stated. Note that in a given physical situation, the three relevant parameters γ , g and τ may be interdependent, in which case the above analysis should be refined.

3. Averaged trajectory.

We first investigate the averaged trajectory of the particle when, at $t = 0$ (i.e. taking t_0 as the origin in time), it is injected into the bath with a velocity v_0 ; v_0 is thus the quantum expectation value of the operator $(p/m) \equiv v$ in the given initial state. Using capital letters for the Laplace transforms ($F_L(s) = \int_0^{+\infty} e^{-st} f(t)$), equation (4) gives for the velocity operator :

$$V_L(s) = [(p/m) - xK_L(s) + A_L(s)] W_L(s) \quad (8)$$

where $W(s) \equiv [s + K_L(s)]^{-1}$ is a *c*-number. From equation (8), one can write :

$$v(t) = w(t)(p/m) - (w^* k)(t) x + (w^* a)(t) \quad (9)$$

where $(f^* g)(t)$ denotes the usual convolution integral $\int_0^t dt' f(t-t')g(t')$; x and p are the

Schrödinger operators. Now, by averaging this expression on all the variables for the given initial state and defining the origin in space as the initial mean position of the particle, we obtain the non-equilibrium expected value of the velocity of the particle as :

$$\langle v(t) \rangle = (2i\pi)^{-1} \int_c e^{st} v_0 W_L(s) \equiv w(t) \langle p/m \rangle. \quad (10)$$

The Laplace inversion introduces three kinds of contributions : exponentially decreasing terms corresponding to the residues, power-law terms $\sim t^\nu$ arising from the integral on both sides of the cut (for δ different from an odd-integer) and a constant describing the asymptotic dynamics coming out from a small circle around the origin. This latter constant vanishes for $\delta < 2$ and is equal to $\rho^{-1} v_0$ for $\delta > 2$, where ρ is given by :

$$\rho = 1 + (2/\pi) g^{\delta-2} M_{\delta-3} = 1 + m^{-1} \Sigma_\nu m_\nu. \quad (11)$$

Note that ρm is the sum of the mass of the particle and of all the bath oscillators, which is

finite for $\delta > 2$ and infinite otherwise. The above final regime can be viewed as the result of an inelastic sticking collision between the particle and the bath, giving the final velocity $v_\infty = \rho^{-1} v_0$ to the particle. Due to the conservation of total momentum, this last result shows that, in the final regime, the whole system moves at the mean constant velocity v_∞ . For $\delta < 2$, v_∞ always vanishes at infinite time, implying that the initial condition is in fact irrelevant as regards to the equilibrium state. On the contrary, for $\delta > 2$, the initial velocity is never forgotten and the particle, for $t \rightarrow \infty$, follows a kinematical motion.

Once realized these rather unexpected features of the dynamics, further details of the motion are best studied by a definite choice of the cut-off function f_c . For instance, for $\delta < 2$, one may take $f_c(x) = (1 + x^2)^{-1}$ since this insures that all quantities of interest are well-defined. Then $K_L(s)$ is given by :

$$K_L(s) = (g^2 - \delta \sin \theta)^{-1} s f_c(is/\gamma) [(s/\gamma)^{\delta-2} - 1] \quad (12)$$

where $\theta = \pi \delta / 2$. The poles of $W(s)$ arise as pairs of complex conjugate numbers and the one having a positive imaginary part is shown in figure 1 for various values of the parameter g (the arrows correspond to δ increasing). It is seen that, when $\delta \rightarrow 0$, both the oscillation frequency (imaginary part of the pole) and the lifetime (inverse of the modulus of the real part) diverge ; this displays the fact that when the low frequency modes are the dominant ones, the particle is more and more strongly bounded by a kind of dynamical potential which develops in the surrounding medium. In the limit $\delta = 0+$, the particle becomes frozen. For $\delta = 1$, the poles are either real (for $g > 4$) or have a constant real part equal to $-\gamma/2$ and a finite g -dependent imaginary part (for $g < 4$) ; in this latter case, which corresponds to a strong coupling, the interaction with the bath introduces a finite frequency, reminiscent of a new dressed particle having an internal eigenmode. For $\delta \rightarrow 2$, all the branches (for various g 's) converge towards a single point.

It is important to note that only those poles having a modulus much smaller than γ can be said *a priori* to be independent of f_c . This is the case when $\delta < 1$ and when $G \gg 1$; in this case, an approximate expression for the poles s_0 in the following :

$$s_0 \approx \tau^{-1} (\sin \theta)^{-1/(2-\delta)} e^{\pm i\varphi} \quad (13)$$

where $\varphi = \pi/(2-\delta)$.

