PHYSICAL REVIEW A VOLUME 32, NUMBER 1 JULY 1985

Quantum theory of a free particle interacting with a linearly dissipative environment

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(Received 11 February 1985)

The quantum-mechanical motion of a free particle coupled to a linearly dissipative environment is analyzed in the Hamiltonian formalism. The total Hamiltonian is diagonalized and its eigenstates displayed. These results are used to discuss the role of initial conditions on the subsequent motion. A widely used initial condition—heat bath uncoupled from particle—is compared with another one in which the initial off-diagonal coherence of the reduced density matrix is comparable to that in the state of thermal equilibrium of the coupled system. Different transient behaviors, on time scales longer than the inverse cutoff frequency of the bath are found. The mean-square momentum of the particle in the steady state is found to depend on this highest bath frequency. An analysis of the correlated states of particle and heat reservoir shows that the latter behaves in some sense like a position-measuring apparatus.

I. INTRODUCTION

In part because of its relevance to the behavior of superconducting tunnel junctions at very low temperatures, there has been a considerable revival of interest recently in the fluctuating (or "Brownian") motion of a quantum degree of freedom q coupled to an environment at a temperature T. The case in which friction is linearly proportional to velocity in the classical regime occurs frequently. Caldeira and Leggett[1,2] have argued that the classical friction force given by

$$\mathbf{F}_{\text{friction}} = -\eta \frac{d\mathbf{q}}{dt} \tag{1}$$

can be modeled by a linear coupling to a suitable distribution of harmonic oscillators. Ambegaokar, Eckern, and Schön[3] and, in a different context, Guinea[4] have shown how electronic reservoirs can lead to the form obtained by Caldeira and Leggett after their elimination of the reservoir coordinates. The resulting model has been applied to different physical situations where the variable q ("particle") tunnels through a potential barrier,[1] oscillates coherently between two potential wells[5] or moves in a periodic potential.[6] Interesting effects due to the environment have been noted. In almost all these studies, the Feynman path-integral method[7] has been used, and the coordinates of the environment have been integrated out to obtain an effective action which describes the modified behavior of the quantum variable q. In particular, the final formula for the time evolution of the reduced density matrix describing the quantum variable is then a special case of the structure derived by Feynman and Vernon,[8] as shown by Caldeira and Leggett.[2] In this paper we study the model proposed by Caldeira and Leggett in a more detailed way, without giving up the possibility of asking questions about the environment. For our purposes it suffices to consider a free particle where the complete Hamiltonian describing the behavior of the particle and the bath can be diagonalized. We carry out this program in Sec. II and give explicit forms for the eigenstates. The results of this exercise are interesting because they allow us to address new questions and to gain some insight—which should remain valid in more complicated situations[6]—into the dynamics of the model. In Sec. III, the possibility of contemplating the state of the bath enables us to show more explicitly than before[9] the relation of this problem with the quantum theory of measurement. By working in the Hamiltonian formalism we stay close to the classical description of measurement.[10] We find that the bath acts like an apparatus which measures the position of the particle with a finite resolution. It is also possible in this formalism to vary the initial condition of the system of particle plus bath. In Sec. IV we obtain the evolution of the reduced density matrix describing the behavior of the particle for an interesting initial state which is different from the one considered by Feynman and Vernon.[8] In Sec. V we relate this initial condition to previous work by computing the influence functional that corresponds to it and displaying differences with the one calculated by Feynman and Vernon[8] and by Caldeira and Leggett.[2] Given the influence functionals, we do the remaining double path integral. In Sec. VI, we compute the time dependences of the reduced density matrix starting from the two initial conditions and show how one can thus calculate the time dependence of position and momentum averages. We compare these results with those of Sec. IV for the thermal initial condition. Section VII contains a summary of results and some concluding remarks. Computational techniques are explained in three appendixes.

II. CALDEIRA-LEGGETT HAMILTONIAN AND ITS DIAGONALIZATION FOR A FREE PARTICLE

The Hamiltonian proposed by Caldeira and Leggett[1] (CL) to model the classical friction force [Eq. (1)] is

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$$H_{\mathrm{CL}} \equiv -\frac{1}{2M}\frac{\partial^2}{\partial q^2} + V(q) - q\sum_\alpha C_\alpha X_\alpha + \sum_\alpha \left[\frac{p_{x_\alpha}^2}{2m_\alpha} + \frac{m_\alpha\omega_\alpha^2}{2}x_\alpha^2\right] + q^2\sum_\alpha \frac{C_\alpha^2}{2m_\alpha\omega_\alpha^2} . \tag{2}$$

The dissipative interaction of the macroscopic variable q with its environment is modeled by a linear coupling to a set ($\{x_\alpha\}$) of harmonic oscillators. The final term in Eq. (2) is included so that there is no shift in the bare potential $V(q)$ due to the coupling. In order to make the physics more transparent, we introduce new coordinates y_α (and their conjugate momenta p_α) for the oscillators

$$x_\alpha = \frac{C_\alpha}{m_\alpha\omega_\alpha^2}y_\alpha, \quad p_\alpha = \frac{C_\alpha}{m_\alpha\omega_\alpha^2}p_{x\alpha}$$

and call μ_α the combination $C_\alpha^2/m_\alpha\omega_\alpha^4$. With these definitions the Hamiltonian becomes

$$H_{\mathrm{CL}} = -\frac{1}{2M}\frac{\partial^2}{\partial q^2} + V(q) + \sum_\alpha \frac{p_\alpha^2}{2\mu_\alpha} + \frac{\mu_\alpha\omega_\alpha^2}{2}(y_\alpha - q)^2 . \tag{3}$$

We see that the friction is obtained by attaching masses μ_α with springs to the particle q. For the classical friction to be described by the force of Eq. (1), the distribution of oscillators must be such that[1,11]

$$J(\omega) \equiv \frac{\pi}{2}\sum_\alpha \frac{C_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha) = \frac{\pi}{2}\sum_\alpha \mu_\alpha\omega_\alpha^3\delta(\omega-\omega_\alpha) = \eta\omega\theta(\omega_c-\omega) \tag{4}$$

(ω_c is an upper cutoff on the frequencies of the bath). For the moment, however, we shall not restrict ourselves to this particular distribution.

In the following we shall only consider a free particle $[V(q)\equiv 0]$. In this case it is obvious that the total momentum of the system (particle and attached springs) is conserved. We take advantage of this fact by using as new variables the particle coordinate q, its conjugate variable, the total momentum $p_q + \sum_\alpha p_\alpha$, the spring elongations $y_\alpha - q$, and their conjugate momenta p_α. To display these variables, it is convenient to introduce the unitary operator

$$U_{1,q} = \exp\left[-iq\sum_\alpha p_\alpha\right] \tag{5}$$

and compute its action on H_{CL} (using the formula $e^A B e^{-A} = B + [A,B]$ valid when $[[B,A],A]=0$):

$$H_1 = U_{1,q}^\dagger H_{\mathrm{CL}} U_{1,q} = \frac{1}{2M}\left[-i\frac{\partial}{\partial q} - \sum_\alpha p_\alpha\right]^2 + \sum_\alpha \left[\frac{p_\alpha^2}{2\mu_\alpha} + \tfrac{1}{2}\omega_\alpha^2\mu_\alpha y_\alpha^2\right] . \tag{6}$$

Now $(1/i)(\partial/\partial q)$ is the total momentum of the system and is manifestly conserved. One can readily check that it commutes with H_1. Therefore the eigenstates of H_1 are of the form

$$|\Psi_p^n\rangle = \int dq\, e^{ipq}|q\rangle \otimes |B_p^n\rangle , \tag{7}$$

where

$$H_1|\Psi_p^n\rangle = E_p^n|\Psi_p^n\rangle . \tag{8}$$

To each momentum corresponds a set of eigenstates (here labeled by n). $|B_p^n\rangle$ describes the state of the bath and is independent of q. It is the nth eigenstate of $H_{1,p}$,

$$H_{1,p} = \frac{1}{2M}\left[p - \sum_\alpha p_\alpha\right]^2 + \sum_\alpha \left[\frac{p_\alpha^2}{2\mu_\alpha} + \frac{\mu_\alpha\omega_\alpha^2}{2}y_\alpha^2\right] , \tag{9}$$

where p is a c-number (the conserved total momentum of the system). So the simple remark that the total momentum is conserved has allowed us to eliminate the explicit dependence on the particle coordinate. It remains to diagonalize an effective Hamiltonian for the bath, which depends on the total momentum of the eigenstate we are considering. In order to obtain explicitly the dependence of E_p^n [Eq. (8)] on p, we translate each p_α by an amount r_α^p and cancel the crossed terms between p and p_α. To achieve this, we introduce a second unitary operator $U_{2,p}$ such that

$$U_{2,p}^\dagger p_\alpha U_{2,p} = p_\alpha + r_\alpha^p \tag{10}$$

with

$$U_{2,p} = \exp\left[i\sum_\alpha r_\alpha^p y_\alpha\right], \quad r_\alpha^p = \frac{\mu_\alpha}{M + \sum_\alpha \mu_\alpha}p . \tag{11}$$

When we use it to transform $H_{1,p}$, we obtain

$$U_{2,p}^\dagger H_{1,p} U_{2,p} = \frac{p^2}{M + \sum_\alpha \mu_\alpha} + H_2 , \tag{12}$$

where H_2 is the Hamiltonian $H_{1,p}$ for $p=0$.

