Dynamics of the dissipative two-state system

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This paper presents the results of a functional-integral approach to the dynamics of a two-state system coupled to a dissipative environment. It is primarily an extended account of results obtained over the last four years by the authors; while they try to provide some background for orientation, it is emphatically *not* intended as a comprehensive review of the literature on the subject. Its contents include (1) an exact and general prescription for the reduction, under appropriate circumstances, of the problem of a system tunneling between two wells in the presence of a dissipative environment to the "spin-boson" problem; (2) the derivation of an exact formula for the dynamics of the latter problem; (3) the demonstration that there exists a simple approximation to this exact formula which is *controlled*, in the sense that we can put explicit bounds on the errors incurred in it, and that for almost all regions of the parameter space these errors are either very small in the limit of interest to us (the "slow-tunneling" limit) or can themselves be evaluated with satisfactory accuracy; (4) use of these results to obtain quantitative expressions for the dynamics of the system as a function of the spectral density $J(\omega)$ of its coupling to the environment. If $J(\omega)$ behaves as ω^s for frequencies of the order of the tunneling frequency or smaller, the authors find for the "unbiased" case the following results: For $s<1$ the system is localized at zero temperature, and at finite T relaxes incoherently at a rate proportional to $\exp-(T_0/T)^{1-s}$. For $s>2$ it undergoes underdamped coherent oscillations for all relevant temperatures, while for $1<s<2$ there is a crossover from coherent oscillation to overdamped relaxation as T increases. Exact expressions for the oscillation and/or relaxation rates are presented in all these cases. For the "ohmic" case, $s=1$, the qualitative nature of the behavior depends critically on the dimensionless coupling strength α as well as the temperature T: over most of the (α,T) plane (including the whole region $\alpha>1$) the behavior is an incoherent relaxation at a rate proportional to $T^{2\alpha-1}$, but for low T and $0<\alpha<\frac{1}{2}$ the authors predict a combination of damped coherent oscillation and incoherent background which appears to disagree with the results of all previous approximations. The case of finite bias is also discussed.

CONTENTS

I. INTRODUCTION

The problem of a quantum-mechanical system whose state is effectively restricted to a two-dimensional Hilbert space is ubiquitous in physics and chemistry. In the simplest examples, the system simply possesses a degree of freedom that can take only two values—for example, the spin projection in the case of a nucleus of spin $\frac{1}{2}$, the strangeness in the case of a neutral K meson, or the polarization in the case of a photon. We shall call such cases "intrinsically" two-state systems. A more common situation is that the system in question actually has a continuous degree of freedom q, for example, a geometrical coordinate, with which is associated a potential energy function $V(q)$ with two separate minima, as illustrated in Fig. 1. Suppose that the barrier height V_0 is large compared to the quantity $\hbar\omega_0$, where ω_0 is of the order of the classical small-oscillation frequencies ω_+ and ω_- in either well separately (ω_+ and ω_- are assumed to be of the same order of magnitude, but not necessarily identical). Then, unless the shape of the potential $V(q)$ is very pathological, the quantum motion in either well separately will be semiclassical, and the separation of the first excited state (of the "isolated" well) from the ground state will be approximately $\hbar\omega_+$ ($\hbar\omega_-$) for the left-hand (right-hand) well, i.e., of order $\hbar\omega_0$ (see Fig. 1). If, moreover, the bias ("detuning") ε between the ground states in the two wells is small compared to ω_0, then we may argue that for $k_BT\ll\hbar\omega_0$ (but k_BT/ϵ arbitrary) the system will be effectively restricted to the two-dimensional Hilbert space spanned by these two ground states. Although we must, of course, take into account the possibility of tunneling between the two wells, a typical matrix element $\hbar\Delta_0$ for this process is, in the limit considered ($V_0\gg\hbar\omega_0$), exponentially small compared to $\hbar\omega_0$, so that the tunneling does not mix the states of this "ground" two-dimensional Hilbert space with the excited states of the system. Examples of such a situation include some types of chemical reaction, the motion of defects in some crystalline solids, and the "two-level systems" believed to be found in many amorphous materials. It is not necessary that the continuous degree of freedom q in question be geometrical; a case in point is the motion of the magnetic flux trapped in an rf SQUID ring for external flux bias near half a flux quantum, which is discussed in detail in Leggett (1984a). (It was, in fact, this example which originally motivated the present work.) For brevity we shall refer to cases of this type, which arise in a system originally described by an extended coordinate, as "truncated" two-state systems.

There are, of course, also well-known problems of a similar type in which the "ground" Hilbert space has dimension N greater than two. Apart from the obvious example of a particle of spin greater than $\frac{1}{2}$, there are again many cases in which the "N-state problem" arises by truncation of an originally more complicated problem involving one or more extended coordinates. For example, the rotation of a deuterated-and-tritiated methyl group (CHDT) in certain types of organic solid possessing a threefold symmetry axis corresponds under certain circumstances to a Hilbert space with dimension three. (For an ordinary CH_3 group, the indistinguishability of the protons leads to complications; see, for example, Hewson, 1982.) A defect in a solid, even if restricted to a single unit cell, may have four, six, or eight possible equilibrium positions, and the "ground" Hilbert space will have the corresponding dimensionality. Finally, perhaps the best-known example of this type is the case of an electron in a periodic solid in the tight-binding approximation: the dimensionality in this case is the number of unit cells in the crystal. Although we believe it to be very probable that many of the results we obtain in this paper may be generalized to these higher-dimensional cases (cf. Schmid, 1983; Bulgadaev, 1984; Fisher and Zwerger, 1985a;

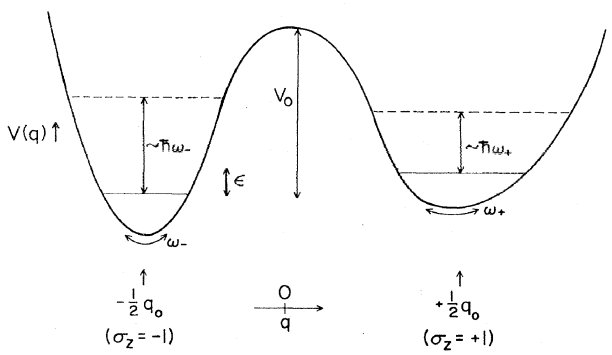

FIG. 1. A double-well system in the "two-state" limit.

Guinea *et al.*, 1985a; Weiss and Grabert, 1985), we shall not consider them explicitly here but shall confine our attention to the two-state problem.

If for the moment we regard our two-state system as totally isolated from its environment, then its motion in the two-dimensional Hilbert space can be completely described by the simple Hamiltonian

$$H = -\tfrac{1}{2}\hbar\Delta_0\sigma_x + \tfrac{1}{2}\varepsilon\sigma_z \ . \tag{1.1}$$

Here the σ_i ($i=1,2,3$) are Pauli matrices, and the basis is chosen so that the eigenstate of σ_z with eigenvalue $+1$ (-1) corresponds to the system's being localized in the right (left) well. The quantity ε is the "detuning" parameter, that is, the difference in the ground-state energies of the states localized in the two wells in the absence of tunneling [note that for $\omega_+ \neq \omega_-$ this is not simply the difference in the values of the potential $V(q)$ at the two minima; see Sec. II]; we have taken the zero of energy as the average of the two ground-state energies. The quantity $\frac{1}{2}\hbar\Delta_0$ is the matrix element for tunneling between the wells, and in the WKB limit is exponentially small compared to ω_0.

It is clear that the Hamiltonian (1.1) is completely equivalent to that of a particle of spin $\frac{1}{2}$ in a magnetic field $\mathbf{H} \equiv -\varepsilon\hat{\mathbf{z}} + \hbar\Delta_0\hat{\mathbf{x}}$, and can be trivially diagonalized, with eigenvalues $\pm(\varepsilon^2+(\hbar\Delta_0)^2)^{1/2}$, by an appropriate rotation of the axis. However, in most cases of practical interest it is not convenient to do this, since the quantity that is directly susceptible to experimental measurement is usually the "coordinate" q, and hence in the two-state approximation σ_z. It is clear that the general nature of the dynamics of σ_z is sensitive only to the ratio $\hbar\Delta_0/\varepsilon$. If this ratio is small, then the eigenstates of $\hat{H}$ are nearly eigenstates of σ_z, i.e., they correspond to states in which the system is nearly localized in one well or other. If, on the other hand, $\hbar\Delta_0/\varepsilon$ is large, then the eigenstates are appreciably delocalized in q; in particular, for $\varepsilon=0$ they are the well-known even- and odd-parity combinations

$$\psi_E = \frac{1}{\sqrt{2}}(\psi_R+\psi_L), \quad \psi_0 = \frac{1}{\sqrt{2}}(\psi_R-\psi_L) \ , \tag{1.2}$$

where ψ_R and ψ_L correspond approximately (to order Δ_0/ω_0) to the ground states in the right or left well separately. The energy splitting E_0-E_E is $\hbar\Delta_0$. In this case the dynamical behavior of σ_z shows spectacular oscillation effects: in fact, if $P(t)$ is the quantity P_R-P_L, where $P_R(P_L)$ is the probability of finding the system in the right (left) well, then if $P(0)=+1$ we find subsequently the behavior

$$P(t) = \cos\Delta_0 t \ , \tag{1.3}$$

a behavior which displays spectacularly the consequences of the phase coherence between the amplitudes for being in the left and right wells, and which has no classical analog. Perhaps the best-known example in which this behavior can be *directly* observed is the "strangeness oscillations" of a neutral K-meson beam (see, for example, Perkins, 1972), a case in which the two-dimensional Hilbert space corresponds to a nongeometrical degree of freedom (namely, strangeness). The best-known case in which oscillations of the form (1.3) occur between spatially separated potential wells is that of the "inversion resonance" of the NH_3 (ammonia) molecule (see, for example, Feynman *et al.*, 1965); however, it is worth noting that in this case the oscillations are rarely if ever observed directly, but are inferred from spectroscopic data.

A major motivation for this work is the hope that there may exist cases where oscillations of the form (1.3) can be directly observed in a system in which the two states in question, ψ_L and ψ_R, not only correspond to different values of an extended coordinate (e.g., the flux in an rf SQUID; see Leggett, 1984a) but are by some reasonable criterion *macroscopically* distinct. Such an experiment, if feasible, would throw considerable light on the conflict, at the macro level, between the quantum-mechanical formalism and "common sense" ideas (see Leggett and Garg, 1985).

In many cases of practical interest, including those relevant to the above goal, the two states in question, ψ_L and ψ_R, are related to some symmetry operation, and the Hamiltonian commutes with this operation, at least to a first approximation. Thus for such cases we have $\varepsilon=0$. Some examples of such cases, with the relevant symmetries and effects likely in practice to break them, are listed in Table I. It should be emphasized that at this point we are concerned only with effects associated with c-number (and constant in time[1]) external fields; as we shall see below, in most cases of practical interest the fluctuating symmetry breaking due to contact with a quantum environment is much more important. In fact, in many cases of practical interest the c-number symmetry-breaking effects are totally negligible. For this reason we shall put most emphasis, in this paper, on the case $\varepsilon=0$, which as we shall see shows the richest variety of behavior.

Provided that the system can be regarded as totally isolated, so that the Hamiltonian (1.1) is a complete description, then its dynamics is of course a trivial problem (for any ε). But in practice this is virtually never the case; almost every real-life two-state system interacts with its environment, and as we shall see this interaction is often strong enough to modify the behavior not only quantitatively but even qualitatively. The main reason for this is as follows: in most cases of experimental interest the principal coupling of the system to its environment is through a term of the form $\sigma_z\hat{\Omega}$, where $\hat{\Omega}$ is some operator of the environment. A coupling of this form means that the state of the environment will be sensitive to the value of σ_z, or to put it in pictorial and not too accurate language, that the environment can "observe" the value of σ_z (i.e., whether the system is in the right or left well).

[1]We could of course also consider the case of c-number external fields that vary in time, but for present purposes there is no great point in doing so.

TABLE I. Summary of results for $P(t)\equiv\langle\sigma_z(t)\rangle$ for bias $\varepsilon=0$.

$H=-\frac{1}{2}\hbar\Delta\sigma_x+\frac{1}{2}q_0\sigma_z\sum_\alpha C_\alpha x_\alpha+H_b(\{m_\alpha\},\{\omega_\alpha\})$,

$J(\omega)\equiv\frac{\pi}{2}\sum_\alpha\frac{C_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha)=A\omega^s e^{-\omega/\omega_c}$ with the conditions $\Delta\ll\omega_c$, $k_BT\ll\hbar\omega_c$.

Other quantities used below: $\alpha\equiv\eta q_0^2/2\pi\hbar$, $\Delta_r=\Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}(\alpha<1)$.

Ohmic dissipation: $J(\omega)=\eta\omega e^{-\omega/\omega_c}$.

$0<s<1$	$T=0$	Localization
	$T\neq0$	exponential relaxation with a rate $\propto\exp[-(T_0/T)^{1-s}]$ (Sec. VI.A)
$s=1$ (ohmic)	$\alpha>1$, $T=0$	Localization
	$\alpha>1$, $T\neq0$ or $\alpha<1$, $\alpha T\gtrsim\Delta_r$ (i.e., region to the right of the curve in Fig. 8)	Exponential relaxation with a rate $\propto T^{2\alpha-1}$ (Sec. V.C)
	$\frac{1}{2}<\alpha<1$, $T\lesssim\Delta r$	Probably incoherent relaxation (Sec. V.E)
	$\alpha=\frac{1}{2}$, all T	Exponential decay with a rate $\pi\Delta^2/2\omega_c$ (Toulouse limit) (Sec. V.B)
	$0<\alpha<\frac{1}{2}$, $\alpha T\lesssim\Delta_r$	Damped oscillations with an incoherent background (Secs. V.D and V.F)
$1<s<2$		Damped oscillations at $T=0$, with a crossover to exponential relaxation at $T=T^*$ (Sec. VI.B); for definition of T^* see Eq. (6.42)
$s>2$		Weakly damped oscillations (Sec. VI.B)

For results for $\varepsilon\neq0$, see Sec. VII.

Now we know from the general concepts of the quantum theory of measurement that if a system is in a linear superposition of states, then any attempt to "observe" which of the two states it is in leads to the destruction of phase coherence between them. Since it is precisely this phase coherence which leads, for example, to the behavior (1.3), it is plausible that a sufficiently efficient coupling, via σ_z, to the environment will destroy this behavior (Simonius, 1978; Zurek, 1981; Joos and Zeh, 1985). We will indeed confirm this result, although as we shall see the question of just when the coupling is "sufficiently efficient" is more subtle than one might infer from some of the literature on this topic.

It may be asked whether we should not also consider the possibilities of coupling of the environment to the operators σ_x and/or σ_y (coupling to the unit matrix in the "ground" two-dimensional space clearly has no effect on the dynamics). There are indeed some problems where such a coupling is realistic; for example, in a typical NMR problem the environment provides fluctuating fields that are in *all* directions relative to the static field, and hence couple to all of σ_x, σ_y, and σ_z. Again, such couplings may have to be taken into account in the theory of tunneling in metallic glasses: see Zawadowski and Zimanyi (1985). However, for most problems involving extended coordinates, where the tunneling takes place in the WKB limit, such couplings are negligible. The reason is that σ_x and σ_y have only nondiagonal matrix elements in the σ_z representation, i.e., they change ψ_L to ψ_R and vice versa. Thus any interaction proportional to them must also be proportional to the overlap of ψ_L and ψ_R in the real coordinate space, i.e., it must be of the order of the exponentially small quantity $\hbar\Delta_0$. That, of course, does not mean that such effects are unimportant. Indeed, it is clear that there may be substantial physical effects which arise from the effect of the environment on the overlap of ψ_L and ψ_R. Consider, for example, a defect trying to tunnel between two equivalent sites in a solid; to do so it will, in general, have to squeeze between the "host" atoms. If now the phonons of the lattice conspire to move these atoms further apart for some small time interval, it will be easier for the defect atom to squeeze through, and we should expect that the effective tunneling matrix element is modified (see, for example, Sethna,

1981,1982, and references therein).[2] However, as we shall indicate in the next section, this effect can be completely taken into account, to within terms of order of the exponentially small ratio Δ_0/ω_0, by a renormalization of the *c-number* tunneling matrix element $\hbar\Delta_0$ (and, in certain circumstances, also of the c-number bias ε). Any residual terms that in effect couple to σ_x and/or σ_y are, as shown there, totally negligible except under very special and unusual circumstances.

In the light of the above considerations, it should be adequate for most purposes to treat the effect of the environment on the two-state system entirely by a Hamiltonian in which the coupling is only to σ_z. Moreover, provided the coupling to any one environmental degree of freedom is sufficiently weak, then arguments similar to that of Caldeira and Leggett (1983), Appendix C, indicate that it should be adequate to represent the environment as a set of harmonic oscillators with a coupling linear in the oscillator coordinates and/or momenta; by an appropriate canonical transformation and related tricks, described in Leggett (1984b), it is possible to ensure that the coupling is only to the coordinates. Thus we reach the Hamiltonian which has become known in the literature as the "spin-boson" Hamiltonian:

$$H_{\rm SB} = -\tfrac{1}{2}\hbar\Delta\sigma_x + \tfrac{1}{2}\varepsilon\sigma_z + \sum_\alpha (\tfrac{1}{2}m_\alpha\omega_\alpha x_\alpha^2 + p_\alpha^2/2m_\alpha) + \tfrac{1}{2}q_0\sigma_z\sum_\alpha C_\alpha x_\alpha \ . \tag{1.4}$$

Here Δ is the "bare" tunneling matrix element (but see below),[3] ε is the c-number bias, x_α, p_α, m_α, and ω_α are, respectively, the coordinate, momentum, mass, and frequency of the αth harmonic oscillator representing the environment, and q_0 is a parameter which, in the case of a system with an extended coordinate, represents the distance between the two potential minima (see Fig. 1); for a system that is "intrinsically" two-state q_0 is superfluous, but it is nevertheless convenient to keep it. C_α is the strength of coupling of the system to the αth oscillator. It will turn out that, for any problem in which a thermal equilibrium statistical average is taken over the initial states of the environment and a sum over the final states, complete information about the effect of the environment is encapsulated in the single "spectral function" $J(\omega)$ defined by the expression

$$J(\omega) \equiv \frac{\pi}{2}\sum_\alpha (C_\alpha^2/m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha) \ . \tag{1.5}$$

Thus our problem is completely defined by the parameters ε, Δ, and the function $J(\omega)$ [the parameter q_0 enters only in the combination $q_0^2 J(\omega)$ and can, if convenient, be incorporated into the definition of J].

In Sec. II we shall examine the problem of obtaining the spin-boson Hamiltonian (1.4) and determining its parameters in the case where the system was originally described by an extended coordinate. In this case it turns out that the form of $J(\omega)$ can be obtained from a knowledge of the *classical* equation of motion of the system, and moreover that the choice of Δ is not independent of the high-frequency behavior of $J(\omega)$. In an "intrinsically" two-state system the values of the parameters must be determined from some *a priori* microscopic knowledge. One assumption we shall make throughout this paper is that $J(\omega)$ is a reasonably smooth function of ω, and moreover that *it is of the form* ω^s *up to some frequency* ω_c *that is large compared to* Δ: in fact, all our quantitative results will be valid to lowest nontrivial order in the ratio Δ/ω_c (and $kT/\hbar\omega_c$ and $\varepsilon/\hbar\omega_c$, see below). We shall see in Sec. II that for a "truncated" two-state system the quantity ω_c enters in a natural way as a cutoff due to the truncation procedure; in this case it would be inconsistent *not* to impose the conditions $\Delta/\omega_c \ll 1$, $kT/\hbar\omega_c \ll 1$, since when they are not fulfilled the truncation procedure is itself invalid.[4]

Even with those restrictions, the Hamiltonian (1.4) has been the subject of innumerable papers in the literature, which have reached widely differing conclusions about the dynamics of the two-state system described by it, ranging from totally undamped oscillation through overdamped (exponential) relaxation to complicated power-law types of behavior to total localization. What seems not to have been clearly recognized until recently is that there *is* no generic "two-state" behavior, and in particular that the system dynamics depends crucially both on temperature and on the behavior of the spectral function $J(\omega)$ for frequencies $\lesssim\Delta$. Let us suppose in particular, as above, that for frequencies less than some cutoff $\omega_c \gg \Delta$, $J(\omega)$ has a simple power-law behavior $J(\omega) = A\omega^s$. We shall call the case $s=1$ (which corresponds, for a truncated system, to a dissipative term linearly proportional to velocity in the classical equation of motion) the "ohmic" case, the case $s>1$ "superohmic," and the case $0<s<1$ "subohmic." (As we shall see in the next section, the case $s\leq 0$ is pathological.) Thus, for example, the case of defect (or electron) tunneling in a solid with coupling to a (three-dimensional) acoustic phonon bath, which has been intensively studied in the context of the polaron problem, is superohmic with $s=3$ or $s=5$,

[2]This effect should be carefully distinguished from the phenomenon discussed, for example, by Teichler and Seeger (1981) under the name of "phonon-assisted tunneling"; the latter occurs even in the limit that Δ is taken to be a c number (see also Sec. VI).

[3]The quantity Δ (which was called Δ_0 in Chakravarty and Leggett, 1984) is already renormalized for higher-frequency effects; see next section.

[4]There is of course no intrinsic reason why, even in a truncated two-state system, the quantity $J_0(\omega)$ [and hence *a fortiori* $J(\omega)$] should not have nontrivial structure on a scale ω_J small compared to ω_c. However, provided $\Delta \ll \omega_J$, we can always adjust ω_c downward until $\omega_J \gg \omega_c$ (see Sec. III.C) and thus make the scale of $J(\omega)$ automatically $\omega_c (\gg\Delta)$. What we do not consider in this paper is the possibility $\omega_J \lesssim \Delta$ (for which see, for example, Garg *et al.*, 1985).

depending on the model used (Flynn and Stoneham, 1970; Teichler and Seeger, 1981; Sethna, 1981, 1982). We note that although most of the cases discussed to date have involved integral s, the case of nonintegral s is not necessarily totally academic, as systems interacting with "fractal" environments (Mandelbrot, 1983) may well possess such a form of $J(\omega)$. What we will find is that the behavior is totally different for the superohmic and subohmic cases, corresponding, crudely speaking, to weakly damped oscillation in the former and complete localization at $T=0$ in the latter. The value 1 of s (corresponding to the "ohmic" case) is therefore a "critical dimensionality" for this problem, and we shall see that by varying the strength of the coupling in this case we can display, in effect, all the possible types of behavior.

The aim of this paper is to explore, as completely as possible, the dynamics of a two-state system described by the spin-boson Hamiltonian (1.4), as a function of Δ, ε, and the function $J(\omega)$, *under two conditions.* (1) We shall always assume that both Δ and $k_B T/\hbar$ (as well as $\varepsilon/\hbar$) are small compared to the characteristic frequency scale ω_c of the environment (defined quantitatively below). (2) We shall be interested in the dynamics at times t which are "not too long"; in particular, if there is some characteristic frequency Δ_r associated with the motion, then we shall assume that $\Delta_r t$ is of order unity rather than of order of some positive power or logarithm of ω_c/Δ. Times of the latter order are irrelevant to most of the real-life experiments that can be performed on such systems. We shall devote most of our effort to the "ohmic" case, which displays the richest variety of behavior as a function of the parameters; the qualitative behavior in the superohmic and subohmic cases can be obtained from rather simple intuitive arguments, and our detailed analysis will confirm these results.

The plan of the paper is as follows. In Sec. II we shall discuss in detail the justification of the spin-boson Hamiltonian for a "truncated" system and derive the form of the parameters occurring in it. (Details of the justification for an initially asymmetric two-well system are relegated to Appendix A.) In Sec. III we formulate precisely the question we wish to ask, and survey a number of qualitative features of the problem and some associated methods of solution that have appeared in the literature. We also discuss in some detail the relationship between the special case of ohmic dissipation and the much-discussed Kondo problem. In Sec. IV we eliminate the environment from the problem and thereby derive a formal expression which is the basis of all our subsequent analysis; as stated above, this expression involves the environment parameters only through the function $J(\omega)$. (Some technical details connected with the derivation are given in Appendix B.) Section V is in a sense the centerpiece of the paper: in it we analyze in detail the dynamics in the ohmic case with zero bias ($\varepsilon=0$), obtaining exact results in some regions of the parameter space and results that we believe to be an extremely good approximation over most of the rest. Much of the detail of the mathematical arguments used in this section is relegated to Appendix D. In Sec. VI we apply our general formalism to the cases of superohmic and subohmic dissipation without bias, and in Sec. VII we generalize some of the results to the case of finite bias. In the conclusion, Sec. VIII, we summarize our results and comment on their significance.

Like so many of the problems discussed in the so-called theoretical physics literature, the topic of this paper is of course formally a problem in applied mathematics. Where the physics comes in is the selection of those features of the solution which one believes it is essential to get qualitatively and/or quantitatively right, as distinct from those regarded as of more marginal relevance. In the present case our main concern is to get a good qualitative, and as far as possible quantitative, account of the dynamics over the time regime (extending, say, for a few times Δ_r^{-1}) for which it has interesting *and potentially experimentally observable* structure: in particular, if we believe the system is going to oscillate, then we would at least like to predict the behavior over the first one or two complete cycles as accurately as possible. [This is particularly important in the context of the problem that originally motivated this work, that of tests of quantum mechanics at the macroscopic level: see Leggett and Garg (1985).] By contrast, we shall be much less interested in the behavior at long times, ($\Delta_r t \gg 1$, even if $\Delta_r t \ll \omega_c/\Delta$), though from a different point of view (e.g., that of phase transition theory) the latter may be of great theoretical interest. The technique used in this paper, which may be described as brute-force analytical, is in some sense intermediate between purely computational studies (which are valuable for specific cases but do not automatically make it easy to see the global picture) and a renormalization-group type of approach, which may give valuable information about the asymptotic behavior but has far more difficulty getting the intermediate-time dynamics right.

A major underpinning of the results of Secs. V–VII of this paper is the observation that the form of the exact formula derived in Sec. IV suggests an approximation to it, which we christen the "noninteracting-blip approximation" and which, unlike many of the approximations made for this problem in the literature, is *controlled,* i.e., such that we can put rigorous bounds on the errors incurred by it and, where necessary, evaluate them systematically. In the case of zero bias ($\varepsilon=0$) and ohmic dissipation, we demonstrate rigorously that the errors vanish, in the limit of interest to us, on the line $\alpha=\frac{1}{2}$, and find explicit bounds on them, and approximations for them, for $0\leq\alpha<\frac{1}{2}$ at $T=0$; we also argue more heuristically that they vanish for sufficiently large α and/or T, and for the superohmic and subohmic cases (i.e., for the vast bulk of the whole parameter space). For nonzero ε we can justify the approximation for a somewhat smaller region of the parameter space. We want to emphasize that while the final formulas which follow from the noninteracting-blip approximation may be obtained in alternative ways (see Sec. VIII), a major advantage of the approach used in this paper is that it allows us to *justify*

this approximation and, where it cannot be justified (as in the ohmic case with $0<\alpha<\frac{1}{2}$), to implement systematic corrections to it.

To summarize our conclusions briefly, we find that even the qualitative behavior of the dissipative two-state system [more specifically, of the quantity $P(t)\equiv\langle\sigma_z(t)\rangle$] is critically sensitive to the low-frequency ($\omega\lesssim\Delta$) behavior of the spectral function $J(\omega)$ defined in Eq. (1.5). For the "subohmic" case ($s<1$) we find that the system is localized at zero temperature in the well it started in, and at finite temperatures relaxes incoherently at a rate proportional to $\exp-(T_0/T)^{1-s}$. For the "superohmic" case with $s>2$ we get coherent underdamped oscillations at all temperatures small compared to $\hbar\omega_c/k_B$, while for $1<s<2$ there is a crossover from coherent oscillation to overdamped relaxation as the temperature is increased. In the ohmic case ($s=1$), where $J(\omega)=\eta\omega$, the behavior depends critically on the dimensionless dissipation parameter $\alpha\equiv\eta q_0^2/2\pi\hbar$ as well as on T. If we define a quantity Δ_r to be $\Delta(\Delta/\omega_0)^{\alpha/(1-\alpha)}$ for $\alpha<1$, and zero for $\alpha>1$, then for *all* regions of the (α,T) plane for which $\alpha k_T T\gg\hbar\Delta_r$ we get incoherent exponential relaxation at a rate proportional to $T^{2\alpha-1}$. In the (very small) region $\frac{1}{2}<\alpha<1$, $k_BT\lesssim\hbar\Delta_r$ we suspect (but cannot rigorously prove) that we get incoherent relaxation at a rate of order Δ_r^{-1}. In the region $0\le\alpha\le\frac{1}{2}$, $T=0$ we show rigorously that $\langle\sigma_z(r)\rangle$ is, in the limit of interest to us, a function only of the variable $\Delta_r t$, and moreover that it can be well approximated for not too long times by a Mittag-Leffler function, i.e., the sum of a damped exponential and an incoherent term nonanalytic in the time, the two terms being in general of comparable importance. Finally, on the line $\alpha=\frac{1}{2}$ the behavior is everywhere a simple exponential relaxation, at a rate $\pi\Delta^2/2\omega_c$. These results are summarized in Table II.

Brief accounts of the method used, and of some of the specific results obtained here, have been given elsewhere (Chakravarty and Leggett, 1984; Fisher and Dorsey, 1985; Garg, 1985; Dorsey *et al.*, 1986). However, the bulk of the material presented in this paper is new.

To conclude this Introduction, we should like to make a few miscellaneous remarks. First, with the exception of Sec. II and the related Appendix A, this paper is entirely devoted to the *two-state* problem described by the standard spin-boson Hamiltonian (1.4). It is *not* concerned (at all) with the problem of tunneling out of a metastable state into a continuum. Although there may be one or two special situations in which the two problems to some extent overlap, for example, in the case of tunneling into a continuum whose floor is only just below the floor of the metastable well (see Weiss *et al.*, 1984), we believe that in general they are quite different and that it only confuses the issue to try to handle them together. In particular, the physical origins of the enhancement of tunneling out of a metastable state with increasing temperature seem to us conceptually quite distinct from the temperature-dependent effects we shall consider in this paper (which can have either sign).

Second, we emphasize that the problem described by the so-called "rotating-wave" Hamiltonian widely used in quantum optics is quite different from ours. To compare the two, it is convenient to rotate the fictitious "spin" coordinates around the y axis by $\pi/2$: the effect is simply to exchange σ_x and σ_z in (1.4) to change the sign of Δ. The rotating-wave Hamiltonian is then obtained by writing

$$\sigma_x\equiv\tfrac{1}{2}[(\sigma_x+i\sigma_y)+(\sigma_x-i\sigma_y)]\equiv(\sigma^+ +\sigma^-)\ ,$$

$$x_\alpha\equiv\frac{1}{\sqrt{2m\omega_\alpha}}(a_\alpha+a_\alpha^+)\ ,$$

where a_α, a_α^+ are the standard oscillator creation and annihilation operators, and discarding the "counterrotating" terms σ^+a^+ and σ^-a. The resulting Hamiltonian, which is essentially equivalent to the Lee model of quantum field theory, has been studied by many authors, in particular by Pfeifer (1982), who obtains some interesting exact results for it and shows that at a certain critical value of the parameters it undergoes a qualitative change in behavior, which he associated with a localization transition superficially similar to the one we shall obtain below for the spin-boson Hamiltonian. We shall discuss Pfeifer's conclusions concerning the spin-boson problem itself in the conclusion; here we want merely to note that the rotating-wave Hamiltonian differs from the spin-boson one (1.4) in a number of important respects, in particular in that the noninteracting ground state (i.e., the state $|0\rangle$ such that $\sigma^-|0\rangle=a_\alpha|0\rangle=0,\forall\alpha$) is always an eigenstate of the *interacting* Hamiltonian for arbitrary coupling strength. For this reason we believe that the results obtained by Pfeifer (and others) for this Hamiltoni-

TABLE II. Some two-state systems with the corresponding symmetry-breaking effects.

System	Symmetry	*C*-number symmetry-breaking effects
Paraelectric impurity in solid	Crystal symmetry	Electric fields
Chiral molecule	Parity	Weak interaction
$K_0-\bar{K}_0$ system	Charge conjugation	Presence of matter
SQUID (in external flux $h/4e$)	Time reversal	Imperfect flux adjustment

an, while interesting in their own right, are not obviously relevant to the qualitatively different spin-boson problem.

Third, we emphasize that when deriving results concerning the temperature dependence of the behavior in this paper we always implicitly assume that the spectral density $J(\omega)$ [Eq. (1.5)] is independent of T. Actually, there are a number of interesting physical exemplifications of a two-state or similar system where the environment cannot be reasonably modeled by a set of linearly coupled oscillators with temperature-independent parameters. As an example, let us consider the case discussed by Harris and Stodolsky (1981, 1982) in which a chiral molecule interacts by collisions with other gas molecules. Since, as they demonstrate, the relevant matrix elements for interaction of the system with its environment sample the velocity distribution of the gas molecules, which is strongly temperature dependent, it is clear that no model with a temperature-independent $J(\omega)$ can reproduce the correct behavior. A second example is the case of rotational tunneling of a methyl group in a solid (see, for example, Hewson, 1982), where a transition of the system must for symmetry reasons necessarily involve absorption as well as emission of a lattice phonon. Although we have no rigorous proof, we believe it is very probable that in each of these cases, and in other similar ones, the effective Hamiltonian at any given environment temperature could, by a sufficiently Procrustean maneuver, be cast in the form (1.4), with, however, $J(\omega)$ an explicit function of temperature. To the extent that this is true, all the formal results of this paper could be taken over verbatim, but of course, the temperature dependence of the behavior might well be quite different from what we describe below.

Finally, a note on citation policy. The problem discussed in this paper has, in effect, been around since the birth of quantum mechanics, and important contributions have been made to it by workers with primary fields of interest as diverse as solid-state physics, chemical physics, quantum optics, quantum measurement theory, particle physics, biophysics, and probably yet others; in many cases, ideas well known in one context have been discovered afresh in another, often in a language sufficiently different that it is not altogether trivial to make the connection. In this situation, to trace the exact ancestry of a particular idea would entail a task equivalent to the writing of a comprehensive review of the topic—something which this paper emphatically does not claim to be. In the present context we take the (probably old-fashioned) point of view that the primary purpose of citation is not to allot credit meticulously among one's colleagues but to help the reader to understand the paper, and the references in the text are chosen with this in mind. However, to help the reader find his or her way through the literature in this field we have included, in Appendix F, a list of some recent papers that we hope are representative of most of the major lines of approach currently being used; we hope that, by following up the references cited in these papers, the reader will be able to trace the ancestry of some of the main themes as far back as he or she cares to go.

II. DERIVATION OF THE SPIN-BOSON HAMILTONIAN FOR AN EXTENDED SYSTEM

In this section we shall explain how, starting from a system described by an extended coordinate q and interacting with its environment, we can reduce ("truncate") the problem (under appropriate conditions; see below) to one described by the Hamiltonian (1.4). For the case of a tunneling defect interacting with phonons in a solid, where the spectral function $J(\omega)$ is proportional to ω^3, this problem has been examined by Sethna (1981, 1982). In the case of "ohmic" dissipation [$J(\omega)\propto\omega$] there are special difficulties (see below), and a possible formulation for this case is given in Chakravarty (1982) and Chakravarty and Kivelson (1983, 1985). The treatment given below is similar in spirit but not quite identical to either of these discussions, and is quite generally applicable. A more detailed discussion of the technique for the ohmic case may be found in Dorsey *et al.* (1986). It should be strongly emphasized that the results of this section are only valid (or only obviously so)[5] in the limit Δ, $k_BT/\hbar$, $\varepsilon/\hbar \ll \omega_0$ [where Δ is the "bare" tunneling matrix element that will eventually enter the Hamiltonian (1.4)]; this condition is fulfilled for the vast majority of cases of interest in physics, although there are chemical problems where it is certainly not met (cf. Garg *et al.*, 1985).

We shall assume that the original extended system interacting with its environment is adequately described by the Lagrangian[6]

$$L(q,\dot{q}:\{x_j,\dot{x}_j\}) = \tfrac{1}{2}\widetilde{M}\dot{q}^2 - \widetilde{V}(q) + \tfrac{1}{2}\sum_j m_j(\dot{x}_j^2 - \omega_j^2 x_j^2) - \sum_j F_j(q)x_j - \sum_j F_j^2(q)/2m_j\omega_j^2 , \tag{2.1}$$

that is, the Lagrangian of a system interacting with a set of linear harmonic oscillators via an interaction linear in the oscillator coordinate, plus a "counterterm" [the last term in Eq. (2.1)]. The quantities $\widetilde{M}$ and $\widetilde{V}(q)$ are the renormalized mass and (conservative) potential energy of the system, which may or may not be identical to these quantities in the absence of any interaction with the environment [see Caldeira and Leggett (1983), Secs. 2 and 3; Leggett (1984b), Sec. IIB]. Although the Lagrangian (2.1) is, of course, not the most general possible description of a system interacting with its environment, we believe that in the present context it is an adequate description of most, if not all, cases of practical interest. The following

[5]This condition is appropriate for light or moderate damping. For very heavy damping the criterion is somewhat different; see Appendix A.

[6]We assume that the number of oscillators in unit frequency range is proportional to some large number N and will eventually let N tend to infinity; then, to preserve the appropriate classical equation of motion, the individual coupling constants $F_j(q)$ must be proportional to $N^{-1/2}$.

considerations may be cited in support of this assertion:

(1) In many cases of interest, such as the case of defect tunneling in a solid, the form (2.1) follows directly from microscopic considerations [the presence or absence of the counterterm is, as discussed in Caldeira and Leggett (1983, Sec. 2), merely a matter of the convention of choice for $\tilde{V}(q)$].

(2) As shown in Leggett (1984b, Sec. IIB), the Lagrangian (2.1), with the special choice $F_j(q)=qC_j$, is a legitimate way of describing any system whose interaction with its environment satisfies the three conditions specified there, namely, (i) small perturbation of any one environmental degree of freedom, (ii) "strict linearity," (iii) time-reversal invariance.

(3) In many cases where condition (i) but not condition (ii) is fulfilled, there are still strong arguments that Eq. (2.1), with a general $F_j(q)$, is a good description. In particular, for the important case of a system interacting by a contact potential with a Fermi sea, the results of Yu and Anderson (1984) and Chang and Chakravarty (1985) make it extremely plausible (though they do not in themselves prove) that such a description is possible, with $F_j(q)$ saturating as a function of q in such a way as to ensure that the dimensionless dissipation coefficient α (defined below) is always less than unity; very recent work by Chen (1986) has put this conjecture on an almost rigorous footing. Again, in the case of an ideal tunnel oxide junction described by the standard tunneling Hamiltonian (where the coordinate q corresponds to the phase difference φ across the junction), the work of Eckern *et al.* (1984) strongly suggests that, at least in the limit described by their Eq. (48), a description of the type (2.1) is legitimate, with two different oscillator baths α and β and the function $F_j(q)\equiv F_j(\varphi)$ given by $\cos\varphi/2$ is the oscillator j is in both α and by $\sin\varphi/2$ if it is in bath β (see especially their remarks on p. 6427).[7] There may well be a few cases where the description (2.1) is not technically legitimate; however, we believe that even in such cases the results obtained in this section are not likely to be qualitatively misleading.

