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Localization and Anomalous Diffusion of a Damped Quantum Particle

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The time evolution of an initially localized state of a quantum particle coupled to a dissipative environment with spectral density $I(\omega) \propto \omega^{\alpha}$ for low frequencies is discussed. At finite temperatures, the width of the state can grow subdiffusively or superdiffusively, depending on α. For $\alpha > 2$, damping becomes ineffective for long times and the state spreads kinematically. At zero temperature the spreading is slower and for $\alpha < 1$ an initially localized state remains localized for all times.

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Recently, there has been a great deal of renewed interest in the problem of how the motion of a quantum particle is affected by the dissipative influence of a heat bath. In the low-temperature regime dissipation was found to lead to novel features such as the exponential suppression of tunneling by dissipation,[1] long-time tails in correlation functions,[2] and most notably dissipative phase transitions.[3,4] The major part of the recent studies was inspired by the work of Caldeira and Leggett,[1] who pioneered a functional-integral approach to the problem. It was mostly assumed that the environmental coupling is such that in the classical regime it leads to a frictional force proportional to the velocity of the particle. This model of frequency-independent or Ohmic damping was studied in detail by Hakim and Ambegaokar[5] for a free particle which is not confined by a potential field. At finite temperatures the variance $\sigma(t) = \langle (q - \langle q \rangle_t)^2 \rangle_t$ of an initially localized state of an Ohmically damped particle grows diffusively proportional to t for large times. At zero temperature, where the spreading is entirely due to quantum fluctuations $\sigma(t)$ grows only proportionally to $\ln(t)$. Clearly, the Ohmic model describes only a special form of the environmental coupling and a rich variety of frequency-dependent damping mechanisms occurs in physical and chemical sciences. Here, we investigate the dynamics of a quantum particle subject to a dissipative influence of arbitrary frequency dependence.

We consider a particle of mass M which interacts with a heat-bath environment. Following Caldeira and Leggett,[1] we assume that the heat bath can be represented by a set of harmonic oscillators coupled bilinearly to the particle. The system is then governed by the Hamiltonian

$$H = \frac{p^2}{2M} + \sum_{n=1}^{N} \left[\frac{p_n^2}{2m_n} + \tfrac{1}{2} m_n \omega_n^2 (x_n - q)^2 \right]. \qquad (1)$$

As pointed out by Hakim and Ambegaokar,[5] this translationally invariant version of the Caldeira-Leggett model[1] can be visualized as a particle with many environmental oscillators attached to it. Now, the heat-bath parameters influence the particle's motion only through the effective spectral density[6]

$$I(\omega) = \frac{\pi}{2} \sum_{n=1}^{N} m_n \omega_n^3 \delta(\omega - \omega_n),$$

in terms of which the frequency-dependent damping coefficient $\hat{\gamma}(\omega)$ takes the form

$$\hat{\gamma}(\omega)=\frac{1}{M}\int_0^\infty \frac{d\omega'}{\pi}\frac{I(\omega')}{\omega'}\frac{2\omega}{\omega^2+\omega'^2}, \qquad (2)$$

where $\hat{\gamma}(\omega)$ is the Laplace transform of the damping kernel occurring in the classical equation of motion. Clearly, Ohmic damping $[\hat{\gamma}(\omega)=\gamma,\ \omega\ll\omega_c]$ arises from a spectral density of the form[1] $I(\omega)=M\gamma\omega$ $(\omega\ll\omega_c)$ where ω_c marks the region above which the frequency dependence of the damping becomes important.

Here we consider a class of models characterized by a spectral density of the form

$$I(\omega)=Mg_\alpha\omega^\alpha \quad \text{for } \omega\ll\omega_c. \qquad (3)$$

We are interested in the motion of the particle on a time scale $t\gg\omega_c^{-1}$ where ω_c is again the frequency where the simple power-law behavior (3) becomes modified. The frequency ω_c may also be looked upon as a cutoff for the spectral density (3) since the precise form of $I(\omega)$ for $\omega>\omega_c$ influences the long-time dynamics of the particle only for $\alpha\geq 2$ in terms of a mass renormalization.[7] Spectral densities of the form (3) have been discussed in connection with particles moving in a fermionic environment leading to Ohmic dissipation $(\alpha=1)$ or in the context of the polaron problem where a d-dimensional phonon bath leads to $\alpha=d$ or $\alpha=d+2$ depending on the model. Nonintegral values of α are of possible interest for diffusion in fractal environments.

