Dynamics of the Two-State System with Ohmic Dissipation

Sudip Chakravarty[a] and Anthony J. Leggett[b]
Laboratory of Atomic and Solid State Physics and The Materials Science Center, Cornell University, Ithaca, New York 14853
(Received 15 August 1983)

The authors study a symmetric two-state system with "bare" tunneling frequency Δ_0, dimensionless Ohmic dissipation coefficient α, and heat-bath cutoff ω_c. Defining $\Delta_r \equiv \Delta_0(\Delta_0/\omega_c)^{\alpha/(1-\alpha)}$ for $\alpha < 1$ and $\Delta_r \equiv 0$ for $\alpha > 1$, they find to lowest order in Δ_r/ω_c, $kT/\hbar\omega_c$ (a) for all $\alpha kT >> \hbar\Delta_r$, incoherent relaxation at a rate $(\Delta_0^2/\omega_c)(\sqrt{\pi}/2)[\Gamma(\alpha)/\Gamma(\alpha+\frac{1}{2})] \times(\pi kT/\hbar\omega_c)^{2\alpha-1}$; (b) for $T=0$, $\frac{1}{2}<\alpha<1$, incoherent relaxation at a rate $\sim\Delta_r$; and (c) for $T=0$, $0<\alpha<\frac{1}{2}$, damped oscillations with frequency $\sim\Delta_r$ and Q factor $\frac{1}{2}\cot[(\pi/2)\alpha/(1-\alpha)]$ plus a power-law background.

PACS numbers: 05.30.-d, 03.65.-w, 71.25.Mg, 74.50.+r

The so-called spin-boson Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\hbar\Delta_0\sigma_x + \sum_\alpha \frac{1}{2}\left(\frac{P_\alpha^2}{m_\alpha} + m_\alpha\omega_\alpha^2 x_\alpha^2\right) + \tfrac{1}{2}q_0\sigma_z\sum_\alpha C_\alpha x_\alpha \qquad (1)$$

(with σ_x and σ_z Pauli matrices) can describe a wide variety of problems in which an effectively two-state system is coupled to its environment, and many authors have used it to study the dynamics of such systems.[1] For this problem all necessary information about the effects of the environment is contained in the spectral density

$$J(\omega) \equiv (\pi/2)\textstyle\sum_\alpha (C_\alpha^2/m_\alpha\omega_\alpha)\,\delta(\omega-\omega_\alpha). \qquad (2)$$

The case of "Ohmic" dissipation [$J(\omega) = \eta\omega$ for $\omega \ll \omega_c$, where ω_c is a cutoff frequency large compared to Δ_0] presents many special features.[2] Here we shall study the system dynamics for this case as a function of temperature T and the dimensionless dissipation coefficient

$$\alpha \equiv \eta q_0^2/2\pi\hbar, \qquad (3)$$

under the assumption[3] $\Delta_0/\omega_c \ll 1$ (the limit of primary interest for the "macroscopic quantum coherence" problem[2]). The problem is the following: Given that for $t<0$ the system is known to be localized in the state corresponding to $\sigma_z = +1$ [e.g., by a sufficiently strong biasing potential $V(t) \equiv -V_0\sigma_z\theta(-t)$], what is the value of $P(t) \equiv \langle\sigma_z(t)\rangle$ for $t>0$, and in particular how far is the characteristic oscillatory behavior $P(t) = \cos\Delta_0 t$ of the uncoupled system preserved for finite α? Our calculation covers wide regions of the (α, T) plane: It reproduces *inter alia* as special cases both the Bray-Moore[2] prediction of exponential relaxation with $\tau \propto T^{-(2\alpha-1)}$ for $\alpha > 1$ (but with a different prefactor) and, in the limit $\alpha \to 0$ only, the high-temperature ($kT \gg \hbar\Delta_0/\alpha$) limit of the predictions of Harris and Silbey[1] (exponential relaxation with $\tau \propto \alpha T$). Some features of our results appear also in the recent work of Zwerger.[2]