In the following we shall discuss explicitly the case of "strictly linear" dissipation, where the coupling coefficients have the simple form

$$F_j(q)=qC_j \ . \tag{2.2}$$

The extension to a more general form of $F_j(q)$ is straightforward and is indicated at the end of this section. In case (2.2) we can define a spectral density $J_0(\omega)$ [distinguished from the $J(\omega)$ of Sec. I for a reason that will shortly become apparent] by the formula

$$J_0(\omega)\equiv\frac{\pi}{2}\sum_j (C_j^2/m_j\omega_j)\delta(\omega-\omega_j) \ . \tag{2.3}$$

The function $J_0(\omega)$ may be obtained, in any specific case, either from *a priori* knowledge of the microscopic interactions or, as described in Leggett [1984b, Eqs. (2.12)—(2.14)], from the classical damped equation of motion. For example, for a system subject to simple "normal ohmic" dissipation (i.e., where the classical equation of motion contains a dissipative term of the form $-\eta\dot{q}$, where η is the classical friction coefficient), we have $J_0(\omega)=\eta\omega$ for all frequencies ω much less than a characteristic cutoff frequency of the order of the inverse Drude relaxation time of the environment; for a defect in a (three-dimensional) solid interacting with acoustic phonons, we have $J_0(\omega)=\text{const}\ \omega^3$ or ω^5 (see above) for frequencies well below the Debye frequency; and so on. In general, the behavior of $J_0(\omega)$ for frequencies of the order of, or greater than, the characteristic microscopic frequencies of the environment (Drude, Debye, etc.) may be complicated, and may not necessarily be inferable in practice either from microscopic considerations or from the (experimentally observable) classical motion; however, the only property we need to postulate for present purposes is that $J_0(\omega)$ falls off at least as some negative power of ω in the limit $\omega\rightarrow\infty$. We shall denote the order of magnitude of the microscopic characteristic frequency of the environment in question generically as ω_{c0}; it is irrelevant to the validity of the procedure to be developed below whether or not ω_{c0} is large compared to the (bare) "attempt frequency" ω_0 [that is, the characteristic frequency of classical motion of a system of mass $\tilde{M}$ in the potential $\tilde{V}(q)$], though in most case of practical interest this is in fact so.[8] It is convenient, moreover, to postulate (though it is not actually needed for the purposes of this section) that $J_0(\omega)$ tends to zero as $\omega\rightarrow 0$ at least as some positive power of ω; note that, together with the restriction placed above on the $\omega\rightarrow\infty$ behavior, this guarantees that the "counterterm" [the last term in Eq. (2.1)] is finite. Models for which the counterterm diverges appear to be pathological and will not be discussed here. Although it is not strictly necessary for the purposes of this section, we shall generally assume that for $\omega\lesssim\Delta$ the function $J(\omega)$ follows a power law and hence can be classified as ohmic, superohmic, etc.

The crucial feature that we need to exploit in order to reduce the problem described by the Lagrangian (2.1) to one described by the spin-boson Hamiltonian (1.4) is the separation of the frequency scales ω_0 on the one hand and Δ, $k_BT/\hbar$ on the other. Intuitively speaking, this means that we can separate the environmental oscillators broadly into two classes, which play two quite different roles: the oscillators of frequency $\gtrsim\omega_0$ affect the process of transition through the potential barrier and thereby renormalize the effective tunneling matrix element, while those of frequency $\lesssim\Delta$ "detune" the two wells [i.e., in effect give the

[7] As noted in Eckern *et al.* (1984), no choice of $F_j(\varphi)$ that makes it independent of j can reproduce their results, even in the limit specified. It is also not immediately obvious (though we believe it is plausible) that a description of the type (2.1) is possible outside this limit.

[8] It is even irrelevant, formally speaking, whether or not ω_{c0} is large compared to the tunneling matrix element Δ that will emerge from the calculation, though if it is not the reduction process is trivial.

bias ε a random fluctuating component; see Leggett (1980), Sec. 5] and thereby tend to destroy the phase coherence between the corresponding amplitudes ψ_L and ψ_R. The spin-boson Hamiltonian (1.4) corresponds to an intermediate stage of the calculation in which the former effect has been incorporated into the renormalized parameters and the latter remains to be taken into account.[9] To make this picture quantitative we introduce an arbitrary cutoff frequency ω_c (not to be confused with the ω_{c0} mentioned above) such that[10] Δ, $k_BT/\hbar \ll \omega_c \ll \omega_0$, and define

$$J_0(\omega) \equiv J(\omega) + J'(\omega) , \tag{2.3'}$$

where the partial spectral densities are defined in such a way that $J(\omega)$ is negligibly small for $\omega \gg \omega_c$ and $J'(\omega)$ negligibly small for $\omega \ll \omega_c$; thus $J(\omega)$ and $J'(\omega)$ in effect represent the contribution of the low- and high-frequency oscillators, respectively. A variety of choices that satisfy this requirement are possible. For our purposes it is convenient to make the specific choice[11]

$$\begin{aligned} J(\omega) &\equiv e^{-\omega/\omega_c} J_0(\omega) , \\ J'(\omega) &\equiv (1 - e^{-\omega/\omega_c}) J_0(\omega) . \end{aligned} \tag{2.4}$$

Note that with the choice (2.4) [as distinct from, say, a sharp cutoff, $J'(\omega) = \theta(\omega - \omega_c) J_0(\omega)$] the high-frequency component does have some weight at $\omega \ll \omega_c$, but the latter tends to zero with ω faster than that of $J(\omega)$ and hopefully will not play a significant role (see below).

Special caution is necessary if the damping of the classical motion is very heavy. For example, in the case of (normal) ohmic dissipation there will then be a characteristic frequency of the classical motion, $M\omega_0^2/\eta$, which is small compared to ω_0. In this case it is necessary to choose ω_c to be small compared to this frequency, so we must require, as a condition for the validity of the truncation, not merely $\Delta \ll \omega_0$ but the more stringent condition $\Delta \ll M\omega_0^2/\eta$. Since, as we shall see below, the quantity Δ decreases at least as a high power of ω_c (proportional to η) for large damping, it is always possible to fulfill this condition. Similar considerations apply *a fortiori* to the nonohmic case (see Sec. III.C).

The calculation now proceeds in two stages. In stage I we consider the "extended" problem described by the Lagrangian (2.1), with $F_j(q) = qC_j$, but with the full spectral density $J_0(\omega)$ [Eq. (2.3)] replaced by its high-frequency component $J'(\omega)$ [Eq. (2.4)]. That is, in effect we set the coupling constants C_j to the low-frequency oscillators equal to zero. Using this "truncated" coupling, we calculate the partition function $Z(\beta)$ of the system in the limit $k_BT/\hbar\omega_c \equiv \beta\hbar\omega_c \ll 1$ by the "instanton" technique (Langer, 1967; Coleman, 1979). After integrating out the environment variables, we can express $Z(\beta)$ in the form (Caldeira and Leggett, 1981, 1983; Chakravarty, 1982)

$$Z(\beta) = \text{const} \int dq \int_{q(0)=q}^{q(\beta\hbar)=q} Dq(\tau) \exp - S_{\text{eff}}[q(\tau)]/\hbar , \tag{2.5}$$

where the effective (Euclidean) action $S_{\text{eff}}[q(\tau)]$ is given (see, for example, Feynman, 1972) by

$$\begin{aligned} S_{\text{eff}}[q(\tau)] \equiv & \int_0^{\beta\hbar} [\tfrac{1}{2}\tilde{M}\dot{q}^2 + \tilde{V}(q)] d\tau \\ & + \tfrac{1}{2} \int_{-\infty}^{\infty} d\tau' \int_0^{\beta\hbar} d\tau \, \alpha(\tau - \tau')[q(\tau) - q(\tau')]^2 , \end{aligned} \tag{2.6}$$

$$\alpha(\tau - \tau') \equiv \frac{1}{2\pi} \int_0^{\infty} J'(\omega) \exp(-\omega \mid \tau - \tau' \mid) d\omega . \tag{2.7}$$

In the evaluation of the last term in (2.6) it is understood that $q(\tau)$ is continued periodically outside the range $0 \le q \le \beta$ by the prescription $q(\tau + \hbar\beta) \equiv q(\tau)$ [see Caldeira and Leggett (1983), Sec. 4]. Since in the calculation of the partition function we are concerned only with paths that satisfy the condition $q(\beta\hbar) = q(0)$, this feature leads to no complications in the limit $\beta\hbar\omega_c \gg 1$ and does not have to be explicitly taken into account.[12]

The details of the evaluation of Eq. (2.5) for an arbitrary (in general asymmetric) two-well system are given in Appendix A. Here for pedagogical simplicity we confine ourselves to the case of a strictly symmetric potential $\tilde{V}(q) = \tilde{V}(-q)$ and briefly review the results of this calculation. As usual, the partition function is dominated in the semiclassical (WKB) limit (which is automatically the relevant limit here, since we assume $V_0 \gg \hbar\omega_0$) by the classical paths $q_{\text{cl}}(\tau)$ available in the inverted potential. If we choose the origin of q so that the potential minima occur at $q = \pm\frac{1}{2}q_0$ (see Fig. 1), then apart from the trivial paths $q(\tau) = \text{const} = \pm\frac{1}{2}q_0$, the only such classical paths available are those built up of well-separated instantons,

[9] However, as we shall see below, in the ohmic or subohmic case the separation cannot be made quite so simply.

[10] Since Δ will be output of the calculation, this is to be done self-consistently.

[11] An important assumption implicit in this procedure of "smoothing" the cutoff is that for a given form of $J_0(\omega)$ it does not matter precisely how the contribution to the right-hand side of Eq. (2.3) is allocated between different oscillators j. Thus we can arbitrarily attribute $J'(\omega)$ to one set of oscillators and $J(\omega)$ to a totally different set. [This avoids having to put back into the problem at stage II (see below) oscillators that have already been integrated out at stage I.] The correctness of the assumption can be verified by writing down formal expressions for the quantities we wish to calculate in functional-integral form and integrating out *all* the oscillators: the resulting expressions manifestly depend only on $J_0(\omega)$, not on the behavior of the individual oscillators. Naturally, once one begins to ask questions of detail about the behavior of the bath in its own right, this procedure (like many other steps in this paper) may break down.

[12] Were we to use the instanton technique to calculate *off-diagonal* elements of the density matrix, this feature would be crucial. See Caldeira and Leggett (1983), Appendix B.

i.e., those in which the system moves backward and forward at rare intervals between the wells, staying a long time at $\pm\frac{1}{2}q_0$ between these moves. A standard summation of the contributions of these paths and the small fluctuations around them, carried out in Appendix A, then gives the simple result

$$Z(\beta)=\cosh(\beta\hbar\Delta)/2\ , \tag{2.8}$$

where Δ is a quantity characterizing a single isolated instanton:

$$\Delta/2\equiv A\exp -S_{\rm cl}[q(\tau)]/\hbar\ . \tag{2.9}$$

Here $S_{\rm cl}[q(\tau)]$ is the effective action taken along the single-instanton classical path, that is, the path which minimizes $S_{\rm eff}[q(\tau)]$ subject to the boundary conditions $q(-\infty)=-q_0/2$, $q_0(+\infty)=+q_0/2$, and A is an appropriate prefactor arising from the small fluctuations around this path in the usual way. It is crucial to the argument of this section that $S_{\rm cl}[q(\tau)]$ be finite: note that for the ohmic and subohmic cases this is so *only* because we have replaced $J_0(\omega)$ by a form $J'(\omega)$, which has a sufficiently sharp low-frequency cutoff [Eq. (2.4)].

The partition function (2.8) evidently describes a simple two-level system with energy splitting $\hbar\Delta$; moreover, in the present (symmetric) case, it follows immediately from the symmetry of the Lagrangian (2.1) [with $F_j(q)=qC_j$] that the two levels must be, respectively, symmetric and antisymmetric with respect to interchange of the two wells. Thus the two lowest-lying states correspond precisely to the Hilbert space and Hamiltonian described by Eq. (1.1) (with $\varepsilon=0$). This completes stage I of the calculation.

An important point about the above maneuvre is that in the superohmic case [$J(\omega)\sim\omega^s$, $s>1$], which is the case predominantly discussed in the literature until recently, the renormalized tunneling parameter Δ is independent of the arbitrary cuttoff ω_c to within terms of relative order $(\omega_c/\omega_b)^m$ and $(\Delta/\omega_b)^m, m>0$, where ω_b is a frequency of the order of the inverse "length" of the isolated instanton. The quantity ω_b may be estimated (for any s) by an obvious generalization of the techniques used in Caldeira and Leggett (1983, Sec. 5); in general it is of the order of the lowest characteristic frequency of classical motion in the metastable well (provided the shape of the potential is not pathological).[13] Since we are explicitly assuming that Δ/ω_b may be taken as small as we like, it is clear that by a suitable choice of ω_c we may make the dependence on it an arbitrary small correction. To verify the above statement, consider the behavior of the quantity

$$\alpha_c(\tau-\tau':\omega_c)\equiv\int_0^\infty d\omega\, J'(\omega:\omega_c)\exp(-\omega\,|\,\tau-\tau'\,|\,) \tag{2.10}$$

as a function of ω_c in various regions of the variable $|\,\tau-\tau'\,|$, where $J'(\omega:\omega_c)$ is defined by the second of Eqs. (2.4). For $|\,\tau-\tau'\,|\ll\omega_c^{-1}$, and in particular for $|\,\tau-\tau'\,|\lesssim\omega_b^{-1}$, the time scale important in the nontrivial parts of the instanton trajectory, it is clear that the ω_c-dependent correction to α_c is of order $(\omega_c/\omega_{c0})^{s+1}$ relative to α_c itself, where ω_{c0} is, as above, the characteristic frequency scale of the original environment spectrum $J_0(\omega)$, and s is the power of ω in $J_0(\omega)$. In the usual case $\omega_{c0}\gtrsim\omega_b$, therefore, the correction in this region is at most of order $(\omega_c/\omega_b)^{s+1}$ (in the opposite case $\omega_{c0}\ll\omega_b$ the simplest prescription is to choose ω_c such that $\omega_{c0}\ll\omega_c\ll\omega_b$, in which case α_c itself can be made arbitrarily small). Now consider the region $|\,\tau-\tau'\,|\equiv t\gg\omega_b^{-1}$, where we have to a good approximation (for almost all of the region) $q(\tau)\cong-q(\tau')\cong\pm\frac{1}{2}q_0$. In this region, assuming again that $\omega_{c0}\gtrsim\omega_b$ (see above for the opposite case), α_c is approximately of the form $t^{-(s+1)}(1-[\omega_c t/(1+\omega_c t)]^{-(s+1)})$. It is clear that the total contribution of the α_c term to $S_{\rm cl}$ [Eq. (2.9)] from this region is of order $q_0^2\omega_s^{s-1}$, while the dependence on ω_c is of order $q_0^2\omega_c^{s-1}$; thus for $s>1$ we can make the relative correction arbitrarily small. Similar arguments show that the factors entering the prefactor A in Eq. (2.9) are only negligibly dependent on ω_c. We conclude that, as stated above, in the superohmic case the dependence of the "bare" tunneling matrix element Δ in the spin-boson Hamiltonian on the arbitrary cutoff ω_c is negligible.

The case of ohmic ($s=1$) or subohmic dissipation needs separate consideration. We shall consider for definiteness the ohmic case (for which the quantity ω_b is of order ω_0 for weak damping and $M\omega_0^2/\eta$ for strong damping; see Caldeira and Leggett, 1983). In this case, while our arguments about the short-time ($|\,\tau-\tau'\,|\lesssim\omega_b^{-1}$) behavior are still valid, the long-time interactions introduce a logarithmically divergent dependence on ω_c. This is easily seen by making the approximation $q(\tau)\cong\frac{1}{2}q_0\,\mathrm{sgn}\tau$ for $\tau\gg\omega_b^{-1}$ (we take the "center" of the instanton trajectory to lie at $\tau=0$). The interaction of the trajectory at large negative times with that at large positive times gives rise to a term in $S_{\rm cl}/\hbar$ of the form $(\eta q_0^2/2\pi\hbar)\ln(\bar\omega_b/\omega_c)$, where $\bar\omega_b$ is a frequency of the order of ω_b and η is defined as the zero-frequency limit of $J_0(\omega)/\omega$. Thus, in this case, Δ depends on ω_c as $\omega_c^{\eta q_0^2/2\pi\hbar}$. (For details, see Dorsey *et al.*, 1986.) If our calculation is to be consistent, it is clearly necessary that this apparent dependence of the results on the value of the arbitrarily chosen parameter ω_c be canceled at a subsequent stage. We shall verify explicitly in Sec. V that this is indeed the case, at least over the overwhelming bulk of the relevant parameter space. Similar considerations ob-

[13] Weiss *et al.* (1984) consider the length of a *bounce* in the limit of a small bias between the wells which tends to zero, and find that it diverges logarithmically in this limit (even for the undamped case). This divergence results entirely from the long time spent by the system at or near the "far" maximum in the inverted potential, and in no way implies that the "instanton" length is divergent. (In fact, in the limit of zero bias the bounce breaks up into two finite-length instantons separated by an infinite "resting time.")

viously apply to the case of subohmic dissipation ($s<1$), for which Δ is proportional to $\exp(-\text{const}\omega_c^{s-1})$.

Now that we have identified the partition function (2.8) as describing a two-dimensional Hilbert subspace of the coupled system and (high-frequency part of) the environment, it is convenient to examine the nature of the corresponding eigenfunctions. It is clear, both on intuitive grounds and by inspection of the form of the path integral leading to (2.8), that to zeroth order in the ratio Δ/ω_c these must have the form

$$\Psi_{\pm}(q:\{x_j\})=\frac{1}{\sqrt{2}}[\Psi_L(q:\{x_j\})\pm\Psi_R(q:\{x_j\})]\ , \tag{2.11}$$

where j labels the modes of the environment that have been included in the sum, analogous to the definition of $J'(\omega)$ [Eq. (2.3)], and $\Psi_L(\Psi_R)$ denotes a wave function in which q is localized in the left-hand (right-hand) well. In fact, to this order we would expect Ψ_L and Ψ_R to be precisely the ground-state wave functions of the "universe" (system plus high-frequency environment) for a damped harmonic oscillator with origin located at $q_0/2$ and $-q_0/2$, respectively. The properties of the reduced system density matrix $\rho(q,q')$ for this wave function are discussed in some detail in Caldeira and Leggett (1983, Appendix B; see also Grabert *et al.*, 1984); note that the existence, in the present problem, of the *low*-frequency cutoff ω_c on the environment spectrum does not affect the zero-temperature form of $\rho(qq')$ appreciably, though it will affect the finite-temperature corrections to it [see Caldeira and Leggett, 1983, Eq. (B9), and below]. In the case of "normal" dissipation (as defined in Leggett, 1984b), the width of the ground-state probability distribution is reduced by the dissipation, and corrections to Eq. (2.11) should therefore be even smaller than in the undamped case. In the (unusual) case of "anomalous" dissipation, the reverse is true. We believe that the corrections to the wave functions (2.11) are in all cases at most of the order of $\Delta/\omega_{\rm cl}$, where $\omega_{\rm cl}$ is the smallest frequency characteristic of the classical motion in either well separately (for nonpathological potentials we have $\omega_{\rm cl}\sim\bar{\omega}_b$); however, it is adequate for our purpose if they are merely of order Δ/ω_c.

Strictly speaking, the above argument is completely clear-cut only in the case where the cutoff on the environment spectrum is sharp, i.e., where the function $(1-e^{-\omega/\omega_c})$ in the definition (2.4) of $J'(\omega)$ is replaced by $\theta(\omega-\omega_c)$. In this case it is intuitively obvious (since the individual oscillator states are perturbed only to order $C_j\sim N^{-1/2}$ by their interaction with the system) that the next lowest excited states have energies of at least $\hbar\omega_c$ relative to the states (2.11); this, of course, is the reason why for $\beta\hbar\omega_c\gg1$ they do not enter the partition function (2.8). There is no reason in principle why we should not use such a sharp cutoff; it would merely make some of the arguments used above about orders of magnitude a little more complicated, and would also be less convenient at stage II of the calculation. If we prefer to use the more convenient smoothed cutoff of Eq. (2.4), then we are left with a finite density of low-frequency oscillators in the spectral function $J'(\omega)$; however, $J'(\omega)$ tends to zero as one higher power of ω than the original spectrum $J_0(\omega)$, i.e., as ω^{s+1}, $s>0$. As we shall verify below (Sec. III), the effect of the coupling of the component of $J'(\omega)$, which has frequency $\omega\lesssim\Delta$, $kT/\hbar$ to the system is negligible [i.e., at most of order $(\Delta/\omega_c)^2$], so it does not invalidate the conclusions reached above. The effect of the oscillators with frequency ω in the range Δ, $kT/\hbar\ll\omega\lesssim\bar{\omega}_c$ is merely to renormalize Δ and has already automatically been taken into account in Eq. (2.9).

We are now in a position to proceed to stage II of the calculation, that is, to take into account the low-frequency environmental oscillators represented by $J(\omega)$ in Eq. (2.4). To do this it is simply necessary to take the matrix elements of the relevant interaction term [i.e., the fifth term in (2.1), with $F_j(q)=qC_j$ and $J(\omega)$ replaced by $J_0(\omega)$] within the subspace spanned by the wave functions (2.11). For $\beta\hbar\omega_c\gg1$, the condition we are assuming throughout this section, this procedure is completely adequate, because (a) the (important) excited states of the stage I Hamiltonian have, as noted above, excitation energies of at least $\hbar\omega_c$ and hence are not appreciably thermally populated and (b) the mixing of these excited states with the states (2.11) by the low-frequency (stage II) terms is negligible in the limit $\omega_c/\omega_b\to0$. [Point (b) is not completely obvious at first sight and requires some consideration of the appropriate matrix elements and energy eigenvalues of the damped-harmonic-oscillator problem. Note however that even if (b) were false, the only effect would be to change the detailed behavior of Ψ_L and Ψ_R in (2.11) somewhat in the regions near their maxima, without changing (appreciably) the long-distance tails of the wave functions which govern the parameters of the two-state problem. On this, see below.]

To project the low-frequency interaction onto the states (2.11), we note that from the symmetry of the problem $(\Psi_L\,|\,q\,|\,\Psi_R)$ is identically zero, while $(\Psi_L\,|\,q\,|\,\Psi_L)$ is equal to $q_0/2$ plus a correction of the order of the deviation of Ψ_L,Ψ_R from strictly harmonic-oscillator behavior, i.e., at most of order Δ/ω_c. It is consistent to neglect this correction, so that we can finally write our two-state Hamiltonian in the form (1.4), with $\varepsilon=0$ and $F_j(q)=qC_j$, the parameters C_j, etc., constrained by the relation

$$\frac{\pi}{2}\sum_j (C_j^2/m_j\omega_j)\delta(\omega-\omega_j)\equiv J(\omega) =J_0(\omega)e^{-\omega/\omega_c}\ , \tag{2.12}$$

and Δ given by Eq. (2.9). We emphasize that the cutoff ω_c is arbitrary within the limits $\Delta\ll\omega_c\ll\omega_b$, and that Δ is in general a function of it; even in the superohmic case, where the correction due to a finite ω_c/ω_b can be made negligibly small relative to Δ itself, it is necessary to keep this dependence if one wishes to get quantitatively correct results (see Sec. VI).

What we claim to have done in this section, subject always to the conditions $\Delta/\omega_b\ll1$, $k_BT/\hbar\omega_b\ll1$, is to have taken a problem involving an extended coordinate q

which has two degenerate *wells,* and converted it into a two-*state* problem of the type described by the Hamiltonian (1.4) , with a prescription for obtaining the parameters of the latter problem which is exact in the above limit. Has anything been left out in this process? At first sight one might worry about the following point: It is known (Grabert *et al.*, 1984; Larkin and Ovchinnikov, 1984) that in the exactly soluble case of the simple damped harmonic oscillator the tail of the probability density distribution is extremely sensitive to the *low*-frequency modes of the environment, and that for the problem of tunneling out of a metastable well into a continuum it is precisely these modes which give the first temperature-dependent corrections to the zero-temperature tunneling rate. Our procedure, which treats Δ as a *c*-number (and hence *a fortiori* as temperature independent), seems to have neglected this phenomenon: is this consistent? We believe that it is, for the following reason: If we examine, for example, the formula for the mean-square displacement (and hence the form of the tail of the probability distribution) for the simple damped harmonic oscillator as given, for example, in Caldeira and Leggett [1983, Eq. (B9)], we see that at zero temperature the contribution of the modes with $\omega<\omega_c$ is (within logarithmic terms) at most of relative order $(\omega_c/\omega_b)^{s+1}$ for $J(\omega)\sim\omega^s$, while at finite temperature the correction is of order $(kT/\hbar\omega_b)^{s+1}$. Since we are assuming that we can make both ratios arbitrarily small, it seems consistent to neglect any correction associated with this effect (see also below, Sec. VI.B).

To conclude this section we note two obvious generalizations to the above results, which were obtained under the assumptions that (a) $V(q)$ is symmetric (and hence $\varepsilon=0$), (b) $F_j(q)$ in Eq. (2.1) has the simple form qC_j. Stage I of the case where (a) is violated but (b) is preserved is discussed explicitly in Appendix A, and as we should expect we find that the calculation (with $\omega_c \gg \varepsilon$) leads to an expression of the form

$$Z(\beta{:}\varepsilon)=2\cosh\frac{\beta}{2}(\hbar^2\Delta^2+\varepsilon^2)^{1/2}\,, \tag{2.13}$$

where the quantity Δ is given by Eq. (2.9) (with a suitable redefinition of the instanton trajectory; see Appendix A) and depends on ε only through terms of relative order $\varepsilon/\hbar\omega_b$. In the rest of this paper we shall assume that $\varepsilon/\hbar\omega_b$ is negligible small (and hence $\varepsilon/\hbar\omega_c$ can be made so) and will therefore treat Δ as a constant that is independent of ε for any given problem.

The generalization to the case where condition (b) is also violated is fairly obvious provided $F_j(q)$ is smooth over the harmonic regions of the potential (which is compatible with its having a range small compared to q_0). We again obtain Eq. (2.9), but the effective instanton action $S_{\rm cl}$ which appears in the latter equation is now given by a more complicated expression [see Caldeira and Leggett, 1983, Eqs. (4.35) and (4.36)]:

$$S_{\rm cl}[q(\tau)]=\int_0^{\beta\hbar}(\tfrac{1}{2}\widetilde{M}\dot{q}^2+\widetilde{V}(q)]d\tau + \tfrac{1}{2}\int_{-\infty}^{\infty}d\tau'\int_0^{\beta\hbar}d\tau\, Z[q(\tau)]\,, \tag{2.14}$$

$$Z[q(\tau)]\equiv\sum_j\frac{e^{-\omega_j|\tau-\tau'|}}{4m_j\omega_j}\{F_j[q(\tau)]-F_j[q(\tau')]\}^2\,, \tag{2.15}$$

where the integral is taken along the classical one-instanton trajectory. All considerations concerning the dependence of Δ on the cutoff go through as above, provided that, in the definition of the "effective" $J'(\omega)$ (for this purpose only), the quantity q_0C_j is replaced by $F_j(\frac{1}{2}q_0)-F_j(-\frac{1}{2}q_0)$. The reason is that while the actual numerical value of $S_{\rm cl}$ is sensitive to the whole instanton trajectory, hence to $F_j(q)$ for all q, the *cutoff dependence* is sensitive only to the behavior at long times, for which we can approximate q by $\pm q_0$. For the more general case, see the last paragraph of Appendix A.

With the above generalization, we now proceed to stage II of the calculation. Since the two lowest stage-I eigenstates are still approximately linear combinations of harmonic-oscillator states (but now in general with different parameters) centered on $\frac{1}{2}q_0$ and $-\frac{1}{2}q_0$, respectively, we obtain all the terms in the spin-boson Hamiltonian (1.4), where, however, the coupling constant C_j is replaced, as above, by $q_0^{-1}[F_j(\frac{1}{2}q_0)-F_j(-\frac{1}{2}q_0)]$, and, as always, only the low-frequency oscillators are taken into account. Since it is only the combination of parameters defined by (2.12) which enters the problem of interest to us, this is equivalent to generalizing the definition of $J(\omega)$ to

$$J(\omega)\equiv\frac{\pi}{2}\sum_j(m_j\omega_j)^{-1}q_0^{-2}[F_j(\tfrac{1}{2}q_0)-F_j(-\tfrac{1}{2}q_0)]^2\delta(\omega-\omega_j)e^{-\omega/\omega_c}\,. \tag{2.16}$$

Note that $J(\omega)$ can now in general no longer be simply related to the parameters of the classical motion (see Caldeira and Leggett, 1983, Appendix C) and that, in the case of short-range coupling to a Fermi bath, if we believe as suggested above that this can indeed be mimicked by an oscillator bath with an appropriate choice of $F_j(q)$, then $J(\omega)$ cannot be arbitrarily large; in particular, for the model studied by Yu and Anderson (1984) and Chang and Chakravarty (1985), it saturates at the value $q_0^{-2}N_s\pi\hbar\omega$, where N_s is the number of spin species in the bath.

In addition to the terms written down in Eq. (1.4), stage II will now in general produce other terms (which vanished in the simple case discussed above on grounds of symmetry). One such term is proportional to $[F_j(\frac{1}{2}q_0)+F_j(-\frac{1}{2}q_0)]x_j$ times the unit matrix in the two-dimensional system space: this can clearly be removed by an appropriate redefinition of the environment

coordinates and is irrelevant to the system dynamics. A less trivial term is of the form[14] $\sigma_x \sum_j \bar{C}_j x_j$ where $\bar{C}_j$ is proportional to the quantity $\langle \Psi_L \mid F_j(q) \mid \Psi_R \rangle$. This quantity corresponds, physically, to the effect of the low-frequency modes of the environment on the actual process of transmission through the barrier, and is evidently at most of order of the overlap of the renormalized ground states, i.e., of order Δ. It seems natural to try to incorporate this term into the stage-I renormalization procedure, and this can be done as follows[15]: We separate each $F_j(q)$ into two functions $F_{1j}(q)$ and $F_{2j}(q)$ in such a way that $F_{1j}(q)$ is equal to $F_j(\frac{1}{2}q_0)$ when $q=\frac{1}{2}q_0$ and $F_j(-\frac{1}{2}q_0)$ when $q=-\frac{1}{2}q_0$, but falls off fast (let us say in a distance l large compared to the width of the harmonic-oscillator ground-state probability distribution but small compared to q_0) when q is different from either of these values. The function $F_{2j}(q)$ is simply the true $F_j(q)$ minus $F_{1j}(q)$, and hence by definition tends to zero for $q \to \pm\frac{1}{2}q_0$. Then we include in stage I also (some) low-frequency oscillators, but with the true coupling constant $F_j(q)$ replaced by $F_{2j}(q)$. Since $F_{2j}(q)$ is effectively zero for the "trivial" parts of the instanton trajectory, it cannot give rise to any divergences in the expression for $S_{\rm cl}$; hence Δ is well defined. Finally, at stage II we couple in the low-frequency oscillators with coupling constant $F_{1j}(q)$, which at this stage can, of course, be replaced by $F_{1j}(\pm\frac{1}{2}q_0)$; thus we obtain once again the simple spin-boson Hamiltonian (1.4), and there are now no nontrivial extra terms.

To summarize the conclusions of this section. Provided that the quantities Δ, ε, and $kT/\hbar$ are small compared to the smallest characteristic classical frequency ω_b of the problem described by the Lagrangian (2.1) (no matter what the ratio of these quantities to one another), then the behavior of the system can be adequately calculated from a standard two-state Hamiltonian of the form (1.4), where the effective tunneling matrix element Δ is given by Eq. (2.9) and the relevant features of the environment are encapsulated in the function $J(\omega)$ defined by Eq. (2.12), or in the general case by (2.16).

III. THE DISSIPATIVE TWO-STATE SYSTEM: STATEMENT OF THE PROBLEM AND QUALITATIVE CONSIDERATIONS

A. Formulation of the problem

Having justified the use of the spin-boson Hamiltonian for realistic problems involving an extended coordinate, in this section we start our consideration of the dynamics of a system described by it. For ease of reference we write out once again the relevant Hamiltonian [Eq. (1.4)]:

$$H\hbar = -\tfrac{1}{2}\hbar\Delta\sigma_x + \tfrac{1}{2}\varepsilon\sigma_z + \sum_\alpha (\tfrac{1}{2}m_\alpha\omega_\alpha^2 x_\alpha^2 + p_\alpha^2/2m_\alpha) + \tfrac{1}{2}q_0\sigma_z \sum_\alpha C_\alpha x_\alpha \ . \tag{3.1}$$

The combination of the parameters entering the last three terms of (3.1) which is relevant for the system dynamics is the spectral density

$$J(\omega) \equiv \frac{\pi}{2}\sum_\alpha (C_\alpha^2/m_\alpha\omega_\alpha)\delta(\omega-\omega_\alpha) \ , \tag{3.2}$$

where $J(\omega)$ is characterized by a high-frequency cutoff, of order ω_c, which we shall generally assume is large compared to Δ. It should be emphasized that none of the formal results to be obtained in the next section depend on the assumption $\Delta/\omega_c \ll 1$; however, the specific forms of behavior obtained in Secs. V–VII are in general valid only to lowest nontrivial order in Δ/ω_c, $kT/\hbar\omega_c$, $\varepsilon/\hbar\omega_c$. Since our derivation of the Hamiltonian (3.1) for an extended system in the last section relied on the assumption that these quantities are small compared to unity, it would in any case be inconsistent in such cases to relax it here.

We shall assume throughout this paper without further explicit remark that the spectrum of oscillator frequencies ω_α is sufficiently dense, and the distribution of masses m_α and coupling constants C_α sufficiently nonpathological, that $J(\omega)$ may be treated as a continuous and fairly smooth function. This, of course, means that we automatically exclude from consideration any "recurrence" phenomena which occur on time scales comparable to, or greater than, the inverse level spacing of the oscillator bath. For spin-bosonlike models involving only a single oscillator mode, such as the Jaynes-Cummings (1963) model in quantum optics, such recurrences are known to be very important (Eberly *et al.*, 1980), and they may well also play a role in those problems of chemical physics where the vibronic degrees of freedom are only few in number; however, whenever the environment with which our system interacts is truly macroscopic, any such effects should be completely negligible on any time scale of practical interest.

We shall consider explicitly the case in which the behavior of the original (untruncated) spectral function $J_0(\omega)$ [Eq. (2.3)] had a simple power-law form for $\omega \lesssim \omega_c$; cases in which it has nontrivial structure in the frequency regime $\Delta \ll \omega \lesssim \omega_c$ can be reduced to this case by a preliminary renormalization of the type indicated in Sec. III.D below. Then, with the choice of cutoff behavior specified by Eq. (2.4), we have

$$J(\omega) = A\omega^s e^{-\omega/\omega_c}, \quad A = \text{const} \ . \tag{3.3}$$

It should be emphasized once again that the (new) "bare" tunneling frequency Δ occurring in (1.4) is in general itself a function of the cutoff ω_c: see Sec. II.

[14]The Lagrangian (2.1) cannot produce any terms in σ_y.

[15]Here the same remarks apply as were made earlier concerning the cutoff smoothing procedure. It should be carefully noted that the procedure outlined here would fail if $F_{1j}(q)$ and $F_{2j}(q)$ turned out to couple to *noncommuting* environment operators [which would, of course, require a Lagrangian more general than Eq. (2.1)]. This is probably why the results of Zawadowski and Zimanyi (1985), who treat just such a case, appear to differ qualitatively from ours.

The important special case which we refer to as "ohmic" dissipation is obtained by setting $s=1$, $A=\eta$ in Eq. (3.3), where [at least in the case of "strictly linear" dissipation; see Caldeira and Leggett (1983)] the quantity η is simply the classically measurable friction coefficient of the extended system. In this case we can form a dimensionless measure of the strength of the system-environment coupling,

$$\alpha \equiv \eta q_0^2/2\pi\hbar \,, \tag{3.4}$$

which is completely independent of the value of the cutoff ω_c. We can therefore treat α and Δ/ω_c as two formally independent dimensionless parameters describing the problem; however, if the Hamiltonian (3.1) was actually obtained from an extended system as described in Sec. II above, we must remember that, for a given (arbitrary) choice of cutoff ω_c satisfying the inequalities $\Delta \ll \omega_c \ll \omega_b$, the quantity Δ itself depends on ω_c as $(\omega_c/\omega_b)^\alpha$; see Dorsey *et al.* (1986). We should expect, therefore, that the dependence of all physical results on ω_c would cancel out by the end of the calculation, and this is indeed what we find, at least for the vast bulk of the parameter space (see Secs. V–VII below).

In the nonohmic case it is clear that the definition of a dimensionless system-environment coupling constant requires reference to some frequency scale. Purely to avoid cluttering up the formulas with more symbols at this stage, we provisionally choose this scale to be ω_c: thus we rewrite (3.3) in the form

$$J(\omega) = A_s \omega^s \omega_c^{1-s} e^{-\omega/\omega_c} \,, \tag{3.5}$$

and the appropriate definition of a dimensionless coupling constant, analogous to α in the ohmic case, is then

$$\beta_s \equiv A_s q_0^2/2\pi\hbar \,. \tag{3.6}$$

However, in inspecting subsequent formulas it should be borne in mind that, unlike α in the ohmic case, β_s has no fundamental significance, and the only physically relevant parameter is the combination $\beta_s \omega_c^{1-s}$. Recall, incidentally, that Δ is a function of ω_c also in the nonohmic case, though for superohmic dissipation ($s>1$) the effect of this is less spectacular.

We now turn to the definition of the problem we wish to solve. Generally speaking, we are not interested in the environment for its own sake, but only because of its effect on the dynamics of the system. Thus we should like to set up the problem by specifying some physically plausible initial conditions on the system *and* the environment, and then ask for the expectation values of the system variables at some later time, without reference to the state of the environment. Moreover, although it is in principle possible to ask questions[16] about the values of σ_x and σ_y for the system, in almost all cases of practical interest (and, in particular, in virtually all "truncated" two-state systems), it is only σ_z which is directly measurable, or on which boundary conditions can be imposed in a realistic experiment; thus it makes sense to restrict ourselves to initial conditions, and subsequent questions, that refer to this variable alone. With these restrictions there are (at least) three different questions we can ask.

(1) Suppose that at all times $t<0$ the system is held at (say) the position $q=+\frac{1}{2}q_0$ (i.e., $\sigma_z=+1$), and the environment is assumed to have come into thermal equilibrium with it. [Such a state of affairs could be achieved, for example, by applying a bias $-|V_0|\theta(-t)\sigma_z$, where V_0 is very large compared to $\hbar\Delta$.] At time zero the constraint is released, so that for $t>0$ the dynamics is governed by the Hamiltonian (3.1). What is the subsequent expectation value of σ_z as a function of t? Call the answer to this question $P^{(1)}(t)$.

(2) Suppose that at time $t=-\infty$ the system and environment are imagined to be uncoupled, and the environment to be in its thermal equilibrium state. At some large negative value of time, t_0, the system-environment interaction is suddenly switched on, but the system is again constrained to be in the state $\sigma_z=+1$ until $t=0$, when the constraint is switched off. In the limit $t_0\to-\infty$, what is the value of $\langle\sigma_z\rangle$ as a function of t for $t>0$? Call the answer $P^{(2)}(t)$.

(3) What is the symmetrized[17] equilibrium correlation function

$$C(t) \equiv \tfrac{1}{2}\langle\{\sigma_z(t),\sigma_z(0)\}\rangle_\beta \equiv \tfrac{1}{2}Z^{-1}\mathrm{Tr}\left[\exp\left[i\frac{\hat{H}}{\hbar}t\right]\sigma_z\left[\exp -i\frac{\hat{H}}{\hbar}t\right]\sigma_z \exp(-\beta\hat{H}) + (t\to -t)\right] \,, \tag{3.7}$$

where $\hat{H}$ is the complete Hamiltonian (3.1) and $Z(\beta)$ the partition function $\mathrm{Tr}(\exp-\beta\hat{H})$?