To determine the time evolution of the density matrix of the damped particle we use a functional-integral method based on the influence-functional theory of Feynman and Vernon.[8] We avoid the commonly used assumption that the initial density matrix factorizes into separate contributions from the particle and the heat bath. This enables us to study, e.g., initial states resulting from perturbations of the equilibrium state or from measurements at $t=0$. A detailed discussion of our approach will be given elsewhere.[9] Here, we consider an initial state of the form

$$\rho(q,q',0)=[2\pi\sigma(0)]^{-1/2}\exp\{-(q+q')^2/8\sigma(0)-[\langle p^2\rangle_\beta/2\hbar^2+1/8\sigma(0)](q-q')^2\},$$

which is localized around $q=0$. The probability distribution of the position is Gaussian with width $\sigma(0)$ and the initial momentum variance $\langle p^2\rangle_0$ exceeds the equilibrium value at $T=1/k_B\beta$ given by

$$\langle p^2\rangle_\beta=\frac{M}{\beta}\left[1+2\sum_{n=1}^\infty\frac{\hat{\gamma}(\nu_n)}{\nu_n+\hat{\gamma}(\nu_n)}\right]$$

as an effect of the position measurement with uncertainty $\sigma^{1/2}(0)$.[5] The density matrix of the particle at time t may now be evaluated exactly for arbitrary forms of the spectral density $I(\omega)$ satisfying the obvious conditions of integrability and $I(0)=0$. Although the model is linear, the explicit evaluation is quite tedious in the general case of frequency-dependent damping. The result may be cast into the form[9]

$$\rho(q,q',t)=[2\pi\sigma(t)]^{-1/2}\exp\left[-\frac{\langle p^2\rangle_\beta}{2\hbar^2}(q-q')^2\right]\exp\left[\frac{1}{2\sigma(t)}\left\{\tfrac14(q+q')^2-\frac{iM}{2\hbar}(q^2-q'^2)\left[\dot{s}(t)+\frac{\hbar^2}{2\sigma(0)}\chi(t)\dot{\chi}(t)\right]\right.\right.$$
$$\left.\left.-\frac{M^2}{4\hbar^2}(q-q')^2\left[\dot{s}^2(t)-\hbar^2\dot{\chi}(t)\left[1-\frac{s(t)}{\sigma(0)}\right]+\frac{\hbar^2}{\sigma(0)}\chi(t)\dot{\chi}(t)\dot{s}(t)\right]\right\}\right]. \qquad (4)$$

Here, $\chi(t)$ is the response function of a damped particle, which has the Laplace transform

$$\hat{\chi}(\omega)=\{M\omega[\omega+\hat{\gamma}(\omega)]\}^{-1},$$

and $s(t)=\langle[q(t)-q(0)]^2\rangle_\beta$ is the mean square displacement evaluated for the homogeneous equilibrium state. The Laplace transform of the mean square displacement and the response function are connected by

$$\hat{s}(\omega)=\frac{2}{\beta}\left[\frac{\hat{\chi}(\omega)}{\omega}+2\sum_{n=1}^\infty(\nu_n^2-\omega^2)^{-1}\left[\frac{\nu_n^2\hat{\chi}(\nu_n)}{\omega}-\omega\hat{\chi}(\omega)\right]\right], \qquad (5)$$

where $\nu_n=2\pi n/\hbar\beta$. This latter relation may also be viewed as a consequence of the fluctuation-dissipation theorem. Finally, the variance of the position, $\sigma(t)$, depends on the response function $\chi(t)$ and the equilibrium mean square displacement $s(t)$ through

$$\sigma(t)=\sigma(0)\left[1+\frac{s(t)}{\sigma(0)}+\frac{\hbar^2}{4}\frac{\chi^2(t)}{\sigma^2(0)}\right].$$

So far, the results presented are *exact* for all values of t.

Let us now discuss the time dependence of the functions $\chi(t)$, $s(t)$, and $\sigma(t)$ for long times $(t\gg\omega_c^{-1})$ for a particle coupled to an environment with spectral density $I(\omega)$ of the form (3). For finite temperatures, the leading long-time dependence of the mean square displacement arises from the first term in (5) and we have

$$s(t)\sim\frac{2}{\beta}\int_0^t du\,\chi(u),\quad T>0,\quad t\to\infty. \qquad (6)$$

TABLE II. Asymptotic long-time dependence at zero temperature of the mean square displacement $s_0(t)$ and the variance of a wave packet $\sigma_0(t)$.