In any case $\delta < 2$, $\delta \neq 1$, the asymptotics of $\langle x(t) \rangle$ is dominated by a power law (Γ is the Euler function) :

$$\langle x(t) \rangle \approx [(\sin \theta)/\Gamma(\delta)] v_0 \tau (t/\tau)^{\delta-1}. \quad (14)$$

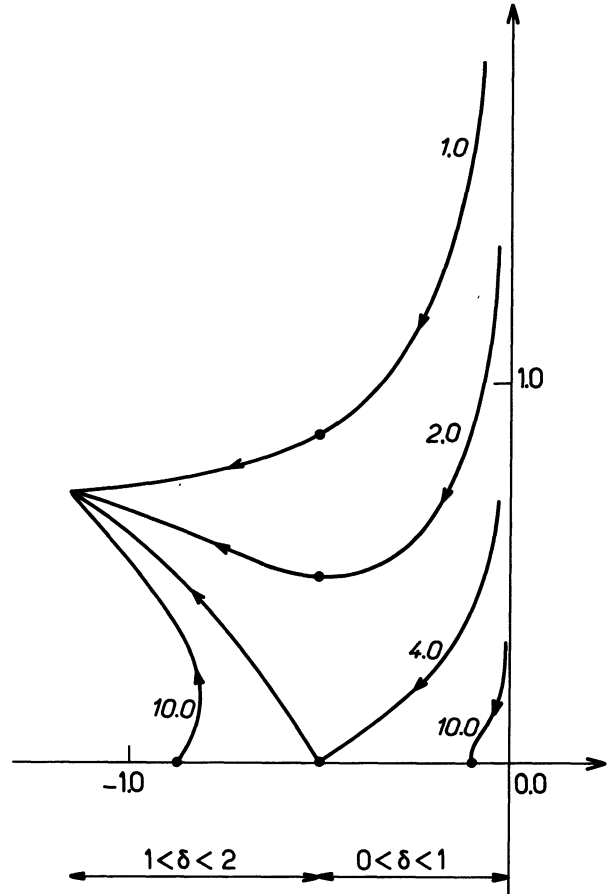


Fig. 1. — Pole (in units of γ) above the real axis for the response function $W_L(s)$ as defined by equation (8) when a Lorentzian cut-off function is used, yielding the expression (12) for $K_L(s)$. Each curve is labelled by the value of the parameter $g = \gamma \tau$. The bold dots correspond to the ohmic case ($\delta = 1$), whereas the arrows indicate the flow when δ increases. All the curves converge towards a single point when $\delta \rightarrow 2$.

This latter equation displays the fact that when $\delta < 1$, $\langle x(t) \rangle$ tends to zero, i.e. that the particle in the mean relaxes towards its initial location, following at intermediate times a damped oscillatory motion. For $\delta > 1$, the particle goes to infinity, whereas its velocity tends towards zero, showing that the net effect of the friction is to slow down the motion as compared to the free one. For $\delta = 1$, $\langle x(t) \rangle$ can be readily (and exactly) written at any time as :

$$\begin{aligned} \langle x(t) \rangle_{\delta=1} = & v_0 \tau - v_0 \tau e^{-\gamma t/2} \times \\ & \times \{ [(\gamma^2 + \gamma'^2)/(2\gamma\gamma')] \\ & \times \sinh(\gamma' t/2) + \cosh(\gamma' t/2) \} \quad (15) \end{aligned}$$

where :

$$\gamma' = \gamma(1 - 4/g)^{1/2}. \quad (16)$$

Only in this case, the particle travels a finite distance equal to $v_0 \tau$, as in the standard Brownian

motion ; moreover, in the limit of an infinite bandwidth ($\gamma \rightarrow \infty$, i.e. strictly ohmic model), one readily recovers the standard result :

$$\langle x(t) \rangle_{\delta=1, \gamma=+\infty} = v_0 \tau [1 - e^{-t/\tau}] \quad (17)$$

For $\delta > 2$, one has :

$$\langle x(t) \rangle \approx v_\infty t [1 + (2/\pi\rho) \Gamma(\delta - 3) \times \cos \theta (t/\tau)^{2-\delta} + \dots] \quad t \rightarrow \infty. \quad (18)$$

The results for the final value of the average coordinate can be summed up as follows :

$$\langle x(+\infty) \rangle = v_0 \tau \begin{matrix} 0 & \delta < 1 \\ \delta = 1 & \delta = 1 \\ +\infty & \delta > 1. \end{matrix} \quad (19)$$