We start by writing down an exact and general expression for $P(t)$ as a power series in Δ_0. For reasons of space we merely sketch the derivation here.[4] We represent $P(t)$ in terms of a double path integral[5] over the possible paths of the system between the two states, and of the environment over its continuum of states. Each transition between different system states is associated with a transition amplitude $\pm i\Delta_0 dt/2$, while the behavior of the environment is described by the usual action factor. Integrating out the environment in the usual way,[5] we obtain a double functional integral over paths $x(t), y(t) = \pm\frac{1}{2}q_0$ of the system, which are now linked by the influence functional.[5] Now comes the crucial step: We rewrite the expression as a *single* path integral over *four* states, corresponding to the four elements of the density matrix. In the contribution associated with a factor Δ_0^{2n}, the system makes transitions at times t_i, $i = 1, 2 \ldots, 2n$, returning finally to its original state $x = y = +q_0/2$. For times between t_{2j-1} and t_{2j} ($j = 1, 2, \ldots, n$) it is in a "nondiagonal" state ($x = -y$): We call such periods "blips"; for times between t_{2j-2} and t_{2j-1} (and initially and finally) it is in a "diagonal" state ($x = +y$) ("sojourns"). After some calculation we find

$$P(t) = \sum_{n=0}^{\infty}(-1)^n\Delta_0^{2n}\int_0^t dt_{2n}\int_0^{t_{2n}} dt_{2n-1}\ldots\int_0^{t_2} dt_1\,\tilde{F}(t_1, t_2, \ldots, t_{2n}), \qquad (4)$$

where the (partially averaged) influence functional $\tilde{F}$ is given by the expression

$$\tilde{F}=\exp\left(-\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}S_j\right)2^{-n}\sum_{\{\zeta_j=\pm1\}}\left[\exp\left(-\frac{q_0^2}{\pi\hbar}\sum_{\substack{j,k=1\\k>j}}^{n}\Lambda_{jk}\zeta_j\zeta_k\right)\prod_{k=0}^{n-1}\cos\left(\frac{q_0^2}{\pi\hbar}\sum_{j=k+1}^{n}\zeta_jX_{jk}\right)\right], \tag{5}$$

and where t_0 equals $-\infty$ by definition. The functions S_j, Λ_{jk}, and X_{jk} are given by

$$S_j\equiv P_{2j,2j-1}, \tag{6a}$$

$$\Lambda_{jk}\equiv P_{2k,2j-1}+P_{2k-1,2j}-P_{2k,2j}-P_{2k-1,2j-1}, \tag{6b}$$

$$X_{jk}\equiv R_{2j,2k+1}+R_{2j-1,2k}-R_{2j,2k}-R_{2j-1,2k+1}, \tag{6c}$$

where $R_{n,m}\equiv Q_1(t_n-t_m)$, $P_{n,m}\equiv Q_2(t_n-t_m)$, and the functions Q_1, Q_2 are

$$Q_1(t)\equiv\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}\sin\omega t, \tag{7a}$$

$$Q_2(t)\equiv\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}(1-\cos\omega t)\coth(\tfrac{1}{2}\beta\hbar\omega). \tag{7b}$$

Note that the case $j=k+1$ in Eq. (6c) produces an effective self-interaction of the jth blip in the limit $t_{2j-1}-t_{2j-2}\to\infty$.

We now observe that under a rather common condition it is possible to make a drastic simplification of the expression (5). Suppose that the characteristic time scale over which $P(t)$ varies appreciably (which must eventually be determined self-consistently as an output of the argument) is some time t_0. Then it is evident that the average length of a blip together with its neighboring sojourn will be of order t_0. Now suppose that in a region $t_s\lesssim t\lesssim t_0$ (where t_s is some time much smaller than t_0) the function $Q_2(t)$ is sufficiently large that the first term in (5) effectively vanishes (a more exact criterion will emerge below). The effect is to limit the integration variable $(t_{2j}-t_{2j-1})$ to a region of order $t_s\ll t_0$. That is, the average length of the blips is now small compared to the spacing between them; they form in effect a "dilute gas." The form of $\tilde{F}$ now simplifies enormously: We can now neglect all interblip interactions, which will contribute at most corrections of the order of t_s/t_0, and also the phase factors X_{jk} [Eq. (6c)] except for the one corresponding to $j=k+1$, which contributes a factor $\cos[(q_0^2/\pi\hbar)Q_1(t_{2j}-t_{2j-1})]$. $\tilde{F}$ is now a simple product of terms of the form $f(t_{2j}-t_{2j-1})$, and the series (4) can be summed explicitly to give the result[6]

$$P(t)=e^{-t/\tau}, \tag{8}$$

where the incoherent relaxation time τ is given by

$$\tau^{-1}=(\Delta_0^2/\omega_c)F_0 \tag{9}$$

and F_0 by

$$F_0\equiv\omega_c\int_0^\infty\cos\left(\frac{q_0^2Q_1(t)}{\pi\hbar}\right)\exp\left(-\frac{q_0^2}{\pi\hbar}Q_2(t)\right)dt. \tag{10}$$