At first sight it seems obvious that $P^{(1)}(t)$ must be identically equal to $P^{(2)}(t)$, on the grounds that in the limit $t_0\to-\infty$, procedure (2) would force the state of the environment to have relaxed, by time zero, to the equilibrium explicitly postulated in (1). This is indeed true for any ergodic environment. However, as is well known, a finite assembly of N harmonic oscillators is not ergodic, and the business of taking the limit $N\to\infty$ in the present context may be quite subtle. Fortunately, we can short-circuit this difficulty by an explicit demonstration (given in Appendix B.1) that the formal expressions for $P^{(1)}(t)$ and $P^{(2)}(t)$ are identical at all positive times. We there-

[16]Such questions can in fact be asked and answered (in principle) by a straightforward generalization of the formal technique of Sec. IV in which the system is allowed to start and/or finish in the configuration called there a "blip."

[17]The quantity $\langle\sigma_z(t)\sigma_z(0)\rangle_\beta$ itself can be related to $C(t)$ via their Fourier transforms in the standard way, as can the various response functions and related quantities.

fore no longer need to distinguish between them, and will henceforth denote them indifferently as $P(t)$. Note that for an asymmetric system $P(t)$ will in general depend on which well we start in: we shall from now on denote this well by convention by $\sigma_z = +1$, so that by Eq. (3.1) a positive (negative) value of ε indicates that this well is the unstable (stable) one.

The relationship between $P(t)$ and $C(t)$ requires some thought, even for an unbiased system ($\varepsilon = 0$). Note first that since the constraint $\sigma_z = +1$ for $t < 0$ (or the application of the strong bias necessary to achieve this) is not a small perturbation, we cannot in general use linear-response-function theory to relate the two quantities. Consider for simplicity the case $\varepsilon = 0$ and define the projection operators $\pi^{\pm} \equiv \frac{1}{2}(1 \pm \sigma_z)$. Then it is clear [see Sec. IV) that both $P(t)$ and $C(t)$ can be defined[18] as the value of $\langle \sigma_z(t) \rangle$ that is attained when the system-plus-environment is described at time zero by an appropriate initial density matrix $\hat{\rho}(0)$ and then allowed to evolve freely under the action of the Hamiltonian $\hat{H}$, Eq. (3.1)]. The unnormalized values $\hat{\rho}_p(0)$, $\hat{\rho}_c(0)$ appropriate, respectively, to the definitions of $P(t)$ and $C(t)$ are

$$\hat{\rho}_p(0) = \pi^+(\exp -\beta \hat{H}')\pi^+, \quad \hat{H}' \equiv \hat{H} + \tfrac{1}{2}\hbar\Delta\hat{\sigma}_x \ , \tag{3.8a}$$

$$\rho_c(0) = \pi^+(\exp -\beta \hat{H})\pi^+ \ . \tag{3.8b}$$

Because of the lack of commutativity of the various operators in $\hat{H}$, Eqs. (3.8a) and (3.8b) are in general not identical, and therefore we have in general no obvious reason to expect $P(t)$ and $C(t)$ to be identical either, even for the unbiased case. In fact, as pointed out by Guinea (1985), the behavior of the low-frequency ($\omega \lesssim \Delta$) oscillators may be quite different in the two cases, and if the contribution of the effects of these oscillators to the system dynamics is important we should therefore not be surprised if the behavior of the two quantities is qualitatively different, in particular at long times. Most previous work on the spin-boson Hamiltonian has calculated $C(t)$ or a related quantity, which is the relevant thing to do if one is interested, for instance, in the neutron-scattering characteristics of the system. We, by contrast, shall concentrate mainly on $P(t)$, which is the quantity directly observed in experiments on "macroscopic quantum coherence" and which is most directly relevant for tests of quantum mechanics versus macrorealism (Leggett and Garg, 1985). However, we shall derive, in the next section, a formal expression for $C(t)$ as well as $P(t)$, and show that to the extent that the "noninteracting-blip approximation" defined there is valid the two expressions coincide (though see the caveat expressed there).

[18]In the case of $C(t)$ this definition exploits the symmetry properties of the system for $\varepsilon = 0$. For the more general case, see Sec. IV.

Before we begin detailed consideration of this problem, one general point should again be emphasized. We shall consider the problem as characterized [for any given value of s in the expression $J_0(\omega) \sim \omega^s$] by four dimensionless parameters, namely, Δ/ω_c, $k_B T/\hbar\omega_c$, $\varepsilon/\hbar\omega_c$, and β_s (or α). Of these, β_s (or α) may take any (positive) value, but the other three parameters, while arbitrary relative to one another, will be assumed unless otherwise stated to be small compared to unity. Now, for any particular set of parameters we shall find that there is a characteristic time scale τ in the problem (or possibly more than one) which is in general at least of order of one of Δ^{-1}, $\hbar/k_B T$, etc., and hence much larger than ω_c^{-1}. Throughout this paper we are primarily interested in obtaining the qualitative, and as far as possible the quantitative, behavior of the system *over times of the general order of* τ. We are not (or at least not primarily) interested in obtaining the behavior either for very short times[19] (e.g., $\sim \omega_c^{-1}$) or for very long ones [e.g., $\sim \omega_c \tau/\Delta$ or $\omega_c \tau^2$, or even $\tau \ln(\omega_c \tau)$]: the former case is uninteresting for most practical purposes, and in the latter the quantity $P(t)$ will generally have already decayed to such small values as to be unobservable in a realistic experiment.

We shall now briefly survey a number of qualitative features of the spin-boson problem, together with the kinds of approximation they suggest; all of them have individually received considerable discussion in the existing literature (though not always in quite the language we use), and we make no claim here to any particular originality. Neither are the three following subsections intended as a complete review of existing approaches to the problem: their only function is as a guide to some of the features to look out for in a formally comprehensive treatment of the kind we shall give in Sec. IV. These three subsections are concerned with the general problem. By contrast Sec. III.E refers explicitly to the special case of ohmic dissipation; in it we shall try to give a careful discussion of one feature of this special case which has been exploited (sometimes, in our opinion, without adequate caution) in the literature, namely, the analogy to the much-studied Kondo problem of solid-state physics. In the course of this discussion we shall return to the question of the relationship between $P(t)$ and the various quantities defined in a linear-response approach. In Sec. III.F we draw some tentative preliminary conclusions.

B. Weak-damping limit[20]

In the limit where the coupling to the environment is sufficiently weak we should expect that it is a good ap-

[19]If this behavior really were of interest, it could in any case be very well approximated by keeping only the first few orders of a perturbative expansion in Δ.

[20]For calculations in the general spirit of this subsection, but at a somewhat more microscopic level, see, for example, Harris and Silbey, 1983; Waxman, 1985.

proximation to treat it as a perturbation. Let us explore the consequences of doing this, starting with the symmetric case ($\varepsilon=0$).

The problem is exactly analogous to that of the nuclear magnetic resonance of a particle of spin $\frac{1}{2}$ in a constant field $\hbar\Delta$ in the **x** (not **z**) direction and an environment that provides fluctuating fields in the z direction only, and it is therefore possible to write down a set of Bloch equations for the motion of the expectation value $\mathbf{S}\equiv\frac{1}{2}\hbar\langle\boldsymbol{\sigma}\rangle$:

$$\frac{dS_x}{dt}=-\frac{(S_x-S_x^{\rm eq})}{T_1}\ , \tag{3.9a}$$

$$\frac{dS_y}{dt}=\Delta S_z-S_y/T_2\ , \tag{3.9b}$$

$$\frac{dS_z}{dt}=-\Delta S_y\ . \tag{3.9c}$$

Note that, in contrast to the standard NMR situation, there is no relaxation term in the equation of motion of S_z, because the fluctuating environmental fields are exclusively along the z direction. In Eq. (3.9a) the quantity $S_x^{\rm eq}$ is the thermal equilibrium value of S_x, that is, $\frac{1}{2}\hbar\tanh(\beta\hbar\Delta/2)$. Eliminating S_z from Eqs. (3.9b) and (3.9c) and noticing that $P(t)$ is simply $S_z(t)$ apart from a constant, we find that the former satisfies the equation

$$\frac{d^2P}{dt^2}+\frac{1}{T_2}\frac{dP}{dt}+\Delta^2P=0\ , \tag{3.10}$$

that is, the equation of a simple damped harmonic oscillator. The lifetimes T_1 and T_2 are determined by processes in which the system makes a transition between the eigenstates of σ_x, i.e., the odd-parity excited state and the even-parity ground state [see Eq. (1.2)], with the emission or absorption of a quantum of the environment. A straightforward perturbation-theoretic calculation shows that, to second order in the system-environment coupling, T_1 and T_2 are equal, as we should expect intuitively, and are given by the expression

$$T_1^{-1}=T_2^{-1}=(q_0^2/2\hbar)J(\Delta)\coth(\beta\hbar\Delta/2)\ . \tag{3.11}$$

We should expect, *prima facie,* that a necessary condition for the above treatment to make sense would be that at zero temperature T_2^{-1} be small compared to Δ. For any s in Eq. (3.3) greater than 1, this condition is automatically fulfilled unless β_s is very large [i.e., of order $(\omega_c/\Delta)^{s-1}$], a case we consider in Sec. III.D below. Excluding this possibility, i.e., assuming that β_s is of order 1 rather than of order (ω_c/Δ), we see that for $s\geq 2$ the system will be underdamped at *all* temperatures much less than $\hbar\omega_c/k_B$ and will perform coherent oscillations with a frequency approximately Δ and damping $\frac{1}{2}T_2^{-1}(\beta)$, where T_2^{-1} is given by Eq. (3.11). For $1<s<2$ the behavior at low temperatures is always underdamped, but as the temperature is raised there is a crossover to overdamped relaxation at a temperature T_0 given by $T_1^{-1}(T_0)=2\Delta$, i.e.,

$$k_BT_0=\hbar\Delta(\pi\beta_s)^{-1}\left[\frac{\omega_c}{\Delta}\right]^{s-1}\ , \tag{3.12}$$

which is large compared to $\hbar\Delta/k_B$ but small compared to $\hbar\omega_c/k_B$.

In the ohmic case we would assume *prima facie* that a necessary condition for the method of this section to apply is $\alpha\ll 1$. In this case the zero-temperature behavior is an underdamped oscillation with frequency approximately Δ and damping $(\pi/2)\alpha\Delta$; note that the Q factor of the oscillation is independent of Δ. As the temperature is raised we get a crossover to overdamped relaxation at the temperature $T_0(\alpha)$ given by

$$k_BT_0(\alpha)=\hbar\Delta/\alpha\pi\ , \tag{3.13}$$

which, if the method is to be consistent, must be large compared with $\hbar\Delta/k_B$. For temperatures much larger than T_0 the behavior is slow overdamped relaxation,[21] $P(t)\cong\exp-t/\tau$ with the relaxation rate τ^{-1} given by the expression

$$\tau^{-1}=\Delta^2T_2=\Delta^2\hbar/2\pi\alpha k_BT\ . \tag{3.14}$$

Note that the relaxation rate *decreases* with increasing temperature: this may be interpreted as the result of the increasing efficiency of the environment in destroying the phase coherence necessary for transitions between wells to occur (cf. Simonius, 1978; Harris and Stodolsky, 1982).

Finally, we note that for the ohmic case with α comparable to or greater than unity, and *a fortiori* for the subohmic case, there is no reason to believe that the approximation of this section will be valid at any temperature.

Let us briefly consider the generalization of the above ideas to the case of nonzero bias ($\varepsilon\neq 0$). Defining $E\equiv+(\varepsilon^2+\hbar^2\Delta^2)^{1/2}$, we rotate the "spin" axes by an angle $\theta=\sin^{-1}(\varepsilon/E)$ so that the first two terms of the Hamiltonian in (3.1) commute with the new x component $S_{x'}$. In this process the fluctuating magnetic field of the environment, which is along the original z axis, acquires an x' component proportional to $\sin\theta$, and its z' component is reduced by a factor $\cos\theta$. If we ignore the correlations between the x' and z' components, the natural generalization of Eq. (3.9a) would seem to be

$$\frac{dS_{x'}}{dt}=-\frac{\cos^2\theta}{T_1'}(S_{x'}-S_{x'}^{\rm eq})\ , \tag{3.15a}$$

$$\frac{dS_{y'}}{dt}=\frac{E}{\hbar}S_{z'}-S_{y'}/T_2'\ , \tag{3.15b}$$

$$\frac{dS_{z'}}{dt}=-\frac{E}{\hbar}S_{y'}-\frac{\sin^2\theta}{T_2'}S_{z'}\ , \tag{3.15c}$$

where $(T_1')^{-1}\equiv(T_2')^{-1}\equiv(q_0^2/2\hbar)J(E/\hbar)\coth\beta E/2$, and the equilibrium value $S_{x'}^{\rm eq}$ of $S_{x'}$ is $\tanh(\beta E/2)$. Evidently

[21] If the initial condition corresponds, say, to $S_y=0$, as it does in our problem, there is also a fast relaxation term (lifetime $\sim T_1$) whose magnitude is, however, very small in this limit.

the behavior of $P(t)$, which is proportional to the *original* $S_z(t)(\equiv\cos\theta S_{z'}-\sin\theta S_{x'})$, will now be a superposition of two terms, one qualitatively similar to that occurring for the unbiased case, the other a pure exponential relaxation with time constant $T_1'\sec^2\theta$. In the limit $\varepsilon/\hbar\Delta\to\infty$, this term dominates the behavior, and the relaxation time tends to infinity, as we should expect since in this limit the eigenstates of the isolated system are localized in one well or the other and the environment cannot induce transitions between them.

Although the above approach has an appealing simplicity, its defects become obvious the moment we try to give it a more rigorous microscopic foundation. For example, suppose we try to derive the Bloch equations, in the case $\varepsilon=0$, by writing the exact operator equation

$$\frac{d\boldsymbol{\sigma}}{dt}=\boldsymbol{\sigma}\times[\Delta\mathbf{x}-\hat{\mathscr{H}}(t)\mathbf{z}],\quad \hat{\mathscr{H}}(t)=q_0\sum_\alpha C_\alpha x_\alpha(t)\ , \tag{3.16}$$

iterating it, and decoupling the resultant equation by setting the operator $\hat{\mathscr{H}}(t)\hat{\mathscr{H}}(t')$ equal to its expectation value in the absence of coupling to the system (i.e., for the "free" environment). After Fourier-transforming the result, we obtain an equation for the Fourier (or Laplace) transform of $P(t)$ which in general does not correspond to the simple equation (3.10), but shows unmistakable effects coming from environment oscillators which have frequencies high compared to Δ.[22] Since these nowhere appear in the calculation leading to (3.10), it is clear that something important has been left out. We now turn to a consideration of the effect of these high-frequency oscillators from a different angle.

C. Adiabatic renormalization

We have set up our problem in such a way that the vast majority of the oscillators that compose the environment have frequencies that are high ($\sim\omega_c$) compared to the bare tunneling frequency Δ. This suggests that we should try, as far as possible, to eliminate these oscillators by an adiabatic (Born-Oppenheimer)[23] type of approximation. We now explore the possibility of doing this; we confine ourselves to the unbiased case and initially consider only zero temperature.

Let us choose a lower cutoff frequency $\omega_l(\Delta)$ that is small compared to the upper cutoff ω_c and equal to $p\Delta$, where p is some number large compared to unity. Then, in the zeroth-order adiabatic approximation, we assume that all oscillators of frequency greater than ω_l adjust instantaneously to the current value of σ_z, that is, that if we ignore for the moment the oscillators of frequency less than $\omega_l(\Delta)$, the two lowest-energy eigenfunctions of the system-plus-environment are of the form [cf. Eq. (2.11)]

$$\Psi_\pm^{(0)}=\frac{1}{\sqrt{2}}(|+\rangle\prod_\alpha|g_{\alpha+}\rangle\pm|-\rangle\prod_\alpha|g_{\alpha-}\rangle)\ , \tag{3.17}$$

where $|+\rangle$, $|-\rangle$ denote, respectively, the states $\sigma_z=\pm1$, $|g_{\alpha\pm}\rangle$ denotes the ground state of the αth oscillator described by the last three terms of (3.1), with σ_z fixed at ±1, respectively, and the product runs over all oscillators with frequency greater than $\omega_l(\Delta)$. Explicitly, the states $|g_{\alpha\pm}\rangle$ are given by

$$\begin{aligned}&|g_{\alpha\pm}\rangle=\exp(\pm\tfrac{1}{2}i\hat{\Omega}_\alpha)|0\rangle_\alpha\ ,\\ &\hat{\Omega}_\alpha\equiv(q_0C_\alpha/\hbar m_\alpha\omega_\alpha^2)\hat{p}_\alpha\ ,\end{aligned} \tag{3.18}$$

with $|0\rangle_\alpha$ the ground state of the corresponding oscillator for vanishing coupling, i.e., without the last term in (3.1). The energy splitting between the even and odd levels (3.17) is entirely due to the term in Δ and is easily seen to have the form $\hbar\Delta'$, where the quantity $\Delta'(\omega_l)$ is given by the expression[24]

$$\Delta'(\omega_l)=\Delta\prod_\alpha\langle g_{\alpha+}|g_{\alpha-}\rangle\ , \tag{3.19}$$

the product running over all oscillators of frequency greater than ω_l. The overlap $\langle g_{\alpha+}|g_{\alpha-}\rangle$ is easily calculated to be $\exp(-q_0^2C_\alpha^2/4\hbar m_\alpha\omega_\alpha^3)$, so using the definition (3.2) of $J(\omega)$ we find

$$\Delta'(\omega_l)=\Delta\exp-\int_{\omega_l}^\infty\frac{q_0^2}{2\pi\hbar}\cdot\frac{J(\omega)}{\omega^2}d\omega\ . \tag{3.20}$$

Since Δ' is less than Δ, we may now iterate the procedure by taking into account oscillators with frequencies in the range $\omega_l(\Delta)>\omega>\omega_l(\Delta')\equiv p\Delta'$, and so on. It is clear that this process will converge to a finite value for the tunneling matrix element provided that there exists a finite frequency ω_t such that for all $\omega<\omega_t$ we can satisfy the condition $d[\ln\Delta'(\omega)]/d(\ln\omega)<1$, i.e.,

$$\frac{q_0^2}{2\pi\hbar}\frac{J(\omega)}{\omega}<1\ \text{ for all }\omega<\omega_t\ . \tag{3.21}$$

If, on the contrary, the structure of $J(\omega)$ is such that for all $\omega\lesssim\Delta$ the inequality (3.21) is reversed, then in general the iteration process can be carried on indefinitely and Δ' can be made as small as we choose. The case in which neither of these conditions is met is more complicated and will not be discussed here. For the simple form (3.3) of $J(\omega)$, the only case in which this can happen is that of subohmic dissipation with $\beta_s\lesssim(\Delta/\omega_c)^{1-s}$, an example of little practical interest.

In the superohmic and subohmic cases (with the excep-

[22]See also, for example, Harris and Silbey (1983); Waxman (1985).

[23]Readers familiar with the chemical physics and/or polaron literature should be warned that our use of these terms, although very natural in the present context, would when applied to these areas describe precisely the opposite limit from that to which they conventionally refer: in the limit considered here the electron would tunnel *slowly* and (most of) the nuclei would follow it adiabatically.

[24]This is, of course, what is usually called the "diagonal" term in polaron theory.

tion of the special case just cited), the situation is simple. In the former the iteration process stops when the renormalized tunneling matrix element Δ' reaches the value $\tilde{\Delta}$ given by

$$\tilde{\Delta}=\Delta\exp-\int_{p\tilde{\Delta}}^{\infty}\frac{q_0^2}{2\pi\hbar}\frac{J(\omega)}{\omega^2}d\omega$$

$$=\Delta_{\mathrm{FC}}[1+0(p\Delta_{\mathrm{FC}}/\omega_c)^{s-1}]\ , \tag{3.22}$$

where Δ_{FC} is the fully renormalized matrix element given by Δ times the Franck-Condon factor e^{-F}:

$$\Delta_{\mathrm{FC}}\equiv\Delta e^{-F},\quad F\equiv\int_0^{\infty}\frac{q_0^2}{2\pi\hbar}\frac{J(\omega)}{\omega^2}d\omega=\beta_s\Gamma(s-1)\ , \tag{3.23}$$

where we used the form (3.5) of $J(\omega)$ and the definition (3.6) of β_s. In the limit of interest to us ($\Delta/\omega_c\to 0$), the difference between $\tilde{\Delta}$ and Δ_{FC} can be ignored. In the subohmic case, by contrast, we can always iterate to zero, and the system can undergo no tunneling at zero temperature, i.e., it effectively localizes in one well or the other.

For the case of ohmic dissipation the situation depends crucially on the value of α. For $\alpha>1$ the inequality (3.21) is always reversed, and the matrix element iterates to zero as in the subohmic case. This is the localization phenomenon that was obtained using renormalization group methods by Chakravarty (1982) and by Bray and Moore (1982). For $\alpha<1$, on the other hand, the iteration converges to a finite value of $\tilde{\Delta}$ given by the self-consistency condition $\tilde{\Delta}=\tilde{\Delta}[\omega_l(\tilde{\Delta})]$, i.e.,

$$\tilde{\Delta}=(p\tilde{\Delta}/\omega_c)^{\alpha}\Delta=\Delta(p\Delta/\omega_c)^{\alpha/1-\alpha}\ . \tag{3.24}$$

Since p is arbitrary apart from being large compared to unity, this indicates intuitively that the effective coherent tunneling rate should be of order $\Delta(\Delta/\omega_c)^{\alpha/1-\alpha}$ for all α less than 1 [cf. Emergy and Luther (1974); Hewson and Newns (1980)].

Before drawing any such conclusion, however, it is necessary to examine the corrections to the zeroth-order adiabatic approximation (3.17).[25] If we denote the correction to the wave function by $\delta\Psi_{\pm}$ and denote by $W_{\pm}$ the ratio of the squared norm of $\delta\Psi_{\pm}$ to that of $\Psi_{\pm}^{(0)}$, then a straightforward calculation, which we shall not reproduce here, shows that the order of magnitude W of $W_{\pm}$ is given by the expression

$$W\sim\tilde{\Delta}^2\int_{p\tilde{\Delta}}^{\omega_c}\frac{q_0^2}{2\pi\hbar}\frac{J(\omega)}{\omega^4}d\omega\ . \tag{3.25}$$

For the superohmic case, W is of the order of $(\tilde{\Delta}/\omega_c)^2$ times some function of $(\tilde{\omega}/\omega_c)$ and can therefore consistently be neglected in the limit of interest to us (and there are no difficulties in taking p to be of order unity). For the subohmic case, if p is taken to be a constant, W diverges as some inverse power of $\tilde{\Delta}/\omega_c$. However, it is easy to see that it is possible to adjust p as a running function of $\tilde{\Delta}$ in such a way that the product $\omega_l=p\tilde{\Delta}$ still iterates to zero, while at the same time W can be made arbitrarily small. Thus the conclusions reached above about this case are unchanged. The same applies to the case of ohmic dissipation with $\alpha>1$. However, in the case of ohmic dissipation with $\alpha<1$ this trick is useless, and on the other hand W is of order αp^{-2} independently of $\tilde{\Delta}$. Thus we cannot in general expect to be able to set p to be of order 1 without serious complications. The tentative conclusion is that while in the superohmic case $\tilde{\Delta}$ can be reasonably identified as the unique frequency scale for the problem, this is so for the ohmic case at best only for small α.

Finally let us consider the generalization to finite temperature. It is now necessary to distinguish between "coherent" transition processes, in which the degree of excitation of all of the oscillators is unchanged, and "incoherent" ones, in which one or more oscillators changes its quantum number.[26] As is well known in the context of polaron theory (see, for example, Mahan, 1980), the effect of temperature on the two processes is quite different: in the expression (3.20) for the coherent transition amplitude Δ' the integrand in the exponent is multiplied by a factor $\coth(\beta\hbar\omega/2)$, so that Δ' is reduced, while the quantity Δ_{inc} whose square gives the incoherent transition probability is given by an expression that is an increasing function of temperature and is qualitatively equivalent to cutting off the integral (3.20) at a lower limit $k_BT/\hbar$ rather than ω_l (for $k_BT\gtrsim\hbar\omega_l$). If we take first the question of coherent tunneling, an argument similar to the one used above indicates that the criterion (in the present case only an order-of-magnitude one) for the relevant matrix element to iterate to a finite value under adiabatic renormalization is

$$\frac{q_0^2}{2\pi\hbar}\frac{J(\tilde{\Delta})}{\tilde{\Delta}}\coth\beta\hbar\tilde{\Delta}/2<1\ , \tag{3.26}$$

where $\tilde{\Delta}$ is the zero-temperature renormalized matrix element. Thus we expect that in the case $s\geq 2$ coherent oscillations persist right up to a temperature of order $\hbar\omega_c/k_B$, while for $1<s<2$ they disappear at a temperature of order $\beta_s^{-1}(\hbar\tilde{\Delta}/k_B)(\omega_c/\tilde{\Delta})^{s-1}$. For the ohmic case with $\alpha<1$, if the argument can be consistently applied and $\tilde{\Delta}$ defined, we would expect that the oscillations disappear at a temperature of order $\hbar\tilde{\Delta}/\alpha k_B$. These conclusions agree qualitatively with those obtained in Sec. III.B, except that the bare tunneling matrix element Δ has

[25] Aficionados of the renormalization group will of course recognize the ensuing argument (and indeed much of this subsection) as a layman's version of an analysis that could be made more elegantly (and perhaps more succinctly) by explicit use of that technique. In the interests of clarity and general accessibility, we have deliberately renounced this option.

[26] In the polaron literature these processes are called "diagonal" and "nondiagonal," respectively.

been replaced by the zero-temperature renormalized quantity $\tilde{\Delta}$. Meanwhile, incoherent processes are always possible, and for the subohmic case and the ohmic case with $\alpha > 1$ are the only processes that can occur. In the subohmic case the appropriate transition "matrix element"[27] $\Delta_{\rm inc}$ depends on temperature as $\exp[-\text{const}(\hbar\omega_c/k_BT)^{1-s}]$, while for the ohmic case it is proportional to $\Delta(k_BT/\hbar\omega_c)^{\alpha}$ (see Bray and Moore, 1982). Were we to assume (dubiously) that when this matrix element was small compared to $k_BT/\hbar$ it could be inserted in place of Δ in the weak coupling formula (3.14), we would get an incoherent transition rate proportional to $\Delta_{\rm inc}^2/k_BT$, i.e., to $(\Delta^2/\omega_c)(k_BT/\hbar\omega_c)^{2\alpha-1}$.

While the arguments above concerning coherent tunneling are relatively clear-cut, those relating to incoherent processes clearly leave much to be desired. It would obviously be desirable to have a conceptually clear-cut approximation which at least handles the incoherent processes consistently. Such an approximation is provided by the "golden rule" approach that we outline in the next section.

D. "Golden rule"

The so-called "golden rule" approach to the spin-boson problem, which has been widely used in chemical physics and in related problems, is based on the idea of doing perturbation theory in the tunneling matrix element rather than, as in Sec. III.B, in the system-environment interaction. In fact, one first handles the latter to all orders and only then considers the tunneling processes.

We first diagonalize the last four terms in the Hamiltonian (3.1) for a given value of $\sigma_z(\equiv\pm1)$. To do this, it is simply necessary to shift each oscillator through a distance $\delta_\alpha\sigma_z$, where

$$\delta_\alpha = -\tfrac{1}{2}q_0C_\alpha/m_\alpha\omega_\alpha^2 . \tag{3.27}$$

The appropriate unitary operator which transforms to the basis of the displaced harmonic-oscillator states is

$$\hat{U} = \exp(-\tfrac{1}{2}i\sigma_z\hat{\Omega}) , \tag{3.28}$$

$$\hat{\Omega} \equiv \sum_\alpha \hat{\Omega}_\alpha , \quad \hat{\Omega}_\alpha \equiv (q_0C_\alpha/\hbar m_\alpha\omega_\alpha^2)\hat{p}_\alpha , \tag{3.29}$$

the factor of 2 being incorporated in the definition of $\hat{\Omega}$ for subsequent convenience. The transformed Hamiltonian $\hat{H}' \equiv \hat{U}\hat{H}\hat{U}^{-1}$ is written, apart from a constant,

$$\hat{H}' = -\tfrac{1}{2}\hbar\Delta(\sigma_+e^{-i\Omega}+\text{H.c.})+\tfrac{1}{2}\varepsilon\sigma_z + \sum_\alpha \tfrac{1}{2}(m_\alpha\omega_\alpha^2x_\alpha^2+p_\alpha^2/m_\alpha) , \tag{3.30}$$

where $\sigma_+ \equiv \frac{1}{2}(\sigma_x+i\sigma_y)$. The result (3.30) is, of course, still exact. Note, moreover, that our formulation of the problem is unchanged, since the value of σ_z is not affected by the transformation generated by $\hat{U}$. [In the calculation of $P^{(1)}(t)$ the initial density matrix of the environment is now simply the Gibbs distribution corresponding to the last two terms of Eq. (3.30), while for $P^{(2)}(t)$ things are rather more complicated.]

We now attempt to treat the first term in Eq. (3.30) by perturbation theory. If the system starts with $\sigma_z=+1$ and the environment is in the above Gibbs distribution, then to second order in Δ the probability $p(t_0)$ that at time t_0 it is still in the state $\sigma_z=+1$ is given by the expression

$$1-p(t_0) = \left[\frac{\Delta}{2}\right]^2 \int_0^{t_0}dt\int_0^{t_0}dt' \sum_m Z_0^{-1}\exp-\beta\varepsilon_m \sum_n \exp[i[(-\varepsilon+(\varepsilon_n-\varepsilon_m)](t-t')/\hbar]\times|\langle m|\exp i\hat{\Omega}|n\rangle|^2 , \tag{3.31}$$

where m and n label the eigenstates of the environment Hamiltonian $\hat{H}_0$ [i.e., the last two terms in (3.30)] and Z_0 is the initial environment partition function, $\sum_m e^{-\beta\varepsilon_m}$. Note that Eq. (3.31) depends in general on the sign of ε.

If the integrand of Eq. (3.31) dies away sufficiently fast as a function of the variable $(t-t')$, then we can define a transition probability Γ per unit time by

$$\Gamma = \left[\frac{\Delta}{2}\right]^2 \int_{-\infty}^{\infty}\exp(-i\varepsilon t/\hbar)\prod_\alpha F_\alpha(t)dt , \tag{3.32}$$

$$F_\alpha(t) \equiv \langle\exp[i\hat{\Omega}_\alpha(0)]\exp[-i\hat{\Omega}_\alpha(t)]\rangle_{H_0} , \tag{3.33}$$

where the angle brackets denote that the expectation value is to be evaluated over the thermal equilibrium distribution specified by the density matrix $Z_0^{-1}\exp-\beta\hat{H}_0$, and where

$$\hat{\Omega}_\alpha(t) \equiv \exp\left[\frac{i}{\hbar}\hat{H}_0t\right]\hat{\Omega}_\alpha\exp\left[-\frac{i}{\hbar}\hat{H}_0t\right] .$$

Writing $\hat{\Omega}_\alpha$ in the form

$$\hat{\Omega}_\alpha = -ig_\alpha(a_\alpha-a_\alpha^+) , \quad g_\alpha \equiv q_0C_\alpha/(2\hbar m_\alpha\omega_\alpha^3)^{1/2} , \tag{3.34}$$

and using a standard result[28] for the harmonic oscillator, we obtain the result

$$F_\alpha(t) = \exp-g_\alpha^2[(N_\alpha+1)(1-e^{-i\omega_\alpha t})+N_\alpha(1-e^{i\omega_\alpha t})] ,$$

where N_α is the Bose occupation factor. Thus, finally, using the definition (3.2) of $J(\omega)$, we can write Γ in the

[27] The concept of $\Delta_{\rm inc}$ is not very well defined (here, at least). See Sec. VI.

[28] See, for example, Mahan (1980), pp. 285 and 273–276.

form

$$\Gamma=\left[\frac{\Delta}{2}\right]^2\int_{-\infty}^{\infty}dt\exp\left[-i\varepsilon t/\hbar+\frac{iq_0^2}{\pi\hbar}Q_1(t)\right]\times\exp[-(q_0^2/\pi\hbar)Q_2(t)]\ , \tag{3.35}$$

where $Q_1(t)$ and $Q_2(t)$ are defined by

$$Q_1(t)\equiv\int_0^{\infty}\frac{J(\omega)}{\omega^2}\sin\omega t\,d\omega\ ,$$
$$Q_2(t)\equiv\int_0^{\infty}\frac{J(\omega)(1-\cos\omega t)}{\omega^2}\coth(\beta\hbar\omega/2)d\omega\ . \tag{3.36}$$

It should be carefully noted that the initial rate of change of the quantity $P(t)$ is, because of its definition, *twice* Γ, and that Γ depends on the sign of ε. If we now assume that the transitions occur incoherently and impose the condition of detailed balance, i.e., require that $\Gamma(\varepsilon)/\Gamma(-\varepsilon)=\exp\beta\varepsilon$ [this can actually be proved directly from Eq. (3.35); see Appendix E], then it is plausible to assume that the correct formula for $P(t)$ at all times is

$$P(t)=P(\infty)+[1-P(\infty)]\exp-t/\tau\ , \tag{3.37}$$

where $P(\infty)\equiv-\tanh\beta\varepsilon/2$ and τ^{-1} is $\Gamma(\varepsilon)+\Gamma(-\varepsilon)$, i.e.,

$$\tau^{-1}\equiv\Delta^2\int_0^{\infty}dt\cos(\varepsilon t/\hbar)\cos[(q_0^2/\pi\hbar)Q_1(t)]\exp-[(q_0^2/\pi\hbar)Q_2(t)]\ , \tag{3.38}$$

with the functions $Q_1(t)$ and $Q_2(t)$ given by Eq. (3.36).

The behavior (3.37) is evidently qualitatively different, in most cases, from what is predicted by the "weak-damping" treatment given in Sec. III.B above: we note, in particular, that for the superohmic case with $s\geq 2$ it can *never* agree with it anywhere in the region of interest ($\Delta, kT/\hbar\ll\omega_c$). In fact, the inadequacy of the assumption of an incoherent decay in this case reveals itself through the divergence of the integral in Eq. (3.38) at long times. (For an appropriate treatment see Sec. VI.B.) Additionally, Eq. (3.37) predicts very bizarre behavior for the case of ohmic dissipation at zero temperature with no bias: as we shall see in Sec. V, the right-hand side of Eq. (3.38) is in this case infinite for $\alpha<\frac{1}{2}$, $\pi\Delta^2/2\omega_c$ for α exactly equal to $\frac{1}{2}$, and zero for $\alpha>\frac{1}{2}$. Finally we note that the above treatment automatically predicts the value $\tanh\beta\varepsilon$ for $P(t)$ in the limit $t\to\infty$, whereas physical intuition would say that for finite bias and not too strong damping $P(t)$ should tend rather to $(\varepsilon/E)\tanh\beta E/2$, where $E\equiv(\varepsilon^2+\hbar^2\Delta_0^2)^{1/2}$.

It is clear that the "golden rule" result rests on two related assumptions: that the integrand in Eq. (3.31) dies away sufficiently fast as a function of $t-t'$ to allow us to extend the limits of integration to infinity, and that the second-order expression for the transition probability, Eq. (3.35), may be iterated to produce the decaying exponential (3.37). In view of the deficiencies noted above, we need an unambiguous way first to determine where these conditions are met, and second to extend the calculation when they are not met. It is, indeed, possible in principle to use the formalism of this subsection and simply work to higher order in Δ (see Arnold and Holstein, 1981), but the formulas rapidly become very cumbersome. Since they must anyway be formally equivalent to the expressions derived in the next section we shall not pursue this approach any further here.

E. Relation to the Kondo problem

In this subsection we shall discuss the relation between the two-state system with ohmic dissipation defined by Eqs. (3.1)—(3.4) and a rather extensively discussed problem in solid-state physics known as the Kondo problem (Kondo, 1964). In its simplest form the Kondo problem is concerned with a single magnetic impurity of spin $\frac{1}{2}$ which interacts via an exchange scattering potential with a band of free electrons. A simple model that is believed to capture the essential physics is given by the so-called Kondo or *s-d* Hamiltonian

$$\hat{H}_K=\sum_{\mathbf{k},\sigma}\varepsilon(\mathbf{k})c_{\mathbf{k}\sigma}^{\dagger}c_{\mathbf{k}\sigma}+J\mathbf{S}\cdot\mathbf{s}(0)\ . \tag{3.39}$$

The operators $c_{\mathbf{k}\sigma}^{\dagger}$ create conduction electrons of wave vector $\mathbf{k}$ and spin index $\sigma=\pm1$. The impurity spin is $\mathbf{S}$, whereas $\mathbf{s}(0)$ denotes the effective spin due to the conduction electrons at the impurity site $\mathbf{r}=0$. The exchange constant J is positive for an antiferromagnetic interaction, which is the usual situation in a real metal.

Compared to the two-state system studied in this work, which introduces dissipation through a coupling to bosons, the Kondo problem may be thought of as a spin-$\frac{1}{2}$ system interacting with a fermionic bath. The relation between the two problems is included here mainly for two reasons. First the analogy actually led to the original understanding of the localization phenomenon in the ohmic two-state problem (Bray and Moore, 1982; Chakravarty, 1982), and it would be interesting to know whether further insight into the dissipative two-state system may be obtained from the Kondo model and vice versa. Second, to the extent that the two models are equivalent, it would provide an interesting demonstration that rather than the detailed microscopic structure of the environment only a few gross features, such as the effective density of states for low-lying excitations, are relevant in determining the system's dynamics at sufficiently low temperature. The notion equivalent will be understood here in the sense that the thermodynamics *and* the real-time dynamics of the spin $\frac{1}{2}$ are at least qualitatively the same in both cases. Since the present work is concerned mainly with dynamical behavior, we shall try in the following to demonstrate the similarity between the Kondo problem and the ohmic two-state system on the basis of

their respective Hamiltonians.[29] However, it should be stressed from the beginning that we shall not derive an exact mapping between the two models. In fact it is at present unclear to what extent—if at all—the arguments supporting their equivalence which are given below can be made more rigorous. Instead we shall try to explain the correspondence in physical terms. The basic idea behind the relation is to realize that the low-lying excitations of the electron gas in the Kondo Hamiltonian may be approximately described by bosons. Thus it will turn out that the oscillators in the two-state system correspond to the spin-density excitations in $\hat{H}_K$. In particular, the density of states and coupling of these excitations [see Eq. (3.62) below] are just such that the function $J(\omega)$ corresponds to ohmic dissipation.

The plan of this section is thus as follows: We shall first show how the equivalence between the two models may be understood on the basis of their Hamiltonians by describing the electron gas in the Kondo problem in terms of its spin- and charge-density excitations. In addition we shall briefly discuss the relation to the so-called resonance level model. The ohmic two-state system will be related to an anisotropic Kondo problem with different amplitudes for spin-flip and nonspin-flip scattering. The same correspondence is shown to follow from the respective partition functions. We shall then introduce Anderson's scaling picture for the thermodynamic properties and indicate some of the results for the Kondo problem obtained from this picture and from the exact solution. These are used to discuss the behavior of the static susceptibility and the localization transition in the ohmic two-state problem as well as its specific heat for $T\to 0$. Finally an exact result for the dynamics of the Kondo problem is shown to have nontrivial consequences for the long-time behavior of the spin-correlation functions.