4. Fluctuations around the mean trajectory.

The autocorrelation of the velocity fluctuations around the mean trajectory is given by :

$$C_{vv}(t', t'') = (1/2) \langle \{ [v(t') - \langle v(t') \rangle] [v(t'') - \langle v(t'') \rangle] + [v(t'') - \langle v(t'') \rangle] [v(t') - \langle v(t') \rangle] \} \rangle$$

and has the expression :

$$\begin{aligned} C_{vv}(t', t'') &= m^{-2} w(t') w(t'') [\langle p^2 \rangle - \langle p \rangle^2] + (1/2) (w^* k)(t') (w^* k)(t'') \langle x^2 \rangle \\ &+ m^{-1} [w(t') (w^* k)(t'') + w(t'') (w^* k)(t')] (1/2) \langle px + xp \rangle \\ &+ \int_0^{t'} dt_1 \int_0^{t''} dt_2 w(t' - t_1) w(t'' - t_2) C_{aa}(t_1 - t_2) \end{aligned} \quad (20)$$

where :

$$C_{aa}(t_1 - t_2) = (1/2) \langle a(t_1) a(t_2) + a(t_2) a(t_1) \rangle \quad (21)$$

is the autocorrelation of the fluctuating force when the uncoupled bath is at equilibrium. Remember that all the averages are taken with the given initial state.

Two kinds of terms can be distinguished. Some of them convey explicit information about the initial state of the particle ; since the convolution $(w^* k)(t)$ always tends to zero when $t \rightarrow +\infty$, whereas $w(t)$ tends towards a constant (vanishing if $\delta < 2$), only the term implying the variance of the momentum $\Delta p^2 \equiv \langle p^2 \rangle - \langle p \rangle^2$ survives at large times in the case $\delta > 2$; due to quantum uncertainty, this term cannot be cancelled by a proper choice of ρ_{part} because then $\langle x^2 \rangle$ would be infinite. On the contrary, for $\delta < 2$, all the information about the initial state for the particle is lost at sufficiently large times. The last term in equation (20) only involves bath operators *via* the autocorrelation function $C_{aa}(t_1 - t_2)$ and, when both times t' and t'' are very large, becomes an even function of the time difference $t' - t''$, as can be seen by replacing each function in the integral by its Laplace transform. In such a limit, this latter contribution can be analysed by a direct Fourier transformation of the equation of motion (4). Summing up, the long-time expression for $C_{vv}(t', t'')$ can be written as :

$$C_{vv}(t', t'') \approx m^{-2} w(t') w(t'') \Delta p^2 + C_{vv}^*(t' - t'') \quad (22)$$

$C_{vv}^*(t' - t'')$ represents the random fluctuation about the mean trajectory, which is diffuse because of the Heisenberg inequalities in the initial state, never forgotten when $\delta > 2$. For $\delta < 2$, $C_{vv}(t', t'')$ does coincide with $C_{vv}^*(t' - t'')$ in the asymptotic regime, once the transient effects have died away.

Since the system is intrinsically linear, $C_{vv}^*(t)$ can be exactly expressed in terms of the response function $\chi(\omega)$ defined as :

$$\chi(\omega) = [\omega^2 + i\omega K(\omega)] \quad (23)$$

where $K(\omega)$ is the Fourier transform of $k(t)$, the properties of which are given in the Appendix A. For instance, $C_{vv}^*(t)$ can be written as :

$$\begin{aligned} C_{vv}^*(t) &= (\hbar\gamma/2 \pi m) \text{Im} \int_0^{+\infty} dz z^2 [\chi(-z) - \\ &- \chi(+z)] \times e^{i\gamma z} \text{cotanh}(\gamma\tau_T z) \end{aligned} \quad (24)$$

where τ_T is the temperature time defined as $\tau_T = \hbar/2 k_B T$. By using equations (24) and (A.6), it is seen that in the classical limit $k_B T/\hbar\gamma \rightarrow +\infty$, $C_{vv}^*(0)$ is equal to $k_B T/m$, independently of the weak coupling assumption, in accordance with the equipartition of energy. Moreover, by using the Mittag-Leffler expansion of the cotanh function in equation (24), one can easily check that, for any temperature, $C_{vv}^*(0)$ tends towards $k_B T/m$ in the limit of weak coupling, as it must be.

The stationary mean square displacement $\Delta x^2(t'', t'')$ is defined as :

$$\Delta x^2(t', t'') \equiv \langle [x(t') - x(t'')]^2 \rangle \quad (25)$$

and, in the limit where t' and t'' are large, can be expressed as :

$$\Delta x^2(t', t'') = \rho^{-2} \Theta(\delta - 2)(t' - t'')^2 + \Delta x^{2*}(t' - t'') \quad (26)$$

where $\Delta x^{2*}(t)$ is obtained from $C_{vv}^*(t)$ by a double time-integration :

$$\Delta x^{2*}(t) = (\hbar \pi m \gamma) \operatorname{Im} \int_0^{+\infty} dz [\chi(-z) - \chi(+z)] \operatorname{coth}(\gamma \tau_T z) (1 - e^{i\gamma t z}). \quad (27)$$

The unit step function in equation (26) is a reminder of the fact that the kinematical term is present only for $\delta > 2$. Note that $\Delta x^2(t', t'')$ is not the variance of the position and, as such, is inadequate for describing quantum localization. In all what follows, we focus the analysis on the starred functions Δx^{2*} and C_{vv}^* .