As could have been expected, the energy is a sum of an internal energy independent of p (eigenvalue of H_2) and the square of the total momentum divided by the total mass of the system. We can write the total mass of the system using the spectral density $J(\omega)$ [Eq. (4)],

$$M + \sum_\alpha \mu_\alpha = M + \frac{2}{\pi}\int d\omega \frac{J(\omega)}{\omega^3} . \tag{13}$$

In the case of Ohmic dissipation, this is

$$M + \frac{2}{\pi}\eta\int d\omega \frac{1}{\omega^2} \tag{14}$$

and we see that the *low-frequency* oscillators give a divergent integral and therefore an infinite mass to the total system. The surprising consequence is that the energy does not depend on the total momentum of the system. We will see below how this affects the spreading of a wave packet.

Now we conclude the diagonalization of our Hamiltonian by going to the normal modes of vibration of H_2. Let us introduce creation and annihilation operators in the usual way

$$a_\alpha = \frac{1}{\sqrt{2\mu_\alpha\omega_\alpha}}(p_\alpha - i\mu_\alpha\omega_\alpha y_\alpha) , \tag{15a}$$

$$a_\alpha^\dagger = \frac{1}{\sqrt{2\mu_\alpha\omega_\alpha}}(p_\alpha + i\mu_\alpha\omega_\alpha y_\alpha) \; . \tag{15b}$$

In terms of $a_\alpha^\dagger$ and a_α, H_2 becomes

$$H_2 = \sum_\alpha \omega_\alpha(a_\alpha^\dagger a_\alpha + \tfrac{1}{2}) + \frac{1}{2M}\left[\sum_\alpha \left[\frac{\mu_\alpha\omega_\alpha}{2}\right]^{1/2}(a_\alpha^\dagger + a_\alpha)\right]^2 . \tag{16}$$

To express H_2 in terms of its normal coordinates we introduce a third (and last) canonical transformation U_3 which mixes a_α and $a_\alpha^\dagger$:

$$U_3^\dagger a_\alpha U_3 = \sum_\beta (A_\beta^\alpha a_\beta^\dagger + B_\beta^\alpha a_\beta) \; . \tag{17}$$

If we choose A_β^α and B_β^α suitable (see Appendix A),

$$A_\beta^\alpha = -\frac{1}{2}\left[\frac{\omega_\alpha\mu_\alpha}{E_\beta}\right]^{1/2}\frac{1}{E_\beta+\omega_\alpha}\left[\sum_\gamma \frac{\mu_\gamma\omega_\gamma^2}{(E_\beta^2-\omega_\gamma^2)^2}\right]^{-1/2} , \tag{18a}$$

$$B_\beta^\alpha = \frac{1}{2}\left[\frac{\omega_\alpha\mu_\alpha}{E_\beta}\right]^{1/2}\frac{1}{E_\beta-\omega_\alpha}\left[\sum_\gamma \frac{\mu_\gamma\omega_\gamma^2}{(E_\beta^2-\omega_\gamma^2)^2}\right]^{-1/2} , \tag{18b}$$

our Hamiltonian is completely diagonalized,

$$U_3^\dagger H_2 U_3 = H_3 = \sum_\beta E_\beta(a_\beta^\dagger a_\beta + \tfrac{1}{2}) \; , \tag{19}$$

where $\{E_\beta\}$ are the energies of vibrations of the normal modes and are given by the positive solutions of the equation

$$1 = \sum_\alpha \frac{\mu_\alpha}{M}\frac{\omega_\alpha^2}{E^2-\omega_\alpha^2} \; . \tag{20}$$

This final step of the diagonalization is performed in detail in Appendix A.

Before proceeding, let us summarize what has been achieved. We have found all the eigenstates of our Hamiltonian [Eq. (3) with $V(q)=0$] and the corresponding energies. They are given by

$$|\epsilon(\{n_\alpha\})\rangle = \int dq\, e^{ipq}\,|q\rangle \otimes U_{1,q}U_{2,p}U_3\,|\{n_\alpha\}\rangle \tag{21}$$

and the corresponding energy is equal to (normalizing the energy of the ground state to zero)

$$\epsilon(\{n_\alpha\}) = \sum_\alpha n_\alpha E_\alpha + \frac{p^2}{M+\sum_\alpha \mu_\alpha} \tag{22}$$

[E_α is given by Eq. (20) and the canonical transformations by Eqs. (5), (11), and (17)].

III. GROUND STATE OF THE SYSTEM AND MEASUREMENT OF THE POSITION

Let us consider the ground state of the system

$$|\epsilon_0\rangle = \int dq\; |q\rangle \otimes U_{1,q}U_3\,|0\rangle \; . \tag{23}$$

This is reminiscent of the state which would describe the system after an interaction of the particle with an apparatus designed to measure its position:[10] to each eigenstate of position $|q\rangle$ is associated a state $|A_q\rangle$ of the apparatus. Here the apparatus is the bath and

$$|A_q\rangle = U_{1,q}U_3\,|0\rangle \; . \tag{24}$$

The resolution of the apparatus is related to the overlap $\langle A_{q_2}|A_{q_1}\rangle$ between states associated with different positions q_1 and q_2 of the particle

$$\begin{aligned}\langle A_{q_2}|A_{q_1}\rangle &= \langle 0|\,U_3^\dagger U_{1,q_2}^\dagger U_{1,q_1} U_3\,|0\rangle \\ &= \langle 0|\,U_3^\dagger U_{1,q_1-q_2} U_3\,|0\rangle \; .\end{aligned} \tag{25}$$

The result is quickly obtained by computing the action of U_3 on U_1 [Eq. (17)] and then taking the vacuum expectation value of the resulting operator which is an exponential of a linear combination of a_β and $a_\beta^\dagger$:

$$\begin{aligned}&\langle A_{q_2}|A_{q_1}\rangle \\ &\quad = \exp\left[-\tfrac{1}{2}(q_1-q_2)^2\sum_\beta \frac{M^2}{2}\left[E_\beta\sum_\gamma \frac{\omega_\gamma^2\mu_\gamma}{E^2-\omega_\gamma^2}\right]^{-1}\right] .\end{aligned} \tag{26}$$

[A similar but more complicated expectation value is computed in Appendix B. Equations (25) and (26) are obtained by putting $t=0$ there.] The sum in the exponent can be written as an integral in the complex plane on a contour encircling the real positive axis, as is shown in detail in Appendix C. In the case of Ohmic dissipation [Eq. (4)], this gives

$$\begin{aligned}\frac{\eta}{\pi}\int_0^{\omega_c} dE\frac{E}{E^2+(\eta^2/M^2)} &= \frac{\eta}{2\pi}\ln\left[1+\frac{M^2\omega_c^2}{\eta^2}\right] \\ &\simeq \frac{\eta}{\pi}\ln\left[\frac{M\omega_c}{\eta}\right]\end{aligned} \tag{27}$$

(the last equality holds in the usual case where the inverse of the cutoff frequency is much shorter than the relaxation time). Furthermore,

$$\langle A_{q_2}|A_{q_1}\rangle = \exp\left[-\tfrac{1}{2}(q_1-q_2)^2\frac{\eta}{\pi}\ln\left[\frac{M\omega_c}{\eta}\right]\right] , \tag{28}$$

so the resolution of the bath is given by the natural friction length $(\hbar/\eta)^{1/2}$ divided by the logarithm of the ratio of the two time scales of the problem. This measurement of the position of the particle is responsible for a nonvanishing mean-square momentum of the particle in the ground state.