In order to demonstrate the relation between the two models we shall first cast the Kondo Hamiltonian (3.39) into a form appropriate to our purposes. Since the exchange interaction is assumed to be pointlike, only s-wave scattering occurs. Thus, expanding the plane-wave electron states $\mathbf{k}$ in spherical waves around the impurity at $\mathbf{r}=0$, we find that the only electrons affected are those with angular momentum quantum numbers $l=m=0$. Therefore we may characterize the relevant states simply by the magnitude $|\mathbf{k}|$ of the wave vector, which reduces the problem to an essentially one-dimensional one.[30] Moreover if, as is indeed the case for the long-time and low-temperature behavior, the dominant excitations are those in the immediate vicinity of the Fermi surface, we may linearize the dispersion relation $\varepsilon(\mathbf{k})$ around the Fermi energy ε_F in the form

$$\varepsilon(\mathbf{k})=\varepsilon_F+\hbar v_F(|\mathbf{k}|-k_F)\ . \tag{3.40}$$

[29]This possibility was first pointed out by Guinea *et al.* (1985b).

[30]More precisely, the system could be called one-half dimensional, since there is only one instead of the usual two Fermi points.

Measuring momentum from its reference value k_F, we obtain the free fermion Hamiltonian in the form

$$\hat{H}_0^F=\hbar v_F\sum_{p\sigma} p c_{p\sigma}^\dagger c_{p\sigma}\ , \tag{3.41}$$

where $c_{p\sigma}^\dagger$ creates an electron with spin σ, momentum $|\mathbf{k}|=p+k_F$, and $l=m=0$. Since p can never be smaller than $-k_F$, this Hamiltonian has to be supplemented with a high-energy cutoff of the order of the bandwidth, which eliminates wave vectors on a scale beyond k_F. As will be discussed below, this may be done by keeping the momenta in the free Hamiltonian unrestricted but introducing a cutoff into the interaction term; this cutoff would then define the energy scale for the coupled problem. Concerning the interaction term, it will turn out to be crucial to generalize the isotropic coupling in the original model to a case where we have a different exchange constant $J_\parallel$ for the S_zs_z term and $J_\perp$ for $S_xs_x+S_ys_y$. Although this has no physical realization in the Kondo context, it was originally introduced (Anderson *et al.*, 1970) as a calculational tool, since the limit $J_\perp=0$ is exactly soluble as an independent electron problem, and $J_\perp$, which induces a nontrivial spin dynamics, can then be treated as a perturbation. In contrast to the genuine Kondo problem, where rotational invariance $J_\parallel=J_\perp$ has always to be imposed at the end of the calculation, it will turn out that for the relation to the spin-boson problem it is essential to keep $J_\parallel$ and $J_\perp$ as two independent parameters. To simplify the notation let us introduce localized Wannier operators for an electron of spin σ at the origin by

$$c_\sigma^\dagger=L^{-1/2}\sum_p c_{p\sigma}^\dagger\ , \tag{3.42}$$

where L is the length of a normalization box, such that the wave vectors $\mathbf{p}$ have values $p=2\pi/L\cdot n$, $n=0,\pm1,\pm2,\ldots$, and the limit $L\to\infty$ is taken according to $L^{-1}\sum_p\to\int dp/2\pi$. If we adjust the units of J such that $\mathbf{S}=\frac{1}{2}\boldsymbol{\sigma}$ and

$$\mathbf{s}(0)=\tfrac{1}{2}\sum_{\sigma\sigma'} c_\sigma^\dagger\boldsymbol{\sigma}_{\sigma\sigma'}c_{\sigma'}\ ,$$

where $\boldsymbol{\sigma}$ is the vector of the 2×2 Pauli matrices $\sigma_{x,y,z}$, the anisotropic Kondo Hamiltonian takes the form

$$\hat{H}_K=\hbar v_F\sum_{p\sigma} p c_{p\sigma}^\dagger c_{p\sigma}+\frac{J_\parallel}{4}\sigma_z\sum_\sigma \sigma c_\sigma^\dagger c_\sigma + \frac{J_\perp}{2}(\sigma_+c_\downarrow^\dagger c_\uparrow+\sigma_-c_\uparrow^\dagger c_\downarrow)\ , \tag{3.43}$$

with $\sigma_\pm=\frac{1}{2}(\sigma_x\pm i\sigma_y)$. Clearly the sign of $J_\perp$ is irrelevant, since a change $J_\perp\to-J_\perp$ may be compensated by a rotation $S_x,S_y\to-S_x,-S_y$ of the impurity spin. The constants $J_\parallel$ and $J_\perp$ now have dimensions of energy times length, and therefore the relevant dimensionless coupling parameters are $\rho J_\parallel$ and $\rho J_\perp$ with

$$\rho=(2\pi\hbar v_F)^{-1} \tag{3.44}$$

as the single spin density of states at the Fermi surface.

As mentioned above, both from a formal and from a physical point of view the Hamiltonian (3.43) makes sense only if there is a high-energy cutoff that sets the scale. Usually the Kondo problem is considered as the large Coulomb repulsion limit of the more general Anderson model (1961), and this scale is then essentially determined by the Coulomb interaction in the localized level. More generally it may be viewed as an effective bandwidth, which is often taken to be of the order of the Fermi energy ε_F. In any case a cutoff in frequency around a given ω_c cuts off the momenta k around k_c with

$$k_c^{-1}=a=v_F/\omega_c \ . \tag{3.45}$$

Physically a is an atomic length, and ω_c^{-1} may be thought of as the time for an electron to pass the local spin. As a low-energy limit of the Anderson model, the Hamiltonian (3.43) makes sense only for $J_{||}=J_\perp$ and small coupling $\rho J \ll 1$. However, as a mathematical model (3.43) may be considered in its own right with $\rho J_{||}$ and $\rho J_\perp$ independent and arbitrarily large. In fact, the formal Hamiltonian (3.43) has been diagonalized exactly by a modified Bethe ansatz for any choice of J's, and we shall use some of the results obtained there later on (for a review of the exact solution, see Tsvelick and Wiegmann, 1983).

To derive the equivalence between (3.43) and the spin-boson problem we essentially follow ideas due to Schotte (1970), who has used bosonization methods to study the thermodynamics of the Kondo problem (see also Emery and Luther, 1974). As mentioned in the beginning of this section, these methods are certainly not rigorous. Their advantage, however, is that they are relatively simple and therefore make it easier to understand the relation between the physics of the two models. Let us introduce charge- and spin-density operators for the fermions by

$$\rho(k)=\sum_{p\sigma} c^\dagger_{p+k\sigma}c_{p\sigma},\quad \rho(-k)=\rho^\dagger(k) \ , \tag{3.46}$$

$$\sigma(k)=\sum_{p\sigma} \sigma c^\dagger_{p+k\sigma}c_{p\sigma},\quad \sigma(-k)=\sigma^\dagger(k) \ , \tag{3.47}$$

with $k>0$. Then for a semi-infinite band with all the states $p<0$ filled, it is straightforward to show that the operators

$$b_k=\left[\frac{\pi}{kL}\right]^{1/2}\rho(-k) \quad \text{and} \quad a_k=\left[\frac{\pi}{kL}\right]^{1/2}\sigma(-k) \tag{3.48}$$

obey Bose commutation rules $[a_k,a_{k'}^\dagger]=[b_k,b_{k'}^\dagger]=\delta_{kk'}$, etc., if acting on the ground state of a filled Fermi sea below $p=0$. The dynamics of these excitations is determined by the commutation rules of $\hat{H}_0^F$ with $\rho(k)$ and $\sigma(k)$, and it is easy to see that using a bosonized form,

$$H_0^B=\hbar v_F\sum_{k>0} k(a_k^\dagger a_k+b_k^\dagger b_k) \ ,$$

for the free Hamiltonian leads to the same dynamics as $\hat{H}_0^F$. The noninteracting electron gas has thus been replaced by its Bose-like charge- and spin-density excitations around the Fermi surface. In the linear spectrum approximation (3.40) these excitations are completely decoupled and constitute two independent Bose fields defined for $k>0$ with a linear spectrum

$$\omega_k=v_F k \ . \tag{3.49}$$

Using $\sum_k \sigma(k)=L\sum_\sigma \sigma c_\sigma^\dagger c_\sigma$ for unrestricted k sums, we may express the $J_{||}\sigma_z$ term in the anisotropic Kondo Hamiltonian (3.43) in terms of the spin-density excitations a_k by

$$\frac{J_{||}}{4}\sigma_z\sum_{k>0}\left[\frac{k}{\pi L}\right]^{1/2}(a_k+a_k^\dagger) \ . \tag{3.50}$$

By contrast, the mixed products $c_\uparrow^\dagger c_\downarrow$ and $c_\downarrow^\dagger c_\uparrow$ that occur in the spin-flip scattering term cannot be linearly related to $\sigma(k)$ and $\rho(k)$. Thus the nontrivial task is to find a nonlinear representation of these combinations by the spin- and charge-density excitations introduced in Eqs. (3.46)—(3.48). The essential idea is to realize that the exponential of a particular combination of Bose operators can be made into an anticommuting Fermi field. Let us define

$$j_\sigma(x)=\sum_{k>0} e^{-ak/2}\left[\frac{2\pi}{kL}\right]^{1/2}(b_{k\sigma}e^{i\sigma kx}-b_{k\sigma}^\dagger e^{-i\sigma kx})$$

$$=-j_\sigma^\dagger(x) \tag{3.51}$$

with Bose operators

$$b_{k\sigma}=\frac{b_k+\sigma a_k}{\sqrt{2}} \tag{3.52}$$

and an exponential cutoff that eliminates k values large compared to the inverse microscopic length a^{-1}. The coefficients in Eq. (3.51) have been chosen such that

$$[j_\sigma(x),j_\sigma(y)]=-i\pi\sigma\,\mathrm{sign}(x-y) \quad \text{for } a\to 0 \ . \tag{3.53}$$

Thus, using $e^Ae^B=e^Be^Ae^{[A,B]}$ if $[A,B]$ is a c number, we find that exponentials of $j_\sigma(x)$ obey the anticommutation relations

$$[\exp\pm j_\sigma(x),\exp\pm j_\sigma(y)]=0 \quad \text{for } x\neq y \ . \tag{3.54}$$

Therefore the operators $\exp j_\sigma(x)$ behave like a Fermi field $\psi_\sigma(x)$; however, different spin operators $\sigma\neq\sigma'$ always commute instead of anticommute. This remains true if $\exp j_\sigma(x)$ is multiplied by an arbitrary constant, and in order to fix the prefactor in the approximate Fermi-Bose relation we require that the expectation value $\langle\psi_\sigma^\dagger(x)\psi_\sigma(x')\rangle$ for $\psi_\sigma(x)=L^{-1/2}\sum_p c_{p\sigma}e^{ipx}$ in the ground state of the noninteracting Fermi or Bose system be identical in both representations. Choosing an exponential cutoff for the fermion momentum distribution

$$\langle c_{p\sigma}^\dagger c_{p'\sigma}\rangle=\delta_{pp'}\theta(-p)\exp(-a\,|p\,|) \ , \tag{3.55}$$

we obtain

$$\langle\psi_\sigma^\dagger(x)\psi_\sigma(x')\rangle=\frac{1}{2\pi}\frac{1}{a-i(x-x')} \ . \tag{3.56}$$

The identical result is obtained by evaluating

$\langle \psi_\sigma^\dagger(x)\psi_\sigma(x')\rangle$ with

$$\psi_\sigma(x)=(2\pi a)^{-1/2}\exp j_\sigma(x) \tag{3.57}$$

in the ground state of the bosons $b_{k\sigma}$. This relation will be used in the following as a boson representation of fermions. We emphasize, however, that Eq. (3.57) does not define two genuine Fermi fields, since it does not reproduce the correct anticommutation relations for different spins, and moreover we have not given a prescription for multiplying operators of the same spin at one point. Although in certain cases these problems may be eliminated in a more complicated representation and an exact bosonization of Fermi fields is possible (see, for instance, Mandelstam, 1975), we shall make no attempt in this direction here. Using Eq. (3.57) it is easy to see that the spin-flip combinations $c_\downarrow^\dagger c_\uparrow$ and $c_\uparrow^\dagger c_\downarrow$ depend again only on the spin-density excitations a_k, whereas the charge-density field is completely decoupled from the problem.[31] In this simple picture the anisotropic Kondo Hamiltonian (3.43) thus becomes equivalent to a boson Hamiltonian,

$$\begin{aligned}\hat{H}_K^B &= \hbar v_F \sum_{k>0} k a_k^\dagger a_k \\ &\quad + \frac{J_\parallel}{4}\sigma_z \sum_{k>0} e^{-ak/2}\left[\frac{k}{\pi L}\right]^{1/2}(a_k + a_k^\dagger) \\ &\quad + \frac{J_\perp}{4\pi a}[\sigma_+ \exp(\xi) + \sigma_- \exp(-\xi)] ,\end{aligned} \tag{3.58}$$

with

$$\xi = \sum_{k>0} e^{-ak/2}\left[\frac{4\pi}{kL}\right]^{1/2}(a_k - a_k^\dagger) . \tag{3.59}$$

Here we have introduced the high-frequency cutoff also in the $J_\parallel\sigma_z$ term. The essential argument why the behavior of the spin degree of freedom in the Kondo Hamiltonian (3.43) and its "bosonized" form (3.58) should be the same at low temperature and in the so-called long-time limit $t \gg \omega_c^{-1}$ is based on the following observation (Schotte, 1970): The dynamics of the Bose operators that multiply the spin variables in $\hat{H}_K^B$ generated by

$$\hat{H}_0^B = \hbar v_F \sum_{k>0} k a_k^\dagger a_k \tag{3.60}$$

is the same as that of the corresponding Fermi operators generated by $\hat{H}_0^F$ Eq. (3.41), provided one evaluates everything in their respective noninteracting ground states and uses the asymptotic form of the bath correlation functions for $t \gg \omega_c^{-1}$. Thus the equivalence should hold at $T=0$ or, more generally, in the so-called Fermi liquid regime of the Kondo problem, where only the very low-lying excitations above the ground state are relevant. As we shall see in Sec. V, this is in fact the most interesting regime for the macroscopic quantum coherence problem. The interesting point about the Hamiltonian $\hat{H}_K^B$ [Eq. (3.58)] is that it can be mapped exactly to an ohmic two-state system as defined in Sec. III.A. Indeed, it is straightforward to show that up to constants the canonical transformation $\hat{S}^{-1}\hat{H}_K^B\hat{S}$ with

$$\hat{S} = \exp(\tfrac{1}{2}\sigma_z\xi) \tag{3.61}$$

leads to

$$\hat{S}^{-1}\hat{H}_K^B\hat{S} = \frac{J_\perp}{4\pi a}\sigma_x + \left[\frac{J_\parallel}{4\pi} - \hbar v_F\right]\sigma_z \sum_{k>0} e^{-ak/2}\left[\frac{\pi k}{L}\right]^{1/2}(a_k + a_k^\dagger) + \hbar v_F \sum_{k>0} k a_k^\dagger a_k . \tag{3.62}$$

Provided we identify

$$-\frac{\hbar\Delta}{2} = \frac{J_\perp}{4\pi a}$$

and

$$-\sqrt{\alpha} = \frac{J_\parallel}{4\pi\hbar v_F} - 1 ,$$

the Hamiltonian (3.62) is identical to the spin-boson Hamiltonian $\hat{H}$ of Eq. (3.1), with

$$J(\omega) = \frac{2\pi\hbar\alpha}{q_0^2}\omega \exp\left[-\frac{\omega}{\omega_c}\right] \quad \text{for} \quad \sum_\alpha \to \sum_{k>0} ,$$

$\omega_k = v_F k$, and the particular choice

$$\frac{C_\alpha}{\sqrt{m_\alpha}} = -\sqrt{\alpha}\frac{2}{q_0}\left[\frac{2\pi\hbar v_F}{L}\right]^{1/2}\omega_\alpha \exp\left[-\frac{\omega_\alpha}{2\omega_c}\right] \tag{3.63}$$

for the coupling constants and oscillator masses. Since the sign of $J_\perp$ is irrelevant, the equivalence may be expressed in dimensionless terms by

$$\frac{\Delta}{\omega_c} = \rho J_\perp , \tag{3.64}$$

$$\alpha = (1 - \tfrac{1}{2}\rho J_\parallel)^2 , \tag{3.65}$$

with $\rho = (2\pi\hbar v_F)^{-1}$ as the density of states. The fact that the relation between $\hat{H}$ and $\hat{H}_K^B$ holds only for a specific choice of ω_α and $C_\alpha/\sqrt{m_\alpha}$ does not affect our previous observation that the only relevant quantity for the spin dynamics is $J(\omega)$. Indeed, the reduced partition function, as well as the time evolution of σ_z, depends in any case only on the dimensionless quantities Δ/ω_c, α, and $k_B T/\hbar\omega_c$, which through Eqs. (3.64) and (3.65) are directly related to the relevant parameters in the anisotropic Kondo problem.

We have thus arrived at an equivalence between the ohmic two-state and the anisotropic Kondo problem, where the oscillators in the spin-boson problem play the role of the spin-density excitations in the Kondo case.

[31] In fact, this decoupling also shows up in the exact solution of the Kondo problem; see Tsvelick and Wiegmann, 1983.

The dimensionless tunneling amplitude Δ/ω_c corresponds directly to the spin-flip exchange constant $\rho J_\perp$ via Eq. (3.64), which is assumed to be small compared to one in both models. The coupling constant α, however, related to $\rho J_\parallel$ by Eq. (3.65), may take arbitrary values, whereas in a proper isotropic Kondo problem $\rho J_\parallel$ and $\rho J_\perp$ have to be equal and small, which means α near 1. The critical coupling $\alpha_c = 1$ separates the corresponding ferromagnetic Kondo problem $\rho J_\parallel < 0$, i.e., $\alpha > 1$ from the antiferromagnetic one $\rho J_\parallel > 0$, i.e., $\alpha < 1$, which is the interesting and difficult case.

Before we proceed to a discussion of some of the properties of the Kondo problem and its consequences for the dissipative two-state system, let us briefly mention another related problem, the so-called resonance level model (Schlottmann, 1982). The Hamiltonian (3.58) arises from the spin-boson model by the canonical transformation $\hat{S}\hat{H}\hat{S}^{-1}$, which is equivalent to a shift $x_\alpha \to x_\alpha + \delta x_\alpha$ of the oscillators, since in the Bose variables $\hat{S}$ may be written as a translation operator,

$$\hat{S} = \exp(\tfrac{1}{2}\xi\sigma_z) = \exp\left[\frac{i}{\hbar}\sum_\alpha \hat{p}_\alpha \delta x_\alpha\right] . \tag{3.66}$$

The $\delta x_\alpha \sim \sigma_z$ and thus ξ has been chosen in such a way that the operators $\exp(\pm\xi)$ that are generated from the tunneling term through

$$\exp(\tfrac{1}{2}\xi\sigma_z)\sigma_x\exp(-\tfrac{1}{2}\xi\sigma_z) = \sigma_+\exp(\xi) + \sigma_-\exp(-\xi) \tag{3.67}$$

could be interpreted as the product of *two* Fermi operators according to Eq. (3.57). In contrast to the previous section, where the interaction term $(q_0/2)\sigma_z\sum_\alpha C_\alpha x_\alpha$ in $\hat{H}$ was transformed away completely [see Eqs. (3.27)–(3.30)], this particular choice of ξ or δx_α leaves a residual term linear in the x_α proportional to $1-\sqrt{\alpha}$, which becomes the $J_\parallel\sigma_z$ term in the Kondo Hamiltonian. The central idea behind the transformation of $\hat{H}$ to the resonance level model is now to choose a different shift of the oscillators, such that the exponential terms multiplying $\sigma_\pm$ in Eq. (3.67) may be reinterpreted as Wannier operators

$$c = \psi(x=0) = L^{-1/2}\sum_p c_p \tag{3.68}$$

of a *single* spinless Fermi field, again using Eq. (3.57). In order to reproduce the anticommutation relations (3.54), these terms have then to be $\exp(\pm\xi/\sqrt{2})$. Compared to Eq. (3.66) the oscillators have thus to be shifted by $\delta x'_\alpha = \delta x_\alpha/\sqrt{2}$, which will leave a residual term linear in the x_α proportional to $\sqrt{1/2}-\sqrt{\alpha}$. Starting from the spin-boson Hamiltonian and the particular choice of coupling constants, masses, and oscillator frequencies defined in Eq. (3.63), we accomplish this by the canonical transformation

$$S^{2^{-1/2}}\hat{H}S^{-2^{-1/2}} = \hbar v_F\sum_{k>0} k a_k^\dagger a_k + \pi\hbar v_F(1-\sqrt{2\alpha})\sigma_z\sum_{k>0} e^{-ak/2}\left[\frac{k}{2\pi L}\right]^{1/2}(a_k + a_k^\dagger)$$
$$-\frac{\hbar\Delta}{2}[\sigma_+\exp(\xi/\sqrt{2}) + \sigma_-\exp(-\xi/\sqrt{2})] . \tag{3.69}$$

The resonance level model arises from this exact rewriting of $\hat{H}$ through our identification of

$$c = (2\pi a)^{-1/2}\exp\frac{\xi}{\sqrt{2}} \tag{3.70}$$

as a localized fermion operator and our interpretation of the oscillator degrees of freedom a_k as the density excitations

$$d(k) = \sum_p c_{p+k}^\dagger c_p, \quad d(-k) = d^\dagger(k) , \tag{3.71}$$

of spinless fermions c_k via

$$a_k = \left[\frac{2\pi}{kL}\right]^{1/2} d(-k) . \tag{3.72}$$

with

$$\sum_{k>0}\left[\frac{k}{2\pi L}\right]^{1/2}(a_k + a_k^\dagger) = L^{-1}\sum_k d(k) \to c^\dagger c - \langle c^\dagger c\rangle , \tag{3.73}$$

where the fermion ground-state expectation value $\langle c^\dagger c\rangle = (2\pi a)^{-1}$ has been subtracted, and with the replacement of $\hat{H}_0^B$ by a free-fermion Hamiltonian we arrive at the resonance level model,

$$\hat{H}_{\rm RL} = \hbar v_F\sum_k k c_k^\dagger c_k + V(\sigma_+ c + \sigma_- c^\dagger)$$
$$+\tfrac{1}{2}U\sigma_z(c^\dagger c - cc^\dagger) , \tag{3.74}$$

where

$$V = \frac{\hbar\Delta}{2}(\rho\hbar\omega_c)^{-1/2} \tag{3.75}$$

and

$$U = (1-\sqrt{2\alpha})/2\rho . \tag{3.76}$$

This Hamiltonian describes a localized level at the Fermi energy with occupation $\frac{1}{2}(1+\sigma_z)$ which hybridizes with a band of spinless fermions and has an additional Coulomb interaction U. If $U=0$, i.e., $\alpha=\frac{1}{2}$, this Hamiltonian may be diagonalized exactly and corresponds to the so-called Toulouse limit of the antiferromagnetic Kondo problem (see below and Appendix C). We emphasize again that

the mapping—at least as we have derived it here—from the spin-boson model to neither the anisotropic Kondo Hamiltonian (3.43) nor the resonance level model (3.74) is exact. Nevertheless these models show a similar behavior for the statics and dynamics of the spin degree of freedom in a certain range of parameters, as will be discussed below.

Let us now discuss some of the basic results known for the Kondo problem (for a recent review see Anderson, 1984). It is known (Kondo, 1964) that the problem cannot be treated by simple perturbation theory. To get a flavor of these difficulties consider, for example, the calculation of the impurity contribution to the static magnetic susceptibility

$$\chi_0 = -\frac{1}{2}\frac{\partial\langle\sigma_z\rangle}{\partial\varepsilon}\bigg|_{\varepsilon=0},$$

which describes the response to a perturbation $\frac{1}{2}\varepsilon\sigma_z$. In the Kondo context this is simply an external magnetic field, whereas in the two-state system ε is a bias energy which makes the minima of the two potential wells inequivalent. The expansion in powers of ρJ for an isotropic Kondo system leads to

$$\chi_0 = \frac{1}{4k_BT}\left[1-\rho J-\left[(\rho J)^2\ln\frac{D}{k_BT}+c_2(\rho J)^2\right]-\left[(\rho J)^3\ln^2\frac{D}{k_BT}+\cdots\right]+\cdots\right], \tag{3.77}$$

where D is a high-energy cutoff of the order of the Fermi energy analogous to the $\hbar\omega_c$ introduced above. In $O(\rho J)^n$, $n\geq 2$, one obtains terms like $(\rho J)^n\ln^{n-1}D/k_BT$, $(\rho J)^n\ln^{n-2}D/k_BT,\ldots$, etc., where the coefficient of the leading logarithm is always unity. Therefore, although at high temperatures χ_0 obeys a Curie law $\sim 1/T$ and the spin is essentially free, this kind of perturbation theory runs into difficulty at a temperature T_K of order

$$k_BT_K = D\exp\left[-\frac{1}{\rho J}\right], \tag{3.78}$$

where all the terms are of the same order of magnitude. Suppose for the moment that one sums the leading logarithms, which give

$$\chi_0 = \frac{1}{4k_BT}\left[1-\frac{\rho J}{1-\rho J\ln\frac{D}{k_BT}}+\text{“less significant terms”}\right]. \tag{3.79}$$

Then for the ferromagnetic case $J<0$ the denominator of the second term cannot vanish, and the summation is meaningful and does indeed give the essentially correct behavior. In particular, the Curie law persists down to zero temperature, thus indicating a degenerate ground state. On the other hand, for the more realistic antiferromagnetic case $J>0$, the denominator in the second term diverges at the so-called Kondo temperature $T=T_K$ defined above, and the summation of the leading logarithms is meaningless. What happens physically in this case is that the impurity spin is compensated by the conduction electron-spin density, and there is a unique singlet ground state. This leads to a saturation of χ_0 in the limit $T\to 0$, in agreement with experimental observations. The first, qualitatively correct, understanding of this behavior came from the work of Anderson, Yuval, and Hamann (1970) and a complete description of the crossover between weak and strong coupling has been obtained through an ingenious numerical solution by Wilson (1975). More recently the Kondo problem has been solved exactly using a modified Bethe ansatz (Andrei, 1980; Wiegmann, 1980). It is thus now understood how the qualitative physics changes as T goes through T_K as an example of a smooth, yet highly complicated, crossover between two distinct physical situations. The essential difficulty in the Kondo problem, which is reflected in the logarithmically divergent terms in Eq. (3.77), is due to the fact that the scattering of the conduction electrons off the impurity is associated with excitations in the electron gas that have arbitrarily small energies. Since the Fermi surface is infinitely sharp at $T=0$, all energy scales from zero up to a cutoff of order D are present, and, due to the large phase space for low-energy excitations, perturbation theory in the number of these excitations becomes impossible. In Wilson's approach the problem of the nonexistence of a characteristic scale is treated by renormalization group methods. These methods focus on the electronic degrees of freedom, which are coupled through the impurity spin. By contrast, the approach of Anderson, Yuval, and Hamann integrates out the electronic degrees of freedom and discusses the resulting reduced path integral for the imaginary-time history of the spin. Here we shall follow the latter approach, since it is directly related to the one used in this work. In fact, the calculation for the system's reduced dynamics given in Sec. IV may be viewed as a real-time generalization of the methods that Anderson *et al.* used for the thermodynamics. Starting from the anisotropic Kondo Hamiltonian (3.43), they showed that when the electrons are eliminated, the reduced partition function for the spin in an expansion in the number of spin flips caused by the $J_\perp$ term is given by

$$\tilde{Z} = \sum_{n=0}^{\infty}\left[\frac{J_\perp\rho}{2}\right]^{2n}\int_0^{\beta\hbar}\frac{d\tau_{2n}}{\tau_c}\int_0^{\tau_{2n}-\tau_c}\frac{d\tau_{2n-1}}{\tau_c}\cdots\int_0^{\tau_2-\tau_c}\frac{d\tau_1}{\tau_c}\exp\left[(2-\bar{\varepsilon})\sum_{i<j}(-)^{i+j}\ln\left|\frac{\beta\hbar}{\pi\tau_c}\sin\frac{\pi(\tau_j-\tau_i)}{\beta\hbar}\right|\right] \tag{3.80}$$

with a short-time cutoff $\tau_c=\omega_c^{-1}$ which takes into account that only the asymptotic form of the conduction-electron Green's function was used to derive this result. This partition function has been written in a form that shows that the complete thermodynamics of the spin depends only on three dimensionless parameters, namely, $J_\perp\rho$, $k_BT/\hbar\omega_c$, and $\bar{\varepsilon}$. The parameter[32] $\bar{\varepsilon}$ is related to the phase shift caused by the $J_\parallel\sigma_z$ term and is given by

$$\bar{\varepsilon}=2\rho J_\parallel-\tfrac{1}{2}(\rho J_\parallel)^2 , \tag{3.81}$$

which reduces to $\bar{\varepsilon}=2\rho J_\parallel$ in the usual case $\rho J_\parallel \ll 1$.[33] As has been realized by one of us (Chakravarty, 1982) and independently by Bray and Moore (1982), the reduced partition function of a spin-boson problem with ohmic dissipation has again precisely the form of Eq. (3.80), provided we identify Δ/ω_c with $\rho J_\perp$ and

$$2-\bar{\varepsilon}=2\alpha . \tag{3.82}$$

This equivalence was the first indication that the behavior of the spin degrees of freedom should be equivalent for the ohmic two-state and the anisotropic Kondo problem. In fact, the correspondences between the two models derived from $\tilde{Z}$ agree precisely with those of our heuristic bosonization approach [Eqs. (3.64) and (3.65)]. As has been discussed in Sec. II and in a somewhat different way by Chakravarty and Kivelson (1985), starting from a physical double-well problem one may derive an effective spin-boson Hamiltonian through a kind of reduction procedure (Chakravarty and Kivelson, 1985; Dorsey *et al.*, 1986), and the effective tunnel splitting that we have called Δ here is related in a nontrivial manner to the bare tunnel splitting in the absence of dissipation.

Having discovered the equivalence between the models again on the basis of their reduced partition functions, let us now discuss the thermodynamic behavior of the Kondo spin as deduced from Eq. (3.80), which will then give immediately the behavior for the ohmic two-state system. The partition function (3.80) may be considered as the classical grand partition of a one-dimensional "Coulomb" gas of alternately positively and negatively charged hard rods of length τ_c on a circle of circumference $\beta\hbar$. The logarithmic term in the exponent of the integrand represents the interaction between the rods as a function of their separation along the circle. The parameter $2\alpha=2-\bar{\varepsilon}$ plays the role of the inverse temperature of this gas and should not be confused with the real physical inverse temperature β. The dimensionless quantity $\rho J_\perp/2$ corresponds to the effective fugacity of the gas. An alternative picture for the same partition function may be obtained by noting that, since the Kondo divergences occur at small energies, it is the large-separation behavior of the interaction that captures the essential physics. Thus instead of treating the variables τ_i as continuous, subject to the restriction $|\tau_i-\tau_j|>\tau_c$, one may take them to assume values that are integral multiples of τ_c; in other words, they form a discrete lattice of spacing τ_c. If we associate an Ising spin ±1 with each lattice point, the places were the original Kondo spin $\sigma_z(\tau)$ flips correspond to local defects in the Ising system (see Fig. 2). Integrating the logarithmic interaction in Eq. (3.80) twice, we may write the partition function in the limit $\beta\to\infty$ as

$$\tilde{Z}=\sum_{\text{paths }\sigma_z(\tau)} \exp\left[-\frac{\alpha}{8}\int_0^\beta d\tau\int_0^\beta d\tau'\frac{[\sigma_z(\tau)-\sigma_z(\tau')]^2}{(\tau-\tau')^2+\tau_c^2}-2n\ln\frac{2}{\rho J_\perp}\right] , \tag{3.83}$$

with $2n$ being the number of spin flips. In this form it becomes evident that $\tilde{Z}$ may also be interpreted as the partition function of a one-dimensional inverse-square Ising model with a short-range ferromagnetic interaction $\ln 2/\rho J_\perp$ and a long-range piece $(i-j)^{-2}$ of strength α (Anderson and Yuval, 1971).

From the statistical-mechanical pictures given above, it is clear that for any finite temperature there should be no singularities in the behavior of the spin, since the corresponding classical system is of finite length. It is only at $T=0$ that a transition as a function of $J_\parallel$ and $J_\perp$ can take place. This is demonstrated very nicely in Anderson's scaling approach (Anderson *et al.*, 1970), which studies how the coupling constants are renormalized if we change the cutoff from τ_c to $\tau_c+d\tau_c$, i.e., if we carry out a partial integration of high-energy degrees of freedom such that the partition function remains form invariant. This leads to a set of differential equations for the change in the parameters known as the scaling equations. The basic idea is that, even if the entire problem exhibits enormous complexity, at each infinitesimal step one has a manageable problem. To lowest order in $\rho J_\perp$ these scaling equations are

$$\frac{d\bar{\varepsilon}}{d\ln\tau}=(2-\bar{\varepsilon})\cdot(\rho J_\perp)^2+O(\rho J_\perp)^4 , \tag{3.84}$$

$$\frac{d(\rho J_\perp)}{d\ln\tau}=\frac{\bar{\varepsilon}}{2}(\rho J_\perp)+O(\rho J_\perp)^3 , \tag{3.85}$$

with τ as the running value of the cutoff. The behavior of these equations is best understood from a plot of the hyperbolic scaling trajectories in the $\bar{\varepsilon},\rho J_\perp$ plane in the vicinity of $\bar{\varepsilon}=0$ shown in Fig. 3. The directions of the arrows are toward increasing τ_c, and the scaling maps a problem with a given $\tau_c/\beta\hbar=k_BT/\hbar\omega_c$ to one of larger $\tau_c/\beta\hbar$ or effectively smaller temperature. If in this process the effective $\rho J_\perp$ becomes smaller, we move further away from any divergence difficulties. As can be seen

[32]Note that our $\bar{\varepsilon}$ is identical with the ε introduced by Anderson *et al.* (1970); we have used an overbar to distinguish it from the bias energy ε.

[33]Equation (3.81) gives the complete result for $\bar{\varepsilon}$ for a regularization of the contact interaction such that the one particle phase shift caused by the $J_\parallel\sigma_z$ term is given by $\delta=(\pi/4)\rho J_\parallel$.

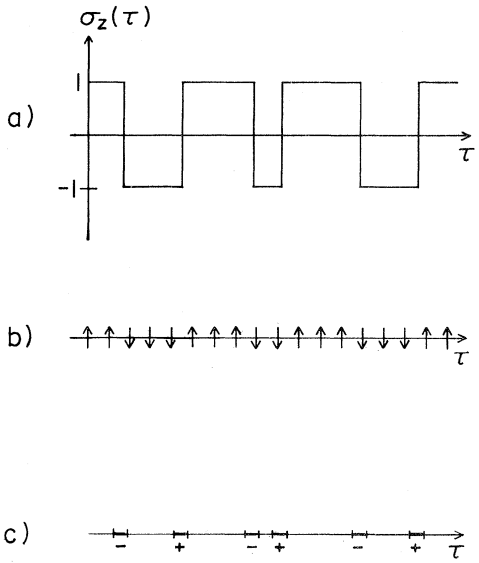

FIG. 2. Equivalence of the partition functions for the Kondo, the one-dimensional $1/r^2$ Ising, and the logarithmic Coulomb gas models. (a) A typical imaginary-time spin-flip trajectory for the Kondo model. (b) The corresponding spin configuration in the equivalent $1/r^2$ Ising model. (c) The corresponding distribution of charged rods in the logarithmic Coulomb gas model.

from the figure, for all initial parameters that lie below the left separatrix, $\rho J_\perp$ scales to zero. Thus for the ferromagnetic Kondo problem $\bar{\varepsilon}<0$ the effective spin-flip amplitude vanishes in the limit $T\to 0$ and the ground state is twofold degenerate, with a Curie susceptibility $\chi_0\sim 1/T$ down to $T=0$. According to Eq. (3.82), $\bar{\varepsilon}<0$ corresponds to $\alpha>1$ in the spin-boson problem and since $\rho J_\perp=\Delta/\omega_c$ this means that for dimensionless friction[34] $\alpha>1$ the effective tunneling amplitude vanishes as $T\to 0$ and the particle is localized in one of the two wells. More precisely, an infinitesimal bias induces a nonzero order parameter $\langle\sigma_z\rangle\neq 0$ which has a discontinuous jump at $\alpha=1$ and reaches its limiting value $\langle\sigma_z\rangle=\pm 1$ only as $\alpha\to\infty$. On the other hand, if the initial parameters are to the right of this separatrix, in particular, if we consider the interesting antiferromagnetic case $\bar{\varepsilon}>0$, i.e., $\alpha<1$ in the spin-boson problem, $\rho J_\perp$ will grow under rescaling and move outside the range of validity of the low-order scaling equations (3.84) and (3.85). In the picture of a gas of flips this gas can then no longer be considered as dilute, since its fugacity $\rho J_\perp$ becomes large.[35] Now although the simple scaling breaks down for $\bar{\varepsilon}>0$, it still gives an indication of what happens in this case. As mentioned earlier, the antiferromagnetic interaction takes advantage of the constant density of states at the Fermi energy to form a bound state, or more properly a resonance, between the local spin and one built from the free-electron states. The binding energy of such a state is of the order of $\Delta E=\hbar\omega_c\exp(-1/\rho J)$, which obviously cannot be obtained by perturbation theory. In the anisotropic case the essential scale on which this nonmagnetic ground state builds up may be "derived" by dropping (3.84) and using only the scaling equation (3.85), which reads $d\ln\Delta=\alpha\, d\ln\omega_c$ in the notation of the spin-boson problem. Integrating this equation from a high-frequency cutoff ω_c, where the tunneling amplitude is Δ, down to a low-frequency value that is self-consistently given by the effective tunneling amplitude Δ itself, we obtain a renormalized Δ_r of order

$$\Delta_r=\Delta\left[\frac{\Delta}{\omega_c}\right]^{\alpha/1-\alpha},\quad \alpha<1\,, \tag{3.86}$$

in agreement with the adiabatic renormalization result (3.24). Its physical significance in the ohmic two-state problem may be understood by noting that the bath oscillators with frequencies smaller than Δ_r have a strongly reduced effective coupling, since they are not able to follow completely the motion of the spin (Emery and Luther, 1974). It should be pointed out that the result (3.86) may break down close to $\alpha=1$.[36] However, as will be shown in Sec. V, it essentially gives the true dynamical scale in the ohmic two-state problem in the interesting regime $\alpha<\frac{1}{2}$ [see Eq. (5.39)]. The characteristic frequency Δ_r determines a corresponding temperature below which the crossover to the strong coupling regime occurs, characterized, for instance, by a static susceptibility that no longer obeys a Curie law but bends over to reach a constant value at $T=0$. To obtain a qualitative understanding of the behavior for $k_BT\ll\hbar\Delta_r$, Anderson *et al.* (1970) argued that the scaling terminates at a strong coupling fixed point $\bar{\varepsilon}=1$ (i.e., $\alpha=\frac{1}{2}$ in the spin-boson language). Now, as we have seen above, the special feature of this value of the coupling is that it corresponds to an exactly soluble problem, namely, the Toulouse Hamiltonian

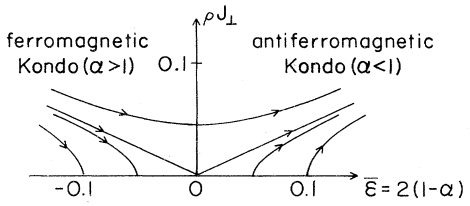

FIG. 3. Scaling trajectories in the Kondo problem in the vicinity of $\bar{\varepsilon}=0$, i.e., $\alpha=1$, and for small $\rho J_\perp$.

[34]The value $\alpha_c=1$ is the result for the critical coupling in the limit $\Delta/\omega_c\to 0$. For finite Δ/ω_c, α_c will be larger than one.

[35]As we shall see in Sec. V, this problem arises again in the corresponding description of the spin's real-time dynamics for $\alpha<1$, in particular, in the regime $\frac{1}{2}<\alpha<1$.