4.1 ZERO-TEMPERATURE CASE. — By looking at equations (A.2), (A.5) and (24), one sees that the behaviour of $C_{vv}^*(t)$ will be quite different according to the location of δ as regards to 2 which is the « order » of the integro-differential equation (4). This comes out from the competition at low frequency between the noise spectrum and the response of the bare particle. For clarity we will separately investigate the two cases. Although the cases $\delta =$ integer can always be obtained by taking the appropriate limits, they are more simply analysed by a separate treatment.

4.1.1 $\delta < 2$. — In this case, the starred and unstarred functions coincide. A simple contour integration shows that two contributions occur in $C_{vv}(t)$. The first one originates from the cut and provides a long time tail, the other one (exponential) comes out from the residues. Only the poles having an imaginary part $\ll \gamma$ yield exponentials (actually oscillating) surviving beyond times $\sim \gamma^{-1}$, thus being universal and independent of the cut-off function. When $g \leq 1$, no such pole exists and $C_{vv}(t)$ essentially follows a power law. On the contrary, for $g \gg 1$, and if $\delta < 1$, a unique pole z_0 , noted $\gamma^{-1}(\Omega_{\text{res}} + iT_R^{-1})$, is obtained satisfying this requirement ; provided that $\delta \gg \delta_1 = (2/\pi g^2) \ll 1$, one can write :

$$T_R \approx \tau (\sin \theta)^{1/(2-\delta)} / \sin \delta \varphi \quad (28)$$

$$\Omega_{\text{res}} \approx \tau^{-1} (\sin \theta)^{-1/(2-\delta)} \cos \delta \varphi. \quad (29)$$

These equations, valid as long as γT_R and $\Omega_{\text{res}}/\gamma$ are small, show that when δ decreases from 1, the relaxation becomes slower and slower. When $\delta \rightarrow 0$, the surrounding medium becomes so gluey and the memory effects so long-lived that the particle is completely frozen. On the other hand, for $\delta \rightarrow 1$, T_R approaches τ , Ω_{res} goes to zero and the

oscillating exponential contribution identically vanishes ; this means that, in the ohmic limit, at zero temperature, $C_{vv}(t)$ only displays a negative long time-tail $\sim -t^{-2}$ in accordance with [3]. Generally, for $t \gg \gamma^{-1}$, one can thus write, for $\delta_1 \ll \delta < 1$:

$$C_{vv}(t) \approx (\hbar/2 \pi m \tau) \times [4 \varphi (\sin \theta)^{-1/(2-\delta)} \cos(\Omega_{\text{res}} t + \delta \varphi) \times \exp(-t/T_R) - 2 \Gamma(3-\delta) \sin^3 \theta (t/\tau)^{-(3-\delta)}]. \quad (30)$$

For $1 < \delta < 2$, no exponential relaxation can be seen beyond times $\gg \gamma^{-1}$, and the only left time-scale governing the dynamics is given by the time τa *priori* introduced in equation (7). In any case, $C_{vv}(t)$ goes to zero at infinite times, a result which implies that $\Delta x^2(t)$ cannot diverge as t^2 or faster ; more precisely, we find :

$$C_{vv}(t) \approx -(\hbar/\pi m \tau) \Gamma(3-\delta) \sin^3 \theta (t/\tau)^{-(3-\delta)}. \quad (31)$$

The mean square displacement $\Delta x^2(t)$ is now obtained from $C_{vv}(t)$ by a double time-integration ; the final value $\Delta x^2(+\infty)$ is easily seen to be infinite for $\delta \geq 1$ and finite for $\delta < 1$. In this last case, we find :

$$\Delta x^2(+\infty) = -(2 \hbar \tau / \pi m) \operatorname{Im} F(\delta, g) \quad (32)$$

where $F(\delta, g)$ is the integral :

$$F(\delta, g) = \int_0^{+\infty} dy y^{-\delta} [y^{2-\delta} + (2/\pi) J_\delta(y/g) + i f_c(y/g)]^{-1}. \quad (33)$$

This integral can be analysed in several limits and yields :

$$\delta \rightarrow 0 : \Delta x^2(+\infty) \approx (\hbar \tau / m) (\pi \delta / 2)^{1/2} \quad (34)$$

$$\delta \rightarrow 1 : \Delta x^2(+\infty) \approx (2 \hbar \tau / \pi m) (1-\delta)^{-1}. \quad (35)$$

Furthermore, in the limit $g \rightarrow +\infty$, which for $\delta < 2$ implies a weak coupling (see Eq. (7)), one has the exact formula :

$$\Delta x^2(+\infty) = (2 \hbar \tau / \pi m) (2 \varphi / \sin 2 \varphi) \times (\sin \theta)^{1/(2-\delta)}. \quad (36)$$

These equations display the fact that the mean squared displacement of the particle is bounded, which, in a classical picture, is characteristic of a spatial confinement. This result by itself does not imply a true quantum localization since, as already quoted, Δx^2 as defined by equation (25) does not represent the mean square dispersion (variance) of the coordinate. This last quantity has been analysed in [12] where it is shown that a true quantum localization occurs for $0 < \delta < 1$.