α	$s_0(t)$	$\sigma_0(t)$
$0<\alpha<1$	const	const
$\alpha=1$	$(2\hbar/\pi M g_1)\ln(t)$	$(2\hbar/\pi M g_1)\ln(t)$
$1<\alpha<2$	$\dfrac{\hbar\sin^2[\frac{1}{2}\pi(2-\alpha)]}{M g_\alpha \Gamma(\alpha)\cos[\frac{1}{2}\pi(2-\alpha)]}t^{\alpha-1}$	$\dfrac{\hbar\sin(\frac{1}{2}\pi\alpha)/2Mg_\alpha\Gamma(\alpha)}{\sigma(0)}t^{2\alpha-2}$
$\alpha=2$	$\dfrac{\pi^2\hbar}{4Mg_2}\dfrac{t}{\ln^2 t}$	$\dfrac{(\pi\hbar/4Mg_2)^2}{\sigma(0)}\dfrac{t^2}{\ln^2 t}$
$2<\alpha<3$	$\dfrac{\hbar M g_\alpha}{M_r^2\Gamma(4-\alpha)\cos[\frac{1}{2}\pi(\alpha-2)]}t^{3-\alpha}$	
$\alpha=3$	$(2\hbar M g_3/\pi M_r^2)\ln(t)$	$[(\hbar/2M_r)^2/\sigma(0)]t^2$
$3<\alpha$	const	

On the other hand, at zero temperature, the thermal frequencies ν_n are continuous and the sum in (5) has to be replaced by an integral yielding

$$s_0(t)=\frac{2\hbar}{\pi}\int_0^\infty du\,\frac{u}{u^2-1}\chi(t/u),\quad T=0. \tag{7}$$

Now, (6) and (7) determine the long-time behavior of the mean square displacement for all temperatures in terms of the long-time behavior of the response function. This latter property can be obtained from the low-frequency behavior of the damping coefficient $\hat{\gamma}(\omega)$ determined by (2) and (3). We find that the cutoff affects the leading-order term only for $\alpha>2$. However, it appears in the corresponding numerical factor only via a renormalized mass.[7] The asymptotic time dependence of $\chi(t)$, $s(t)$, and $\sigma(t)$ may be worked out explicitly. The results are summarized in Tables I and II.

For $\alpha>2$, the response function $\chi(t)$ is proportional to $t^{\alpha-1}$ for long times. Hence, in the Ohmic case ($\alpha=1$) a constant driving force leads to a constant asymptotic velocity of the damped particle. In the sub-Ohmic case ($\alpha<1$) the particle coordinate grows for constant driving force but the velocity becomes arbitrarily small. In the super-Ohmic case ($\alpha>1$) the particle responds to a constant force with an ever increasing velocity. For $\alpha>2$ the damping effectively vanishes for long times and a constant force F results in an acceleration F/M_r of the particle where M_r is the renormalized mass. In the special case $\alpha=2$ we find the non-power-law behavior $\chi(t)\propto t/\ln(t)$. The asymptotics of $\chi(t)$ does not change at $T=0$ while this case must be discussed separately for $s(t)$ and $\sigma(t)$.

At finite temperatures and for $\alpha\le 2$ the long-time behavior of the variance $\sigma(t)$ of the initially localized state (4) is completely determined by the growth of the mean square displacement $s(t)$. Both quantities increase $\propto t^\alpha$ for $\alpha<2$. This gives diffusive long-time behavior $\propto t$ in the Ohmic case while for $\alpha<1$ and $1<\alpha<2$ the behavior is subdiffusive and superdiffusive, respectively. Again $\alpha=2$ yields a nonanalytic growth $\propto t^2/\ln(t)$ while for $\alpha>2$ both the mean square displacement and the variance grow $\propto t^2$, but the prefactors differ because in this case the response function also contributes to the variance. This difference is due to quantum effects and vanishes in the classical limit $\hbar\to 0$.