This result is generally true when the condition stated above is satisfied: It does not depend on the assumption $\Delta_0/\omega_c\ll1$, nor on the particular form of $J(\omega)$.

Let us now specialize to the case of Ohmic dissipation. For convenience we choose the cutoff behavior of $J(\omega)$ to have the form[7]

$$J(\omega)=\eta\omega\exp(-\omega/\omega_c). \tag{11}$$

With the choice (11) the functions $Q_1(t)$ and $Q_2(t)$ are given by the following expressions:

$$Q_1(t)=\eta\tan^{-1}(\omega_ct), \tag{12}$$

$$Q_2(t)=\tfrac{1}{2}\eta\ln(1+\omega_c^2t^2)+\eta\ln\left(\frac{\beta\hbar}{\pi t}\sinh\frac{\pi t}{\beta\hbar}\right). \tag{13}$$

Substituting (12) and (13) into (10), we find for all α

$$F_0\equiv F(\alpha,\beta)=\frac{\sqrt{\pi}}{2}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left(\frac{\pi kT}{\hbar\omega_c}\right)^{2\alpha-1}. \tag{14}$$

We note that the coefficient of the power law in (14) tends to $(2\alpha)^{-1}$ for $\alpha\to0$ and to $\pi/2$ for $\alpha=\frac{1}{2}$.

We now examine the self-consistency of our procedure. It will be self-consistent if the effective cutoff on the length of a blip, which from (10)–(13) can be seen to be of order $\beta\hbar/\alpha$, is small compared to the time τ calculated from (9). Defining the renormalized tunneling frequency Δ_r by the relation

$$\Delta_r\equiv\begin{cases}\Delta_0(\Delta_0/\omega_c)^{\alpha/(1-\alpha)}, & \alpha<1,\\ 0, & \alpha>1,\end{cases} \tag{15}$$

we see that the condition for self-consistency is, for $\alpha<1$,

$$\frac{kT}{\hbar}\gg\Delta_r\left(\frac{\Gamma(\alpha)}{\alpha\Gamma(\alpha+\frac{1}{2})}\right)^{1/2(1-\alpha)}, \tag{16}$$

i.e., roughly, $\alpha kT/\hbar\gg\Delta_r$. For $\alpha>1$, the condition is satisfied for all T.

Let us now turn to the case where (16) is not satisfied. We shall discuss here[4] only the zero-temperature case, which should show most of the interesting features. First we consider the region $\frac{1}{2} < \alpha < 1$. Here an argument similar to the above, but with the integral (10) defining F_0 cut off at an upper limit of the order of the (to be determined) relaxation time τ, would predict incoherent relaxation at a rate $\Delta_r h(\alpha)$, where $h(\alpha)$ is generally of order unity. However, a Laplace-transform analysis due to Garg[8] indicates that there is in addition a power-law background algebraically identical to that found below for $\alpha < \frac{1}{2}$. We plan to discuss this in more detail elsewhere.

Finally we turn to the region of most practical interest in the "quantum coherence" problem,[2] namely zero temperature and $0 \leq \alpha \leq \frac{1}{2}$. Substitution of formulas (12) and (13) (with $\beta = \infty$) into (6a)–(6c) gives the influence functional (5). Now the time scale of the problem is certainly no shorter than Δ_0^{-1} and hence is very large compared to ω_c^{-1}. Hence for $\alpha < \frac{1}{2}$ we may ignore the 1 in the logarithm in (13) by comparison with $\omega_c^2 t^2$, and also take $Q_1(\tau) = \pi/2$ for values of τ other than zero [recall that the last term in X_{jk} is $Q(0)$ when $j = k + 1$]. Then by introducing new variables $z_i \equiv t_i/t$, we can immediately conclude that $P(t)$ can be a function only of the dimensionless variable $(\Delta_r t)^{1-\alpha}$. In fact, incorporating some α-dependent factors into the variable for subsequent convenience, we can write