It is worthwhile to observe that the main contribution to the final value comes out from the pole in the integrand of equation (33) ; this corresponds to the resonance Ω_{res} in χ , the quality factor of which increases as δ decreases. This resonance has a width $\sim T_R^{-1}$ and is clearly related to memory effects, since in the case of an instantaneous dynamical equation (for instance for $\delta = 1$ and $\gamma = +\infty$) one should simply have :

$$\chi_{\text{inst}}(\omega) = [\omega(\omega + iT_R^{-1})]^{-1} \quad (37)$$

which does not display any resonance for ω finite. Its existence implies that the modes having a frequency $\sim \Omega_{\text{res}}$ are in fact much more coupled to the particle

than all the others and indeed, an effective $\chi(\omega)$ could be here written, near the resonance, as

$$C^{\text{ste}} \times [\omega(\omega - \Omega_{\text{res}} + iT_R^{-1})]^{-1}.$$

It may be said that some dynamical potential develops in the surrounding medium which pulls the particle back towards its initial location, as if the latter had left some hole behind it.

The dynamics of relaxation towards $\Delta x^2(+\infty)$ is found by integrating the asymptotic regime of $C_{\text{vv}}(t)$; thus, $\Delta x^2(t)$ displays the same features as $C_{\text{vv}}(t)$, namely an oscillating exponential regime implemented by a long-time tail. In the limit of very large time :

$$\Delta x^2(t) \simeq \Delta x^2(+\infty) - (2\hbar\tau/\pi m) \sin^3 \theta \Gamma(1-\delta)(t/\tau)^{-(1-\delta)} \quad (0 < \delta < 1) \quad (38)$$

$$\Delta x^2(t) \simeq (2\hbar\tau/\pi m) \sin^3 \theta |\Gamma(1-\delta)| (t/\tau)^{\delta-1} \quad (1 < \delta < 2) \quad (39)$$

Equation (38) shows the approach towards localization in the broad sense ($\Delta x^2(+\infty) < +\infty$), whereas equation (39) displays the so-called subdiffusive regime since $\Delta x^2(t)$ diverges at infinite time more slowly than in a purely diffusive regime. When $\delta \rightarrow 1$, the relaxation dynamics becomes slower and slower and eventually provides a $\ln(t/\tau)$ for $\delta = 1$, in accordance with [3, 12].

This confinement is reminiscent of the tendency already found for a particle in a periodic potential (see [11] and references therein). Similarly, for a damped non-ohmic particle in a symmetric double-well potential, localization is found for $\delta < 1$ [1b, 13].

The case $\delta = 2$ deserves a separate study ; in that case, $J_\delta(z)$ can be written as $-\ln z +$ regular function at $z = 0$; this implies that :

$$C_{\text{vv}}(t) \simeq -(\pi^2 \hbar/4 m \tau)(t/\tau)^{-1} [\ln(t/\tau)]^{-3} \quad (40)$$

$$\Delta x^2(t) \simeq (\pi^2 \hbar\tau/4 m)(t/\tau) [\ln(t/\tau)]^{-2} \quad (41)$$

in accordance with [12].

4.1.2 $\delta > 2$. — In this case, the expression for χ near $z = 0$ is the following :

$$\chi^{-1}(z) \simeq \rho z^2 + i g^{\delta-2} z |z|^{\delta-1} \quad (42)$$

where ρ is defined in equation (11). Equation (41) shows that one effect of the bath is to produce a mass renormalization $m_{\text{ren}} = \rho m$.

The precise variation of this mass correction as a function of δ depends on the value of the coupling constant g and of the chosen cut-off function. With an exponential cut-off, the behaviour at large δ is dominated by the moment $M_{\delta-3} = \Gamma(\delta-2)$ which goes to infinity when $\delta \rightarrow +\infty$; on the contrary, for a sharp cut-off, $f_c(x) = \Theta(1-x)$, the renormalized mass goes to zero in that limit and one then recovers the free particle [12b]. As anticipated in the introduction, one here explicitly observes the qualitative effect of the cut-off function for large δ , which goes beyond a simple numerical factor of order unity.