IV. EVOLUTION OF A REDUCED DENSITY MATRIX WITH NONFACTORIZED INITIAL CONDITION

We want to compute the evolution of the reduced density matrix which describes the time development of all quantities pertaining to the particle only. It depends, of course, on the initial state from which the system evolves. Caldeira and Leggett, following Feynman and Vernon, have used a factorized initial condition where the bath is initially in the thermal state of the free oscillators and the coupling to the particle is switched on at $t=0$. This is by no means the only possible initial condition and it is very different from the equilibrium state of the total system since even far-away points are initially quantum mechanically very coherent. The results obtained with this initial condition are given explicitly in Sec. VI. Here the dynamics will be studied starting from another initial condition (thermal initial condition) which differs less from the equilibrium state. We denote by $\rho_{\text{eq}}(q_1,q_2,Q_1,Q_2)$ the equilibrium density matrix of the total system where q_1 and q_2 are two different spatial coordinates for the particle and Q_1 and Q_2 are two different configurations of the bath. Then the thermal initial condition we consider is given by

$$\rho_{\text{th}}(q_1,q_2,Q_1,Q_2)=\rho_0(q_1,q_2)\rho_{\text{eq}}(q_1,q_2,Q_1,Q_2)\ , \tag{29}$$

where $\rho_0(q_1,q_2)$ is an arbitrary function of q_1 and q_2. This initial condition has the feature that its off-diagonal elements are suppressed as in thermal equilibrium. One thereby avoids transients due to the switching on of the coupling at $t=0$ and to the relaxation of the uncoupled state of the bath to its real ground state.

Given the initial condition (29), the state of the system at time t is (at $T=0$)

$$\rho_{\text{th}}(t)=\int\int dq_1\,dq_2\,\rho_0(q_1,q_2)e^{-iH_{\text{CL}}t}|\,q_1\rangle\otimes|\,Aq_1\rangle\langle Aq_2\,|\otimes\langle q_2\,|\,e^{iH_{\text{CL}}t}\ . \tag{30}$$

We use our previous results by expressing H_{CL} [Eq. (3)] in terms of $H_{1,p}$ [Eq. (9)] and $\rho_0(q_1,q_2)$ in terms of its Fourier components $[\rho_0(q_1,q_2)=\int\int e^{ip_1q_1-p_2q_2}\widetilde{\rho}_0(p_1,p_2)dp_1dp_2]$. Then the reduced density matrix at time t is

$$\rho_{\text{th}}(q_1,q_2,t)=\int\int dp_1\,dp_2 e^{i(p_1q_1-p_2q_2)}\widetilde{\rho}_0(p_1,p_2)\langle 0\,|\,U_3^\dagger e^{+iH_{1,p_2}t}U^\dagger_{1,q_2}U_{1,q_1}e^{-iH_{1,p_1}t}U_3\,|\,0\rangle\ . \tag{31}$$

At finite temperatures, the expectation with respect to the ground state is replaced by the average in the thermal-equilibrium state. Note that the real energies of the interacting system will appear in this thermal average in contrast to what happens with the factorized initial condition. Another interesting difference is that with this initial condition there exists a stationary reduced density matrix; if we choose $\widetilde{\rho}_0(p_1,p_2)=\delta(p_1)\delta(p_2)$, then as $H_{1,p=0}$ is equal to H_2 [Eq. (12)] we get

$$\begin{aligned}\rho_0(q_1,q_2,t)&=\langle 0\,|\,U_3^\dagger U^\dagger_{1,q_2}U_{1,q_1}U_3\,|\,0\rangle\\&=\langle A_{q_2}\,|\,A_{q_1}\rangle\end{aligned} \tag{32}$$

which is independent of time and reflects the correlation between states of the bath corresponding to different positions of the particle in the ground state of the Hamiltonian (or more generally, in the thermal-equilibrium state). The density matrix given by Eq. (32) is also obtained at $t=+\infty$ with the factorized initial condition. But there it is not a stationary state of the equation of motion because the ground state of the interacting system is different from the ground state of the free oscillators (see Sec. VI).

The average (in the thermal state) which appears in Eq. (31) is computed in detail in Appendix B for an arbitrary number of oscillators. The result is

$$\begin{aligned}\langle\,U_3^\dagger e^{iH_{1,p_2}t}U^\dagger_{1,q_2}U_{1,q_1}e^{-iH_{1,p_1}t}U_3\,\rangle_\beta=&\exp\{i[A(t)(p_1^2-p_2^2)+(p_1+p_2)(q_1-q_2)B(t)]\\&\times\exp[-C(t)(p_1-p_2)^2+D(t)(q_1-q_2)(p_2-p_1)-(q_1-q_2)^2F]\}\ .\end{aligned} \tag{33}$$

As shown in Appendix C, the functions A, B, C, D, and F can be expressed as integrals and in the case of Ohmic dissipation are given by

$$A(t)=\frac{1}{2\eta}(e^{-\eta t/M}-1)\ , \tag{34a}$$

$$B(t)=\tfrac{1}{2}(e^{-\eta t/M}-1)\ , \tag{34b}$$

$$C(t)=\frac{\eta}{\pi M^2}\int_0^\infty dE\frac{\coth(\beta E/2)}{E^3+(\eta^2/M^2)E}[1-\cos(Et)]\ , \tag{34c}$$

$$D(t)=\frac{\eta}{\pi M}\int_0^\infty dE\frac{\coth(\beta E/2)}{E^2+\eta^2/M^2}\sin(Et)\ , \tag{34d}$$

$$F=\frac{1}{2}\frac{\eta}{\pi}\int_0^{\omega_c}dE\frac{\coth(\beta E/2)}{E^2+\eta^2/M^2}\ . \tag{34e}$$

Equation (31), together with Eqs. (33) and (34), gives us the final formula expressing the reduced density matrix at time t as a function of the initial condition. It is given in terms of new variables $x=\frac{1}{2}(q_1+q_2)$, $y=q_1-q_2$ by

$$\begin{aligned}\rho(x_f,y_f,t)=&\int\int dx_i\,dy_i\,J(x_f,y_f,t;x_i,y_i,0)\\&\times\rho_0(x_i+\tfrac{1}{2}y_i,x_i-\tfrac{1}{2}y_i)\ ,\end{aligned} \tag{35a}$$

where

$$\begin{aligned}J(x_f,y_f,t;x_i,y_i,0)=&\frac{1}{4\pi\,|\,A(t)\,|}\exp\left[-i\left[\frac{y_fe^{-\eta t/M}-y_i}{2A(t)}\right](x_f-x_i)\right]\\&\times\exp\left[-C(t)\left[\frac{y_fe^{-\eta t/M}-y_i}{2A(t)}\right]^2-D(t)y_f\left[\frac{y_fe^{-\eta t/M}-y_i}{2A(t)}\right]-y_f^2F\right]\ .\end{aligned} \tag{35b}$$

We specialize these results to the propagation of a Gaussian wave packet

$$\rho_0(q_1,q_2)=\frac{1}{\sigma_0\sqrt{\pi}}\exp\left[ip_0(q_1-q_2)-\frac{q_1^2+q_2^2}{2\sigma_0^2}\right] . \tag{36}$$

Let us first compute the diagonal part of the reduced density matrix at time t, $\rho(q,q,t)$. Substituting Eq. (36) into Eq. (35) we obtain

$$\rho(q,q,t)=\frac{1}{\sigma(t)\sqrt{\pi}}\exp\left[-\frac{[q+2A(t)p_0]^2}{\sigma_{\mathrm{th}}^2(t)}\right] \tag{37}$$

with

$$\sigma_{\mathrm{th}}^2(t)=\sigma_0^2+4\frac{A(t)}{\sigma_0^2}+4C(t) . \tag{38}$$

The center of the wave packet follows the classical trajectory

$$q(t)=-2A(t)p_0=\frac{p_0}{\eta}(1-e^{-\eta t/M}) . \tag{39}$$

At zero temperature, the spreading of the wave packet is only logarithmic since

$$[C(t)]_{T=0}=\frac{\eta}{\pi M^2}\int_0^\infty dE\frac{1}{E^3+(\eta^2/M^2)E}[1-\cos(Et)]$$
$$\sim\frac{1}{\pi\eta}\ln\left[\frac{\eta}{M}t\right] . \tag{40}$$

For high temperatures, we find the usual classical diffusive behavior

$$[C(t)]_{T\gg\omega_c}=\frac{2\eta}{\pi M^2\beta}\int_0^\infty dE\frac{1}{E^3+(\eta^2/M^2)E}\frac{1-\cos(Et)}{E}$$
$$\sim\frac{1}{\eta\beta}t . \tag{41}$$

We can also compute the evolution of momentum moments using off-diagonal terms of the reduced density matrix. The first two are given by

$$\langle p\rangle=p_0[1+2B(t)]=p_0e^{-\eta t/M} , \tag{42a}$$

$$\langle p^2\rangle=p_0^2[1+2B(t)]^2+2F . \tag{42b}$$

The mean value of p follows the classical equation. The mean value of p^2 does not vanish at $t=\infty$ but goes to the inverse of the resolution length of the bath according to the Heisenberg uncertainty relation. This shows that the upper cutoff frequency of the bath is actually measurable by looking only at the particle and, surprisingly, does not disappear completely.