$$P(t) = f([\Gamma(1-2\alpha)\cos\pi\alpha]^{1/2}(\Delta_r t)^{1-\alpha}), \tag{17}$$

where the function $f(x)$ is defined by the power-series expansion

$$f(x) \equiv \sum_{n=0}^{\infty} (-1)^n \tilde{K}_{2n}(\alpha) x^{2n}, \tag{18}$$

$$\tilde{K}_{2n}(\alpha) \equiv [\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \int_0^{z_{2n}} dz_{2n-1} \cdots \int_0^{z_2} dz_1 \prod_{j=1}^{n} (z_{2j} - z_{2j-1})^{-2\alpha} \times \Big(2^{-n} \sum_{\{\zeta_j = \pm 1\}}\Big) \prod_{\substack{j,k=1 \\ k>j}}^{n} \left[\frac{(z_{2k} - z_{2j-1})(z_{2k-1} - z_{2j})}{(z_{2k} - z_{2j})(z_{2k-1} - z_{2j-1})}\right]^{-2\alpha\zeta_j\zeta_k}. \tag{19}$$

Let us call the value of $\tilde{K}_{2n}(\alpha)$ which would be obtained by neglecting the second (interblip correlation) factor in (19) $K_{2n}^{(0)}(\alpha)$, and the form of $f(x)$ so obtained $\varphi(x)$. Moreover let us define the quantities

$$q(\alpha) \equiv \left\{ \lim_{n\to\infty} \left(\frac{\tilde{K}_{2n+2}(\alpha)/\tilde{K}_{2n}(\alpha)}{K_{2n+2}^{(0)}(\alpha)/K_{2n}^{(0)}(\alpha)} \right) - 1 \right\}, \tag{20}$$

$$A(\alpha) \equiv \lim_{n\to\infty} \tilde{K}_{2n}(\alpha)/[1+q(\alpha)]^n K_{2n}^{(0)}(\alpha). \tag{21}$$

Evidently $q(\alpha)$ tends to 0 [and $A(\alpha)$ to 1] both to first order in α and for $\alpha \to \frac{1}{2}$. We have strong though not rigorous arguments[4] to indicate that $q(\alpha)$ is at most a few percent for all α. Then $f(x)$ is equal to $A(\alpha)\varphi(x[1+q(\alpha)])$ plus a function $S(x)$ which is a sum of powers of x whose coefficients oscillate in sign and decrease with n faster than $K_{2n}(0)$, and which vanishes with $q(\alpha)$. Since the physical meaning of $P(t)$ implies that $S(x)$ must tend to zero for large x (cf. below), we can presumably safely assume that S vanishes for large x faster than $\varphi(x)$; since it is anyway of order $q(\alpha)$, it should not play a major role [this assumption could be checked by computing the first few $\tilde{K}_{2n}(\alpha)$ numerically]. Now it is straightforward to show that $K_{2n}^{(0)}(\alpha) = \Gamma^{-1}(2n(1-\alpha)+1)$, and so from the above argument we have

$$P(t) = A(\alpha) \sum_{n=0}^{\infty} (-1)^n y^{2n(1-\alpha)}/\Gamma(2n(1-\alpha)+1) + \Delta P(t), \tag{22}$$

$$y \equiv \{[1+q(\alpha)](\cos\pi\alpha)[\Gamma(1-2\alpha)]\}^{1/2(1-\alpha)} \Delta_r t \equiv \Delta_{\rm eff} t, \tag{23}$$

where $\Delta P(t)$ is the contribution arising from $S(x)$. The infinite series in (22) may be evaluated by using an integral representation of the inverse Γ function[9] and closing the contour in the upper half-plane. As a result we find

$$P(t) = \frac{A(\alpha)}{1-\alpha} \cos\left\{\left[\Delta_{\rm eff} \cos\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right] t\right\} \exp\left\{-\left[\Delta_{\rm eff} \sin\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right] t\right\} + P_{\rm inc}(t) + \Delta P(t), \tag{24}$$