The dynamics at large times can be found by the same techniques as in the preceding section. We successively find :

$$C_{\text{vv}}^*(t) \simeq (\hbar/\pi m \tau \rho^2) \Gamma(\delta-1) \sin \theta (t/\tau)^{-(\delta-1)} \quad (43)$$

$$\Delta x^{2*}(t) \simeq (2\hbar\tau/\pi m \rho^2) \Gamma(\delta-3) \sin \theta (t/\tau)^{3-\delta} \quad (2 < \delta < 3) \quad (44)$$

$$\Delta x^{2*}(t) \simeq \Delta x^{2*}(+\infty) + (2\hbar\tau/\pi m \rho^2) \Gamma(\delta-3) \sin \theta (t/\tau)^{(3-\delta)} \quad (\delta > 3) \quad (45)$$

Note that for $\delta = 4, 6, 8, \dots$, the amplitude of the tail vanishes and one has to go one step further in the asymptotic series ; this gives $C_{\text{vv}}^*(t) \sim t^{-\delta}$ and so on. As already observed in the symmetric double-well potential [13], the dominant exponent can have

jumps. For $\delta = 2$ (resp. 3), $\Delta x^{2*}(t)$ behaves like $(t/\tau)[\ln(t/\tau)]^{-2}$ (resp. $\ln(t/\tau)$).

The constant $\Delta x^{2*}(+\infty)$ is approximately given by :

$$\Delta x^{2*}(+\infty) \simeq (2\hbar\tau/\pi m) g^{\delta-3} (M_{\delta-4}/\rho^2). \quad (46)$$

When $\delta \rightarrow 3$ from above, $\Delta x^{2*}(+\infty)$ diverges as $(\delta - 3)^{-1}$ because of the $M_{\delta-4}$ moment. The ρ^2 factor can be viewed as originating first from the mass renormalization and secondly from a rescaling of the time τ introduced at the beginning.

Exactly as for the case $\delta < 2$, a new time scale arises; more precisely, when one analyses χ , it is seen that a new pole arises every time that δ crosses an odd integer value; the largest of all these times is still called T_R and is given by:

$$T_R = \gamma^{-1} \rho^{-1/(\delta-2)}/\sin \varphi \quad (47)$$

T_R tends to γ^{-1} when $\delta \rightarrow 3$ and diverges when δ goes to infinity, showing that the dynamics slows down when δ increases beyond 3.

Equations (31), (40) and (43) show that $C_{vv}^*(t)$ has

a negative long-time tail for $1 < \delta < 3$. Generally speaking, this is to be related with some « cage effect » which occurs here when the particle is in a subdiffusive regime.

4.2 FINITE TEMPERATURE CASE. — The dynamics at finite temperature is nearly the same as at $T = 0$ for all times much smaller than τ_T . This implies that only the final step ($t \gg \tau_T$) of the dynamics is changed due to the presence of $\cotanh(\beta \hbar \gamma z/2)$ and is independent of the ratio $k_B T/\hbar \gamma$. This final regime involves the small neighbourhood $z \sim 0$ where the $\cotanh z$ can be replaced by $1/z$. On the other hand, the possible finite limit of $\Delta x^{2*}(t)$, which integrates the whole dynamics, will be dependent of the ratio $k_B T/\hbar \gamma$. Thus we find:

$$C_{vv}^*(t) \simeq + (k_B T/m)[\sin \theta/\Gamma(\delta - 1)](t/\tau)^{-(2-\delta)} \quad (\delta < 2, \delta \neq 1) \quad (48)$$

$$C_{vv}^*(t) \simeq - (2 k_B T/\pi m \rho^2) \cos \theta \Gamma(\delta - 2)(t/\tau)^{(2-\delta)} \quad (\delta > 2, \delta \neq 3). \quad (49)$$

As emphasized before, when the coefficient of the above long time-tails vanishes, one has to go one step further in the asymptotic series (however, for $\delta = 1$ only a final exponential tail appears [3], as it is the case for $\delta = 3$). Equations-(48) and (49) display the fact that $C_{vv}^*(t)$ always goes to zero at infinite times, implying that $\Delta x^{2*}(t)$ can never grow as t^2 or faster. For the same reasons as in the zero-temperature case, the exponents have jumps occurring now for $\delta = 5, 7, \dots$ For $0 < \delta < 4$, $\Delta x^{2*}(t)$ is found diverging at large times more slowly than t^2 , namely:

$$\Delta x^{2*}(t) \simeq (2 k_B T \tau^2/m)[(\sin \theta)/\Gamma(\delta + 1)](t/\tau)^\delta \quad (0 < \delta < 2) \quad (50)$$

$$\Delta x^{2*}(t) \simeq (4 k_B T \tau^2/\pi m \rho^2) |\cos \theta \Gamma(\delta - 4)| (t/\tau)^{4-\delta} \quad (2 < \delta < 4). \quad (51)$$

In the marginal cases $\delta = 2$ and $\delta = 4$, one respectively has $\Delta x^{2*}(t) \sim t^2/[\ln(t/\tau)]$ and $\sim \ln(t/\tau)$. The diffusive regime occurs only for $\delta = 1$ and 3.