[36]In fact, the analogy to the $1/r^2$ Ising model suggests that Δ_r, which corresponds to the inverse correlation length in the Ising model, vanishes as $\exp(-\text{const}/\sqrt{1-\alpha})$ for $\alpha\to 1^-$.

$$\hat{H}_T=\hbar v_F\sum_k kc_k^\dagger c_k+V(\sigma_+c+\sigma_-c^\dagger)\ , \tag{3.87}$$

with $V=\hbar\Delta/2(\rho\hbar\omega_c)^{-1/2}$. This model describes a resonance level of width $\hbar\tilde{\Delta}=\pi V^2\rho=\frac{1}{4}\pi\hbar\Delta_r(\alpha=\frac{1}{2})$ and has a finite zero-temperature susceptibility $\chi_0=[(\pi^2/4)\hbar\Delta_r]^{-1}$. Qualitatively this picture has been confirmed though Wilson's numerical solution, which gave the complete behavior in the complicated crossover regime, and later by the exact diagonalization of the problem.

Instead of discussing the Kondo problem further, we shall in the remainder of this section briefly indicate some of the consequences for the spin-boson problem which follow from the analogy. What we have seen so far may be summarized as follows.

(1) There is a correspondence $\rho J_\perp\to\Delta/\omega_c$ and $2-\bar{\varepsilon}\to 2\alpha$ between the anisotropic Kondo and the ohmic two-state problem, which leads to a localized twofold-degenerate ground state for $\alpha>1$ similar to the behavior of a ferromagnetically coupled Kondo spin $\bar{\varepsilon}<0$.

(2) In the antiferromagnetic case $\bar{\varepsilon}>0$, i.e., $\alpha<1$ we expect a unique nondegenerate ground state with a finite zero-temperature static susceptibility χ_0 of order $(\hbar\Delta_r)^{-1}$. By continuity this should hold in the whole range $0\le\alpha<1$, which means it is valid in the formal anisotropic Kondo problem beyond the Toulouse limit, i.e., for $\bar{\varepsilon}>1$.

(3) For $\alpha<1$ the expansion in the number of spin flips in the partition function does not lead to a dilute gas of flips for $k_BT\ll\hbar\Delta_r$, which reflects the basic difficulty that the exact ground state is orthogonal (Emery and Luther, 1974) to that for a static spin $\Delta=0$. In addition we mention the following result, which is well known in the Kondo context.

(4) The spin contribution C_i to the specific heat is not Schottky-like as for an uncoupled two-state system, but will vanish linearly in temperature as $T\to 0$. This is in fact a special example of the general result (Fisher and Zwerger, 1985b), that for a spin-boson model with coupling $J(\omega)\sim\omega^s$ for $\omega\to 0$ we have $C_i(T)\sim T^s$ for $T\to 0$. It demonstrates again that the fermionic bath in the Kondo case is equivalent to an ohmic coupling $J(\omega)\sim\omega$. From the Fermi liquid picture of the Kondo problem (Nozières, 1974) it is known that

$$\lim_{T\to 0}\frac{C_i}{T\chi_0}=\text{const}\ . \tag{3.88}$$

This relation should continue to hold in the spin-boson case; however, the constant obviously has to vanish as $\alpha\to 0$, where $C_i\sim\alpha T$ and $\chi_0\to(2\hbar\Delta)^{-1}$.

Since our main interest in this work lies in the dynamic properties of the spin degrees of freedom, let us discuss some of those properties, which can be inferred from the Kondo analogy. The complete linear response and the equilibrium spin-correlation functions are determined by the imaginary part of the dynamic susceptibility

$$\chi''(\omega)=(2\hbar)^{-1}\int_{-\infty}^{\infty}dt\,e^{i\omega t}\langle[S_z(t),S_z(0)]\rangle_\beta\ , \tag{3.89}$$

which is a real and odd function of ω. It determines the static susceptibility via

$$\chi_0=\frac{2}{\pi}\int_0^\infty d\omega\frac{\chi''(\omega)}{\omega}\ . \tag{3.90}$$

Let us first discuss the qualitative behavior expected for a dissipative two-state system. For vanishing coupling, $\alpha=0$, the symmetric function $\chi''(\omega)/\omega$ consists of two δ peaks at $\omega=\pm\Delta$ which describe the spin's undamped coherent oscillations. For finite but small α (the crucial question is obviously how small α has to be) these peaks will shift and broaden to give a damped oscillatory behavior, characterized by a transverse relaxation time T_2 in the NMR language of Sec. III.B. In addition there may be incoherent contributions. If α is increased further, the maxima around $\omega=\pm\Delta_r$ will eventually disappear and the spin will show only a relaxational dynamics. Such a behavior is expected in the whole region $\alpha\ge\frac{1}{2}$, since from the analogy to the Toulouse Hamiltonian, where $\chi''(\omega)$ may be calculated exactly as (Zwerger, 1985; Guinea, 1985)

$$\frac{\chi''(\omega)}{\omega}=\frac{2\tilde{\Delta}^2}{\hbar\pi}\frac{1}{\omega^2+4\tilde{\Delta}^2}\left[\frac{1}{\omega\tilde{\Delta}}\tan^{-1}\left[\frac{\omega}{\tilde{\Delta}}\right]+\frac{1}{\omega^2}\ln\left[1+\frac{\omega^2}{\tilde{\Delta}^2}\right]\right] \tag{3.91}$$

with $\tilde{\Delta}=(\pi/4)\Delta^2/\omega_c$, it follows that already at $\alpha=\frac{1}{2}$ (and $T=0$) all coherence is lost and σ_z relaxes incoherently. Thus for $\alpha\ge\frac{1}{2}\chi''(\omega)/\omega$ will be concentrated around $\omega=0$ and its width—which has been called T_1^{-1} in the Kondo context (Götze and Schlottmann, 1974)—will be of order Δ_r^{-1}. If α approaches 1 from below, this relaxation slows down dramatically as $\Delta_r(\alpha)$ goes to zero and the peak of $\chi''(\omega)/\omega$ around $\omega=0$ becomes increasingly sharp. For $\alpha>1$ and $T=0$, $\chi''(\omega)/\omega$ has a δ function contribution at zero frequency that is proportional to the order parameter $\langle\sigma_z\rangle\neq 0$, and the spin is no longer ergodic.

Since χ_0 is finite for $\alpha<1$, we conclude from Eq. (3.90) that $\chi''(\omega)$ has to vanish in the limit $\omega\to 0$. The way it does so is determined by an exact relation that has been proven for the general Anderson model by Shiba (1975), namely,

$$\lim_{\omega\to 0}\frac{\chi''(\omega)}{\omega}=2\pi\chi_0^2,\quad T=0\ . \tag{3.92}$$

This relation will hold for the usual Kondo problem (i.e., Δ/ω_c and $1-\alpha$ small) as a limit of the Anderson model, and shows that $\chi''(\omega)$ vanishes linearly as $\omega\to 0$. Although its proof is essentially based on a particle number conservation law, for which no direct analog seems to exist in our spin-boson problem, we expect the behavior

$$\lim_{\omega\to 0}\frac{\chi''(\omega)}{\omega}=\text{const} \tag{3.93}$$

to hold in this case too, whenever $\alpha<1$. This belief is based on the observation that Eq. (3.93) is simply a reflection of the fact that the system is subject to ohmic dissi-

pation. Indeed, it is clear that the identical behavior characterizes a damped harmonic oscillator with a general frequency-dependent damping $\eta(\omega)$ precisely if $\lim_{\omega\to 0}\eta(\omega)=\text{const}$. As for the specific-heat relation (3.88), the factor 2π in Eq. (3.92), which holds in the limit $\alpha\to 1^-$, will be replaced by a constant that vanishes as $\alpha\to 0$. It is, however, extremely likely that $\chi''(\omega)$ does behave as in Eq. (3.93) in the whole range $0<\alpha<1$.

The conclusions that may be drawn from these observation for the long-time dynamics of σ_z are the following.

(1) Let us assume that we may replace the expectation value $P(t)=\langle\sigma_z(t)\rangle$, which starts out at $P(t=0)=1$, i.e., far from its equilibrium value $\langle\sigma_z\rangle_\beta=0$, by its linear-response approximation $P(t)\approx\varphi(t)$ (Zwerger, 1983a, 1983b) where the normalized relaxation function is given by[37]

$$\varphi(t)=\frac{2}{\pi}\int_0^\infty d\omega\frac{\chi''(\omega)}{\omega\chi_0}\cos\omega t\ . \tag{3.94}$$

Then from $\chi''(\omega)\sim\omega$ for $\omega\to 0$ we may conclude that $\langle\sigma_z(t)\rangle$ relaxes faster than t^{-1} in the limit $t\to\infty$.

(2) Alternatively, as discussed in Sec. III.A, $P(t)$ may be approximated by the symmetrized correlation function

$$\begin{aligned}C(t)&=\tfrac{1}{2}\langle[\sigma_z(t),\sigma_z]\rangle_\beta\\&=\mathrm{Re}\langle\sigma_z(t)\sigma_z(0)\rangle_\beta\ .\end{aligned}\tag{3.95}$$

Its Fourier transform is given by the fluctuation-dissipation theorem

$$C(\omega)=\hbar\omega\coth\frac{\beta\hbar\omega}{2}\cdot\frac{\chi''(\omega)}{\omega}\underset{T\to 0}{\to}\hbar\,|\omega|\cdot\frac{\chi''(\omega)}{\omega}\ . \tag{3.96}$$

Then, concentrating on the limit $T=0$, which will be the most difficult case to treat from the point of anomalously slow relaxation, we find that a finite χ_0 implies that $C(\omega)$ vanishes as $\omega\to 0$, and thus $C(t)$ has to decay faster than t^{-1} in the limit $t\to\infty$. The more restrictive condition (3.93), however, leads to

$$C(\omega\to 0)=\text{const}\,|\omega|+O(\omega^{1+\varepsilon})\ . \tag{3.97}$$

Thus, at $T=0$ and for all $\alpha<1$, $C(t)$ will asymptotically behave as $-t^{-2}$ and no slower-decaying contribution can occur.[38] Now in the simple noninteracting-blip approximation of Sec. IV.C we find that $P(t)$ and $C(t)$ are the same. If this were true generally, the power law $t^{-2(1-\alpha)}$ which is found for this function in Sec. V could not hold asymptotically as $t\to\infty$.[39]

At this point, however, several comments should be made. First, and most important, it should be emphasized that the problems that have been studied in the Kondo context are quite different from those in the present work. Whereas in the Kondo case the interest has always concentrated mainly on thermodynamic properties, our main concern here is the dynamical behavior of the spin at intermediate times, where $P(t)$ has not yet decayed to almost zero. In fact, it may be seen from the Laplace transform equation (4.32) of $P(t)$ that the methods used below for determining the spin's dynamics are equivalent to summing up a short-time expansion to infinite order. It is therefore not too surprising that these methods may fail in the limit of very long times. From the point of view of the macroscopic quantum coherence problem, however, this failure is likely to be irrelevant. Second it is important to note that $P(t)$ cannot be obtained from any equilibrium correlation function of the system, since the initial condition $\sigma_z=+1$ at $t=0$ corresponds to a large perturbation. Thus no restriction on $P(t)$ can be derived from a linear-response argument. It is intuitively very plausible, however, that the normalized relaxation function $\varphi(t)=\langle\sigma_z(t)\rangle/\langle\sigma_z(t=0)\rangle$, which describes the relaxation of σ_z after a *small* deviation $\langle\sigma_z(t=0)\rangle\ll 1$ from equilibrium has been created by a small bias

$$\varepsilon(t)=\varepsilon(0)\lim_{\eta\to 0}e^{\eta t}\theta(-t)\ ,$$

i.e., an adiabatic switching procedure, will have the same qualitative behavior as the exact $P(t)$. In this case the argument above indicates that the simple noninteracting-blip approximation would asymptotically fail only in the incoherent regime $\frac{1}{2}<\alpha<1$. Contrary to $\varphi(t)$, the long-time tails in the symmetrized correlation function $C(t)$ are in a way an artifact of the definition of this function. As we may see from the fluctuation-dissipation theorem (3.96), $C(t)$ has a $-t^{-2}$ long-time tail at $T=0$ even for a completely analytic response function $\chi''(\omega)\sim\omega$ for $\omega\to 0$, such as that for a damped harmonic oscillator or at $\alpha=\frac{1}{2}$. Thus within a description in terms of linear response and correlation functions it seems more natural to work with $\varphi(t)$.

In conclusion, we have shown in this section that there is an interesting relation between the anisotropic Kondo and the ohmic two-state problem. This analogy has several consequences for the static and the long-time behavior of our spin-boson problem, and in particular it gave the first indication that coherent oscillations of the spin may be expected only for $\alpha<1$. Indeed, as the relation to the resonance level model shows, we must have $\alpha<1/2$. Unfortunately the few existing results about the low-T dynamics of both the anisotropic Kondo and the resonance level model only cover either $t\to\infty$ properties, as in Eq. (3.92), or the behavior for $\alpha>\frac{1}{2}$, where the spin is essentially relaxing incoherently with a typical time scale of order Δ_r^{-1}, however complicated the actual behavior may be in this regime. It would therefore be quite interesting to investigate to what extent the relation between the Hamiltonians can be put on a more rigorous basis and whether the physics described by the formal an-

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[37]This approach can obviously be used only if χ_0 is finite, which also guarantees ergodicity, i.e., $\varphi(t)$ vanishes as $t\to\infty$.

[38]This is true even at $\alpha=\frac{1}{2}$, whereas from an exact calculation within the Toulouse Hamiltonian both $P(t)$ (see Sec. V.B and Appendix C) and $\varphi(t)$ relax exponentially at large times, although they are not identical.

[39]See also the discussion in Secs. V.C and V.D below.

isotropic Kondo Hamiltonian (3.43) beyond the Toulouse limit ($\bar{\varepsilon} > 1$) or the resonance level model (3.74) for $U > 0$ does in fact eventually become similar to that in the ohmic two-state problem for $\alpha < \frac{1}{2}$, in the sense that the spin starts to oscillate, or whether the analogies are strictly valid only close to $\alpha = 1$ or $\alpha = \frac{1}{2}$, respectively. Recent work in this direction has been done (Guinea, 1985); however, many questions are still open.

F. Summary

Collecting together the results of the various approaches used in this section, one may plausibly make the following conjectures about the behavior of the dissipative two-state system as a function of the form of the environment spectral density $J(\omega)$:

(1) In the case of *superohmic* dissipation ($s > 1$), we expect that at zero temperature the system will perform weakly damped coherent oscillations with a renormalized frequency given by Eq. (3.23) and a damping calculated from Eq. (3.11) with $\beta = \infty$, but with Δ replaced by $\Delta_{\rm FC}$. At finite temperatures, for $s \geq 2$ the situation will be different only in that the damping is now temperature dependent according to Eq. (3.11). For $1 < s < 2$, however, we shall get a crossover to overdamped behavior at a temperature of order of $\hbar\Delta_{\rm FC} \cdot \beta_s^{-1} (\omega_c / \Delta_{\rm FC})^{s-1}$.

(2) In the case of *subohmic* dissipation ($s < 1$), the system is localized at zero temperature provided we are in the limit $\Delta/\omega_c \to 0$. At finite temperature we expect incoherent relaxation at a rate whose principal temperature dependence is $\exp[-\text{const}(\hbar\omega_c / k_B T)^{1-s}]$. We should expect that in this case the golden rule formula (3.37) would always be valid, since it is precisely set up to handle incoherent processes.

(3) The case of *ohmic* dissipation ($s = 1$) is particularly difficult. For $\alpha > 1$ the situation is qualitatively similar to that in the subohmic case, except that the relaxation rate should now increase as a power of T rather than exponentially. For $\alpha < 1$ none of the arguments developed in this section is entirely convincing, though it is plausible that for $\alpha \ll 1$ (but $\alpha \ln \omega_c / \Delta$ possibly large) the quantity $\tilde{\Delta} \equiv \Delta (\Delta/\omega_c)^{\alpha/1-\alpha}$ acts as an effective renormalized coherent tunneling rate and that in this limit the treatment of Sec. III.B is a fairly good approximation, provided we replace Δ by $\tilde{\Delta}$. For larger coupling the behavior of τ^{-1} mentioned in Sec. III.D indicate a qualitative change in the zero-temperature dynamics at $\alpha = \frac{1}{2}$ and $\alpha = 1$. This is confirmed in Sec. III.E by the analogy of the ohmic two-state and the Kondo problems. In particular, it has been shown there that for $\alpha > 1$ the ground state is localized (again provided $\Delta/\omega_c \ll 1$) and the spin dynamics is not ergodic. Furthermore, the equivalence between the case $\alpha = \frac{1}{2}$ and the Toulouse problem makes it extremely plausible that for any $\alpha \geq \frac{1}{2}$ coherence is completely destroyed by the bath coupling even at $T = 0$, and thus $\alpha < \frac{1}{2}$ is at least a necessary condition for finding oscillatory behavior. To the extent that $P(t)$ can be qualitatively approximated by the normalized relaxation function $\varphi(t)$ we found that at long times $P(t)$ should decay faster than t^{-1}, whereas the symmetrized correlation function $C(t)$ will asymptotically behave as $-t^{-2}$ for all $0 < \alpha < 1$ and $T = 0$. At finite temperature we expect the relaxation to become incoherent if $k_B T$ is large compared to the characteristic scale $\hbar\Delta_r(\alpha)$. None of the approaches discussed so far however gives an indication for the structure of $P(t)$ at intermediate times in the interesting regime $\alpha < \frac{1}{2}$ and small temperatures, in particular where in the α, T-plane coherence is lost.

Our aim in the rest of the paper is thus to give a method that covers in a unified way both incoherently relaxing and oscillatory regimes for arbitrary $J(\omega)$ and that provides precise conditions for their respective ranges of validity. In particular, for the special case of ohmic dissipation, we shall derive detailed results in essentially the complete range of parameters and determine explicitly the conditions necessary for such a system to show coherent oscillations.

IV. EXACT FORMAL EXPRESSIONS FOR THE SYSTEM DYNAMICS: THE "NONINTERACTING-BLIP APPROXIMATION"

In this section we shall derive exact formal expressions, in the form of power series in Δ, for the quantities $P(t)$ and $C(t)$, for a system whose Hamiltonian is given by Eq. (3.1). The formal solution is expressed in terms of the spectral function $J(\omega)$ [Eq. (3.2)] and is valid quite independently of the form of this function; thus, in particular, the results of Secs. IV.A and IV.B of this section do *not* depend on the assumptions $\Delta/\omega_c \ll 1$, etc. These results may well be formally equivalent to some already written down in the literature, but they are arranged in a way that is particularly convenient for some approximations we shall make in later sections. In particular, they suggest rather naturally a particular form of approximation, which we call the "noninteracting-blip" approximation, that will be used rather widely below. We therefore take time in Sec. IV.C of this section to explain this approximation and go through the necessary algebra, which is then applied to specific cases in subsequent sections.

A. Formal expression for $P(t)$

Since our environment consists entirely of harmonic oscillators, there are any number of different techniques available for eliminating them from the problem; here we choose to use the "influence-functional" method[40] of Feynman and Vernon (1963), and will calculate explicitly the quantity $P^{(2)}(t)$ as defined in Sec. III [the equivalence of $P^{(1)}(t)$ and $P^{(2)}(t)$ is demonstrated in Appendix B]. If at an initial negative time $t = t_0 < 0$ a system with coordi-

[40] An alternative derivation of the formula for $P^{(2)}(t)$ is given in Appendix B.2, using a possibly more familiar form of many-body perturbation theory.

nate $x(t)$ starts with a value x_i, and the environment starts in a state of thermal equilibrium with respect to its own Hamiltonian [i.e., in this case the bilinear terms in the brackets in (3.1)], then the probability $p(x_f{:}t)$ for the system to have arrived at a coordinate x_f at a subsequent time t, irrespective of the state of the environment at this time [i.e., the element $\rho(x_f,x_f{:}t)$ of the reduced density matrix] is

$$p(x_f{:}t)=\int Dx(\tau)\int Dy(\tau')A[x(\tau)]A^*[y(\tau')]F[x(\tau),y(\tau')]\ , \tag{4.1}$$

where the double path integral runs over all paths $x(\tau),y(\tau')$ such that $x(t_0)=y(t_0)=x_i$, $x(t)=y(t)=x_f$, $A[x(\tau)]$ is the amplitude for the system's following the path $x(\tau)$ in the absence of the environment (see below), and the quantity $F[x(\tau),y(\tau')]$ is the influence functional. If the physical conditions of the problem are such that we know with certainty that the system was at position x_i not only at time t_0 but for all $t\le 0$, then the paths in Eq. (4.1) must be restricted by the constraints

$$x(\tau)=x_i,\ \ \tau\le 0;\ y(\tau')=x_i,\ \ \tau'\le 0\ . \tag{4.2}$$

It is essential to note that the condition (4.2) does *not* mean that we can neglect the contribution to the path integral (4.1) of the negative-time parts of the paths: As we shall see, the influence functional couples the negative- and positive-time behavior.

For an environment of harmonic oscillators, the influence functional can be calculated exactly and has the form (Feynman and Vernon, 1963)

$$F[x(\tau),y(\tau')]=\exp-\frac{1}{\hbar}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}ds\,[x(\tau)-y(\tau)][\gamma(\tau-s)x(s)-\gamma^*(\tau-s)y(s)]\ , \tag{4.3}$$

where the function $\gamma(\tau-s)$ is given by

$$\gamma(\tau-s)\equiv\sum_\alpha(C_\alpha^2/2m_\alpha\omega_\alpha)\left[\exp-i\omega_\alpha(\tau-s)+\frac{2\cos\omega_\alpha(\tau-s)}{\exp(\beta\hbar\omega_\alpha)-1}\right]\ . \tag{4.4}$$

Using the definition (3.21) of $J(\omega)$, we can write F equivalently in the form

$$F[x(\tau),y(\tau')]=\exp-\frac{1}{\pi\hbar}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}ds\{-iL_1(\tau-s)[x(\tau)-y(\tau)]\cdot[x(s)+y(s)]+L_2(\tau-s)[x(\tau)-y(\tau)]\cdot[x(s)-y(s)]\}\ , \tag{4.5}$$

where the functions L_1,L_2 are defined

$$L_1(\tau-s)\equiv\int_0^\infty d\omega\,J(\omega)\sin\omega(\tau-s)\ , \tag{4.6a}$$

$$L_2(\tau-s)\equiv\int_0^\infty d\omega\,J(\omega)\cos\omega(\tau-s)\coth\beta\hbar\omega/2\ . \tag{4.6b}$$

One general point that is important to note for future reference is that the influence functional is always bounded above by unity;[41] this can be seen most easily by noting that the Fourier transform of L_2 is always positive, and hence so is the second term in the curly brackets in Eq. (4.5).

For the two-state problem the variables $x(\tau),y(\tau')$ can take only the two discrete values $\pm\frac{1}{2}q_0$. Equation (4.1) is therefore an integral over all possible *pairs* of paths, each of which jumps between *two* states. For our purposes, however, it is more convenient to visualize it as an integral over a *single* path that jumps between *four* states. In fact, since in the path integral τ and τ' as well as x and y are dummy variables, we can specify the pair of paths completely by specifying, for each time τ, the pair $[x(\tau),y(\tau)]$. Let the states corresponding to $\{+,+\}$, $\{+,-\}$, $\{-,+\}$, and $\{-,-\}$ (where $+\equiv\frac{1}{2}q_0$, etc.) be labeled A,B,C,D, respectively. Then the influence functional can be rewritten in the form

$$F[\xi(\tau),\chi(\tau')]=\exp-\frac{q_0^2}{\pi\hbar}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}ds[-iL_1(\tau-s)\xi(\tau)\chi(s)+L_2(\tau-s)\xi(\tau)\xi(s)]\ , \tag{4.7}$$

where $\xi(\tau)\equiv q_0^{-1}[x(\tau)-y(\tau)]$ is 0 for states A and D, $+1$ for B, and -1 for C, while $\chi(\tau')\equiv q_0^{-1}[x(\tau')+y(\tau')]$ is 0 for B and C, $+1$ for A, and -1 for D. It is evident that $\xi(\tau)\equiv 0$ for all times $\tau<0$, so the lower limit of the integration over τ (but *not* that over s) can be taken to zero if we wish. Intuitively speaking, states A and D correspond to the diagonal elements of the reduced density matrix, and states B and C to the off-diagonal ones: Note that, as indicated by the last (positive) term in the square brackets in Eq. (4.7), spending time in the off-diagonal elements always tends to suppress the weight of the path in question. This is in agreement with the phenomenological arguments often used in the context of quantum measurement theory about the de-

[41] This is of course a general property of influence functionals (whether or not arising from a harmonic-oscillator bath), as can be verified from an obvious Schwarz inequality.

struction of phase coherence by the environment (see, for example, Simonius, 1978).

Let us now consider the structure of the "bare" amplitudes $A[x(\tau)]$. For definiteness we shall, as in Sec. III, choose our convention for the sign of q so that the state occupied by the system for $t<0$ was $+\frac{1}{2}q_0$ (so that the four-state path was in state A); moreover, we choose the zero of energy so that this state has energy $+\varepsilon/2$ (where ε may, of course, have either sign). Now, the total bare amplitude $A[x(\tau)]$ for a given (two-state) path may be broken up into small pieces each of length dt. The amplitude to stay in the state $+\frac{1}{2}q_0$ $(-\frac{1}{2}q_0)$ during time dt is $\exp[-i(\varepsilon/2\hbar)dt][\exp i(\varepsilon/2\hbar)dt]$, while the amplitude to switch between the two states (in either direction) is $i(\Delta/2)dt$. Applying these prescriptions to the four-state path and neglecting terms of order $(dt)^2$, we see that the amplitude to stay in the same state is $\exp[-i\varepsilon\xi(t)dt]$, while the amplitude to switch states is $i\lambda(\Delta/2)dt$, where λ is 0 for $A\rightleftarrows D$ and $B\rightleftarrows C$, -1 for $A\rightleftarrows B$ and $D\rightleftarrows C$, and $+1$ for $A\rightleftarrows C$ and $B\rightleftarrows D$.

Consider now a definite four-state path that starts in state A at time zero and returns to it at time t, making a total of $2n$ transitions ("flips") along the way. Clearly any such path will contain a factor $(-1)^n(\Delta/2)^{2n}$ coming from the $2n$ flips [it is easily verified that any specific sequence starting and terminating at A, e.g., $A\rightarrow B\rightarrow D\rightarrow C\rightarrow A$, does indeed have a factor $(-1)^n$ irrespective of how many times D is visited]. At any "odd" flip the system can go either to B or to C, and at any "even" flip except the last either to A or to D. Consider a particular path for which the mth transition occurs at t_m. It is convenient to assign to each of the interval $t_{2j-1}<t<t_{2j}$ a label ζ_j, which is $+1(-1)$ if the system spends the interval in state B (state C), and similarly to each of the intervals $t_{2j}<t<t_{2j+1}$ a label η_j, which is $+1$ or -1 according to whether the interval is spent in state A or state D; note that by construction we have $\eta_0\equiv\eta_n\equiv+1$. We can now evaluate the influence functional (4.7) for the path in question as a function $\tilde{F}_n$ of the quantities $\{t_m\}$, $\{\zeta_i\}$, and $\{\eta_i\}$. It is convenient to include in the definition of the $\tilde{F}_n$ as well the factor $\exp -i\varepsilon\int_0^t\xi(t)dt$ from the asymmetry of the states. Then we can write the probability $p(t)$ for finding the system in state A at time t in the form of a series in Δ^2:

$$p(t)=1+\tfrac{1}{2}\sum_{n=1}^{\infty}(-1)^n\Delta^{2n}K_n(t)\,, \tag{4.8}$$

$$K_n(t)\equiv 2^{-(2n-1)}\sum_{\{\zeta_j,\eta_j\}}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1\tilde{F}_n(t_1,t_2\cdots t_{2n};\zeta_1\zeta_2\cdots\zeta_n;\eta_1\eta_2\cdots\eta_{n-1})\,. \tag{4.9}$$

Correspondingly, the expression for $P(t)\equiv\langle\sigma_z(t)\rangle\equiv 2p(t)-1$ is given by

$$P(t)\equiv\sum_{n=0}^{\infty}(-1)^n\Delta^{2n}K_n(t)\,, \tag{4.10}$$

where $K_0(t)$ is 1 by definition.

We now consider the explicit form of $\tilde{F}_n$. Substituting the expressions

$$\chi(\tau)=\sum_{j=0}^{n}\eta_j[\theta(\tau-t_{2n})-\theta(\tau-t_{2n+1})],\quad \xi(\tau)\equiv\sum_{j=1}^{n}\zeta_j[\theta(\tau-t_{2j-1})-\theta(\tau-t_{2j})]\,, \tag{4.11}$$

in Eq. (4.7), we find that the term bilinear in $\xi(\tau)$ produces a factor of the form

$$\exp-\frac{q_0^2}{\pi\hbar}\left[\sum_j Q_2(t_{2j}-t_{2j-1})+\sum_{\substack{j,k\\ j>k}}\zeta_j\zeta_k[Q_2(t_{2j}-t_{2k-1})+Q_2(t_{2j-1}-t_{2k})-Q_2(t_{2j}-t_{2k})-Q_2(t_{2j-1}-t_{2k-1})]\right], \tag{4.12}$$

where Q_2 is the second integral of $L_2(t)$ (see below). The treatment of the imaginary part of the exponent in Eq. (4.7) calls for some care, because of the special role of the initial period before t_1. This part is

$$i\left[-\frac{\varepsilon}{\hbar}\sum_{j=1}^{n}\zeta_j(t_{2j}-t_{2j-1})+\frac{q_0^2}{\pi\hbar}\sum_{k=0}^{n-1}\sum_{j=k+1}^{n}\eta_k\zeta_jX_{jk}\right], \tag{4.13}$$

$$X_{jk}\equiv Q_1(t_{2j}-t_{2k+1})+Q_1(t_{2j-1}-t_{2k})-Q_1(t_{2j}-t_{2k})-Q_1(t_{2j-1}-t_{2k+1})\,, \tag{4.14}$$

where Q_1 is the second integral of $L_1(t)$ (see below), and t_0, we recall, is a large negative time that will eventually be allowed to tend to $-\infty$.

We may now simplify the expression for K_n by summing over the possible values ±1 of the $\eta_k(k=1,2,\ldots,n-1)$. Clearly this summation yields a factor in $K_n(t)$ of the form

$$2^{n-1}\prod_{k=1}^{n-1}\cos\left[\frac{q_0^2}{\pi\hbar}\sum_{j=k+1}^{n}\zeta_jX_{jk}\right]. \tag{4.15}$$

We can also turn the remainder of the expression whose argument is (4.13) into a cosine by exploiting the fact that the

remaining factor in K_n, i.e., Eq. (4.12), as well as the factor (4.15), is invariant under simultaneous reversal of the signs of *all* the ζ_j ($j=1,\ldots,n$). This yields a factor

$$\cos\left[\sum_j \zeta_j \left[(t_{2j}-t_{2j-1})\frac{\varepsilon}{\hbar}-\frac{q_0^2}{\pi\hbar}X_{j0}\right]\right] . \tag{4.16}$$

Collecting all these factors and definitions, and writing $Q_1(t)$ and $Q_2(t)$ explicitly in terms of $J(\omega)$, we reach the following final expression for $P(t)$:

$$P(t)=\sum_{n=0}^{\infty}(-1)^n\Delta^{2n}K_n(t) , \tag{4.17}$$

$$K_n(t)\equiv 2^{-n}\sum_{\{\zeta_j\}}\int_0^t dt_{2n}\int_0^{t_{2n}} dt_{2n-1}\cdots\int_0^{t_2} dt_1 F_n(t_1 t_2\cdots t_{2n};\zeta_1\zeta_2\cdots\zeta_n;\varepsilon) , \tag{4.18}$$

$$F_n\{t_m,\zeta_i;\varepsilon\}\equiv F_1\{t_m\}F_2\{t_m,\zeta_i\}F_3\{t_m,\zeta_i\}F_4\{t_m,\zeta_i,\varepsilon\} , \tag{4.19}$$

where the four factors entering F_n are given by the expressions

$$F_1\equiv\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}S_j\right] , \tag{4.20a}$$

$$F_2\equiv\exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{k=1}^{n}\sum_{j=k+1}^{n}\zeta_j\zeta_k\Lambda_{jk}\right] , \tag{4.20b}$$

$$F_3\equiv\prod_{k=1}^{n-1}\cos\left[\frac{q_0^2}{\pi\hbar}\sum_{j=k+1}^{n}\zeta_j X_{jk}\right] , \tag{4.20c}$$

$$F_4\equiv\cos\left[\sum_{j=1}^{n}\zeta_j\left[(t_{2j}-t_{2j-1})\frac{\varepsilon}{\hbar}-\frac{q_0^2}{\pi\hbar}X_{j0}\right]\right] . \tag{4.20d}$$

The quantities S_j,Λ_{jk},X_{jk} occurring in Eq. (4.19) are functions of the $\{t_m\}$ and are defined in terms of the spectral density $J(\omega)$ by the expressions

$$S_j=Q_2(t_{2j}-t_{2j-1}) , \tag{4.21a}$$

$$\Lambda_{jk}\equiv Q_2(t_{2j}-t_{2k-1})+Q_2(t_{2j-1}-t_{2k})-Q_2(t_{2j}-t_{2k})-Q_2(t_{2j-1}-t_{2k-1}) , \tag{4.21b}$$

$$X_{jk}\equiv Q_1(t_{2j}-t_{2k+1})+Q_1(t_{2j-1}-t_{2k})-Q_1(t_{2j}-t_{2k})-Q_1(t_{2j-1}-t_{2k+1}) , \tag{4.21c}$$

where Q_1 and Q_2 are the second integrals of L_1 and L_2 from 0 to t, that is, the expressions

$$Q_1(t)\equiv\int_0^{\infty}\frac{J(\omega)}{\omega^2}\sin\omega t\, d\omega , \tag{4.22a}$$

$$Q_2(t)\equiv\int_0^{\infty}\frac{J(\omega)}{\omega^2}(1-\cos\omega t)\coth(\beta\hbar\omega/2)d\omega . \tag{4.22b}$$

Note that $Q_1(t)$ and $Q_2(t)$ are well defined for all t, provided that, as ω tends to zero, $J(\omega)$ tends to zero, at least as fast as $\omega^n, n>0$, and is cut off at the higher-frequency end as described earlier.

Equation (4.17), with the definitions (4.18)—(4.22), forms the basis of all our subsequent work in this paper. Note that for $\varepsilon=0$ these formulas reduce, apart from trivial notational differences, to Eqs. (5)—(7) of Chakravarty and Leggett (1984). Before embarking on a detailed analysis (in the next three sections) of Eq. (4.17), it is convenient to develop a graphical representation of the paths and some useful terminology, and to examine the significance of the various factors (4.20) in F_n.

To represent a path, we draw a line that runs along the x axis when the system is in a "diagonal" state (A or D) and above and parallel to it when it is in a "nondiagonal" state (B or C); see Fig. 4. The label $\zeta_j(=\pm 1)$, which distinguishes B from C, is added separately (or we could, if preferred, reflect the B line in the x axis). We shall refer to the periods when the line is along the x axis as "sojourns" and the periods when it is above it as "blips"; thus, the "jth blip" is the period $t_{2j-1}<t<t_{2j}$, and the "kth sojourn" is (by convention) the period $t_{2k}<t<t_{2k+1}$. With this convention, therefore, the kth blip precedes the kth sojourn.

It is clear that the various factors in Eq. (4.17) can now be regarded as "interactions" between the blips, and between blips and sojourns; in the former case we call an interaction "repulsive" if it tends to decrease F_n, "attractive" if it increases it. The term F_1 [Eq. (4.20a)] is the self-interaction of the blips: this is always repulsive for any form of $J(\omega)$, as can be seen by returning to the original influence-functional expression (4.7). The term F_2 is an interaction between different blips which depends on the relative signs ζ_j,ζ_k. It is not possible in general to

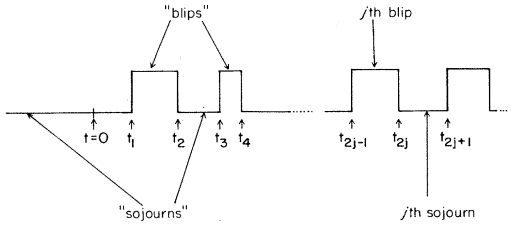

FIG. 4. Graphical representation of Eq. (4.17).

make any statement about the "sign" of this term by itself, but it is important to notice that, quite generally, the expression $(\sum_j S_j + \sum_{jk} \zeta_j \zeta_k \Lambda_{jk})$ is always positive where both sums go over the same subset of the blips [again, this follows from Eq. (4.7)]. The term F_3 expresses the interference between processes in which the system goes, say, from B to A to B and from B to D to B: it appears as an interaction between a given blip and *previous* sojourns only. A case of special interest is the case $j=k+1$: if we can neglect the contribution of all the other $X_{jk}(j \geq k+2)$, then this term produces an effective self-interaction of the form $\cos[(q_0^2/\pi\hbar)Q_1(t_{2j}-t_{2j-1})]$ for the jth blip in the limit that the length of the $(j-1)$th sojourn tends to infinity. Finally, the term F_4 not only modulates (for $\varepsilon \neq 0$) the contribution of the self-interaction of the blips, but gives an interaction of all the blips with the zeroth sojourn (which, we recall, extends back to the initial time t_0, which we allow to tend to $-\infty$). This term is not usually particularly important in the unbiased case, but in the case of finite bias ($\varepsilon \neq 0$) it is essential to keep it if one is to get sensible behavior in the limit $t \to \infty$; it is the only term that is sensitive to the sign of ε, i.e., to whether we started in the upper or the lower well, and we clearly would expect on intuitive grounds that $P(t)$ [which, we recall, is defined relative to the initial state, i.e., as $\langle \sigma_z(t) \rangle$ where $\sigma_z(0) \equiv +1$] should behave quite differently in the two cases, in the limit $t \to \infty$.