V. THE NEW INITIAL CONDITION WITHIN THE PATH-INTEGRAL FORMALISM AND ITS RELATION TO THE INFLUENCE FUNCTIONAL OF FEYNMAN AND VERNON

We want to compare the evolution of the reduced matrix following two different initial conditions: the Feynman-Vernon one used by Caldeira and Leggett[2] and the thermal one introduced in the last section. We shall find that differences persist for times larger than the inverse cutoff frequency. Before carrying out this program in the next section, we shall here compute the influence functional corresponding to the initial condition introduced in the previous section, in the hope of clarifying its relation to the usual one.

As explained in Ref. 7 it is possible to give a path-integral representation for the evolution of the reduced density matrix

$$\rho(q_1,q_2,t)=\int\int dq_1'\,dq_2'\,K(q_1,q_2,t;q_1',q_2',0) , \tag{43}$$

where

$$K(q_1,q_2,t;q_1',q_2',0)$$
$$=\int\int D\{q_1\}D\{q_2\}\exp\left[i\frac{S_0(q_1)}{\hbar}\right]\exp\left[-i\frac{S_0(q_2)}{\hbar}\right]$$
$$\times F(\{q_1\},\{q_2\}) . \tag{44}$$

S_0 is the action of the particle alone and the integration is over all particle paths connecting the specified initial and final coordinates. The functional $F(\{q_1\},\{q_2\})$ describes the influence of the bath on the propagation of the particle (it is not yet what is usually called the influence functional because we have included the initial density matrix in it). It is determined by the dynamics of the bath, when the particle follows the classical paths $\{q_1\}$ and $\{q_2\}$. Looking at Eq. (3) it is seen that the path of the classical particle acts like a time-dependent force $F_\alpha(t)$ on each oscillator of the bath

$$F_\alpha(t)=\mu_\alpha\omega_\alpha^2q(t) . \tag{45}$$

The required dynamics of a forced harmonic oscillator is given by a unitary operator $V_\alpha(t)$ relating the wave function at time t to the wave function at time zero:

$$|\Psi_\alpha(t)\rangle=V_\alpha(t)|\Psi_\alpha(0)\rangle , \tag{46}$$

where

$$V_\alpha(t)=e^{i\phi_\alpha(t)}e^{-iH_\alpha^0t}U_\alpha(t) , \tag{47a}$$

$$U_\alpha(t)=\exp\left[\frac{1}{\sqrt{2\mu_\alpha\omega_\alpha}}\left[a_\alpha^\dagger\int_0^tF_\alpha(u)e^{i\omega_\alpha u}\right.\right.$$
$$\left.\left.-a_\alpha\int_0^tF_\alpha(u)e^{-i\omega_\alpha u}\right]\right] , \tag{47b}$$

$$\phi_\alpha(t)=\frac{1}{2\mu_\alpha\omega_\alpha}\int_0^tdu\int_0^uds\,F(u)F(s)\sin[\omega_\alpha(u-s)] , \tag{47c}$$

and where H_α^0 is the Hamiltonian of the αth harmonic oscillator. Then the evolution of the whole set of harmonic oscillators when the particle traverses the path $q(\tau)$ is described by the unitary operator $V_{\{q(\tau)\}}(t)$,

$$V_{\{q(\tau)\}}(t)=\prod_\alpha V_\alpha(t) . \tag{48}$$

Now it is possible to write an expression for the functional

$F(q_1,q_2)$ for a general initial state of the total system described by a density matrix $\rho(q_1',Q_1;q_2',Q_2)$ (here q_1',q_2' refer to the particle and Q_1,Q_2 to the environment) as follows:

$$F(\{q_1\},\{q_2\},t)=\mathrm{Tr}_Q[\rho(q_1';q_2')V^\dagger_{\{q_2\}}(t)V_{\{q_1\}}(t)]\ . \qquad (49)$$

The initial condition considered by Caldeira and Leggett[2] is

$$\rho_{\mathrm{CL}}(q_1',Q_1;q_2',Q_2)=\rho_0(q_1',q_2')\rho_B(Q_1,Q_2)\ , \qquad (50)$$

where $\rho_0(q_1',q_2')$ is the density operator of the particle alone and $\rho_B(Q_1,Q_2)$ is the thermal density matrix of the bath when it is not interacting with the particle. The initial condition of the previous section corresponds to

$$\rho_{\mathrm{th}}(q_1',Q_1;q_2',Q_2)=\rho_0(q_1',q_2')\rho_{\mathrm{eq}}(q_1',Q_1;q_2',Q_2)\ , \qquad (51)$$

where ρ_{eq} is the equilibrium density matrix for the *coupled* system at temperature T. Using these equations in the expression for $F(\{q_1\},\{q_2\})$ given by [Eq. (49)], one obtains

$$F(\{q_1\},\{q_2\},t)=\rho_0(q_1',q_2)\mathscr{F}(\{q_1\},\{q_2\},t)\ . \qquad (52)$$

In the case of Caldeira and Leggett, the influence functional $\mathscr{F}$ is

$$\mathscr{F}_{\mathrm{CL}}(\{q_1\},\{q_2\},t)=\langle V^\dagger_{\{q_2\}}(t)V_{\{q_1\}}(t)\rangle\ , \qquad (53)$$

where the average is in the thermal equilibrium state of the uncoupled harmonic oscillators. The initial condition (51) gives (at $T=0$)

$$\begin{aligned}\mathscr{F}_{\mathrm{th}}(\{q_1\},\{q_2\},t)&\\ &=\langle A_{q_2'}\,|\,V^\dagger_{\{q_2\}}(t)V_{\{q_1\}}(t)\,|\,A_{q_1'}\rangle\\ &=\langle 0\,|\,U_3^\dagger U^\dagger_{1,q_2'}V^\dagger_{\{q_2\}}(t)V_{\{q_1\}}(t)U_{1,q_1'}U_3\,|\,0\rangle \qquad (54)\end{aligned}$$

[see Eqs. (23) and (24)]. More generally the average is taken in the thermal state of the total system at temperature T. These expectation values are not difficult to compute using the method of Appendix B. They are given by the exponential of an expression which has a real and an imaginary part. The imaginary parts are the same for $\mathscr{F}_{\mathrm{CL}}$ and $\mathscr{F}_{\mathrm{th}}$ [actually there is one more term in $\mathscr{F}_{\mathrm{th}}$ but it exactly cancels a term neglected by Caldeira and Leggett[2] (second term of their formula 3.35)]. The difference lies in the real part. For $\mathscr{F}_{\mathrm{th}}$ it is given by

$$\exp\left[-\sum_\alpha \tfrac{1}{2}\coth(\tfrac{1}{2}\beta E_\alpha)\left|\sum_\gamma(\tfrac{1}{2}\mu_\gamma\omega_\gamma)^{1/2}(A^\gamma_\alpha I_\gamma-B^\gamma_\alpha I^*_\gamma)\right|^2\right] \qquad (55)$$

where

$$I_\gamma=i(q_2'-q_1')+\omega_\gamma\int_0^t[q_1(u)-q_2(u)]e^{i\omega_\gamma u}du\ . \qquad (56)$$

The sums over energy eigenvalues can be performed using the techniques of Appendix C. After having done that carefully, the real part of $\mathscr{F}_{\mathrm{th}}$ is given by

$$\exp\left[-\frac{\eta}{2\pi}\int_0^{\omega_c}d\omega\,\omega\coth(\tfrac{1}{2}\beta\omega)\int_0^t du\int_0^t ds\,y(u)y(s)\cos[\omega(u-s)]\right]$$
$$\times\exp\left[-\frac{\eta}{2\pi}\int_0^{\omega_c}d\omega\frac{\omega\coth(\tfrac{1}{2}\beta\omega)}{\omega^2+\eta^2/M^2}\left[y_i^2+y_i\int_0^t du\,y(u)[2(\eta/M)\cos(\omega u)-2\omega\sin(\omega u)]\right]\right]\ , \qquad (57)$$

where we have introduced $y_i=q_1'-q_2'$. In contrast, the real part of $\mathscr{F}_{\mathrm{CL}}$ is only given by the first exponential [their Eqs. (3.10) and (6.4)]. The entire difference between the two initial conditions is contained in the second exponential of Eq. (57).