For $\delta > 4$, $\Delta x^{2*}(t)$ does have a finite value at $t = +\infty$. When the $k_B T$ is much smaller than $\hbar \gamma$, by expanding $\cotanh z$ as $1 + 2 \sum_{n=0}^{+\infty} e^{-2nz}$ we find

for $\delta > 3$:

$$\begin{aligned} \Delta x^{2*}(+\infty; T) &\simeq \Delta x^{2*}(+\infty; 0) \times \\ &\times \{1 + [\Gamma(\delta - 3) \zeta(\delta - 3)/M_{\delta-4} \rho^2] \times \\ &\times (k_B T/\hbar \gamma)^{\delta-3}\} \end{aligned} \quad (52)$$

where $\zeta(x)$ denotes the Riemann function. Due to the presence of this function, the temperature correction is thus divergent for $3 < \delta < 4$, in agreement with the fact that, at $T = 0$, Δx^{2*} is indeed finite at infinite time. On the other hand, for $k_B T/\hbar \gamma \gg 1$, $\cotanh z \sim 1/z$ in the whole relevant integration interval and one has:

$$\begin{aligned} \Delta x^{2*}(+\infty; T) &\simeq 2(M_{\delta-5}/M_{\delta-4}) \times \\ &\times (k_B T/\hbar \gamma) \Delta x^{2*}(+\infty; 0). \end{aligned} \quad (53)$$

Thus, although Δx^{2*} has a finite limit, its final value is very large at high temperature where classical effects are dominant. Note that formula (53) is in fact independent of \hbar and we thus find a classical anomalous diffusion, while the equipartition is satisfied since $C_{vv}^*(t=0) = k_B T/m$.

The approach to equilibrium is independent of $k_B T/\hbar \gamma$ and, for $\delta > 4$, is given by:

$$\begin{aligned} \Delta x^{2*}(t; T) &\simeq \Delta x^{2*}(+\infty; T) - (4 k_B T \tau^2/\pi m \rho^2) \times \\ &\times \cos \theta \Gamma(\delta - 4)(t/\tau)^{-(\delta-4)}. \end{aligned} \quad (54)$$

Finally, one can remark that in the range $0 < \delta < 1$, where confinement disappears at finite T , one obtains subdiffusive regimes; this is also displayed by the negative long-time tails in $C_{vv}^*(t)$, again related to cage effects. On the other hand, for $1 < \delta < 3$, Δx^{2*} follows a superdiffusive law.

5. Summary and conclusions.

We have shown that the quantum dynamics of a damped free particle is extremely sensitive to the behaviour at low frequency of the effective coupling

strength with the bath, assumed to be of the form ω^δ , and to memory effects.

We first determined the averaged trajectory of the particle, resulting from an external percussion. For $\delta < 2$, this initial velocity fluctuation always dies out at infinite times. In addition, for $\delta < 1$, the particle relaxes in the mean towards its initial location due to the friction with the low-frequency modes and to very long-lived memory effects. In this case, the surrounding medium develops a kind of dynamical potential pulling back the particle; in the limit $\delta \rightarrow 0$, the particle is completely frozen. For $1 < \delta < 2$, the particle goes to infinity, the net effect of the bath being to slow down of the motion, governed at large times by a sub-diffusive regime characterized by $\langle x(t) \rangle \sim t^{\delta-1}$. When $\delta = 1$ (ohmic case), the particle travels a finite distance before stopping, as in ordinary Brownian motion and the dynamics exactly follows an exponential law at all times. For $\delta > 2$, the system is not ergodic in the sense that the initial velocity is never forgotten and the particle recovers in the mean, at large times, a pure kinematical motion with a renormalized mass. The final motion of the system is the same as that of two massive particles which have aggregated through a sticking inelastic collision.

We subsequently analysed the long-time correlations starting from a non-equilibrium factorized state. At $T = 0$ and for $\delta < 1$, the mean square displacement of the coordinate, Δx^2 , is bounded at infinite times, indicating that, in the mean, the particle does not go to infinity (confinement); this results from the friction with the dominant low-frequency modes and reminds what is observed in a symmetric double well potential [1b, 13]. The approach to the final value follows a law of the form $t^{-(1-\delta)}$. On the contrary, for $1 < \delta < 2$, Δx^2 is found to diverge as t^ν where the exponent ν is always smaller than 1. In the marginal case $\delta = 2$, $\Delta x^2 \sim t/(\ln t)^2$. For δ greater than 2, the dominant effect is the kinematical term arising as well as for the one-time average values; the next subdominant term is $\sim t^{-(\delta-3)}$.