At zero temperature the direction of energy flow can only be from the particle into the heat bath. Hence, the mean square displacement grows slower than at finite temperatures. The variance of the wave packet, however, depends also on the temperature-independent re-

TABLE I. Asymptotic long-time dependence at finite temperatures $T=1/k_B\beta$ of the response function $\chi(t)$, the mean square displacement $s(t)$, and the variance of a wave packet $\sigma(t)$. The results for $\chi(t)$ remain valid for $T=0$.

α	$\chi(t)$	$s(t)$	$\sigma(t)$
$0<\alpha<2$	$[\sin(\frac{1}{2}\pi\alpha)/Mg_\alpha\Gamma(\alpha)]t^{\alpha-1}$	$[2\sin(\frac{1}{2}\pi\alpha)/M\beta g_\alpha\Gamma(\alpha+1)]t^\alpha$	$[2\sin(\frac{1}{2}\pi\alpha)/M\beta g_\alpha\Gamma(\alpha+1)]t^\alpha$
$\alpha=2$	$(\pi/2Mg_2)t/\ln(t)$	$(\pi/2M\beta g_2)t^2/\ln(t)$	$(\pi/2M\beta g_2)t^2/\ln(t)$
$2<\alpha$	$(1/M_r)t$	$(1/M_r\beta)t^2$	$[1/(M_r\beta+\hbar^2)/4\sigma(0)M_r^2]t^2$

sponse function which dominates the long-time behavior of $\sigma(t)$ for $\alpha > 1$. Because of the high density of low-frequency environmental modes the mean square displacement approaches a constant in the sub-Ohmic case ($\alpha < 1$). Since in this regime the response function vanishes asymptotically the width of the wave packet is finite for all times. Hence, an initially localized state remains localized even though the particle is not confined by an external potential. The localization length

$$\xi = \sigma^{1/2}(t \to \infty) = (\sigma(0) + \{2\hbar/(2-\alpha)M \sin[\pi/(2-\alpha)]\}[\sin(\tfrac{1}{2}\pi\alpha)/g_\alpha]^{1/(2-\alpha)})^{1/2}$$

diverges as the Ohmic case is approached. In the Ohmic case the mean square displacement grows $\propto \ln(t)$ for large t which also determines the long-time behavior of the variance $\sigma(t)$. In the region $1 < \alpha < 2$ the mean square displacement grows algebraically $\propto t^{\alpha-1}$. The fastest asymptotic growth is found for $\alpha = 2$ where $s_0(t) \propto t/[\ln(t)]^2$ while for $2 < \alpha < 3$ the rate of growth decreases with increasing α yielding $s_0(t) \propto t^{3-\alpha}$. Logarithmic growth of the mean square displacement is found again for $\alpha = 3$ whereas for $\alpha > 3$ it approaches a constant. This decrease of the asymptotic value of $s_0(t)$ is connected with the fact that the ground state of the damped particle approaches the zero-momentum state of a free particle for large α.

In summary, we have investigated the quantum diffusion of a particle for a wide range of environmental couplings. We have studied a simplified model allowing for the derivation of exact results. However, the type of asymptotic long-time behavior found here can be expected to remain unchanged for most values of α when the particle moves in a periodic potential. In this case the particle is localized at $T = 0$ for Ohmic damping provided the damping constant is large enough.[4] In contrast, the localization found here for a free particle and $\alpha < 1$ persists for arbitrarily small coupling to the heat bath. Some of our findings are also of interest in view of the polaron problem. While the Hamiltonian (1) can only describe the absorption and emission of phonons, the effect of phonon scattering vanishes as $T = 0$ is approached so that the heat bath can model the influence of phonons at very low temperatures except for very long times. Finally, we mention that our results for $T = 0$ are not purely academic since the zero-temperature behavior is also found for low finite temperatures for intermediate times $\omega_c^{-1} \ll t \ll \hbar/k_B T$.

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[6]This form of $I(\omega)$ is obtained when the coupling constants c_n of the Caldiera-Leggett model (Ref. 1) are chosen as $c_n = m_n \omega_n^2$. This choice is always possible, since only $I(\omega)$ appears in the final expressions.

[7]For $\alpha \geq 2$ the long-time behavior of an initially localized state can be shown to depend on the cutoff only in terms of the renormalized mass $M_r = M + (2/\pi)\int_0^\infty d\omega\, I(\omega)/\omega^3$ which is just the sum of the masses of the particle and the environmental oscillators.

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