B. Expression for $C(t)$

We now indicate more briefly how to obtain an expression similar to Eq. (4.17) for the symmetrized correlation function

$$C(t) \equiv \frac{1}{2Z} \mathrm{Tr}\{[\sigma_z(t)\sigma_z(0) + \sigma_z(0)\sigma_z(t)] \exp -\beta \hat{H}\}$$

$$\equiv \tfrac{1}{2} \langle \{\sigma_z(t), \sigma_z(0)\} \rangle_\beta \,, \tag{4.23}$$

where Z is the partition function, and the operator $\sigma_z(t)$ is taken in the Heisenberg representation with respect to the full Hamiltonian $\hat{H}$, i.e.,

$$\sigma_z(t) \equiv \exp(i\hat{H}t/\hbar)\sigma_z \exp(-i\hat{H}t/\hbar) \,. \tag{4.24}$$

We first relate $C(t)$ to the joint probabilities $P(\sigma'\sigma{:}t)$ defined as follows. Suppose we start at $t=0$ with the system-plus-environment in a thermal equilibrium state (i.e., with a density matrix proportional to $\exp -\beta\hat{H}$). Now suppose that at $t=0$ the system is observed to have a value $\sigma(=\pm 1)$ of σ_z, the environment being undisturbed by the observation. The system is again observed at some subsequent time t and found to have a value σ' of σ_z. The probability for this sequence of events is defined to be $P(\sigma',\sigma{:}t)$. To relate it to $C(t)$ we define, as in Sec. III, projection operators $\hat{\pi}_\pm \equiv \frac{1}{2}(1 \pm \hat{\sigma}_z)$, and note the identities $\hat{\pi}_+ + \hat{\pi}_- \equiv \hat{1}$, $\hat{\pi}_+ - \hat{\pi}_- = \hat{\sigma}_z$. It is then obvious[42] that we have

$$\sum_{\sigma'} \sigma' P(\sigma', \pm \,|\, {:}t) = \mathrm{Tr}[\hat{\pi}_\pm \exp(-i\hat{H}t)(\hat{\pi}_+ - \hat{\pi}_-)\exp(i\hat{H}t)\hat{\pi}_\pm \exp -\beta\hat{H}]/Z \equiv \langle \hat{\pi}_\pm \sigma_z(t) \hat{\pi}_\pm \rangle_\beta \tag{4.25}$$

(where in the first equality we used the cyclic invariance of the trace). Subtracting the relation for $\sigma=-1$ from that for $\sigma=1$, and writing $\hat{\pi}_- = 1 - \hat{\pi}_+$, we get

$$\sum_{\sigma,\sigma'} \sigma\sigma' P(\sigma',\sigma{:}t) = -\langle \sigma_z \rangle + \langle \hat{\pi}_+ \sigma_z(t) + \sigma_z(t)\hat{\pi}_+ \rangle \tag{4.26}$$

and a similar relation obtained by interchanging the $+$ and $-$ indices. Subtracting one relation from the other and using the definition (4.23) of $C(t)$, we find the intuitively rather obvious result

$$C(t) = \sum_{\sigma\sigma'} \sigma\sigma' P(\sigma',\sigma{:}t) \,. \tag{4.27}$$

For simplicity we shall discuss explicitly from here on the case of an unbiased system; the generalization is trivial. In this case the symmetry implies that $C(t)$ is just the expectation value of σ_z at time t, given that at time zero the system is known to be in the state $\sigma_z=+1$ and that apart from this we have thermal equilibrium [i.e., the density matrix of the "universe" is proportional to $\hat{\pi}_+ \exp(-\beta\hat{H})\hat{\pi}_+$]. The quantity $C(t) \equiv C^{(1)}(t)$ defined in this way is clearly analogous to the $P^{(1)}(t)$ defined in Sec. III. It is also possible to define a $C^{(2)}(t)$ that is the analog of $P^{(2)}(t)$, as follows: We assume that before some negative time t_0, which is eventually allowed to approach $-\infty$, the system and environment were uncoupled and were in their (independent) thermal equilibrium states. At time t_0 the coupling was switched on, and thereafter the system and environment were left alone except that at $t=0$ the system was observed to have the value $\sigma_z=+1$. Strictly speaking, the quantities $C^{(1)}$ and $C^{(2)}$ are obviously identical only if we assume that the behavior of the coupled system-environment complex is ergodic. We shall make this assumption,[43] or at least the assumption $C^{(1)}=C^{(2)}$ (which is actually rather weaker; see the discussion of $P^{(1)}$ and $P^{(2)}$ in Sec. III.A). Thus we shall take $C(t)$ to be given by $C^{(2)}(t)$ whenever it is convenient to do so.

[42] Here we implicitly assume, in accordance with the usual considerations of quantum measurement theory (see, for example, d'Espagnat, 1976, Sec. 14.4), that the effect of an "observation" is to project the density matrix that described the system just prior to observation onto the manifold corresponding to the appropriate eigenvalue of the observed quantity.

[43] In cases (if any) where this assumption does not hold, a discussion of the thermal equilibrium correlation functions is likely to be of somewhat academic interest anyway, since it is then not clear how one would prepare the thermal equilibrium state in real life.

It is now clear that $P(t)$ and $C(t)$ are just special cases, defined by the limits $t_c \to -\infty$ and $t_c \to 0$, respectively, of a more general quantity $P(t:t_c)$ defined as the expectation value of σ_z at a time $t > 0$, where the coupling is switched on in the way described above at a time t_0 which tends to $-\infty$ and the system is known to have been in the state $\sigma_z = +1$ for the period $t_c \le t \le 0$. It is clear that this quantity has a path-integral representation that is identical to the one derived in Sec. IV.A for its special case $P(t)$, except that an arbitrary combination of blips and sojourns is allowed to occur at any time before t_c (while for $t_c \le t \le 0$ the path is, of course, in state A). It is very straightforward to write down explicitly the resulting power-series expansion in Δ, but there is little point in doing so here. We merely note that in general the effect is not simply to multiply the series for $P(t)$ by a second power series, since the interaction between blips (and sojourns) at positive and negative times cannot be factorized in a simple way. However, we shall see in the next subsection (with a proviso) that, to the extent that a certain simple approximation for power series of the type found for $P(t)$ is valid, the quantities $P(t)$ and $C(t)$ are in fact equal.

C. Noninteracting-blip approximation

Equations (4.17)—(4.22), while exact, are exceedingly cumbersome. We shall now describe an approximation, which we call the "noninteracting-blip approximation," that simplifies them enormously. This approximation turns out to be exact (to lowest order in Δ/ω_c, etc.) in some regions of the parameter space and very good in most of the rest.

The approximation consists in two simple prescriptions:

(1) Set all the factors X_{jk} in Eqs. (4.20c) and (4.20d) equal to zero for $k \neq j-1$, and put $X_{j,j-1} = Q_1(t_{2j} - t_{2j-1})$.

(2) Set all the factors Λ_{jk} in Eq. (4.20b) equal to zero.

To motivate these prescriptions,[44] we note that with a spectral density $J(\omega) \sim \omega^s$ ($s \neq 1$) the functions $Q_1(t)$ and $Q_2(t)$ at zero temperature are simply proportional to the imaginary part and a constant-plus-the-real-part, respectively, of $(1 - i\omega_c t)^{1-s}$: This remains true of Q_1 (but not Q_2) at finite temperature. We also note that the length of a "typical" *sojourn* occurring in Eq. (4.18) is always at least of order Δ^{-1}. This is almost intuitively obvious, since the typical length of a blip-sojourn pair is of order t/n, which for the dominant terms in the series (4.17) is at least of order Δ, and since blips tend to be suppressed relative to sojourns because of the self-interaction term (4.20a). Consider first the justification of approximation (1). In the superohmic case $s > 1$ this is clearly extremely plausible, since $Q_1(t)$ is of order of (at most) some negative power of ω_c/Δ for typical configurations whenever t refers to a time difference that includes the length of a sojourn, while $Q_1(0)$ is zero identically. The case $s < 1$ is slightly more tricky: here we have to argue that the self-interaction term (4.20a) suppresses long blips to the extent that the average blip length is of order ω_c^{-1}, rather than (like the average sojourn length) of order at least Δ^{-1}. Now it is the *difference* of Q_1's that occurs in X_{jk}, and this difference is, by the above argument, of order $\omega_c^{-1}(d/dt)(\omega_c t)^{1-s}|_{t \sim \Delta^{-1}} \sim (\Delta/\omega_c)^s$, so the quantity X_{jk} should again be negligible for $j \neq k+1$ [and by the same reasoning $X_{j,j-1}$ should be well approximated by $Q_1(t_{2j} - t_{2j-1})$]. Finally, in the case of ohmic dissipation $Q_1(t)$ tends to a constant in the limit of large $\omega_c t$, so the same argument again goes through. Approximation (1) will be misleading only if either (a) there are strong cancellations in the multiple integral (4.18), which means that terms of relative order $(\Delta/\omega_c)^l (l > 0)$ have to be taken into account in the expressions (4.18) for the $K_n(t)$ themselves or (b) the corrections, though of relative order $(\Delta/\omega_c)^l$ in each individual K_n, add up in the series (4.17) so as to give a substantial contribution for large t. In case (b) we should expect important effects only for $t \gtrsim (\omega_c/\Delta)^l \tau$ (where τ is the typical time scale as defined in Sec. III), a regime not of interest to us. Case (a) can be discounted in any case for which the integrand of Eq. (4.18) is positive definite (as it is, for example, for the ohmic case with $\alpha < \frac{1}{2}$; see Appendix D.1); it appears exceedingly unlikely to arise, for the unbiased case, in any regime except possibly the ohmic one with $\frac{1}{2} < \alpha < 1$ (and then only dubiously; see Sec. V.E). Thus, with this one possible exception, it seems very probable that for $\varepsilon = 0$ approximation (1) is always valid for our purposes. For the biased case the situation is a little more problematic; see Sec. VII.

The justification of approximation (2) is not quite so general. With the same caveats as above, it should hold if (and only if) the length of a typical sojourn is large enough, and $Q_2(t)$ fall off fast enough, that all the Q_2's are small compared to 1 for $j \neq k$. Now $Q_2(t)$ increases, for ohmic and subohmic dissipation, as a function of t; hence these conditions are not guaranteed in the general case. Approximation (2) can, however, be justified in at least three different cases.

(a) Extreme weak-coupling case: because of the sum over the $\{\zeta_j\}$, it is clear that the effect of the factor F_2 [Eq. (4.20b)] is of the order of the square of the coupling constant β_n (or α), whereas the terms kept in the noninteracting-blip approximation give nontrivial effects of order β_n. Thus in the limit $\beta_n \to 0$ it is consistent to make this approximation.

(b) Superohmic case: for $s > 1$ at zero temperature, and $s > 2$ at finite temperature, the difference from its asymptotic value of quantity $Q_2(t)$ is very small for $t \gtrsim \Delta^{-1}$, which is a lower limit on the typical length of a sojourn. The asymptotic value merely renormalizes Δ; see Sec. VI. Thus the noninteracting-blip approximation is justified in this case.

[44] The arguments given below are presented in more detail, and sometimes with more rigor, in the context of specific parameter regimes in Secs. V and VI and Appendix D.

(c) "Golden-rule" limit: If the function $Q_2(t)$ *increases* with t, then the factor F_1 [Eq. (4.20a)] suppresses long blips to the extent that a typical blip is very much shorter than a typical sojourn. Because it is the *differences* of the Q_2's that enter the factor F_2, it then turns out that this factor can be set equal to unity with negligible error, again justifying the approximation. In this case [but *not* in cases (a) and (b)] the resulting expression turns out to coincide with that obtained from the "golden-rule" approach of Sec. III.D. It turns out that case (c) occurs in the subohmic case, in the ohmic case for large enough dissipation and/or temperature, and also in the case $1<s<2$ for high enough temperature.

Thus the noninteracting-blip approximation gives essentially exact results in three physically quite different limits. Because most of the rest of the parameter space is in some sense intermediate between these limits, it is very natural to expect that it would give results that are not qualitatively misleading almost everywhere. We shall verify in subsequent sections that this is so. We return in the Conclusion to a discussion of the physical meaning of this approximation.

Use of the noninteracting-blip approximation simplifies the expression for the influence functions F_n [Eq. (4.18)] very drastically and reduces the problem of finding $P(t)$ to the calculation and inversion of Laplace transforms. Let us consider the case $\varepsilon=0$, for which the situation is particularly simple (the case of finite bias is discussed in Sec. VII). The integrand F_n of Eq. (4.18) is now given by the simple product

$$F_n(t_1\cdots t_{2n})=\prod_{j=1}^{n}\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t_{1j}-t_{2j-1})\right]\exp-\frac{q_0^2}{\pi\hbar}Q_2(t_{2j}-t_{2j-1})\ , \tag{4.28}$$

and hence the expression for $P(t)$, Eq. (4.17), becomes

$$P(t)=\sum_{n=0}^{\infty}(-1)^n\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1\prod_{j=1}^{n}f(t_{2j}-t_{2j-1})\ , \tag{4.29}$$

$$f(t)\equiv\Delta^2\cos\left[\left[\frac{q_0^2}{\pi\hbar}\right]Q_1(t)\right]\exp-\left[\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ . \tag{4.30}$$

The formal similarity of Eq. (4.29) to the partition function of a system of particles in a one-dimensional, fixed volume suggests that we switch to the analog of an isobaric ensemble. This is done by taking the Laplace transform:

$$\tilde{P}(\lambda)=\int_0^\infty e^{-\lambda t}P(t)dt\ . \tag{4.31}$$

A few changes of the orders of integration yield

$$\begin{aligned}\tilde{P}(\lambda)&=\sum_{n=0}^{\infty}(-1)^n\int_0^\infty dt\int_0^\infty dt_1\cdots\int_0^\infty dt_{2n}e^{-\lambda(t_1+t_2\cdots+t_{2n})}\prod_{j=1}^{n}f(t_{2j})\\&=\sum_{n=0}^{n}(-1)^n[f(\lambda)]^n/\lambda^{n+1}=[\lambda+(f)\lambda]^{-1}\ ,\end{aligned} \tag{4.32}$$

where $f(\lambda)$ is the Laplace transform of $f(t)$

$$f(\lambda)\equiv\Delta^2\int_0^\infty\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp-\left[\lambda t+\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ . \tag{4.33}$$

Thus, in principle, $f(\lambda)$ can be calculated for any form of $J(\omega)$. The transform can then be inverted to obtain $P(t)$

$$\begin{aligned}P(t)&=\frac{1}{2\pi i}\int_C e^{\lambda t}\tilde{P}(\lambda)d\lambda\\&\equiv\frac{1}{2\pi i}\int_C e^{\lambda t}[\lambda+f(\lambda)]^{-1}d\lambda\ ,\end{aligned} \tag{4.34}$$

where C is the standard Bromwich contour, i.e., any contour from $-i\infty$ to $+i\infty$ lying entirely to the right of all singularities of $\tilde{P}(\lambda)$. In cases where explicit inversion is difficult, it is clear that much can nevertheless be learned from a study of the singularities of $\tilde{P}(\lambda)$.

Equation (4.34), with the definitions (4.33) and (4.22), gives a complete solution to the dynamics of the unbiased spin-boson problem within the noninteracting-blip approximation. [The slight generalization necessary in the case of finite bias ($\varepsilon\neq0$) is discussed in Sec. VII.] We note, further, that within this approximation $C(t)$ and $P(t)$ are identical for $\omega_c t\gg1$, since there is now no "interaction" in $C(t)$ between the positive- and negative-time parts of the path. However, this remark needs to be treated with some caution: the fact that the interblip interactions are negligible in the calculation of $P(t)$ in a given parameter regime does not rigorously imply that they are also negligible for $C(t)$, although it would certainly be very odd if their effect was dramatic.

V. OHMIC DISSIPATION: UNBIASED CASE

In this section we shall apply the formal results of Sec. IV to a calculation of the behavior of $P(t)$ for the case of zero bias ($\varepsilon=0$) an an ohmic form of dissipation, that is,

with $J(\omega)$ given by the expression [cf. Eq. (3.3)]

$$J(\omega)=\eta\omega\exp-\omega/\omega_c\ , \tag{5.1}$$

where ω_c is an arbitrary cutoff as described in Sec. II. As above, we define a dimensionless dissipation coefficient α by

$$\alpha\equiv\eta q_0^2/2\pi\hbar\ . \tag{5.2}$$

The characteristic frequencies of the problem, apart from $k_BT/\hbar$, are the "bare" tunneling frequency Δ in the Hamiltonian (3.1) and the cutoff ω_c; we recall that in most physically realistic problems, where the two-state model arises as a result of the (arbitrary) truncation of a two-well problem, these two parameters are not totally independent, in the sense that Δ is proportional to a constant times ω_c^α (see Sec. II). We reemphasize that in this paper we are always interested in the limiting behavior of the system in the limit of a small value of the ratio Δ/ω_c, and moreover that we shall not be interested in the behavior at very short times ($\lesssim\omega_c^{-1}$) nor at times so long that $P(t)$ is already negligibly small. Thus our problem is the behavior, for small Δ/ω_c and "interesting" times, of the quantity $P(t)$ as a function of the dimensionless dissipation coefficient α and the temperature T.

Before we embark on the details of the calculation, one general remark should be made. With the quantity Δ proportional to ω_c^α, there is only one quantity we can form with the dimensions of frequency from Δ and ω_c that is independent of ω_c, namely,

$$\Delta_r\equiv\Delta\left[\frac{\Delta}{\omega_c}\right]^{\alpha/(1-\alpha)}\ . \tag{5.3}$$

If, therefore, the whole idea of transforming our original two-well problem into a two-state problem is to make sense, we should expect $P(t)$ to be a function of Δ and ω_c only in the combination (5.3). If there are any regions of the parameter space where this is not the case, then we should expect that the behavior in these regions might be sensitive to details of the original two-well problem that are not necessarily reflected in the two-state model. With these preliminaries we now turn to the detailed form of $P(t)$ in the unbiased ohmic case.

A. General formulas

From the definitions (4.22), the functions $Q_1(t)$ and $Q_2(t)$ are given for the form (5.1) of $J(\omega)$ by

$$Q_1(t)=\eta\tan^{-1}\omega_c t\ , \tag{5.4a}$$

$$Q_2(t)=\tfrac{1}{2}\eta\ln(1+\omega_c^2t^2)+\eta\ln\left[\frac{\beta\hbar}{\pi t}\sinh\frac{\pi t}{\beta\hbar}\right]\ , \tag{5.4b}$$

where as usual we have set $\beta\equiv1/k_BT$. It is convenient until further notice to measure time in units of ω_c^{-1}. Thus the quantity $f(t)$, Eq. (4.30), which would give the contribution to the influence function of a totally isolated blip,[45] is given by

$$f(t)\equiv\cos[(q_0^2/\pi\hbar)Q_1(t)]\exp[-(q_0^2/\pi\hbar)Q_2(t)]$$
$$=\cos[2\alpha\tan^{-1}t]\left[\frac{(\pi t/\beta\hbar\omega_c)\mathrm{cosech}(\pi t/\beta\hbar\omega_c)}{(1+t^2)^{1/2}}\right]^{2\alpha}\ . \tag{5.5}$$

We note that in the limit $\beta\to\infty$ the quantity $f(t)$ may be written more succinctly as $\mathrm{Re}(1-it)^{-2\alpha}$. An important point to notice is that, irrespective of the value of β, $f(t)$ is positive for all t provided we have $\alpha\le\frac{1}{2}$. For $\alpha>\frac{1}{2}$, on the other hand, $f(t)$ oscillates in sign.

It is interesting to consider the integral

$$F(\alpha,\beta)\equiv\int_0^\infty f(t:\alpha,\beta)dt \tag{5.6}$$

which occurs in the golden rule expression (3.88) (with $\varepsilon=0$). In the limit $\beta\to\infty$ this quantity has rather unusual properties: as may be easily verified from the complex representation noted above, it is infinite for $\alpha<\frac{1}{2}$, equal to $\pi/2$ for α exactly equal to $\frac{1}{2}$, and zero for $\alpha>\frac{1}{2}$. At finite temperature the value of $F(\alpha,\beta)$ is always finite, and in the limit $\beta\hbar\omega_c\gg1$ of interest to us it is given, for all values of α, by

$$F(\alpha,\beta)=\frac{\sqrt{\pi}}{2}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left[\frac{\pi k_BT}{\hbar\omega_c}\right]^{2\alpha-1}\ . \tag{5.7}$$

Note that on the line $\alpha=\frac{1}{2}$, $F(\alpha,\beta)$ is independent of temperature and equal to $\pi/2$.

To obtain the complete expression for $P(t)$, we substitute Eqs. (5.4) into Eq. (4.20) and set $\varepsilon=0$. Incorporating the simplified F_4 for notational simplicity into F_3, we find that the three factors F_1,F_2,F_3 in the influence function $F_n(\{t_i\},\{\zeta_i\}:0)$ are given by

$$F_1=\prod_{j=1}^{n}[f'(b_j)]^{2\alpha}\ , \tag{5.8a}$$

$$F_2=\prod_{k=1}^{n}\prod_{j=k+1}^{n}\left[\frac{f'(b_j+b_k+u_{jk})f'(u_{jk})}{f'(b_j+u_{jk})f'(b_k+u_{jk})}\right]^{2\alpha\zeta_j\zeta_k}\ , \tag{5.8b}$$

$$F_3=\prod_{k=0}^{n-1}\cos\left[2\alpha\sum_{j=k+1}^{n}\zeta_jX_{jk}\right]\ . \tag{5.8c}$$

Here we have introduced the notation b_j,s_j for the length of the jth blip and the subsequent sojourn, respectively, and also defined the quantity

$$u_{jk}\equiv t_{2j-1}-t_{2k}\equiv s_k+\sum_{l=k+1}^{j-1}(b_l+s_l) \tag{5.9}$$

[45] It is convenient to redefine $f(t)$ at this point so as to omit the factor Δ^2 that was included in Eq. (4.30).

(so that $u_{j,j-1}\equiv s_{j-1}$); see Fig. 5 for a pictorial representation of these quantities. The quantity $f'(t)$ [which differs from $f(t)$ in Eq. (5.5)] occurring in Eqs. (5.8a) and (5.8b) is defined by

$$f'(t)=(1+t^2)^{-\alpha}\left[\frac{\beta\hbar\omega_c}{\pi t}\sinh\frac{\pi t}{\beta\hbar\omega_c}\right]^{-2\alpha}, \qquad [f(t)\equiv\cos(2\alpha\tan^{-1}t)\times f'(t)] , \tag{5.10}$$

and the quantity X_{jk} in Eq. (5.8c) is given by

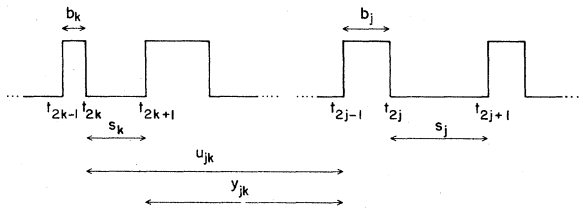

FIG. 5. Definition of the quantities appearing in Eqs. (5.8)–(5.11).

$$X_{jk}\equiv\tan^{-1}(t_{2j}-t_{2k+1})+\tan^{-1}(t_{2j-1}-t_{2k})-\tan^{-1}(t_{2j}-t_{2k})-\tan^{-1}(t_{2j-1}-t_{2k+1})$$
$$=\tan^{-1}\left[\frac{b_j s_k(b_j+s_k+2y_{jk})}{\{[1+y_{jk}(y_{jk}+s_k)][1+(y_{jk}+b_j)(y_{jk}+b_j+s_k)]+s_k^2\}}\right], \tag{5.11a}$$

where for subsequent convenience we define the quantity

$$y_{jk}\equiv t_{2j-1}-t_{2k+1}\equiv u_{jk}-s_k . \tag{5.11b}$$

Note that $y_{j,j-1}\equiv 0$. Also recall that t_0 is by convention to be taken equal to $-\infty$, so that we have, for all j,

$$X_{j0}=\tan^{-1}\left[\frac{b_j}{1+y_{j0}(y_{j0}+b_j)}\right] . \tag{5.12}$$

An alternative representation of the influence functions F_n that does not involve an explicit cosine is sometimes helpful. Omitting the tedious but straightforward algebra necessary to obtain it, we simply note the result: introducing a dummy variable $\eta_i=\pm 1$ for $i=0,1,\ldots,n-1$, we have

$$F_n\{t_i,\zeta_i;0\}=2^{-n}\sum_{\{\eta_i=\pm 1\}}[\Phi\{t_i,\zeta_i,\eta_i\}]^{2\alpha} , \tag{5.13}$$

$$\Phi\{t_i,\zeta_i,\eta_i\}\equiv\prod_{j=1}^{n}\frac{g(b_j)[1+y_{j0}(y_{j0}+b_j)+i\eta_0\zeta_1\zeta_j b_j]}{(1+b_j^2)}\prod_{k=1}^{j-1}[(D_{jk}+i\eta_k\zeta_j\zeta_{k+1}E_{jk})G_{jk}^{(\zeta)}M_{jk}^{(\zeta)}] , \tag{5.14}$$

where we have used the notation

$$D_{jk}\equiv[1+y_{jk}(y_{jk}+s_k)][1+(y_{jk}+b_j)(y_{jk}+b_j+s_k)]+s_k^2 , \tag{5.15a}$$

$$E_{jk}\equiv b_j s_k(b_j+s_k+2y_{jk}) , \tag{5.15b}$$

$$M_{jk}^{(\zeta)}\equiv\left[\frac{g(y_{jk}+b_j+b_k+s_k)g(y_{jk}+s_k)}{g(y_{jk}+b_j+s_k)g(y_{jk}+b_k+s_k)}\right]^{\zeta_j\zeta_k} , \tag{5.15c}$$

$$G_{jk}^{(\zeta)}\equiv\{[1+(y_{jk}+s_k)^2][1+(y_{jk}+b_j+b_k+s_k)^2]\}^{-1} \text{ if } \zeta_j=\zeta_k$$
$$\equiv\{[1+(y_{jk}+b_j+s_k)^2][1+(y_{jk}+b_k+s_k)^2]\}^{-1} \text{ if } \zeta_j=-\zeta_k , \tag{5.15d}$$

$$g(t)\equiv\frac{\pi t}{\beta\hbar\omega_c}\operatorname{cosech}\frac{\pi t}{\beta\hbar\omega_c} . \tag{5.15e}$$

When $j=1$ the curly bracket in Eq. (5.14) is defined to be unity. Clearly at zero temperature the factor $M_{jk}^{(\zeta)}$ is just unity. The expansion (5.13) is completely equivalent to Eqs. (5.8a)–(5.8c), and is more convenient for some purposes, particularly when α takes integral or half-integral values.

We shall now apply the formulas we have obtained to calculate $P(t)$ in various regions of the (α,T) plane. The level of mathematical rigor varies somewhat among the next five subsections: in Sec. V.B (the line $\alpha=\frac{1}{2}$), where we claim completely exact[46] results, and in Sec. V.D ($T=0$, $0<\alpha<\frac{1}{2}$), where the results are claimed to be exact up to a certain point, we have tried to be completely rigorous; in Sec. V.C, on the other hand (large α and/or large T), we have proceeded somewhat more intuitively, although we are confident that the results could if neces-

[46]In the sense specified there.

sary be put on a more rigorous footing. In Sec. V.E ($T=0, \frac{1}{2}<\alpha<1$) we would have liked, but have so far failed, to find a rigorous way of doing things; in Sec. V.F, having observed that the noninteracting-blip approximation gets things exactly right in Secs. V.B and V.C and at least qualitatively right in Sec. V.D, we go on to apply it to the whole of the (α,T) plane without any pretense of further justification.

B. The line $\alpha=\frac{1}{2}$

For the special value $\frac{1}{2}$ of α, the integrals in the expressions for the coefficients $K_n(t)$ in Eq. (4.18) are products of polynomial and (at $T\neq 0$) hyperbolic functions of the variables t_i, and this permits a brute-force evaluation of $P(t)$ to lowest order in the ratio Δ/ω_c (see below for the precise meaning of this statement). We start with the case of zero temperature, so that we can put the quantities $g(t)$ and $M_{jk}^{(\zeta)}$ in Eq. (5.15) equal to unity.

We recall that we are always interested in times large compared to ω_c^{-1}, so that in the dimensionless units being used the region of integration over the times t_i in Eq. (4.18) is very large compared to unity. Before embarking on the general argument we first consider the first three coefficients $K_n(t)$ in Eq. (4.17) for $P(t)$ explicitly. The first two are trivial: K_0 is identically unity and K_1 is given by

$$K_1(t)\equiv \int_0^t dt_2 \int_0^{t_2} dt_1 (1+b_1^2)^{-1} \quad (b_1\equiv t_2-t_1)$$
$$= t\tan^{-1}t-\tfrac{1}{2}\ln(1+t^2)\ . \tag{5.16}$$

It is clear that in the limit of large t the value of K_1 is just $(\pi/2)t$, the first correction being of order $\ln t$. The case of K_2 is slightly less trivial; from the general formula (5.15) (or directly) the integrand I_2 is, after summation over the η_i and ζ_i,

$$I_2=\frac{1}{2}\left[\frac{1+b_2(b_2+s_1)+s_1^2}{(1+b_1^2)(1+b_2^2)}\left[\frac{(b_1+s_1)(b_1+b_2+s_1)+1-b_1b_2}{(1+s_1^2)[1+(b_1+b_2+s_1)^2]}+\frac{(b_1+s_1)(b_1+b_2+s_1)+1+b_1b_2}{[1+(b_1+s_1)^2][1+(b_2+s_1)^2]}\right]\right], \tag{5.17}$$

where as usual $b_1\equiv t_2-t_1$, $s_1\equiv t_3-t_2$, $b_2\equiv t_4-t_3$. This expression is to be integrated, according to the usual prescription (4.18), over the variables $t_1\cdots t_4$, or equivalently over positive values of b_1,b_2,s_1, and the fourth variable s_2 subject to the constraint $b_1+s_1+b_2+s_2\leq t$.

The crucial point, now, is that the denominators in Eq. (5.17) always contain at least two more powers of the b's then the numerators, while the same is not true for s_1. Thus, if we wish to obtain from the three integrals over b_1, b_2, and s_1 something proportional to t, we must keep only those terms that contain an equal number of powers (four) of s_1 in the numerator and the denominator; we easily verify that any term with fewer than four powers of s_1 in the numerator will give at most a contribution of order $(\ln t)^2$. Moreover, in the terms we keep, the dominant contribution clearly comes from the region $s_1\gg 1$, $b_1,b_2\lesssim 1$, so that the denominators in the brackets can be approximated simply by s_1^4. Consequently I_2 reduces to the simple form

$$I_2=(1+b_1^2)^{-1}(1+b_2^2)^{-1}\ . \tag{5.18}$$

Further, because of the rapid convergence at large values of b_i, the upper limit of the integrations over the b_i can be taken to infinity, corrections again being at most of order $(\ln t)^2$. As a result we get $K_2(t)\cong\frac{1}{2}(\pi t/2)^2$.

It is now clear how to proceed in the general case. First, inspection of Eq. (5.14) reveals that there is a class of terms with the same number of powers of the s_j's [namely,[47] $4n(n-1)$] in the numerator and denominator. Since the integrand of K_n is everywhere positive (see above), these terms will contribute to K_n a term proportional to t^n. All other terms have at least one less power of the s_j's in the numerator than in the denominator, and also at least one less power of each b_j; hence such terms can contribute at most a term of order $t^{n-1}(\ln t)^2$, and hence are *prima facie* negligible for $t\gg 1$ (but see below). Thus we keep only the terms with the maximum number of powers of the s_j's in the numerator; this immediately means that the term in E_{jk} can be dropped for all j,k except when $j=k+1$ (as can the term in $i\eta_0\zeta_1\zeta_j b_j$ for $j\neq 1$), and since the sum over the η_j can now be taken independently, the remaining terms $E_{j,j-1}$ also drop out of the problem entirely, as does the term in η_0. Second, since the important region of integration is now clearly that of large s_j but small $b_j(\lesssim 1)$, the 1's and the b_j's in the expressions $G_{jk}^{(\zeta)}$ can be neglected; the quantity $G_{jk}^{(\zeta)}$ then becomes independent of the ζ_j, and if we define

$$R_{jk}\equiv\sum_{l=k+1}^{j-1} s_l \quad (j\geq k+2) \tag{5.19}$$

(so that $R_{j,j-2}\equiv s_{j-1}$), we have in this approximation

$$D_{jk}/G_{jk}^{(\zeta)}=(R_{jk}/R_{j,k-1})^2,\quad j\geq k+2$$
$$D_{jk}/G_{jk}^{(\zeta)}=s_{j-1}^{-2},\quad j=k+1\ . \tag{5.20}$$

Thus Eq. (5.19) for $F\{t_i,\zeta_i{:}0\}$ becomes independent of the ζ_i and is given simply by

$$F_n\{t_i,\zeta_i{:}0\}\equiv F_n\{t_i\}$$
$$=\prod_{j=1}^{n}\left[\frac{1}{1+b_j^2}\cdot\frac{R_{j0}^2}{s_{j-1}^2}\prod_{k=1}^{j-2}\left[\frac{R_{jk}}{R_{j,k-1}}\right]^2\right]$$
$$\equiv\prod_{j=1}^{n}(1+b_j^2)^{-1}\ , \tag{5.21}$$

[47] Note that since $y_{j,j-1}\equiv 0$, the term $D_{j,j-1}$ in Eq. (5.14) contributes only *two* powers of s_k to the numerator, not 4 as do the other D_{jk}. The remaining two powers are supplied by the term y_{j0}^2.

which is, of course, precisely the result we would have obtained by making the "noninteracting-blip approximation" from the start. What the above argument has shown is that the relative correction to each of the $K_n(t)$ from the terms neglected in this approximation is rigorously of order, at most, $t^{-1}\ (\ln t)^2$ in the limit of large t (where t is measured in units of ω_c^{-1}). Furthermore, the error in the value of K_n caused by taking the limits of integration over the b_j's to infinity is again obviously at most of relative order $t^{-1}\ (\ln t)^2$. Thus we reach the conclusion (restoring the units of time)

$$K_n(t)=\left[\frac{\pi}{2}\right]^n\frac{(\omega_c t)^n}{n!}[1+0(\ln^2\omega_c t/\omega_c t)]\quad t\to\infty\ . \tag{5.22}$$

If we neglect the correction terms, then the series (4.17) for $P(t)$ can be trivially summed to yield the strikingly simple result[48]

$$P(t)=\exp\left[-\frac{\pi}{2}\frac{\Delta^2}{\omega_c}t\right]\ . \tag{5.23}$$

It is very tempting, in the light of the above remarks, to assert that the result (5.23) is *exact* "in the limit $\omega_c\to\infty$." However, this statement needs careful definition if it is to be claimed as rigorously demonstrated by the above argument. From the fact that the corrections to each K_n individually are of relative order (roughly) $(\omega_c t)^{-1}$ in the limit $t\to\infty$ it does *not* follow that the corrections to the whole (oscillating) series for $P(t)$ are of the same relative order. All that we can show rigorously (see below) is that the corrections to Eq. (5.23) for $P(t)$ are negligible until this expression has itself fallen to a value of order Δ/ω_c. It may well be highly plausible that even for times larger than this the corrections to (5.23) are negligible, but it would require a separate argument to demonstrate this in a mathematically rigorous way. We return to this point at the end of this subsection.

It is clear that finite temperatures cannot affect the above argument (so long as we maintain the condition $\beta\hbar\omega_c\gg 1$, of course). The only difference now is that the expression for $\Phi\{t_i,\zeta_i,\eta_i\}$ [Eq. (5.14)] is multiplied by a product of extra single-blip terms $g(b_j)$ and a series of extra blip-interaction factors of the form $M_{jk}^{(\zeta)}$ [Eq. (5.15c)]. It is easy to prove [using the convexity upward of the function $\ln(\sinh z)-\ln z$] that the function $\sinh(x+a+b)\sinh x/\sinh(x+a)\sinh(x+b)$ is bounded below by the expression $x(x+a+b)/(x+a)(x+b)$, and (using the exponential representation of the sinh function) that it is bounded above by unity. Hence the factor $M_{jk}^{(\zeta)}$ lies between unity and

$$\left[\frac{(y_{ji}+b_j+s_k)(y_{jk}+b_k+s_k)}{(y_{jk}+b_j+s_k+b_k)(y_{jk}+s_k)}\right]^{\zeta_j\zeta_k},$$

and clearly cannot affect the argument developed above about the powers of the b_j's and s_j's. Furthermore, in the region of large s_j, $M_{jk}^{(\zeta)}$ can be simply set equal to unity. Hence the only effect of finite temperatures for large t is to multiply each of the factors $(1+b_j^2)^{-1}$ in the integrand of K_n by a factor $g(b_j)$. However, we already saw [Eq. (5.7)] that the integral of the function $g(b_j:T)(1+b_j^2)^{-1}$ from zero to infinity, i.e., the function $F(\alpha,\beta)$ for the special value $\alpha=\frac{1}{2}$, is actually completely independent of T for $\beta\hbar\omega_c\gg 1$. Hence Eq. (5.23) remains true along the whole line $\alpha=\frac{1}{2}$ in the (α,T) plane with the same accuracy[49] as at zero temperature.

At this point we digress to sketch a possible alternative approach to the dynamics, which is perhaps more elegant, although it requires even more algebra (which is given, for the case of zero temperature, in Appendix C). It is based on the idea that, provided we can neglect terms "of order ω_c^{-1}," there should be an equivalence between the spin-boson problem and a class of problems concerning *Fermi* systems (Guinea *et al.*, 1985b; see also Sec. III.E). For the special case $\alpha=\frac{1}{2}$ we can make the correspondence in a particularly simple way. In fact, consider the so-called Toulouse (1969) Hamiltonian

$$H_T=\sum_k\varepsilon_k c_k^\dagger c_k+V\sum_k(d^\dagger c_k+c_k^\dagger d)\ . \tag{5.24}$$

Here the operator[50] $d^\dagger(d)$ represents the creation (destruction) of a d electron in a localized state which is situated at exactly the Fermi energy, while $c_k^\dagger(c_k)$ creates an electron in a Bloch state k in this band; spin is neglected and all energies are measured from the Fermi energy. The density of conduction-band states $\rho(E)$ is assumed symmetric around the Fermi energy and tends to zero for large $|E|$ in a way that for the moment need not be specified in detail; it is sufficient to know that $\rho(E)$ is effectively constant for an energy range large compared to V. Concerning the system described by the Hamiltonian (5.24), we can pose the following question, which is precisely analogous to the one defining $P(t)$ in the spin-boson problem: Given that at time $t=-\infty$ the "environment" (i.e., the conduction electrons) was in its thermal equilibrium state, and that for all times $t\le 0$ the "system" (i.e., the d state) is known to have occupation number $n_d=1$, what is the quantity $\tilde{P}(t)\equiv 2\langle n_d(t)\rangle-1$ at a later (positive) time t? It is straightforward to calculate $\tilde{P}(t)$ as an infinite series in V (Appendix C). We then compare this series with the series for $P(t)$ in the spin-boson problem at $\alpha=\frac{1}{2}$ and show that, provided we (a) keep in the numerators of the expressions only those terms which give the leading contribution in the limit $\omega_c t\to\infty$ (cf. above) and (b) choose the density of states $\rho(E)$ in the Toulouse problem to have the specific form

$$\rho(E)=\rho_0\exp-|E|/\hbar\omega_c^{(T)}\ , \tag{5.25}$$

[48]This result was obtained in Chakravarty and Leggett (1984) as the $\alpha\to\frac{1}{2}$ limit of the formula for $0\le\alpha<\frac{1}{2}$.

[49]A more detailed examination shows that the accuracy of Eq. (5.23) actually increases with increasing temperature, since the latter tends to reduce the typical length of a blip (see Sec. V.C).

[50]In Sec. III.E this operator was written $\sigma^+(\sigma^-)$. For present purposes the two representations are completely equivalent.

then the two series have, term by term, exactly the same structure and are numerically identical if we make the correspondences [see Eq. (3.75)]

$$\omega_c = \omega_c^{(T)}, \quad \Delta = 2\hbar^{-1} V(\rho_0 \hbar \omega_c)^{1/2} . \tag{5.26}$$

Thus, with the choices (5.25) and (5.26), it may be plausibly argued (Guinea *et al.*, 1985b, though see below) that the dynamics of the Toulouse problem is identical for times $t \gg \omega_c^{-1}$ with that of the spin-boson problem on the line $\alpha = \frac{1}{2}$.

A *prima facie* advantage of this approach is that the Toulouse problem, being bilinear in the fermion operators, can be exactly diagonalized, and thus we would expect the behavior of $P(t)$ to be given by

$$\tilde{P}(t) = \exp -t/\tau, \quad \tau^{-1} = \frac{2\pi}{\hbar} V^2 \rho_0 , \tag{5.27}$$

which agrees precisely with Eq. (5.23).