Given these expressions for the influence functional, the formula [Eqs. (43) and (44)] expressing the reduced density matrix at time t in terms of the initial condition is given by

$$\rho(x_f,y_f,t)=\int\int dx_i dy_i D\{x\}D\{y\}e^{i(S_1+iS_2)}\rho_0(x_i,y_i)\ , \qquad (58)$$

where it is again convenient, following previous authors, to use sum and difference variables $x=\frac{1}{2}(q_1+q_2)$ and $y=q_1-q_2$. S_1 is given by the action of the free particle plus the imaginary part of the influence functional and is the same for the two initial conditions,

$$S_1=\int_0^t du(M\dot{x}\dot{y}-\eta\dot{x}y)\ , \qquad (59)$$

$\exp(-S_2)$ is given by Eq. (57), or only the first exponential in that equation, depending upon which initial condition we use.

The path integral in (58) may be easily evaluated.[2,12] There are two reasons for this, one obvious and the other not quite obvious: (1) the integrals are Gaussian and therefore present no difficulties of principle, (2) because of the form of S_1 it is a useful tactic to take as a reference the paths that make S_1 an extremum. To clarify the latter remark, we first note that an expansion about paths that are not the extremum paths for the full action S_1+iS_2 leaves an *inhomogeneous* Gaussian functional integral to be done. The relevant general formula is

$$\begin{aligned}\int D\mathbf{V}\exp(-\tfrac{1}{2}\mathbf{V}^T\underline{M}\mathbf{V}+i\,\mathbf{A}^T\mathbf{V})&\\ &=(\det\underline{M})^{-1/2}\exp(-\tfrac{1}{2}\mathbf{A}^T\underline{M}^{-1}\mathbf{A})\ . \qquad (60)\end{aligned}$$

Here $\mathbf{V}$ and $\mathbf{A}$ are N-dimensional real (column) vectors. $\underline{M}$ is a real, symmetric, nonsingular matrix and $D\mathbf{V}$ means $\prod_i(dV_i/\sqrt{2\pi})$. For the case at hand let V be $(\delta x_i,\delta y_j)$ where δx_i and δy_j are derivations from the path determined by $\delta S_1=0$, at discrete times denoted by the subscripts. Then, note that Eq. (58) when expanded about the extremum of S_1 leads to a structure of the form (60), in which, however, the quadratic piece has no terms of the form $\delta x_i\delta x_j$, and the linear part comes solely from S_2 and so does not contain any terms in δx. Symbolically, then, in the space spanned by $(\delta x, \delta y)$ we have the structures

$$\mathbf{A}=\begin{bmatrix}0\\ a\end{bmatrix}, \quad \underline{M}=\begin{bmatrix}\underline{0} & \underline{p}\\ \underline{\tilde{p}} & \underline{r}\end{bmatrix} . \tag{61}$$

It follows that $\underline{M}^{-1}$ *has a zero in the lower right-hand corner and, thus, that* $\mathbf{A}^T\underline{M}^{-1}\mathbf{A}=0$. This fact greatly simplifies the calculation. There is a good reason for the zeros in Eq. (61).[13] Paths for which $y\equiv 0$ are paths for which $q_1(t)=q_2(t)$. Now the action in Eq. (58) comes from (1) terms in the Hamiltonian which act on the particle coordinate alone, (2) terms coming from the influence functional. In terms of type (1) the action involves $S_0(q_1)-S_0(q_2)$ which is clearly zero if $q_1(t)=q_2(t)$. For the other terms the argument is also simple. The influence functional [Eq. (49)] involves the comparison at time t between states of the bath that have evolved subject to the external forces specified by $q_1(t)$ and $q_2(t)$ [Eq. (45)]. For $q_1(t)=q_2(t)$ these states are identical and the influence functional is equal to one. Thus everything in the exponent of (53) and (54) must, and does, go to zero for paths $y(t)\equiv 0$. This condition, plus the fact that S_1 and S_2 are quadratic, requires the structures (61).

The condition $\delta S_1=0$ leads to the equations

$$\ddot{x}+\gamma\dot{x}=0 , \tag{62a}$$

$$\ddot{y}-\gamma\dot{y}=0 . \tag{62b}$$

(Here $\gamma=\eta/M$. Note that this is twice the γ used by Caldeira and Leggett.)

Because of the zero in the upper left-hand corner of $\underline{M}$ [Eq. (61)] the functional determinant in (60) is also easy to evaluate. By considering the finite matrix for discrete time steps, one can deduce that $\det\underline{p}\equiv d(t)$ obeys the differential equation (62a) and the boundary conditions $d(0)=0$, $\dot{d}(0)=1$. Since $\det\underline{M}=(\det\underline{p})^2$, this completes the evaluation of the path integral in (58). The extremum value of the action S_1 can be expressed—via an integration by parts and exploitation of the equation of motion [(62a) and (62b)]—in terms of values at the endpoints. After these steps (58) becomes

$$\rho(x_f,y_f,t)=\frac{M}{2\pi d(t)}\int\int dx_i\,dy_i\exp[iM(\dot{x}_f y_f-\dot{x}_i y_i)]$$
$$\times\exp[-S_2(\{y_{\rm cl}\})]\rho_0(x_i,y_i) . \tag{63}$$

Here $S_2(\{y_{\rm cl}\})$ is the action S_2 evaluated along the path $y_{\rm cl}(t)$, i.e., the solution of (62b) with $y_{\rm cl}(0)=y_i$ and $y_{\rm cl}(t)=y_f$, and $\dot{x}_i,\dot{x}_f$ are the initial and final velocities associated with (62a) subject to the boundary conditions $x(0)=x_i$, $x(t)=x_f$. Explicitly one finds

$$d(t)=\frac{1}{\gamma}(1-e^{-\gamma t}),\quad \gamma=\frac{\eta}{M} , \tag{64a}$$

$$\dot{x}_i=(x_f-x_i)/d(t) , \tag{64b}$$

$$\dot{x}_f=e^{-\gamma t}\dot{x}_i , \tag{64c}$$

$$y_{\rm cl}(u)=y_i+\frac{d(u)}{d(t)}(y_f-y_i)\exp[\gamma(u-t)] . \tag{64d}$$

When these equations are substituted in Eq. (63) and the expression (57) is used for S_2 we recover the previously deduced evolution of the reduced density matrix [Eqs. (35)]. When we use only the first exponential of Eq. (57) for S_2 we obtain the evolution of the reduced density matrix corresponding to the initial condition chosen by Caldeira and Leggett. It is worth noting here that the two influence functionals are very similar. Their imaginary parts are exactly the same. This should be true in general in order to obtain the classical equations of motion. The differences in their real parts come only from a contribution proportional to the initial coordinates. In the next section this will enable us to give a unified treatment of the time dependence of various averages, starting from both initial conditions.

VI. COMPARISON OF THE EVOLUTION OF THE REDUCED DENSITY MATRIX FROM THE TWO INITIAL CONDITIONS

In this section we calculate and compare the time development of position and momentum moments using the uncoupled initial condition of Caldeira and Leggett[2] and the thermal one introduced in Sec. IV. We also consider explicitly the propagation of a Gaussian wave packet. We study first the time dependence of position moments (and come back to usual units by restoring the missing $\hbar$'s).

For a general function of position, we have

$$\langle F(x)\rangle_t=\int dx_f\,F(x_f)\rho(x_f,y_f=0,t) , \tag{65}$$

since setting $y_f=0$ is the same[14] as integrating over final momenta. The integrals are straightforward and one finds

$$\langle F(x)\rangle_t=\int\int dx_i\,dy_i[F((i\hbar/M)d(t)\partial/\partial y_i)\delta(y_i)]$$
$$\times e^{i[M/\hbar d(t)x_i y_i]}$$
$$\times e^{-y_i^2 f(t)}\rho(x_i,y_i) . \tag{66}$$

Here we have used Eqs. (63) and (64). In the factorized case we have simply written S_2 in Eq. (63), for $y_f=0$, as $y_i^2 f_{\rm CL}(t)$. For the thermal initial condition, as $\rho_0(x_i,y_i)$ is only proportional to the initial density matrix at $t=0$, we have written (for $y_f=0$)

$$-y_i^2 f_{\rm th}(t)=S_2-y_i^2 F$$

[F is given by (34e) and comes from the equilibrium density matrix in Eq. (51)].