At finite temperature, the confinement effect found above for $\delta < 1$ is lost; for $\delta < 2$, Δx^2 diverges always slower than t^2 , namely $\Delta x^2 \sim t^\delta$. For $\delta > 2$, $\Delta x^2 \sim t^2$.

A few final comments may be made concerning the kinematical arising effect for $\delta > 2$. It is seen that two kinds of supplementary effects can occur, either an additional divergent spreading ($2 < \delta < 3$ and $T = 0$ or $2 < \delta < 4$ and $T \neq 0$) or a bounded spreading in all other cases. For a classical particle, one can always choose the initial state so as to suppress the kinematical term. Then, for $\delta > 3$ and $T = 0$ or $\delta > 4$ and $T \neq 0$, the effect of the bath is a confinement of the particle in a region of space, albeit possibly large at high temperature.

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Appendix A.

We here analyse in some details mathematical and general properties of the various quantities defined in the main text. The Fourier transform of $k(t)$ is $K(\omega) = \int_{-\infty}^{+\infty} dt k(t) e^{i\omega t}$ (in the following, capital letters are used for Fourier transforms: $F(\omega) \leftrightarrow f(t)$). Clearly, for ω a real number, one must have $K(-\omega) = K(\omega)^*$ since $k(t)$ is a real function; this implies that $K_1(\omega) \equiv \text{Re } K(\omega)$ is even, whereas $K_2(\omega) \equiv \text{Im } K(\omega)$ is odd. Furthermore, by just looking at equation (7), one sees that $K_1(z) = \gamma g^{\delta-2} z^{\delta-1} f_c(z)$ for $z = \omega/\gamma$ real positive; thus, for any z real:

$$K_1(z) = \gamma g^{\delta-2} |z|^{\delta-1} f_c(z). \quad (\text{A.1})$$

This equation has interesting consequences; it shows that, except for the odd-integer values of δ , $K_1(z)$ has a singularity at $z = 0$ which is clearly a branching point. The imaginary part of $K(z)$ can be obtained by the Cauchy theorem (leading to dispersion relations) using the fact that $k(t)$ vanishes identically for $t < 0$; we thus find the following final form for $K(z)$ for any real z :

$$K(z) = \gamma g^{\delta-2} [|z|^{\delta-1} f_c(z) - i(2z/\pi) \times |z|^{\delta-2} J_\delta(z)] \quad (\text{A.2})$$

with:

$$J_\delta(z) = P \int_0^{+\infty} dZ f_c(zZ) Z^{\delta-1} / (Z^2 - 1) \quad (\text{A.3})$$

where P denotes the Cauchy principal value. It is readily seen that:

$$J_\delta(0) = -(\pi/2) \cotang(\pi\delta/2) \quad (\delta < 2). \quad (\text{A.4})$$

For $\delta = 2, 4, 6, \dots$, a logarithm is to occur in K_2 , whereas for δ real and non-integer the multiform function $z^{\delta-1}$ is present. This implies that the long-time behaviour of $k(t)$ is exponential (and dominated by the smallest pole) only for the very special values $\delta = 1, 3, 5, \dots$; in all other cases, $k(t)$ displays a long-time tail which identically vanishes when δ recovers an odd-integer value.

From equations (A.2) and (A.3), the leading behaviour of K_2 for z real and $|z| \ll 1$ is found to be:

$$\begin{aligned} \delta < 2 & K_2(z) \sim z |z|^{\delta-2} \\ \delta = 2 & K_2(z) \sim z \ln |z| \\ \delta > 2 & K_2(z) \sim z. \end{aligned} \quad (\text{A.5})$$

Note that, for an harmonic oscillator with the frequency ω_0 , the only change in equation (23) is to replace ω^2 by $\omega^2 - \omega_0^2$; so, when $\omega K(\omega)$ is finite when $\omega \rightarrow 0$, $\chi(\omega)$ has then a finite limit (the same is to be expected for any confined particle). So, the spectacular effects found for the free particle are in this case hidden by the built-in confining potential. Moreover, when one is interested in transport properties, the simplest and most exemplifying case is clearly that of the free particle.

From the analytical properties of $\chi(z)$, it is readily seen that the following sum rule holds :

$$\int_{-\infty}^{+\infty} dz z \chi(z + i0) = -i\pi. \quad (\text{A.6})$$

For this relation to be true, it is required that $K(z)$ is an analytic function devoid of any singularity in the open upper half-plane, the modulus of which being strictly bounded by $|z|$ at infinity; this is insured here by the presence of the smooth cut-off function. (A.6) in turn is equivalent to the conservation of the canonical relations; as an example, it can be readily checked that $[x, p] = i\hbar$ is satisfied at any time, as it must be in an Hamiltonian model.

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