We now return to the question of the corrections to $P(t)$ at long times. It should be emphasized that the correspondence with the Toulouse problem is (*prima facie* at least) of no help in determining these, since to make the correspondence we had to drop terms of relative order (roughly) $(\omega_c t)^{-1}$ in each $K_n(t)$ individually, and it is precisely the effect of dropping such terms that we wish to investigate. We may, however, make a *very conservative* estimate of the shortest times at which $P(t)$ is liable possibly to deviate from Eq. (5.23), as follows. Apart from the terms we kept to obtain Eq. (5.23), namely, those containing as many powers of the s_j in the numerator as in the denominator, the "most dangerous" terms are those in which one power of one of the s_j only is replaced by a power of one of the b_j [e.g., the term in Eq. (5.17) with $b_2 s_1$ replacing s_1^2 in the first factor in the numerator]. Each of these terms can at worst make a contribution of order $\ln^2(\omega_c t)/(\omega_c t/n)$ relative to the terms originally kept,[51] and there are at most of order n^3 such terms. Thus the correction δK_n to the value $K_n^{(0)}$ of K_n given by Eq. (5.22) can at worst be of order $[n^4(\ln^2\omega_c t)/(\omega_c t)]K_n^{(0)}$, and the correction to the whole expression for $P(t)$ can at worst be of order $(\Delta/\omega_c)^2 z^3 e^z$, where $z \equiv (\pi\Delta^2/2\omega_c)t$. Thus, to leading order in the small quantity Δ/ω_c, the correction to $P(t)$ can become comparable to $P(t)$ itself, if at all, only when the condition $z \gtrsim \ln(\omega_c/\Delta)$ is satisfied. By this time $P(t)$ is already at most of order Δ/ω_c, so that we can conclude that $P(t)$ is indeed correctly given by Eq. (5.23) until that expression has itself decreased at least to a value of order Δ/ω_c. It is in this sense, only, that we can justify rigorously the claim that Eq. (5.23) is exact "in the limit $\omega_c \to \infty$." Of course, it is entirely possible that Eq. (5.23) is in fact exact to within corrections of relative order $(\omega_c t)^{-1}$ [or, perhaps $(\ln^2\omega_c t)/(\omega_c t)$] for all t. However, while this may well be very plausible on physical grounds, we do not have at the time of writing a rigorous proof, and contrary to some claims that appear to be at least implicit in the literature we do not believe any such proof has yet been given.

[51]The corrections coming from the extension of the integrations over the b_j to infinity are of similar order.

C. The limit of high temperatures and/or strong dissipation

The argument of this subsection, and implicitly at least some of that of succeeding subsections, is based on the observation that the characteristic length of the blip-sojourn pairs that contribute appreciably to $K_n(t)$ is of order t/n. This follows because, while there are effects that tend to limit the length of the blips (see below), there is nothing to limit the length of the *sojourns*. As we see from Eq. (5.8), the factor F_1 in the influence function is independent of the sojourn length, and the factors F_2 and F_3 tend to constant values in the limit that the s_k tend to infinity for fixed finite b_j. Thus, on phase-space grounds alone, we see that the dominant contribution will come[52] from pairs of length of order t/n. Now, we recall that we are interested, not in totally arbitrary times, but in times such that $P(t)$ shows interesting structure and is not negligibly small. Suppose, for example, that we guess that as a result of our calculation we shall find $P(t)$ has an exponentially decay form $P(t) \sim e^{-t/\tau}$. Then, in the series for $P(t)$, the nth term becomes important approximately when $t \sim n\tau$. Thus we can say that the characteristic length of a blip-sojourn pair is simply of order τ. More generally, the length will be of order of the shortest characteristic time (other than ω_c^{-1}) associated with the series equation (4.17) for $P(t)$. This time must of course be determined self-consistently, by calculating the series under the above assumption.

Now, because of the factor F_1 in the influence function, all blips with a length much greater than $\beta\hbar/\alpha$ contribute an exponentially small amount [see Eq. (5.5)]. It is easy to verify that the factors F_2 and F_3 cannot cancel this small factor. Thus, whenever $2\alpha\beta\hbar/\pi$ is much less than the typical time scale defined, above, it is *prima facie* legitimate, in evaluating Eq. (4.18) for $K_n(t)$, to take all blip lengths negligibly short compared to the sojourn lengths. Under these conditions the formula simplifies enormously: the factor F_2 is unity, and the X_{jk} becomes zero except for $X_{j,j-1}$, which is equal to $\tan^{-1} b_j$. Thus the influence function has the simple form

$$F_n\{t_i, \zeta_i; 0\} = \prod_{j=1}^{n} f(b_j) \quad (b_j \equiv t_{2j} - t_{2j-1}) , \tag{5.28}$$

[52]This argument could fail if, because of near-exact cancellations or for some other reason, the contribution of these pairs were anomalously small. This might happen in the regime $T \to 0$, $\frac{1}{2} < \alpha < 1$ (see Sec. V.E); however, there seems no reason to believe it is likely to happen anywhere else in the (α, T) plane for $\varepsilon = 0$ (in particular, we in effect exclude it rigorously for $\alpha < \frac{1}{2}$, $T = 0$ in Appendix D.1, and it seems very probable that the proof could be generalized to finite T).

where $f(t)$ is the function defined by Eq. (5.5) (and we revert to measuring time in units of ω_c^{-1}). This is, of course, precisely the form postulated in the non-interacting-blip approximation introduced in Sec. IV.C. Moreover, since the length of the blip is by hypothesis limited by the strongly decreasing factor $f(b_j)$ to a value much less than the characteristic length of a blip-sojourn pair, in doing the integration over $b_j \equiv t_{2j} - t_{2j-1}$ we can extend the upper limit of integration to infinity. Then each blip-sojourn pair (b_j, s_j) contributes a factor proportional to $t_{2j} - t_{2j-2}$, and since we must of course still take into account the mutual exclusion of the pairs, the remaining integrations over the t_{2j} give a series that sums to a simple exponential formula. Thus we obtain, using Eqs. (5.6) and (5.7), the simple result (where we restore dimensional units for the time)

$$P(t) = \exp -t/\tau \,, \tag{5.29}$$

$$\tau^{-1} = (\Delta^2/\omega_c) F(\alpha,\beta) = (\Delta^2/\omega_c) \frac{\sqrt{\pi}}{2} \frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})} \left[\frac{\pi k T}{\hbar \omega_c} \right]^{2\alpha-1} . \tag{5.30}$$

This is, of course, nothing but the "golden-rule" result that was written down in Sec. III.D [Eqs. (3.37) and (3.38)] specialized to the case of ohmic dissipation and zero bias. We emphasize, however, that we have demonstrated *explicitly* (rather than assuming) that the correct expression $P(t)$ at arbitrary time is obtained by exponentiating the second-order perturbation-theoretic expression for the transition probability; this point is not entirely trivial, as we shall see when we come to discuss the case of finite bias in Sec. VII.

It is instructive to rewrite Eq. (5.30), for $\alpha < 1$, in terms of the renormalized tunneling frequency Δ_r defined by Eq. (5.3) [$\Delta_r \equiv \Delta(\Delta/\omega_c)^{\alpha/1-\alpha}$]:

$$\tau^{-1} = \frac{\sqrt{\pi}}{2} \frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})} \frac{\Delta_r^2}{k_B T/\hbar} \left[\frac{\pi k_B T}{\hbar \Delta_r} \right]^{2\alpha} . \tag{5.31}$$

We see that τ depends only on Δ_r and is therefore independent of the arbitrary truncation cutoff ω_c, as expected. For $\alpha \geq 1$ the quantity Δ_r is not defined, but it is easily checked that Eq. (5.3)) is still independent of ω_c. We note that the numerical coefficient $(\pi/\sqrt{2})[\Gamma(\alpha)/\Gamma(\alpha+\frac{1}{2})]$ tends to $(2\alpha)^{-1}$ for $\alpha \to 0$ and to $\frac{1}{2}\sqrt{\pi/\alpha}$ for $\alpha \to \infty$, and for $\alpha = \frac{1}{2}$ is equal to $\pi/2$. Thus, along the line $\alpha = \frac{1}{2}$, we recover the exact result of Sec. V.B, while in the limits $\alpha \to 0$ and $\alpha \to \infty$ our results agree, apart possibly from α-dependent constants in τ^{-1}, with those obtained by other methods (see Secs. III.B and III.C). It is amusing to note that the temperature dependence of the relaxation rate given by Eq. (5.30) changes sign at $\alpha = \frac{1}{2}$; this may be qualitatively understood as indicating that, for weak damping, thermal noise tends to "observe" the system and hence inhibit tunneling (cf. Simonius, 1978; Harris and Stodolsky, 1981, 1982), while for strong damping it increases the relaxation by providing an extra activation mechanism.

Let us now examine the self-consistency of the procedure used to obtain Eq. (5.29). Our basic assumption was that the characteristic length of the blips, which is of order $\beta\hbar/\alpha$, was much smaller than the characteristic time defined by the series of $P(t)$. Thus, for self-consistency, $\beta\hbar/\alpha$ must be much less than the τ defined by Eq. (5.30). Dropping numerical factors of order unity, we find that this condition reduces for $\alpha < 1$ to the inequality

$$\frac{k_B T}{\hbar} \gg \Delta_r \left[\frac{\Gamma(\alpha)}{\alpha \Gamma(\alpha+\frac{1}{2})} \right]^{1/2(1-\alpha)} . \tag{5.32}$$

For $\alpha \ll 1$ we have $\Gamma(\alpha) \sim \alpha^{-1}$, and the exponent of the bracket is nearly $\frac{1}{2}$, while for larger values of α the dependence of the quantity in large parentheses is relatively weak, except close to $\alpha = 1$. Hence, generally speaking, the condition for the results to hold is approximately

$$\alpha k_B T/\hbar \gg \Delta_r \quad (\alpha < 1) \,, \tag{5.33}$$

though this condition is too stringent near $\alpha = 1$. (A somewhat better—and weaker—criterion is given in Sec. V.F.) For $\alpha > 1$, since by hypothesis both Δ and $k_B T/\hbar$ are small compared to ω_c, the criterion is automatically fulfilled for any temperature, so that Eq. (5.29) should be valid everywhere to the right of the line $\alpha = 1$, in agreement (apart from the prefactor) with the results of Bray and Moore (1982). However, it is important to observe that they are also valid for the vast bulk of the portion of the plane to the *left* of this line, despite the fact that the physics involved is radically different in the two extremes.

D. $T = 0$, $0 \leq \alpha < \frac{1}{2}$

We next study the case of zero temperature and α in the range between zero and $\frac{1}{2}$. Since we should expect, on rather general grounds, that the deviation from the simple oscillating behavior of the uncoupled system is an increasing function both of α and of T, this region is the most promising, in an ohmically dissipative system, for the observation of oscillations. Thus, for example, in the context of the so-called macroscopic quantum coherence phenomenon (Leggett and Garg, 1985) this is the region of primary interest.

The exact expression for the quantity $P(t)$ is obtained by inserting Eqs. (5.8a)—(5.8c) into Eqs. (4.17)—(4.19), with F_4 incorporated into F_3 as noted above and the function $f'(t)$ now simply equal to $(1 + \omega_c^2 t^2)^{-1/2}$. The resulting formula is quite complex in appearance: see Appendix D, Eqs. (D1)—(D3). Let us, however, imagine for a moment that we could set, in Eq. (5.8), $F_2 = F_3 = 1$. Then we would have, in the expression for the coefficients $K_n(t)$ in the power series (4.17), a multiple integral of the form

$$\int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1} \cdots \times \int_0^{t_2} dt_1 \prod_j [1 + \omega_c^2 (t_{2j} - t_{2j-1})^2]^{-\alpha} . \tag{5.34}$$

It is evident that for $\alpha < \frac{1}{2}$ and $\omega_c t \gg 1$ the major contribution to such an integral will come from regions where both the blips and the sojourns have lengths very much greater than ω_c^{-1}. Consequently, provided we have[53] $\omega_c t \gg 1$, it is extremely plausible that in the true expression [Eq. (D2)] for $K_n(t)$ we can make the following approximations:

(1) Replace everywhere the factor $[1+\omega_c^2(\delta t)^2]$ by $\omega_c^2(\delta t)^2$ (where δt is an interval between any pair of t's).

(2) Replace the quantity X_{jk} by zero for any pair j,k other than $k=j-1$.

(3) Replace the quantity $X_{j,j-1}$ by $\pi/2$.

These replacements were made, on intuitive grounds, in Chakravarty and Leggett (1984) and have also been made, for the more general case of ε not necessarily zero, in Grabert and Weiss (1985). However, it is by no means trivial to justify them rigorously for the "interesting" values of t, which crudely speaking are of order Δ_r^{-1} (see below). In Appendix D we do in fact justify them rigorously "in the limit $\Delta/\omega_c \to 0$" by which we mean the following: Given any finite value of t in units of the "interesting" time scale $\Delta_{\rm eff}^{-1}$ ($\sim \Delta_r^{-1}$, see below), then we can always find a value of Δ/ω_c such that the error induced by the above replacements is arbitrarily small, either compared to 1 or compared to the value of $P(t)$ calculated by making them. We emphasize that the proof is by no means trivial, that it *fails* for the case of finite bias ($\varepsilon \neq 0$), and that we have *not* proved that given some small number δ we can find a value of Δ/ω_c that will make the error introduced smaller than δ for *all* t. However, for practical purposes the result stated above is quite adequate, since it guarantees that in the limit $\Delta/\omega_c \to 0$ the behavior of $P(t)$ may be calculated by the above approximations until its envelope has fallen to a value that tends to zero in this limit.[54] In the future, when we refer to our results for $P(t)$ as "exact in the limit $\Delta/\omega_c \to 0$" we shall be using the words in the above precisely defined sense.

The expression for $P(t)$ that results from making the above approximations is

$$P(t)=\sum_{n=0}^{\infty}(-1)^n\Delta^{2n}K_n(t)\ , \tag{5.35}$$

$$K_n(t)\equiv 2^{-n}\sum_{\{\xi_m=\pm 1\}}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}\cdots\int_0^{t_2}dt_1 F_n(t_1,t_2\cdots t_{2n};\xi_1,\xi_2\cdots\xi_n)\ , \tag{5.36}$$

$$F_n\{t_i,\xi_m\}\equiv(\cos\pi\alpha)^n\prod_{j=1}^{n}[\omega_c(t_{2j}-t_{2j-1})]^{-2\alpha}\prod_{k=1}^{n}\prod_{j=k+1}^{n}\left[\frac{(t_{2j}-t_{2k})(t_{2j-1}-t_{2k-1})}{(t_{2j}-t_{2k-1})(t_{2j-1}-t_{2k})}\right]^{2\alpha\xi_j\xi_k}\ . \tag{5.37}$$

Let us introduce the dimensionless time variable

$$y\equiv\Delta_{\rm eff}t\ , \tag{5.38}$$

where the effective inverse time scale $\Delta_{\rm eff}$ is given by

$$\Delta_{\rm eff}\equiv[\Gamma(1-2\alpha)\cos\pi\alpha]^{1/2(1-\alpha)}\Delta_r\quad[\Delta_r\equiv\Delta(\Delta/\omega_c)^{\alpha/1-\alpha}]\ . \tag{5.39}$$

Note that $\Delta_{\rm eff}$ is always of order Δ_r, in particular being equal to Δ_r in the limit $\alpha\to 0$ and to $(\pi/2)\Delta_r$ in the limit $\alpha\to\frac{1}{2}$. The factor $\Gamma(1-2\alpha)$ is introduced into the definition for subsequent convenience: when it is included, $\Delta_{\rm eff}$ is indeed the true time scale, as we shall verify. It is now evident that $P(t)$ is a function only of the dimensionless variable y, being given by the expression (Chakravarty and Leggett, 1984).

$$P(t)=P_r(y)\equiv P_r(\Delta_{\rm eff}t)\ , \tag{5.40}$$

where the function $P_r(y)$ is defined by the infinite series

$$P_r(y)\equiv\sum_{n=0}^{\infty}(-1)^n\tilde{K}_n(\alpha)y^{2n(1-\alpha)}\ , \tag{5.41}$$

$$\tilde{K}_n(\alpha)\equiv[\Gamma(1-2\alpha)]^{-n}\times\int_0^1 dz_{2n}\int_0^{z_{2n}}dz_{2n-1}\cdots\int_0^{z_2}dz_1\prod_{j=1}^{n}(z_{2j}-z_{2j-1})^{-2\alpha}\times 2^{-n}\sum_{\{\xi_j=\pm 1\}}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}\left[\frac{(z_{2j}-z_{2k})(z_{2j-1}-z_{2k-1})}{(z_{2j}-z_{2k-1})(z_{2j-1}-z_{2k})}\right]^{2\alpha\xi_j\xi_k}\ . \tag{5.42}$$

[53]For $\omega_c t \lesssim 1$ it is clear that the corrections to 1 in $P(t)$ are of order $(\Delta/\omega_c)^2$ at most, so this region is of little interest.

[54]As in the case $\alpha=\frac{1}{2}$, our formal argument does not rigorously exclude the possibility that at even larger times $P(t)$ has nontrivial behavior, conceivably even rising again to a magnitude of order 1; however, this possibility seems so remote as to be negligible in practice.

We want to emphasize that, for $\alpha<\frac{1}{2}$ and in the limit $\Delta/\omega_c\to 0$, the result (5.40) is *rigorous*: it is *not* a result of making the noninteracting-blip approximation or any other approximation. Thus the problem is reduced, in principle, to the evaluation of the numbers $\tilde{K}_n(\alpha)$ and the summation of the resultant series.

It is of course entirely conceivable that the function $P_r(y)$ defined by Eq. (5.41) is some simple well-known function that we have been unable to recognize. Assuming this is not so, we should like to obtain a reasonable approximation to $P_r(y)$ for, at least, the first few cycles: in particular, for the study of the macroscopic quantum coherence phenomena and the related question of tests of quantum mechanics versus macroscopic realism (Leggett and Garg, 1985), it should be adequate to find an approximation that is valid to, say, one percent over the first cycle or so. For this purpose, a numerical computation of the coefficients $\tilde{K}_n(\alpha)$ for, say, $n\leq 20$ should be quite sufficient.[55] We have not attempted, at the time of writing, such a numerical computation; instead, we shall investigate how much information about the function $P_r(y)$ can be obtained by analytical means.

Suppose, first, that we decided to ignore the "interblip correlation" term in Eq. (5.42), that is, to set the factor in large parentheses equal to one everywhere. Let the resulting expression for $P_r(y)$ be denoted $P_r^{(0)}(y)$. It is very easy to show that the corresponding expression for the coefficients $\tilde{K}_n(\alpha)$, which we denote $\tilde{K}_n^{(0)}(\alpha)$, is simply

$$\tilde{K}_n^{(0)}(\alpha)=\Gamma^{-1}[2n(1-\alpha)+1]\ . \tag{5.43}$$

The series (5.41) can then be summed by using Hankel's contour integral representation (Gradshteyn and Ryzhik, 1980, p. 935, 8.315) for the reciprocal of the Γ function, summing over n, and evaluating the resultant integral by deformation of the contour. Alternatively, the function $P_r^{(0)}(y)$ can be evaluated by taking the Laplace transform explicitly (see Sec. V.F, below) or by recognizing (Grabert and Weiss, 1985) that when expressed in terms of the variable $(-y)^{2(1-\alpha)}$ it is just a known special function, namely, the Mittag-Leffler function (Erdelyi *et al.*, 1955, p. 206). In any event the result is

$$P_r^{(0)}(y)=P_{\rm coh}(y)+P_{\rm inc}(y)\equiv\psi(y)\ , \tag{5.44a}$$

$$P_{\rm coh}(y)\equiv\frac{1}{1-\alpha}\cos\left\{\left[\cos\left[\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right]\right]y\right\}\times\exp-\left\{\left[\sin\left[\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right]\right]y\right\}, \tag{5.44b}$$

$$P_{\rm inc}(y)\equiv-\frac{\sin 2\pi\alpha}{\pi}\int_0^\infty dz\frac{z^{2\alpha-1}e^{-zy}}{z^2+2z^{2\alpha}\cos 2\pi\alpha+z^{4\alpha-2}}\ . \tag{5.44c}$$

A number of features of Eq. (5.44) should be noted. (1) The Q factor of the coherent oscillations given by (5.44b) is completely independent of the time scale $\Delta_{\rm eff}^{-1}$ and is given by $\cot[\pi/2(\alpha/1-\alpha)]$. Hence the system is completely undamped in the limit $\alpha\to 0$ and becomes overdamped at $\alpha=\frac{1}{2}$. (2) If we take the limit $\alpha\to\frac{1}{2}$, we obtain the simple result $\psi(y)=\exp-y$, which is identical to that obtained in Sec. V.B [Eq. (5.23)], since for $\alpha=\frac{1}{2}$ we have $y=(\pi/2)\Delta_r t=(\pi\Delta^2/2\omega_c)t$. (3) Not only is $\psi(0)$ unity, as of course it must be, but $(d\psi/dt)_{t=0}$ is zero for $\alpha<\frac{1}{2}$ [this follows directly from Eq. (5.41)]. (4) For $t\gg\Delta_{\rm eff}^{-1}$ and not too small α, $\psi(y)$ is dominated by the "incoherent" part, Eq. (5.44c), which is always negative and is asymptotically given by

$$\psi(y)\approx\pi^{-1}\sin(2\pi\alpha)\Gamma(2-2\alpha)y^{-2(1-\alpha)}\ . \tag{5.45}$$

Note that the coefficient of this term vanishes[56] in the limit $\alpha\to\frac{1}{2}$. (5) Even for quite small t the incoherent part can in general be quite comparable to the oscillating term. For example, for $\alpha=\frac{1}{3}$ the former actually exceeds the latter after the first half-cycle.[57]

We now turn to the rather delicate question of the corrections to the approximation $\psi(y)$ for $P_r(y)$ introduced by the interblip correlations, that is, the second factor in the integrand of (5.42). Let us first look at the question somewhat intuitively. First, because of the sum over the values ± 1 of the ζ_j, the difference between $P_r(y)$ and $\psi(y)$ must vanish[58] as α^2 in the limit $\alpha\to 0$. Second, consider the behavior in the limit $\alpha\to\frac{1}{2}$. For this purpose it is convenient to consider a single term (j,k) in the product in Eq. (5.42), choose specific values of ζ_j and ζ_k, and set as above

$$z_{2j}-z_{2j-1}\equiv b_j,\quad z_{2k}-z_{2k-1}\equiv s_k\ ,$$
$$z_{2j-1}-z_{2k}\equiv u_{jk}\quad(\equiv s_k \text{ for } j=k+1)\ .$$

Then the interblip correlation term in question is of the form

$$\left[1+\frac{b_j b_k}{u_{jk}(b_j+b_k+u_{jk})}\right]^{2\alpha\zeta_j\zeta_k} \tag{5.46}$$

and multiplies, in the integrand of Eq. (5.42), factors of $b_j^{-2\alpha}$ and $b_k^{-2\alpha}$. Now, in general we would expect a "typical" length of a blip-sojourn *pair* to be of order n^{-1}, and

[55] An alternative, and possibly better, approach might be to refine our numerical calculation of the amplitudes A_m and frequencies e_m [see Eqs. (5.47) and Appendix D.3] by including further-neighbor correlations.

[56] However, the contribution of the "incoherent" part does not vanish in this limit: it becomes $(-\frac{1}{2})$ times the "coherent" part.

[57] For $\alpha=\frac{1}{4}$, on the other hand, the effect at this point is quite small, which shows how sensitive the qualitative behavior is to α. For completeness we should note that in each case the term with $m=2$ in Eq. (5.47b) below nearly cancels the contribution of $P_{\rm inc}$ at this particular value of t (one half-cycle); however, since this term is nearly constant over the first few cycles, it clearly cannot restore anything like a simple damped oscillation.

[58] Because there is no sum over independent values ± 1 of the combination $\zeta_j\zeta_k$, this result is in fact not completely obvious. It is established rigorously in Appendix D.

hence a typical value of u_{jk} is at least $(j-k-1)n^{-1}$. On the other hand, if we were to neglect the correlations, the principal contribution to the integral, near $\alpha=\frac{1}{2}$ where the factor $b_k^{-2\alpha}$ rises steeply for small b_k, would come from blips of length of order $(1-2\alpha)n^{-1}$. Hence the second term in large parentheses in (5.46) is "typically" of order $[(1-2\alpha)/(j-k-1)]^2$. The nearest-neighbor pairs need special consideration: in this case the correction to unity can be large, if $u_{jk}\equiv s_k$ is small. However, it is clear that this region will give a negligible contribution if $\zeta_j=-\zeta_k$, while for $\zeta_j=+\zeta_k$ it gives a contribution smaller[59] by a factor of order $(1-2\alpha)$ than the leading contribution [which corresponds to setting the quantity in large parentheses in Eq. (5.46) equal to one]. Thus we would conjecture (a) that the corrections to $P_r^{(0)}(y)\equiv\psi(y)$, that is, to a calculation that completely neglects all interblip correlations, would be of order α^2 as $\alpha\to 0$ and of order $(1-2\alpha)$ as $\alpha\to\frac{1}{2}$ and (b) that corrections to a calculation that completely takes into account nearest-neighbor correlations but neglects all others—call the result of such a calculation $P_r^{(1)}(y)$—should be of order α^2 as $\alpha\to 0$ and of order $(1-2\alpha)^2$ as $\alpha\to\frac{1}{2}$.

In Appendix D.2 we confirm these conjectures as regards the $\alpha\to 0$ limit by deriving a rigorous upper limit [Eq. (D34)] to the corrections to each $\tilde{K}_n$ from *all* interblip correlations [hence to the correction to $P_r^{(0)}(y)$], which tends to zero as α^2 in the limit $\alpha\to 0$. This limit is not very useful in the present context[60] in the limit $\alpha\to\frac{1}{2}$, as it merely implies that $\tilde{K}_n$ is bounded above by the expression $(2^n)\tilde{K}_n^{(0)}$, not that it tends to $\tilde{K}_n^{(0)}$ itself. However, we have also been able to show (Appendix D.2) that the corrections to $\tilde{K}_n^{(0)}$ and hence to $P_r^{(0)}(y)$ are of order $(1-2\alpha)$ in the limit $\alpha\to\frac{1}{2}$, and that the corrections from the non-nearest-neighbor interactions not included in $P_r^{(1)}(y)$ are of order $(1-2\alpha)^2$ in the same limit. Finally, we can make an explicit formal expansion of the $\tilde{K}_n(\alpha)$ in terms of the variables α and $\gamma\equiv 1-2\alpha$, and show that the lowest-order correction to the values obtained in the nearest-neighbor calculation is indeed of order $\alpha^2\gamma^2$. Of course, none of these arguments demonstrates that $P_r^{(1)}(y)$ is an accurate approximation to $P_r(y)$ for all values of y however large: the relative error in $\tilde{K}_n(\alpha)$ increases with n, and hence for large y could be very important [see also the discussion below of the difference between $P_r^{(1)}(y)$ and $P_r^{(0)}(y)$]. However, these arguments do establish that for any finite value of y it is possible to choose a value of α close enough to zero that the corrections to $P_r^{(1)}(y)$ [or $P_r^{(0)}(y)\equiv\psi(y)$, which coincides with it in this limit] are negligible; they also make it overwhelmingly plausible that a similar statement holds with respect to a choice of α close to $\frac{1}{2}$, and that for times within the first few cycles, at least $P_r^{(1)}(y)$ is a very good approximation to $P_r(y)$ for all α in the range $0\le\alpha<\frac{1}{2}$.

The expression $P_r^{(1)}(y)$ for $P_r(y)$, which results if we keep, in the second term in the integrand of Eq. (5.42), only nearest-neighbor correlations, is calculated in Appendix D.3, by a transfer matrix method. If we neglect the problematical constant term discussed there, it has the strikingly simple structure

$$P_r^{(1)}(y)=\sum_{m=1}^{\infty}A_m(\alpha)\psi\{[e_m(\alpha)]^{1/(2-2\alpha)}y\} \tag{5.47a}$$

or, equivalently,

$$\begin{aligned}P^{(1)}(t)&=\sum_{m=1}^{\infty}A_m(\alpha)\psi(\Delta_m t)\ ,\\ \Delta_m(\alpha)&\equiv\Delta_{\rm eff}[e_m(\alpha)]^{1/(2-2\alpha)}\ ,\end{aligned} \tag{5.47b}$$

where $e_m(\alpha)$ are the eigenvalues of the transfer matrix corresponding to the nearest-neighbor interactions, and $A_m(\alpha)$ are the corresponding amplitudes. The numerically computed values of $A_m(\alpha)$ and $e_m(\alpha)$ are given in Table III; we note that in the limit $\alpha\to 0$ and $\alpha\to\frac{1}{2}$ the coefficients A_m vanish except for $m=1$, while A_1 and $e_1(\alpha)$ both tend to unity; thus we recover the expression $\psi(y)$ in these limits. [It further turns out, upon inspection of the numbers in the table, that the corrections are of order α^2 and $(1-2\alpha)$, respectively, in accordance with our conjecture (a) above.] For intermediate values of α, the coefficient $A_1(\alpha)$ of the leading term is always close to unity, while A_2 is never greater than about 0.06 and the higher A_m's are much smaller.

It is clearly intuitively tempting to conjecture that the result of considering further-neighbor interactions would be simply to reproduce Eq. (5.47), with, however, the expressions for $A_m(\alpha)$ and $\Delta_m(\alpha)$ somewhat modified. At the time of writing we have been unable either to prove or to disprove this conjecture, and will just make a few remarks in this connection.

(1) Not only is the expression for $P(t)$ given by Eq. (5.40) an arbitrarily good approximation to its true value in the limit $\Delta/\omega_c\to 0$ (as we have seen above), but the approximate form of (5.40) given by summing only lth-neighbor interactions is also an arbitrarily good approximation to the value of $P(t)$ which would be obtained by keeping only lth-neighbor interactions in the exact expression (5.8).[61]

(2) It is shown at the end of Appendix D.3 that the result of summing interactions up to lth neighbors in Eq. (5.41) is to produce an expression of the form (5.47) *plus* a polynomial $\Delta P^{(l)}(t)$ of order $l-1$ in t.

(3) Equation (5.47) clearly tends to zero in the limit $t\to\infty$. From considerations (1)—(3) it follows immediately that *if* the lth-neighbor approximation $P^{(l)}(t)$ to the true form of $P(t)$ is guaranteed to be bounded in magnitude by unity for all t (and, in particular, in the limit $t\to\infty$), then for any finite l the polynomial $\Delta P^{(l)}(t)$ must

[59] This is because each introduction of the correction cancels two terms ($b_j^{-2\alpha}$ and $b_k^{-2\alpha}$) that would otherwise each give a factor $(1-2\alpha)$.

[60] However, the fact that we can obtain a rigorous bound (for all $\alpha<\frac{1}{2}$) on $\tilde{K}_n$ relative to $\tilde{K}_n^{(0)}$ at all is crucial to the argument of Appendix D.1.

[61] How we treat the cosine factors is clearly irrelevant to the present argument.

TABLE III. The first two eigenvalues of the transfer matrix $\hat{\kappa}$ and the associated amplitudes.

α	$e_1(\alpha)$	$A_1(\alpha)$	$e_2(\alpha)$	$A_2(\alpha)$
0.01	1.000 150	0.9998	5.274×10^{-4}	1.11×10^{-4}
0.02	1.000 603	0.9994	2.106×10^{-3}	4.35×10^{-4}
0.1	1.012	0.988	5.251×10^{-3}	9.13×10^{-3}
0.2	1.039	0.962	2.180×10^{-2}	2.83×10^{-2}
0.25	1.052	0.950	3.500×10^{-2}	3.90×10^{-2}
0.3	1.06	0.94	5.25×10^{-2}	4.8×10^{-2}
0.4	1.06	0.94	1.05×10^{-1}	5.3×10^{-2}
0.45	1.05	0.95	1.45×10^{-1}	4.0×10^{-2}
0.495	1.01	0.99	1.95×10^{-1}	6.0×10^{-3}

vanish identically except possibly for its constant term. It would then follow immediately that the true $P(t)$ is indeed given by an expression, apart possibly from a constant, of the form (5.47), where the $e_m(\alpha)$ and $A_m(\alpha)$ are given by calculating them for increasing finite l and taking the limit $l\to\infty$.[62]

Unfortunately, while it follows directly from the unitarity property that the *true* $P(t)$ must be bounded in magnitude by unity for all t, it is not at all obvious that this property is preserved by the approximate forms $P^{(l)}(t)$ for finite l. Thus we cannot exclude the possibility that the quantity $\Delta P^{(l)}(t)$, Eq. (D61), is finite for all finite l and in the limit $l\to\infty$ tends to an infinite oscillating series, which, in the limit $t\to\infty$, tends either to a constant of magnitude ≤ 1 or (more probably) to zero.

If our conjecture is correct, we find the final result

$$P(t)=\sum_{m=1}^{\infty} A_m(\alpha)\psi(\Delta_m t)+C\ ,$$
$$\Delta_m\equiv\Delta_{\rm eff}[e_m(\alpha)]^{1/2-2\alpha}\ , \tag{5.48}$$

where $\psi(y)$ is the function given by Eq. (5.44), C is the constant term (if any) of $\Delta P^{(l)}(t)$ in the limit $l\to\infty$, and the amplitudes $A_m(\alpha)$ and eigenvalues $e_m(\alpha)$ can in principle be determined to any desired accuracy either by solving the lth-neighbor eigenvalue problem for increasing integral l or by computing the quantities $\tilde{K}_n(\alpha)$ [Eq. (5.42)] numerically for $n\leq l$ and using the relation

$$\tilde{K}_n(\alpha)=\sum_{m=1}^{\infty} A_m(\alpha)[e_m(\alpha)]^n/\Gamma[2n(1-\alpha)+1],\quad n\geq 1 \tag{5.49}$$

to fix approximate values for increasing numbers of e_m and A_m. It is virtually certain that the constant C in Eq. (5.48) vanishes, i.e., that Eq. (5.49) holds also for $n=0$, but at the time of writing we have not constructed a totally rigorous proof of this, even within the framework of our conjecture.[63] We believe that the values of the $A_m(\alpha)$ and $e_m(\alpha)$ computed by using the nearest-neighbor approximation, and tabulated in Appendix D.3, are likely to be an excellent approximation for most practical purposes; in particular, they are exact to lowest nontrivial order in α and, very probably, also in $(1-2\alpha)$.

The form (5.48) for $P(t)$, if correct, also illustrates that, unless there are independent reasons for believing otherwise, it may be dangerous if not altogether wrong to draw conclusions about the asymptotic behavior of the "true" $P(t)$ on the basis of the noninteracting-blip approximation, even after we ignore what might be termed "finite-ω_c effects." By these we mean the effects that cause $P(t)$ to deviate significantly from the approximation (5.40) and that, as argued in Appendix D.1, do not come into play until ultralong times, of order $\Delta_{\rm eff}^{-1}$ times a positive power or logarithm of $(\omega_c/\Delta_{\rm eff})$. It is clear that the higher-m terms dominate Eq. (5.48) (assuming $C=0$) at time scales that are not quite so long but are still much longer than $\Delta_{\rm eff}^{-1}$. Further, the asymptotic behavior of Eq. (5.48) is *not* of the form $t^{-2(1-\alpha)}$, and is in fact extremely complicated, depending intricately on the m dependence of A_m and e_m for large m. All this is perhaps not surprising in view of the close connections between the two-state problem in the ohmic case and the Kondo problem (see Sec. III.E) and the well-known difficulty "all frequency scales are coupled together in the Kondo problem." We emphasize this point here because it is useful to see directly how this difficulty is reflected in the nonequilibrium time-dependent behavior, as opposed to the equilibrium thermodynamic properties, which have been the object of most existing studies of the Kondo problem.

We finally note the relationship between the conclusions obtained here and those of Chakravarty and Leggett (1984). It is clear that the first two terms in Eq. (24) of that reference correspond to the term $m=1$ of Eq. (5.48), where we can now identify the quantity $q(\alpha)$ with $e_1(\alpha)-1$ and $A(\alpha)$ with $A_1(\alpha)$ The correction term $\Delta P(t)$ of Chakravarty and Leggett (1984) is the sum of the remaining terms in Eq. (5.48). As noted above, contrary to the "presumption" of this reference, these terms dominate the behavior of $P(t)$ at very long times. It should be emphasized, however, that in the context of fundamental tests of quantum mechanics [which typically require $\alpha\lesssim 0.1$ and $\Delta_1 t\lesssim 2\pi/3$; see Leggett and Garg (1985)], these terms are almost totally negligible: in this context the approximation of keeping only the $m=1$

[62] We implicitly assume, of course, that this process converges.

[63] It seems very probable that such a proof could be constructed by exploiting the fact that, on all but a set of measure zero of paths contributing to $P(t)$, the influence functional decreases continually in the limit $t\to\infty$. Needless to say there are also various rigorous bounds that we do not bother to write out here, on C in terms of the coefficients $\tilde{K}_n$; in particular, it is easy to show that for $\alpha\to 0$, C (if not identically zero) must vanish at least as fast as α^2.

term in Eq. (5.48) should be an excellent one. Note, moreover, that in that context the fact that the argument of this term is $\Delta_1 t$ rather than $\Delta_{\rm eff} t$ is of little significance, since in any realistic case we are likely to have to take the value of Δ_1 from experiment anyway; it is the dependence of $\psi(y)$ on the dimensionless variable y which is all important (see Leggett and Garg, 1985).

E. $T=0$, $\frac{1}{2}<\alpha<1$

Although the region of the parameter space corresponding to $\frac{1}{2}<\alpha<1, kT \lesssim \hbar\Delta(\Delta/\omega_c)^{\alpha/1-\alpha}$ (so that we are not in the limit discussed in Sec. V.C) is a very small fraction of the whole, it is of considerable conceptual interest, in particular, because it is here that contact is most easily made with the Kondo problem (see Sec. III.E). Unfortunately, it is also the region in which it is most difficult to evaluate the expression for $P(t)$ with any reliability. Here we shall confine ourselves to the case of zero temperature and give plausible, but not rigorous, arguments for the form of $P(t)$.

The basic problem about the region $T=0$, $\frac{1}{2}<\alpha<1$ is that the one-blip contribution, namely,

$$f(t) \equiv \frac{\cos[2\alpha \tan^{-1}(\omega_c t)]}{(1+\omega_c^2 t^2)^{\alpha}} \tag{5.50}$$

is not uniformly positive in this region. In fact, as we saw in Sec. III.C, the integral of $f(t)$ from zero to infinity is rigorously zero. This makes it extremely difficult to obtain rigorous limits on the contributions of different regions to the integrals $\tilde{K}_n$. However, we can plausibly argue as follows.[64] First, if we could neglect the interblip correlations, then the only reason why the expression for $\tilde{K}_n$ is not rigorously zero would be the interblip exclusion, i.e., the fact that the integral of $f(t)$ will typically be cut off at a value of t of the order of the (to be determined) characteristic inverse frequency scale (see the first paragraph of Sec. V.C). Call this frequency scale $\bar{\delta}$. Then the value of the integral over the single-blip length, i.e., the integral of $f(t)$, will be positive and of order

$$[\,|\cos\pi\alpha|\,/(2\alpha-1)]\bar{\delta}^{\,2\alpha-1}\omega_c^{-2\alpha} \sim \bar{\delta}^{\,2\alpha-1}\omega_c^{-2\alpha}\,.$$

If we could proceed according to the "golden rule" technique (Sec. III.D), we would therefore have a transition rate of the order of $\Delta^2\bar{\delta}^{\,2\alpha-1}\omega_c^{-2\alpha}$. Since this rate must be precisely the frequency scale $\bar{\delta}$, we put $\bar{\delta}\sim\Delta^2\bar{\delta}^{\,2\alpha-1}\omega_c^{-2\alpha}$ and solve to obtain $\bar{\delta}\sim\Delta_r \equiv \Delta(\Delta/\omega_c)^{\alpha/1-\alpha}$. Thus the contribution of a single blip of length $\sim\Delta_r$ and its associated sojourn to the multiple integral for $\tilde{K}_n$, for $t\sim n\Delta_r$ (see Sec. V.C) will be $\sim\Delta_r^2$. This argument is of course far from rigorous, but we shall see below that within the noninteracting-blip approximation the behavior of $P(t)$, though not described by the golden rule (exponential relaxation) expression, is nevertheless indeed characterized by a frequency scale $\sim\Delta_r$.