It follows from (66) that

$$\langle x\rangle_t=\langle x\rangle_0+\frac{d(t)}{M}\langle p\rangle_0 , \tag{67a}$$

$$\langle x^2\rangle_t=\langle x^2\rangle_0+2f(t)\frac{\hbar^2 d^2(t)}{M^2}+\frac{d^2(t)}{M}\langle p^2\rangle_0$$
$$+\frac{d(t)}{M}\langle(xp+px)\rangle_0 . \tag{67b}$$

In these equations only $f(t)$ is dependent on the initial condition. It is instructive to compare these formulas [Eqs. (67)] with those for a noninteracting particle:

$$\langle x\rangle_t=\langle x\rangle_0+\frac{t}{M}\langle p\rangle_0\,, \tag{68a}$$

$$\langle x^2\rangle_t=\langle x^2\rangle_0+\frac{t^2}{M^2}\langle p^2\rangle_0+\frac{t}{M}\langle (xp+px)\rangle_0\,. \tag{68b}$$

Comparing (67) and (68) we see that the environment has two effects. Because it causes the time t in (68) to be replaced by $d(t)$, [Eq. 64a)], it quenches the quantum-mechanical spreading of a free-particle wave packet after a time on the order of the relaxation time γ^{-1}. There is an additional physical effect associated with the second term on the right side of Eq. (67b). This is a diffusion which dominates for times greater than γ^{-1}. The function $f(t)$ which controls this effect is evaluated by substituting (64d), with $y_f=0$, into S_2 in (63) and using Eq. (57) [or only the first exponential in (57) for the factorized initial condition]. One thus finds, for the Caldeira-Leggett initial condition,

$$f_{\rm CL}(t)=\frac{M\gamma}{\hbar(1-e^{-\gamma t})^2}\int_0^{\omega_c}d\omega\frac{\omega}{2\pi}\coth(\tfrac{1}{2}\hbar\beta\omega)\left[\frac{4\gamma^2}{\omega^2(\omega^2+\gamma^2)}\sin^2(\omega t/2)+\frac{(1-e^{-\gamma t})^2}{\gamma^2+\omega^2}-\frac{2\gamma(1-e^{-\gamma t})}{\omega(\omega^2+\gamma^2)}\sin(\omega t)\right]. \tag{69a}$$

In the case of the thermal initial condition f is given by

$$f_{\rm th}(t)=\frac{M\gamma}{\hbar(1-e^{-\gamma t})^2}\int_0^{\omega_c}d\omega\frac{\omega}{2\pi}\coth(\tfrac{1}{2}\hbar\beta\omega)\left[\frac{4\gamma^2}{\omega^2(\omega^2+\gamma^2)}\sin^2(\omega t/2)-\frac{(1-e^{-\gamma t})^2}{\omega^2+\gamma^2}\right]. \tag{69b}$$

These functions depend on three dimensionless parameters: time, $\tau\equiv\gamma t$; inverse temperature, $b\equiv\beta\hbar\gamma$; and the upper-frequency cutoff, $\Omega\equiv\omega_c/\gamma$. In the classical limit $b\Omega\ll 1$, $\Omega\gg 1$, one finds for both initial conditions after a short time transient on the scale $t\sim\omega_c^{-1}$ the expression

$$\frac{\hbar}{M\gamma}f(\tau,b,\Omega)=\frac{1}{b(1-e^{-\tau})^2}[\tau-(1-e^{-\tau})-\tfrac{1}{2}(1-e^{-\tau})^2]\,. \tag{70}$$

For long times $\tau\gg 1$, this reduces to

$$\frac{\hbar}{M\gamma}f\to\frac{1}{b}(\tau-\tfrac{3}{2})\,. \tag{71}$$

The linear dependence on time describes classical diffusion, and (67b) shows that the coefficient obeys the Einstein relation between diffusivity and viscosity. At zero temperature ($b=\infty$) one finds a different behavior for long times, $\tau\gg 1$, namely, $\hbar f/m\gamma\to\pi^{-1}\ln\tau$. The logarithmic dependence changes to a linear one at any finite temperature for time greater than $\hbar\beta$. Here one again recovers the linear diffusive behavior, with the Einstein coefficient, but with a different offset. The crossover time $\hbar\beta$ is the period of the most rapid classical environmental oscillation. Figure 1 is a plot of $f_{\rm CL}$ for parameter values chosen to illustrate the various regimes.

It is now also straightforward to calculate the behavior of momentum moments. For these, the general formula is

$$\langle F(p)\rangle_t=\int dx_f\,F((\hbar/i)\partial/\partial y_f)\rho(x_f,y_f,t)\Big|_{y_f=0}\,. \tag{72}$$

Integrating (63) over x_f and x_i, one obtains the simple formula

$$\rho(y_f,t)=\exp[-S_2(\{y_{\rm cl}\}_{y_i=y_fe^{-\gamma t}})]\rho_0(y_i=y_fe^{-\gamma t})\,, \tag{73}$$

where $\rho(y)\equiv\int dx\,\rho(x,y)$ and S_2 should be evaluated along a classical trajectory such that $y_i=y_fe^{-\gamma t}$. For the initial condition of Caldeira and Leggett, one has

$$[S_2(\{y_{\rm cl}\}_{y_i=y_fe^{-\gamma t}})]_{\rm CL}=\frac{M\gamma k_BT}{\hbar^2}y_f^2e^{-2\gamma t}\times\int_{-\omega_c}^{\omega_c}d\omega\frac{K(\omega)}{2\pi(\omega^2+\gamma^2)}[1+e^{2\gamma t}-2e^{\gamma t}\cos(\omega t)]\,, \tag{74a}$$

where $K(\omega)$ is $(\hbar\omega/2k_BT)\coth(\hbar\omega/2k_BT)$. For the thermal initial condition, S_2 is simply given by

$$[S_2(\{y_{\rm cl}\}_{y_i=y_fe^{-\gamma t}})]_{\rm th}=\frac{M\gamma k_BT}{\hbar^2}y_f^2\int_{-\omega_c}^{\omega_c}d\omega\frac{K(\omega)}{2\pi(\omega^2+\gamma^2)}(1-e^{-2\gamma t})\,. \tag{74b}$$

From Eqs. (74) it follows that for both initial conditions

$$\langle p\rangle_t=e^{-\gamma t}\langle p\rangle_0\,. \tag{75}$$

Thus, in both cases, the mean momentum of the particle follows the classical equation of motion.

The evolution of the mean-square momentum, for the factorized initial condition, is given by

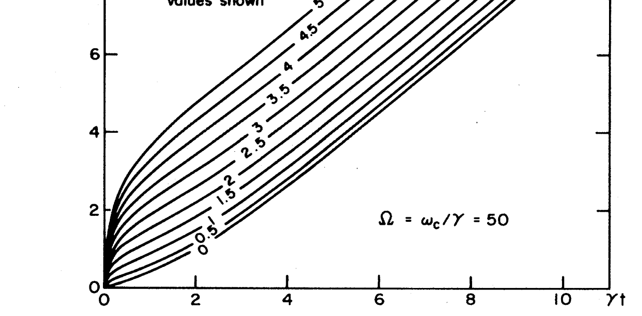

FIG. 1. Curves illustrating the quantum corrections to classical diffusion, as given by Eq. (69a).

$$\langle p^2\rangle_t = e^{-2\gamma t}\langle p^2\rangle_0 + 2M\gamma k_B T\int_{-\omega_c}^{\omega_c} d\omega \frac{K(\omega)}{2\pi(\omega^2+\gamma^2)}[1+e^{-2\gamma t}-2e^{-\gamma t}\cos(\omega t)] \,. \tag{76a}$$

For the thermal initial condition, its evolution is

$$\langle p^2\rangle_t = e^{-2\gamma t}\langle p^2\rangle_0 + 2M\gamma k_B T\int_{-\omega_c}^{\omega_c} d\omega \frac{K(\omega)}{2\pi(\omega^2+\gamma^2)}(1-e^{-2\gamma t}) \,. \tag{76b}$$

In the classical limit $K(\omega)\to 1$, $\omega_c\to\infty$ and both evolutions reduce to

$$\langle p^2\rangle_t = e^{-2\gamma t}\langle p^2\rangle_0 + Mk_B T(1-e^{-2\gamma t}) \,.$$

This shows that equipartition, i.e., $\langle p^2\rangle = Mk_B T$, is both the long-time and stationary solution. However in the quantum case the long-time solution

$$\langle p^2\rangle = Mk_B T\int_{-\omega_c}^{\omega_c} d\omega \frac{K(\omega)}{\pi(\omega^2+\gamma^2)} \tag{77}$$

is only a stationary solution of the evolution (76b) corresponding to the thermal initial condition. It is not a stationary solution of (76a), a fact which reflects the uncoupled initial condition [Eq. (50)] imposed by Caldeira and Leggett. The long-time limit [Eq. (77)] corresponds of course to the mean value of the square momentum of the particle in thermal equilibrium [Eqs. (42b) and (34e)]. Now we specialize these results to the propagation of a Gaussian wave packet

$$\rho_0(x_i,y_i) = \frac{1}{\sigma\sqrt{\pi}}\exp\left[ip_0 y_i - \frac{x_i^2+y_i^2/4}{\sigma_0^2}\right] . \tag{78}$$