where $P_{\rm inc}(t)$ is a "cut" contribution which is negative for all t and at large t gives a power-law decay, $P_{\rm inc}(t) \approx -\pi^{-1}\sin(2\pi\alpha)\Gamma(2-2\alpha)(\Delta_{\rm eff} t)^{-2(1-\alpha)}$. [This "incoherent" contribution vanishes for $\alpha \to 0$, and its power-law tail vanishes for $\alpha \to \frac{1}{2}$, leaving a term $\sim \exp(-\Delta_{eff}t)$.] Although for sufficiently long times this term will of course dominate the behavior (except for $\alpha = 0$ and $\alpha = \frac{1}{2}$), from the perspective of the "macroscopic quantum coherence" problem[2] (which primarily motivated this work) the important point is that at relatively short times the coherent oscillations of the undamped system persist for finite $\alpha < \frac{1}{2}$ with a Q factor which is determined, independently of the unknown factor $q(\alpha)$, to be exactly $\frac{1}{2}\cot[(\pi/2)\alpha/(1-\alpha)]$.

We thank J. E. Lukens and R. de Bruyn Ouboter for persistently pressing us to solve this problem, and A. Carlsson, S. Kivelson, N. Rivier, J. Samson, S. Trugman, D. Waxman, P. G. Wolynes, W. Zwerger, and especially A. K. Garg for helpful discussions and/or preprints. We also thank the Laboratory of Atomic and Solid State Physics, Cornell University, for the hospitality which made this collaboration possible. One of us (S.C.) would also like to thank the Alfred P. Sloan Foundation for a fellowship. This work was supported in part by the National Science Foundation through Grant No. DMR-8301510 and also through the facilities of the Materials Science Center at Cornell University, Grant No. DMR-8020429.

[(a)] Present and permanent address: Department of Physics, State University of New York at Stony Brook, Stony Brook, N.Y. 11794.

[(b)] On leave of absence from University of Sussex, Brighton, United Kingdom and University of Illinois, Urbana, Ill. 61801. Present and permanent address: Department of Physics, University of Illinois, Urbana, Ill. 61801.

[1] For example, L. M. Sander and H. B. Shore, Phys. Rev. B 3, 1472 (1969); R. Pirc and P. Gosar, Phys. Kondens. Mater. 9, 377 (1969); N. Rivier and T. J. Coe, J. Phys. C 10, 4471 (1976); S. V. Maleev, Zh. Eksp. Teor. Fiz. 79, 1995 (1980) [Sov. Phys. JETP 52, 1008 (1980)]; R. A. Harris and R. Silbey, J. Chem. Phys. 78, 7330 (1983), and references cited therein.

[2] S. Chakravarty, Phys. Rev. Lett. 49, 681 (1982); A. J. Bray and M. A. Moore, Phys. Rev. Lett. 49, 1546 (1982); S. Chakravarty and S. Kivelson, Phys. Rev. Lett. 50, 1811 (1983), and 51, 1109(E) (1983); W. Zwerger, Z. Phys. B (to be published). (Note that Bray and Moore's q_0 is half ours and Zwerger's α is twice ours.)

[3] We shall not be interested here in any "critical region," presumably of width $\sim (\Delta_0/\omega_c)^n$, $n > 1$, which may occur at $\alpha = 1$.

[4] We intend to give further details and extensions of this work elsewhere.

[5] R. P. Feynman and F. L. Vernon, Jr., Ann. Phys. (N.Y.) 24, 118 (1963).

[6] Formulas (8)–(10) are of course nothing but the "golden rule" result [see, e.g., G. D. Mahan, *Many-Particle Physics* (Plenum, New York, 1980), pp. 527–536], which is obtained by diagonalizing the last three terms in Eq. (1), treating the first by second-order perturbation theory and exponentiating the result. (We thank P. G. Wolynes for pointing this out to us.) We are unaware of a previous demonstration that this procedure is exact under the condition stated.

[7] This choice is not restrictive, since problems with a different cutoff behavior can be treated (Ref. 4) by an initial renormalization of the "bare" matrix element Δ_0.

[8] A. K. Garg, private communication.

[9] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals Series and Products* (Academic, New York, 1965), p. 935, 8.315-3.