For the diagonal part of the reduced density matrix at time t we obtain, for the factorized initial condition,

$$\rho(x_f,0,t) = \frac{1}{\sigma_{\rm CL}(t)\sqrt{\pi}}\exp\left[-\frac{[x_f-p_0 d(t)/M]^2}{\sigma_{\rm CL}^2(t)}\right] \tag{79}$$

with

$$\sigma_{\rm CL}^2(t) = \sigma_0^2 + \frac{d^2(t)}{\sigma_0^2 M^2} + \frac{4d^2(t)}{M^2} f_{\rm CL}(t) \,. \tag{80}$$

This should be compared with our previous results [Eqs. (37) and (38)] for the thermal initial condition $[d(t)=2M\,|A(t)|=(1/\gamma)(1-e^{-\gamma t})]$. Here as before the center of the mass follows the classical equation of motion, but the evolutions of the widths of the wave packets are different:

$$\sigma_{\rm CL}^2 - \sigma_{\rm th}^2 = \frac{4}{M\gamma\hbar}\int_0^{\omega_c} d\omega \frac{\omega}{2\pi}\coth\left[\frac{\beta\hbar\omega}{2}\right] \times\left[\frac{(1-e^{-\gamma t})^2}{\gamma^2+\omega^2} - \frac{2\gamma(1-e^{-\gamma t})}{\omega(\omega^2+\gamma^2)}\sin(\omega t)\right] . \tag{81}$$

The long-time logarithmic behavior of the widths are exactly the same but the subleading terms differ. It is interesting to note that for the thermal initial condition the behavior of $\sigma_{\rm th}^2$ is well behaved when $\omega_c\to\infty$, contrary[15] to $\sigma_{\rm CL}^2$. This happens because the initial cutoff-dependent initial mean-square momentum cancels exactly the cutoff-dependent term in $f_{\rm th}(t)$ [see Eq. (67b)].

For the evolution of momenta averages there are also some differences, since for the factorized initial condition,

$$\langle p^2\rangle = e^{-2\gamma t}p_0^2 + M\gamma\int_0^{\omega_c} d\omega \frac{\omega\coth(\frac{1}{2}\hbar\beta\omega)}{2\pi(\omega^2+\gamma^2)} \times[1+e^{-2\gamma t}-2e^{-\gamma t}\cos(\omega t)] \,, \tag{82}$$

whereas for the thermal initial condition [Eqs. (64)],

$$\langle p^2\rangle = e^{-2\gamma t}p_0^2 + M\gamma\int_0^{\omega_c} d\omega \frac{\omega\coth(\frac{1}{2}\hbar\beta\omega)}{2\pi(\omega^2+\gamma^2)} \,. \tag{83}$$

They differ by a transient which lasts a time of the order of the relaxation time.

VII. CONCLUSION

In the present paper we have studied in great detail the model proposed by Caldeira and Leggett, when there is no external potential and the model is completely soluble, in the hope of exhibiting some of its features which may also be relevant in more general cases. We have obtained the eigenstates of the total Hamiltonian and shown more explicitly that the bath is, in some sense, measuring the position of the particle. This has given a nice explanation of the residual mean-square momentum of the particle in equilibrium and explained why it is related to the upper cutoff, and it also has the somewhat surprising consequence that the upper cutoff of the bath is theoretically a directly measurable quantity. We have compared the evolution of the particle according to different initial conditions. We have introduced a nonfactorized initial condition where the bath has already "measured" the position of the particle in the sense that off-diagonal terms of the reduced density matrix are as suppressed as in thermal equilibrium. We have also worked out explicitly the time dependence of position and momentum averages according to an initial condition used previously in the work of Caldeira and Leggett. Contrary to previous expectations, the difference between the two different initial conditions is very long lived, being governed by the relaxation time, which is also the scale of the evolution of the system. The importance of the initial condition seems therefore worth studying in other models like two-level systems. Finally, the results of this paper may be useful in trying to understand tunneling by matching wave functions in different regions, although this approach appears rather complicated at the moment.

ACKNOWLEDGMENTS

We are particularly grateful to A. Caldeira and F. Guinea for many helpful discussions. We would also like to thank J. Deutsch, J. P. Sethna, and W. Zurek for interesting conversations. This work was supported by the National Science Foundation under Grant No. PHY-77-27084 supplemented by funds from the U. S. National Aeronautics and Space Administration (NASA). V. Hakim is also very grateful to Professor R. Schrieffer for his hospitality at the Institute for Theoretical Physics (Santa Barbara), when he was partially supported by the NSF under Grant No. DMR-82-16285. One of us (V.A.) was partially supported by the U. S. Office of Naval Research (ONR) under Grant No. N00014-78-C-0666. During the time when the major part of this work was performed, V.A. gratefully acknowledges support from the John Simon Guggenheim Memorial Foundation.

APPENDIX A: DIAGONALIZATION OF H_2

We want to show in this Appendix how we perform the transformation to the normal modes of H_2 [Eqs. (18), (19), and (20)]:

$$H_2=\sum_\alpha \omega_\alpha(a_\alpha^\dagger a_\alpha+\tfrac{1}{2}) +(1/2M)\left[\sum_\alpha(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2}(a_\alpha^\dagger+a_\alpha)\right]^2 . \tag{A1}$$

The equations of motion of a_α and $a_\alpha^\dagger$ are

$$\frac{da_\alpha}{dt}=i[H,a_\alpha] =i\left[-\omega_\alpha a_\alpha-(1/M)(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2} \times\sum_\beta(\tfrac{1}{2}\mu_\beta\omega_\beta)^{1/2}(a_\beta^\dagger+a_\beta)\right] , \tag{A2a}$$

$$\frac{da_\alpha^\dagger}{dt}=i[H,a_\alpha^\dagger] =i\left[+\omega_\alpha a_\alpha^\dagger+(1/M)(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2} \times\sum_\beta(\tfrac{1}{2}\mu_\beta\omega_\beta)^{1/2}(a_\beta^\dagger+a_\beta)\right] . \tag{A2b}$$

We are looking for linear combinations $b_\alpha^\dagger$ of a_α and $a_\alpha^\dagger$ which are eigenvectors of these equations with eigenvalues E_α. We find

$$a_\alpha=\sum_\beta A_\beta^\alpha b_\beta^\dagger+B_\beta^\alpha b_\beta , \tag{A3a}$$

$$a_\alpha^\dagger=\sum_\beta B_\beta^\alpha b_\beta^\dagger+A_\beta^\alpha b_\beta , \tag{A3b}$$

and A_β^α and B_β^α are solutions of

$$-\omega_\alpha A_\beta^\alpha-(1/M)(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2}\sum_\gamma(\tfrac{1}{2}\mu_\gamma\omega_\gamma)^{1/2}(A_\beta^\gamma+B_\beta^\gamma) =E_\beta A_\beta^\alpha , \tag{A4a}$$

$$+\omega_\alpha B_\beta^\alpha+(1/M)(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2}\sum_\gamma(\tfrac{1}{2}\mu_\gamma\omega_\gamma)^{1/2}(A_\beta^\gamma+B_\beta^\gamma) =E_\beta B_\beta^\alpha . \tag{A4b}$$

Let us call K_β the sum

$$K_\beta=(1/M)\sum_\gamma(\tfrac{1}{2}\mu_\gamma\omega_\gamma)^{1/2}(A_\beta^\gamma+B_\beta^\gamma) . \tag{A5}$$

Then from Eqs. (A4) we readily obtain

$$A_\beta^\alpha=\frac{-K_\beta}{E_\beta+\omega_\alpha}(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2},\quad B_\beta^\alpha=\frac{K_\beta}{E_\beta-\omega_\alpha}(\tfrac{1}{2}\mu_\alpha\omega_\alpha)^{1/2} \tag{A6}$$

and (A5) gives us the consistency relation

$$1=\sum_\alpha\frac{\mu_\alpha}{M}\frac{\omega_\alpha^2}{E_\beta^2-\omega_\alpha^2} \tag{A7}$$

which is the eigenvalue equation [Eq. (20) in the main text]. In order to have proper canonical commutation for the b and $b^\dagger$'s A_β^α and B_β^α should be normalized such as to satisfy

$$1=\sum_\beta(-A_\beta^\alpha A_\beta^\alpha+B_\beta^\alpha B_\beta^\alpha) . \tag{A8}$$

This will be verified for K_β [Eq. (A6)] given by

$$K_\beta=\left[\sum_\gamma\frac{2\mu_\gamma\omega_\gamma^2E_\beta}{(E_\beta^2-\omega_\gamma^2)^2}\right]^{-1/2} . \tag{A9}$$

When we put this last expression into Eq. (A6) we obtain the expression for A_β^α and B_β^α given in the main text [Eqs. (18)].

APPENDIX B: COMPUTATION OF THERMAL AVERAGES AND OVERLAPS

Here we want to show how we have computed the thermal average of the product of operators that appear in the time evolution of the reduced density matrix. Specifically we want to compute

$$F(p_1,p_2,t)=\langle U_3^\dagger e^{iH_{1,p_2}t}U_{1,q_2}^\dagger U_{1,q_1}e^{-iH_{1,p_1}t}U_3\rangle_\beta . \tag{B1}$$

For $t=0$, this is also the overlap $\langle A_{q_2}\,|\,A_{q_1}\rangle$ between two states of the bath associated with positions q_1 and q_2 of the particle [see Eq. (25)].

Using the result of our diagonalization we firstly express (B1) as

$$F(p_1,p_2,t) =\langle(U_3^\dagger U_{2,p_2}U_3) \times(e^{iH_3t}U_3^\dagger U_{2,p_2}^\dagger U_{1,q_1-q_2}U_{2,p_1}U_3e^{-iH_3t}) \times(U_3^\dagger U_{2,p_1}^\dagger U_3)\rangle_\beta . \tag{B2}$$

This seems cumbersome until it is noticed that the three terms in parenthesis are easily computed since we know the action of U_3 on a_q and $a_q^\dagger$ [Eq. (17)] and their evolution in time. Thus,

$$U_3^\dagger U_{2,p} U_3 = \exp\left[\sum_\beta f_\beta^p (a_\beta^\dagger - a_\beta)\right] . \tag{B3}$$

With

$$\begin{aligned} f_\beta^p &\equiv \sum_\alpha \frac{r_\alpha^p}{\sqrt{2\omega_\alpha \mu_\alpha}} (B_\beta^\alpha - A_\beta^\alpha) \\ &= \frac{p}{\sqrt{2E_\beta} E_\beta \left[\sum_\gamma [\omega_\gamma^2 \mu_\gamma / (E_\beta^2 - \omega_\gamma^2)^2]\right]^{1/2}} \end{aligned} \tag{B4}$$

[r_α^p is defined in Eq. (11), A_β^α and B_β^α in Eqs. (18)]. In the same way we get for the middle term

$$\begin{aligned} & e^{iH_3 t} U_3^\dagger U_{2,p_2}^\dagger U_{1,q_1-q_2} U_{2,p_1} U_3 e^{-iH_3 t} \\ &\quad = \exp\left[-\tfrac{1}{2} i \sum_\alpha [(q_1 - q_2) r_\alpha^{p_2+p_1}]\right] \exp\left[\sum_\beta [f_\beta^{p_1-p_2} e^{iE_\beta t} - i(q_1-q_2) g_\beta e^{iE_\beta t}] a_\beta^\dagger \right. \\ &\qquad \left. - [f_\beta^{p_1-p_2} e^{-iE_\beta t} + i(q_1-q_2) g_\beta e^{-iE_\beta t}] a_\beta \right] \end{aligned} \tag{B5}$$

and we have defined

$$\begin{aligned} g_\beta &= \sum_\alpha (\tfrac{1}{2} \mu_\alpha \omega_\alpha)^{1/2} (A_\beta^\alpha + B_\beta^\alpha) \\ &= \frac{M}{\sqrt{2E_\beta}} \frac{1}{\left[\sum_\gamma [\omega_\gamma^2 \mu_\gamma / (E_\beta^2 - \omega_\gamma^2)^2]\right]^{1/2}} . \end{aligned}$$

Now the three terms between parenthesis in Eq. (B2) are exponentials of linear combinations of a_α and $a_\alpha^\dagger$. We express them as a single exponential using the simplified version of the Baker-Hausdorff formula

$$e^A e^B = e^{A+B+[A,B]/2} , \tag{B6}$$

valid when $[A,[A,B]] = [B,[A,B]] = 0$, and we compute the thermal average of the resulting expression with a formula of Bloch:[16]

$$\langle \exp(t a_\alpha^\dagger + u a_\alpha) \rangle_\beta = \exp[\tfrac{1}{2} t u \coth(\tfrac{1}{2} \beta E_\alpha)] .$$

The result of these manipulations is

$$\begin{aligned} F(p_1,p_2,t) = {} & \exp\left[i \sum_\beta f_\beta^{p_1+p_2} f_\beta^{p_2-p_1} \sin(E_\beta t) + f_\beta^{p_2+p_1} g_\beta (q_1-q_2) [\cos(E_\beta t) - 1]\right] \\ & \times \exp\left[-\tfrac{1}{2} \sum_\beta \coth\left[\frac{\beta E_\beta}{2}\right] | f_\beta^{p_2-p_1} (1 - e^{iE_\beta t}) + i(q_1-q_2) g_\beta |^2 \right] . \end{aligned} \tag{B7}$$

APPENDIX C: SUMS OVER ENERGIES AS INTEGRALS

The result of many computations are given by sums over the energy eigenvalue of the Hamiltonian [see, for example, Eqs. (B4) and (B6)]. We want to show how to express them as integrals to simplify their computation. Specifically, we want to compute the sum S_f

$$S_f = \sum_\beta \frac{M f(E_\beta)}{2E_\beta^2 \sum_\gamma [\omega_\gamma^2 \mu_\gamma / (E_\beta^2 - \omega_\gamma^2)^2]} , \tag{C1}$$

where E_β are the positive solutions of Eq. (A7),

$$1 = \frac{1}{M} \sum_\alpha \frac{\mu_\alpha}{M} \frac{\omega_\alpha^2}{E_\beta^2 - \omega_\alpha^2} . \tag{C2}$$

If we choose a contour C encircling the real positive axis (see Fig. 2), we can write S_f as

$$S_f = \frac{1}{2\pi i} \int_C dz \frac{f(z)}{z \left[1 - \sum_\alpha \left[\frac{\mu_\alpha}{M} \frac{\omega_\alpha^2}{z^2 - \omega_\alpha^2}\right]\right]} . \tag{C3}$$

We introduce the spectral density of oscillators $J(\omega)$ [Eq. (4)] and write the denominator as

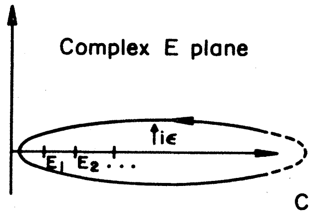

FIG. 2. Contour used in evaluating Eq. (C3).

$$1-\sum_{\gamma}\frac{\mu_\gamma}{M}\frac{\omega_\gamma^2}{z^2-\omega_\gamma^2}=1-\frac{2}{\pi M}\int_0^\infty d\omega\frac{J(\omega)}{\omega(z^2-\omega^2)}$$

$$\overset{\text{O.D.}}{=}1+\frac{\eta}{ME}i\,\mathrm{sgn}(\epsilon)\ . \qquad \text{(C4)}$$

The last equality is only valid in the case of Ohmic dissipation (we have also written z as $z=E+i\epsilon$). We finally obtain the expression we were looking for,

$$S_f=\frac{\eta}{\pi M}\int_0^{\omega_c}dE\frac{f(E)}{E^2+\eta^2/M^2}\ . \qquad \text{(C5)}$$

This allows us to write $F(p_1,p_2,t)$ computed in Appendix B in terms of integrals [see (B1) and (B7)]. The result is

$$F(p_1,p_2,t)=\exp\{\,i[A(t)(p_1^2-p_2^2)+(p_1+p_2)(q_1-q_2)B(t)]\}$$
$$\times\exp\{-[C(t)(p_2-p_1)^2-D(t)(q_1-q_2)(p_2-p_1)+(q_1-q_2)^2F]\}\ ,$$

where

$$A(t)=-\frac{\eta}{\pi M^2}\int_0^\infty dE\frac{1}{E^2+\eta^2/M^2}\frac{\sin(Et)}{E}$$
$$=\frac{1}{2\eta}(e^{-\eta t/M}-1)\ ,$$

$$B(t)=\frac{\eta}{\pi M}\int_0^\infty dE\frac{\cos(Et)-1}{E^2+\eta^2/M^2}=\tfrac{1}{2}(e^{-\eta t/M}-1)\ ,$$

$$C(t)=\frac{\eta}{\pi M^2}\int_0^\infty dE\frac{\coth(\beta E/2)}{E^3+(\eta^2/M^2)E}[1-\cos(Et)]\ ,$$

$$D(t)=\frac{\eta}{\pi M}\int_0^\infty dE\frac{\coth(\beta E/2)}{E^2+\eta^2/M^2}\sin(Et)\ ,$$

$$F=\frac{1}{2}\frac{\eta}{\pi}\int_0^{\omega_c}dE\frac{\coth(\beta E/2)}{E^2+\eta^2/M^2}E\ .$$

(We have replaced ω_c by ∞ in all integrals except the last one, since they are convergent.)

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