Now consider the effect of interblip interactions. If, for all time intervals δt involved, the quantity $\omega_c\delta t$ is $\gg 1$, then all the quantities X_{jk} in Eq. (5.6) are effectively zero except for the term $j=k+1$, which is already included in the single-blip contribution [Eq. (5.41)]. Moreover, the factor F_2 [Eq. (5.56)] is a product of *ratios* of the blip and sojourn lengths, and is independent of ω_c in this limit. Thus, while this factor may affect the detailed form of $P(t)$, it cannot change its general frequency scale (cf. case $\alpha<\frac{1}{2}$). What remains, therefore, is to check whether consideration of *short* blips and/or sojourns ($\delta t \lesssim \omega_c^{-1}$) would give a contribution greater than the one so far considered. Suppose, for example, we consider two blips and their associated sojourns in a time interval, $\sim\Delta_r^{-1}$. In the approximation of no interblip interaction the contribution has already been taken into account. To get appreciable effects from the interaction, the intermediate sojourn must itself be of order ω_c^{-1} in length. Thus *three* of the four integrals are confined to a time interval $\sim\omega_c^{-1}$, and the resulting contributions cannot be longer than $\sim\Delta_r^{-1}\omega_c^{-3}$, compared to the noninteracting-blip contribution, which, from the considerations above, is $\sim\Delta_r^{-4}$. Thus the contribution of short blips and/or sojourns should be negligible.

The conclusion of this (far from rigorous) argument is that in this regime the result obtained by neglecting all interblip interactions is probably qualitatively correct, though the detailed form of $P(t)$ will probably be affected by the interaction terms in F_2 [Eq. (5.56)]. In particular, the frequency scale, in this regime as elsewhere, is simply $\Delta_r \equiv \Delta(\Delta/\omega_c)^{\alpha/1-\alpha}$. This is a cause for relief, if true, since we saw in Sec. II that it is only if the cutoff ω_c enters into the formulas precisely in this way that our conclusions, for a system which actually has an extended coordinate, are independent of the precise point at which we truncate to a two-state system.

We shall see in the next subsection that the results of the noninteracting-blip calculation in this regime are a simple extension of those for $\alpha<\frac{1}{2}$. In fact, the expression for $P(t)$ is formally identical to Eq. (5.44c) [with $y\equiv\Delta_{\rm eff}t$: note that the factor $(\cos\pi\alpha)\Gamma(1-2\alpha)$ is always positive]. Note (a) that $P(t)$ is always *positive* for $\frac{1}{2}<\alpha<1$; (b) that as $\alpha\to 1$, $P(t)$ behaves like $t^{-2(1-\alpha)}$ for *all* t; (c) that if we were to identify $P(t)$ with the correlation function $C(t)$, we would find the static susceptibility to be infinite for all values of α in this range, despite the fact that there is no localization. This result, which appears surprising in view of the fact that for the closely related problem of the antiferromagnetic Kondo system the susceptibility is known to be perfectly finite, might induce a certain scepticism about the validity of the

[64] This is a more explicit version of the argument used in Chakravarty and Leggett (1984).

noninteracting-blip approximation in this regime, and this scepticism is strengthened by the fact that an attempt (Garg, 1984) to extend the "nearest-neighbor" calculation of the last subsection to the case $\alpha > \frac{1}{2}$ runs into technical difficulties that indicate (contrary to the intuitive reasoning given above) that short sojourns may after all be playing an important role, so that Δ_r may not be the only relevant time scale. In view of these difficulties we must regard the true behavior of $P(t)$ in the regime $T=0$, $\frac{1}{2} < \alpha \leq 1$ as a currently unresolved problem.

F. Results for the whole parameter space in the noninteracting-blip approximation

In the foregoing subsections we have shown that the "noninteracting-blip approximation" gives exact results in the limit $\alpha kT/\hbar \gg \Delta_r$ as well as, for arbitrary T, on the line $\alpha = \frac{1}{2}$. It is also qualitatively very good (at least for not too long t) at $T=0$ for all α between 0 and $\frac{1}{2}$, and may or may not give qualitatively correct behavior for $T=0$, $\frac{1}{2} < \alpha < 1$. Since all other regions of the (α, T) plane are intermediate between these extreme cases, it is extremely plausible that the approximation may be applicable to the whole of the parameter space. We shall now apply the approximation in a unified way, obtaining along the way as special cases the results already quoted (and in some cases derived by an alternative method) in earlier subsections.

In the noninteracting-blip approximation, the expression for $P(t)$ is quite generally given by Eq. (4.32), with $f(\lambda)$ defined by Eq. (4.33). For the ohmic case, $f(\lambda)$ is given by[65]

$$f(\lambda)=\Delta^2 \int_0^\infty e^{-\lambda t}\left[\frac{2\gamma t}{2\sinh(\gamma t)}\right]^{2\alpha}\frac{\cos[2\alpha \tan^{-1}(\omega_c t)]}{(1+\omega_c^2 t^2)^\alpha}dt\ , \tag{5.51}$$

where

$$\gamma = \pi kT/\hbar\ . \tag{5.52}$$

Since we are interested in the behavior of $P(t)$ for times much larger than ω_c^{-1}, it suffices to know $f(\lambda)$ asymptotically for $|\lambda/\omega_c| \ll 1$. To find this, we write the temperature-independent factor in $f(t)$ as $\mathrm{Re}(1-i\omega_c t)^{-2\alpha}$. Then, after some elementary manipulations, we get (for real λ)

$$f(\lambda)=\mathrm{Re}\frac{\Delta^2}{(-i\omega_c)^{2\alpha}}e^{i\lambda/\omega_c}\lambda^{2\alpha-1}\int_{i\lambda/\omega_c}^\infty \frac{e^{-z}}{z^{2\alpha}}\left[\frac{(\gamma/\lambda)(z-i\lambda/\omega_c)}{\sinh[(\gamma/\lambda)(z-i\lambda/\omega_c)]}\right]^{2\alpha}dz\ . \tag{5.53}$$

This can now be expanded by standard methods. The leading term in particular, which is mainly what we shall be interested in, is obtained by setting λ/ω_c to zero in both the integrand and the limit of integration; the resulting integral is tabulated in Gradshteyn and Ryzhik (1980; formula 3.541.1). The final result is

$$f(\lambda)\approx\frac{\Delta^2}{\omega_c}\left[\left[\frac{2\gamma}{\omega_c}\right]^{2\alpha-1}\cos\left[\alpha\pi+\frac{\lambda}{\omega_c}\right]\frac{\Gamma(1-2\alpha)\Gamma(\alpha+\lambda/2\gamma)}{\Gamma(1-\alpha+\lambda/2\gamma)}+(1-2\alpha)^{-1}\sin(\lambda/\omega_c)\right.$$
$$\left.-(2-2\alpha)^{-1}(\gamma/\omega_c)\cos(\lambda/\omega_c)+O(\lambda/\omega_c)^{2,1+2\alpha}\right]\ . \tag{5.54}$$

Note that this expression is finite in the limits $\alpha \to \frac{1}{2}$, $\alpha \to 1$, and $\gamma \to 0$, etc. It is inconsistent with the spirit of the noninteracting-blip approximation, however, to retain the terms of order $\lambda(\Delta/\omega_c)^2$, and so we shall use the following approximation to $f(\lambda)$, which is valid for all values of α not too close to an integer:

$$f(\lambda)\approx\Delta_{\mathrm{eff}}(2\gamma/\Delta_{\mathrm{eff}})^{2\alpha-1}\frac{\Gamma(\alpha+\lambda/2\gamma)}{\Gamma(1-\alpha+\lambda/2\gamma)}$$
$$+O\left[\lambda\left[\frac{\Delta}{\omega_c}\right]^2\right]\ . \tag{5.55}$$

It is now a simple matter to show that Eq. (5.55), along with Eqs. (4.32) and (4.33), yields the results obtained in earlier subsections, as indeed it must. Thus, for $\alpha=\frac{1}{2}$, we have $f(\lambda)=\Delta_{\mathrm{eff}}$, which leads to $P(t)=\exp(-\Delta_{\mathrm{eff}}t)$. Similarly, for high enough temperatures, $f(\lambda)$ is seen to vary on a scale set by γ, allowing a Taylor expansion near $\lambda=0$:

$$f(\lambda)\simeq f(0)\left[1-\frac{\pi}{2\gamma}\cot(\pi\alpha)\lambda+\cdots\right]\ . \tag{5.56}$$

It is easy to show that $f(0)$ is identical to τ^{-1} defined in Eq. (5.30), so that

$$P(t)\approx\left[1-\frac{\hbar}{2kT\tau}\cot\pi\alpha\right]^{-1}$$
$$\times\exp\{-t/[\tau-\hbar(\cot\pi\alpha)/2kT]\}\ . \tag{5.57}$$

The terms involving $(kT\tau/\hbar)^{-1}$ are the first corrections

[65] Note that we have restored the factor Δ^2 in the definition of $f(t)$.

to the results (5.29) and (5.30), and since they arise from the second term in the Taylor expansion of $f(\lambda)$, we can obtain a criterion for what constitutes a "high" temperature simply by demanding that they be small:

$$\frac{kT}{\hbar} \gg \Delta_r \left| \frac{\pi\Gamma(\alpha)}{(\tan\pi\alpha)\Gamma(\alpha+1/2)} \right|^{1/(2-2\alpha)} . \quad (5.58)$$

This is essentially identical to Eq. (4.32) except near $\alpha=\frac{1}{2}$: for $\alpha=\frac{1}{2}$, it is satisfied for all temperatures, in accord with our earlier results.

For zero temperature, Eq. (5.55) must be interpreted by using Stirling's formula for the gamma function of large arguments. Doing this, we get[66]

$$f(\lambda)=\Delta_{\rm eff}^{2(1-\alpha)}\lambda^{2\alpha-1}+O[\lambda(\Delta/\omega_c)^2] \quad (T=0) . \quad (5.59)$$

With this result, $\tilde{P}(\lambda)$ is now seen to be the Laplace transform of the Mittag-Leffler function (Erdelyi *et al.*, 1955, Vol. 3, p. 206). The Laplace inversion is very useful in understanding the behavior of $P(t)$ for nonzero values of temperature, and so, rather than refer the reader to the literature, we summarize the salient features of how it is done.

For $\alpha<\frac{1}{2}$, $\tilde{P}(\lambda)$ has three singularities (see Fig. 6): a branch point at $\lambda=0$, and a complex-conjugate pair of simple poles at

$$\lambda_{0\pm}=\Delta_{\rm eff}\exp[\pm i\pi/2(1-\alpha)] . \quad (5.60)$$

The contributions to the Bromwich contour integral arising from the poles and the branch cut are easily seen to be the "coherent" and "incoherent" parts, respectively, of Eq. (5.44).

For $\frac{1}{2}<\alpha<1$, the poles given by Eq. (5.60) are not on the principal λ sheet, and $P(t)$ is given (subject to all the caveats discussed in Sec. V.E) entirely by the branch-cut contribution, which is algebraically identical to $P_{\rm inc}(t)$ given by Eq. (5.44c).

For $\alpha>1$, the leading term in the expansion of $f(\lambda)$ is not the one varying as $\lambda^{2\alpha-1}$, but the one linear in λ. Since, however, we are neglecting all corrections to $P(t)$ of order $(\Delta/\omega_c)^l$ where l is any positive number, we should write $\tilde{P}(\lambda)=\lambda^{-1}$, which leads to $P(t)=1$ for all t. This is, of course, the localization phenomenon of Chakravarty (1982) and Bray and Moore (1982).

The real usefulness of Eq. (5.55) lies not in its permitting a clean evaluation of $P(t)$ in the various limiting cases discussed above, but in the fact that it allows one to obtain quantitative approximations to $P(t)$ for "interesting" times for intermediate temperature values. This consideration is particularly important in the context of the macroscopic quantum coherence question, where an observation/nonobservation of oscillatory behavior would be of fundamental significance to our understanding of quantum mechanics. With this point in mind, we note that since there is no "coherent" behavior for $\alpha>\frac{1}{2}$, even at $T=0$, it is very unlikely that there would be any for $T>0$.[67] We shall restrict ourselves, therefore, to an examination of $P(t)$ for intermediate temperature values for $\alpha<\frac{1}{2}$.

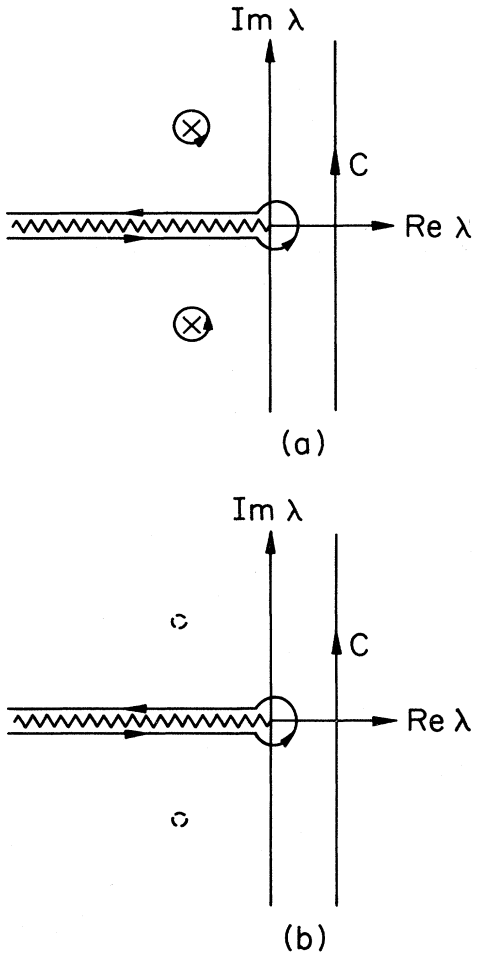

FIG. 6. Singularities of $\tilde{P}(\lambda)$ and the Bromwich contour: (a) $\alpha<\frac{1}{2}$; (b) $\frac{1}{2}<\alpha<1$.

Since the gamma function has no branch points, neither does $\tilde{P}(\lambda)$, and the only singularities it can have are poles, given by the solutions to the equation

$$\Gamma(\alpha+u)/\Gamma(1-\alpha+u)=-(2\gamma/\Delta_{\rm eff})^{2-2\alpha}u , \quad (5.61)$$

where we have defined $u=\lambda/2\gamma$. To solve this equation, we use a graphical procedure. Figure 7 shows a sketch of the left-hand side of Eq. (5.61) and the right-hand side for three temperatures, T_1, T^*, and T_2, with $T_2>T^*>T_1$. Note that the poles of the function $\Gamma(\alpha+u)/\Gamma(1-\alpha+u)$ lie to the left of the zeros, giving it a negative slope for all u.

Let us now follow the behavior of the poles of $\tilde{P}(\lambda)$ as

[66]With the usual proviso that α not be too close to an integer.

[67]Arguments analogous to those given below support this conclusion.

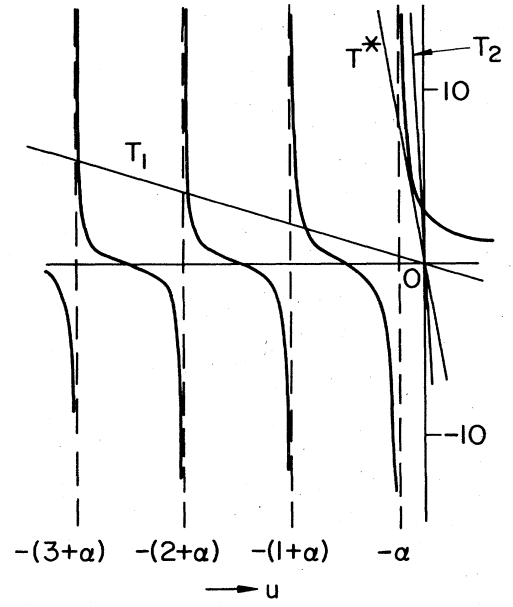

FIG. 7. Graphical solution of Eq. (5.61) for $\alpha < \frac{1}{2}$.

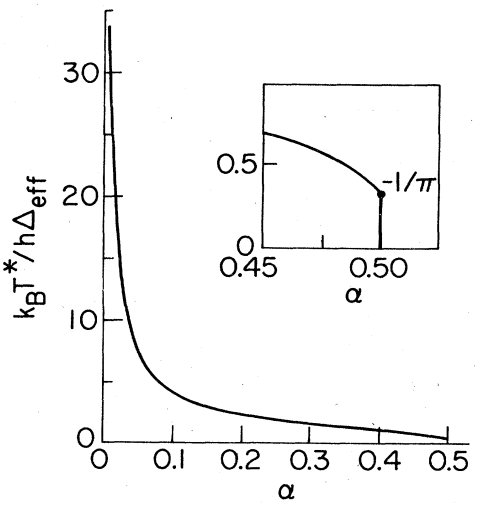

FIG. 8. Dependence on α of the temperature $T^*(\alpha)$ for crossover to incoherence. The inset shows the behavior near $\alpha = \frac{1}{2}$.

the temperature increases. For $T = T_1$, there is a real solution in the range $-(m+\alpha) < u < -m+\alpha$; $m = 1,2,\ldots$. This remains true as T increases, until $T = T^*$, at which point the two sides of Eq. (5.61) become tangential to one another for some value $-\alpha < u < 0$, corresponding to a real, negative, double pole of $\tilde{P}(\lambda)$. For $T > T^*(\alpha)$, the double pole breaks up into two simple poles, one moving toward $u = -\alpha$, the other toward $u = 0$.

Since Eq. (5.61) varies smoothly with γ, one cannot create or destroy any poles of $\tilde{P}(\lambda)$ as the temperature is varied. This very strongly suggests the following. As the temperature is increased from zero, the two complex-conjugate poles given by Eq. (5.60) move toward the negative real axis, hitting it at $T = T^*$, after which they move along it in opposite directions. As for the branch cut found at $T = 0$, it breaks up into a series of unevenly spaced poles on the negative real axis, with a spacing that grows linearly with temperature on the average. It is also clear from Fig. 5(a) that, for $T < T^*$, the residues from the poles on the real axis are all negative, which agrees with the fact that $P_{\rm inc}(t)$ is negative at $T = 0$ and $\alpha < \frac{1}{2}$ for all values of t. This continues to hold for $T > T^*$. In addition, the contribution to $P(t)$ from the pole nearest the origin is positive, and from the remaining poles is negative. Since[68] $P(0) = 1$, it follows that for $T > T^*(\alpha)$, $P(t)$ can vanish only as $t \to \infty$; i.e., $P(t)$ does not show oscillatory behavior.

The temperature $T^*(\alpha)$ is thus of special interest for the problem of macroscopic quantum coherence, since it provides an excellent approximation to the temperature above which coherent oscillations cannot be seen.[69] It is obtained by requiring that Eq. (5.61) and its first u derivative hold simultaneously. This leads to the result

$$2\pi k T^*(\alpha)/\hbar\Delta_{\rm eff}(\alpha) = \left[-\frac{1}{u^*} \frac{\Gamma(\alpha+u^*)}{\Gamma(1-\alpha+u^*)} \right]^{1/2(1-\alpha)} , \tag{5.62}$$

where u^* is given by the solution of the equation

$$u^*[\psi(\alpha+u^*) - \psi(1-\alpha+u^*)] = 1 , \tag{5.63}$$

where $\psi(z)$ is the digamma function.

We have solved Eqs. (5.62) and (5.63) numerically; the results are plotted in Fig. 8. Note that $T^*(\frac{1}{2})$ is nonzero. The limiting behavior of $T^*(\alpha)$ and the position $\lambda^*(\alpha)$ of the double pole, as $\alpha \to 0$, are given by

$$[2\pi k T^*/\hbar\Delta_{\rm eff}(\alpha)] \approx 2/\alpha + 2\ln\alpha^{-1} + O(\alpha\ln\alpha) , \tag{5.64a}$$

$$\lambda^*/\Delta_{\rm eff}(\alpha) \approx -1 + \alpha\ln\alpha + O(\alpha^2\ln\alpha) . \tag{5.64b}$$

Similarly, as $\alpha \to \frac{1}{2}$,

$$2\pi k T^*(\alpha)/\hbar\Delta_{\rm eff}(\alpha) \approx 2 + 8(\tfrac{1}{2} - \alpha)^{1/2} + O(1-2\alpha) , \tag{5.65a}$$

[68] To see that this is true even when $f(\lambda)$ is approximated by Eq. (5.55), use the series Eq. (4.32) for $\tilde{P}(\lambda)$, and the convolution theorem to invert it term by term.

[69] The reader may object that this conclusion is based on the noninteracting-blip approximation. Note, however, that as the temperature increases, the "self-energy" S_j of a blip [see Eq. (4.21a)] increases, causing the mean blip length to decrease. This in turn means that the interblip effects become less and less important as the temperature increases, and since even at $T = 0$, as seen in subsection D, they never result in more than a 5% correction to $P(t)$ for interesting values of t, the noninteracting-blip approximation should be more than adequate for temperatures of the order of $T^*(\alpha)$.

$$\lambda^*/\Delta_{\rm eff}(\alpha)\approx -1-2(\tfrac{1}{2}-\alpha)^{1/2}+O(1-2\alpha)\ . \quad (5.65b)$$

It is clear from Fig. 8 that $T^*(\alpha)$ drops very rapidly as α increases. [It should be kept in mind that $\Delta_{\rm eff}(\alpha)$ itself drops quite rapidly with α.] Given currently available cryogenic technology and SQUIDS, it is very likely that for an experimental test of macroscopic quantum coherence, very low values of α will be required. It is therefore useful to explore this region further and to obtain as much quantitative information about $P(t)$ as possible. First of all, recall that at $T=0$, $P_{\rm inc}(t)$ is of order α. It requires some algebra to show that, at $T=T^*$, the contribution to $P(0)$ from the double pole differs from unity by a term of order α^3, and since $P(0)$ equals unity, this means that the contribution from the other poles, which we continue to call $P_{\rm inc}$ is of order α^3. To a first approximation, then, it is reasonable to neglect $P_{\rm inc}(t)$ altogether. The remaining contribution to $P(t)$, which we denote by $P_{\rm osc}(t)$, can clearly be written as the solution of a damped harmonic oscillator with temperature-dependent frequency and damping. Since the weak-damping approximation of Sec. III.B results in precisely such an equation, one might wonder how well the solutions to Eqs. (3.10) and (3.11) compare with $P_{\rm osc}(t)$, even after the most glaring flaw, namely, the lack of frequency renormalization, is put in by hand. [That is to say, Δ is replaced by $\Delta_{\rm eff}$ everywhere in Eqs. (3.10) and (3.11).] Figure 2 of Garg (1985) shows a plot of the real and imaginary parts of the complex frequency associated with $P_{\rm osc}(t)$ and the approximation of Sec. III.B (with the frequency renormalization) as a function of T for $\alpha=0.05$. It is amusing that while the damping rate is virtually identical for the two approximations, the true oscillation frequency [which should be very accurately given by $P_{\rm osc}(t)$], and, therefore, the true Q factor, is higher than that given by the weak-damping approximation.

VI. NONOHMIC SPECTRAL DENSITIES: THE UNBIASED CASE

In this section the discussion of Sec. V is extended to include the behavior of two-state systems with nonohmic dissipation. As stated in Secs. III we shall concern ourselves with simple spectral densities of the form

$$\frac{q_0^2}{2\pi\hbar}J(\omega)=\beta_s\tilde{\omega}(\omega/\tilde{\omega})^s e^{-\omega/\omega_c} \quad (6.1)$$

for general $s\neq 1$,[70] where ω_c is the usual upper cutoff frequency. In addition, we shall focus attention on the unbiased ($\varepsilon=0$) case, leaving the discussion of the biased two-state system to Sec. VII. We shall be interested in calculating $P(t)$ using the exact formal power-series expansion that was derived in Sec. IV, Eqs. (4.17)—(4.22). Explicit results for $P(t)$ are obtained by making a series of controlled approximations on the exact expression. It will become apparent that the qualitative behavior of $P(t)$ (i.e., underdamped versus overdamped) is quite sensitive to the low-frequency behavior of $J(\omega)$, as was emphasized in Sec. III. In fact, most of the results of this section are wholly equivalent to the results obtained by more heuristic methods in Sec. III. What we hope to show is that a unified framework exists for discussing all of the different types of behavior. The utility and ubiquity of the noninteracting-blip approximation will soon become apparent; this approximation was already extensively applied to the ohmic case in Sec. V.

Before delving into the nature of the approximations of this section, we should first like to comment on the level of rigor involved in this section and in Sec. VII. Since the primary motivation for this work has been the study of macroscopic quantum coherence, the study of nonohmic dissipation is of somewhat less importance for our purposes. In addition, ohmic dissipation provides for the richest possible behavior. For these reasons we shall not embark on a detailed analysis here, as was done for the ohmic case in Sec. V and Appendix D. Our goal here is rather less ambitious—to provide what we believe to be some rather intuitive approximations to the formal results of Sec. IV, thereby confirming the heuristic results of Sec. III in the appropriate limits.

A. The subohmic case ($0<s<1$)

We begin our discussion of the nonohmic spectra by considering the subohmic case, $s<1$. As we shall see, it is in this regime that the noninteracting-blip approximation, as discussed in Sec. IV.C, can easily be justified. The reader may find it instructive to compare the ensuing discussion with that of the $\alpha>1$ (or $\alpha<1$ for $T\gg\alpha^{-1}\Delta_r$) ohmic case presented in Sec. V. We show below that, for the subohmic case, $P(t)$ exhibits overdamped behavior, so that $P(t)=\exp(-\Gamma t)$, with a relaxation rate Γ. This is completely equivalent to the golden rule result, Eqs. (3.37) and (3.38).

We should first like to motivate the use of the noninteracting-blip approximation for the subohmic case. We start by examining the behavior of the quantities $Q_1(t)$ and $Q_2(t)$, which were defined in Sec. III. For convenience we repeat these definitions here:

$$Q_1(t)\equiv\int_0^\infty \frac{J(\omega)}{\omega^2}\sin\omega t\, d\omega\ , \quad (6.2a)$$

$$Q_2(t)\equiv\int_0^\infty \frac{J(\omega)}{\omega^2}(1-\cos\omega t)\coth\beta\hbar\omega/2\, d\omega\ . \quad (6.2b)$$

For $J(\omega)$ given by (6.1), at long times ($\omega_c t\gg 1$) and at zero temperature, these functions behave as $Q_1(t)\sim(\text{const})\beta_s(\tilde{\omega}t)^{1-s}$, $Q_2(t)\sim(\text{const})\beta_s(\tilde{\omega}t)^{1-s}$. Since $Q_2(t)\to\infty$ as $t\to\infty$, the term F_1 [Eq. (4.20a)] in the power-series expansion becomes negligible for long times. Thus we conclude that configurations with long blips will make

[70] For the nonohmic spectra, an arbitrary frequency scale $\tilde{\omega}$ must be introduced to define a dimensionless coupling parameter β. We note, however, that $\tilde{\omega}$ has no fundamental significance, since the only physically relevant parameter is the combination $\beta_s\tilde{\omega}^{1-s}$.

exponentially small contributions to the sum (4.17); the important configurations will be those for which the blip width is small compared to the interblip separation. (We shall make this statement more precise below.) Now that we have argued that the blips form a dilute "gas," we may ask whether the interblip interactions may be safely ignored. The interaction terms Λ_{jk} and X_{jk} defined by Eqs. (4.21b) and (4.21c) behave roughly as $\Lambda \sim \partial^2 Q_2/\partial t^2$ and $X \sim \partial^2 Q_1/\partial t^2$, so that both Λ and X decay as $(\tilde{\omega}t)^{-(1+s)}$ for $\omega_c t \gg 1$. Since the blips are dilute, and the interactions between blips decay algebraically, the interblip interactions can be ignored. Thus, for $s<1$, the noninteracting-blip approximation is expected to be valid; we shall examine its self-consistency below.

Within the noninteracting-blip approximation the following expressions for $P(t)$ were derived in Sec. IV:

$$P(t)=\frac{1}{2\pi i}\int_C e^{\lambda t}\tilde{P}(\lambda)d\lambda\ , \tag{6.3a}$$

$$\tilde{P}(\lambda)=\frac{1}{\lambda+f(\lambda)}\ , \tag{6.3b}$$

$$f(\lambda)\equiv\Delta^2\int_0^\infty \cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\lambda t-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]dt\ , \tag{6.3c}$$

where the contour C in Eq. (6.3a) is the standard Bromwich contour. Consider expanding $f(\lambda)$ in a power series about $\lambda=0$:

$$f(\lambda)=f_0+f_1\lambda+\cdots$$

with

$$f_0=\lim_{\lambda\to 0^+}f(\lambda),\quad f_1=\lim_{\lambda\to 0^+}\frac{\partial}{\partial\lambda}f(\lambda)\ . \tag{6.4}$$

For $s<1$, the expansion for $f(\lambda)$ is easily obtained by expanding $\exp(-\lambda t)$ in a power series and integrating term by term; all of the resulting integrals for the coefficients f_n are convergent, and we obtain

$$f_0=\Delta^2\int_0^\infty \cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]dt\ , \tag{6.5a}$$

$$f_1=-\Delta^2\int_0^\infty t\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]dt\ . \tag{6.5b}$$

If we assume for the moment that $|f_1|\ll 1$, then $\tilde{P}(\lambda)$ has a simple pole at $-f_0$; performing the Laplace inversion then gives

$$P(t)=\exp(-\Gamma t),\quad \Gamma=f_0\ . \tag{6.6}$$

This is identical to the golden rule result, Eq. (3.38), with $\varepsilon=0$.

We should now like to show that the condition $|f_1|\ll 1$ is precisely what is needed for the blips to form a dilute gas. First, we note that the typical distance between blips is $\Gamma^{-1}=f_0^{-1}$. This can be seen by expanding $P(t)$;

$$P(t)=\sum_{n=0}^{\infty}(-\Gamma t)^n/n\ .$$

At a given time t, the dominant term in this series has $n\simeq\Gamma t$ blip-sojourn pairs, and so the typical length of a blip and its neighboring sojourn is $\Gamma^{-1}=t/n$. Next, we observe that $|f_1|/f_0\equiv t_b$ provides an estimate of the typical blip width. To see this, recall that the factor $F_1=\exp(-q_0^2Q_2/\pi\hbar)$ in Eq. (4.20a) controls the width of a blip; we expect that the first moment of this function will provide an estimate of the typical blip width. Aside from the additional cosine factors, $|f_1|/f_0$ is just the first moment of F_1. Hence the statement that $|f_1|\ll 1$ is equivalent to $\Gamma t_b\ll 1$; the typical blip width must be much less than the typical distance between blips. If this condition is met, then we are correct in ignoring the interblip interactions.

A straightforward order-of-magnitude calculation of f_1, using the long-time behavior of Q_1 and Q_2 from Eq. (6.2), gives

$$f_1=0\left[\left[\frac{\Delta}{(\beta_s\tilde{\omega}^{1-s})^{1/(1-s)}}\right]^2\right]\ , \tag{6.7}$$

so that $|f_1|\ll 1$ requires

$$\Delta/\omega_c\ll[\beta_s(\tilde{\omega}/\omega_c)^{1-s}]^{1/(1-s)}\ . \tag{6.8}$$

Notice that Δ/ω_c can always be chosen sufficiently small so that condition (6.8) is satisfied.

Equations (6.5a) and (6.6) are our desired results for $P(t)$. It remains for us to evaluate (6.5a) for a particular form of the cutoff function in order to get explicit results for Γ. As usual, we choose an exponential cutoff, so that $J(\omega)$ is given by Eq. (6.1).

Evaluating $Q_1(t)$ and $Q_2(t)$ at zero temperature, we find

$$\frac{q_0^2}{2\pi\hbar}Q_1(t)=\beta_s\frac{\Gamma(s)}{1-s}\left[\frac{\tilde{\omega}}{\omega_c}\right]^{1-s}\mathrm{Im}(1+i\omega_c t)^{1-s}\ , \tag{6.9a}$$

$$\frac{q_0^2}{2\pi\hbar}Q_2(t)=-\beta_s\frac{\Gamma(s)}{1-s}\left[\frac{\tilde{\omega}}{\omega_c}\right]^{1-s}[1-\mathrm{Re}(1+i\omega_c t)^{1-s}]\ . \tag{6.9b}$$

By substituting these expressions into Eq. (6.5a) and performing the integration exactly, it can be shown that $\Gamma=0$ at $T=0$. Thus at zero temperature the particle remains in the well it started in; this is in accordance with the adiabatic renormalization arguments given in Sec. III.C. At finite temperatures, there is an additional contribution $\Delta Q_2(t)$ to $Q_2(t)|_{T=0}$. This is given by

$$\frac{q_0^2}{2\pi\hbar}\Delta Q_2(t)=\int_0^\infty\frac{q_0^2}{2\pi\hbar}J(\omega)\frac{(1-\cos\omega t)[\coth(\beta\omega/2)-1]}{\omega^2}d\omega\ . \tag{6.10}$$

We only need to evaluate this function for values of t

such that $t \lesssim 1/(\tilde{\omega}\beta_s^{1/(1-s)})$, since $Q_2(t)\,|_{T=0}$ cuts off the integral f_0 for values of t greater than this. In addition, the $[\coth(\beta\hbar\omega/2)-1]$ factor in Eq. (6.10) cuts off the ΔQ_2 integral at frequencies of order $\hbar\omega \simeq k_B T$. Thus, if the combination $\omega t \sim k_B T/\hbar\tilde{\omega}\beta_s^{1/(1-s)} \ll 1$, then the $(1-\cos\omega t)$ term in Eq. (6.10) may be safely expanded; the remaining integral for $\Delta Q_2(t)$ is easily evaluated,[71] and we get

$$\frac{q_0^2}{2\pi\hbar}\Delta Q_2(t)=\beta_s\left[\frac{kT}{\hbar\tilde{\omega}}\right]^{1+s}\Gamma(s+1)\zeta(s+1)(\tilde{\omega}t)^2 . \quad (6.11)$$

Substituting Eqs. (6.11), (6.9a), and (6.9b) into (6.5a), we arrive at an expression for Γ that may be evaluated asymptotically as $\beta_s(\hbar\tilde{\omega}/kT)^{1-s}\to\infty$. This evaluation is carried out using the method of steepest descents; we quote only the final result, which is

$$\Gamma=\frac{[B(\omega_c)\Delta]^2}{2\tilde{\omega}}\left[\frac{\hbar\tilde{\omega}}{kT}\right]^{(1+s)/2}\left[\frac{\pi}{2(1+s)^2\Gamma(s)\zeta(1+s)\beta_s}\right]^{1/2}$$
$$\times\exp\left[-\frac{1+s}{1-s}\Gamma(s)\left[\frac{1}{2(1+s)\zeta(1+s)}\right]^{(1-s)/(1+s)}\beta_s\left[\frac{\hbar\tilde{\omega}}{k_B T}\right]^{1-s}\right], \quad (6.12)$$

where

$$B(\omega_c)=\exp[\beta_s\,|\,\Gamma(s-1)\,|\,(\tilde{\omega}/\omega_c)^{1-s}] . \quad (6.13)$$

Notice that as the temperature goes to zero, Γ vanishes with an essential singularity in T. This should be contrasted with the results for the ohmic case ($s=1$), with $\alpha>1$, where the tunneling rate Γ vanishes according to a power law, $T^{2\alpha-1}$ [see Eq. (5.30)]. In fact, this $T^{2\alpha-1}$ behavior can be obtained from Eq. (6.12) by carefully considering the limit $s\to 1^-$.

We should like to emphasize that ω_c (the unphysical cutoff frequency introduced in truncating the original double-well problem to the spin-boson form) does not appear explicitly in Eq. (6.12). All of the cutoff dependence has been absorbed into the function $B(\omega_c)$. However, recall that Δ also depends on ω_c, since it contains the renormalizing effects of the high-frequency oscillators. To lowest order in $\beta_s(\tilde{\omega}/\omega_c)^{1-s}$, this dependence is given[72] by $\Delta=\Delta_0[\text{const}B^{-1}(\omega_c)]$, where Δ_0 is the level splitting in the original double well in the absence of a dissipative environment. Thus the leading dependence of Δ on ω_c is exactly canceled by the ω_c dependence of the function B defined above. Therefore the decay rate is independent of ω_c (to leading order) as required.

B. The superohmic case

We now study the behavior of $P(t)$ for superohmic spectral densities of the form (6.1) with $s>1$. The analysis again proceeds by employing the formally exact and completely general expression for $P(t)$, Eqs. (4.17)—(4.22), derived in Sec. IV. We consider first the properties of $P(t)$ when $T=0$, before generalizing to finite temperatures below. When $T=0$, $Q_1(t)$ and $Q_2(t)$, defined as integrals over the spectral density $J(\omega)$ in Eq. (4.22), are given by

$$\frac{q_0^2}{2\pi\hbar}Q_1(t)=A_s\,\mathrm{Im}\left[\frac{1}{1-i\omega_c t}\right]^{s-1}, \quad (6.14a)$$

$$\frac{q_0^2}{2\pi\hbar}Q_2(t)=A_s\left[1-\mathrm{Re}\left[\frac{1}{1-i\omega_c t}\right]^{s-1}\right]$$
$$\equiv A_s-\frac{q_0^2}{2\pi\hbar}Q_3(t) , \quad (6.14b)$$

with A_s, a dimensionless measure of the damping strength, defined by

$$A_s\equiv\frac{q_0^2}{2\pi\hbar}\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}=\beta_s\Gamma(s-1)(\omega_c/\tilde{\omega})^{s-1} . \quad (6.15)$$

In Eq. (6.14b) we have defined $Q_3(t)$, the *time-dependent* piece of $Q_2(t)$; as an integral over the spectral density it is given (at $T=0$) by

$$Q_3(t)\equiv\int_0^\infty\frac{d\omega}{\omega^2}J(\omega)\cos\omega t . \quad (6.16)$$

The important point that distinguishes the superohmic from the subohmic case, $s<1$, is that $Q_2(t)$ now approaches a finite constant as $t\to\infty$ [cf. Eq. (6.9)]. As a result, the factor F_1 in Eq. (4.20a), which for a blip of length t contributes a factor proportional to $\exp[-(q_0^2/\pi\hbar)Q_2(t)]$, is no longer effective in suppressing the widths of the blips. Thus we do not expect the blips to form a dilute gas as they did in the subohmic case. Nevertheless, as we now argue, the noninteracting-blip approximation as described at the end of Sec. IV can in fact still be justified.

We first remark that, in the absence of any damping at all, both the typical blip width and typical sojourn width will be roughly Δ^{-1}. This can be deduced from Eqs. (4.17) and (4.18) by observing that with no damping the term in the sum with n blips and n sojourns is $(-1)^n(t\Delta)^{2n}/(2n)$. For a given time t the dominant term then has $n\equiv t\Delta$ blip-sojourn pairs, implying that a typical time per pair is Δ^{-1}. Since blips and sojourns are on

[71] Gradshteyn and Ryzhik (1980), p. 360, 3.551.3.

[72] This may be shown by an extension of the argument of Dorsey *et al.* (1986).

equal footing (with no damping) on average they will have the same width. In the presence of superohmic damping (at $T=0$), since $Q_2(t)$ does not suppress blips appreciably, we expect that blips and sojourns will still have roughly the same typical width, given now by a renormalized level splitting (see below) $\tilde{\Delta}^{-1}$.

Since Q_1 and Q_3 [the time-dependent piece of $Q_2(t)$; see Eq. (6.16)] decay to zero as $t\to\infty$ if $\tilde{\Delta}^{-1}$ is large enough, it is possible that the dimensionless quantity

$$\frac{q_0^2}{\pi\hbar}Q_1(t=\tilde{\Delta}^{-1}),\ \frac{q_0^2}{\pi\hbar}Q_3(t=\tilde{\Delta}^{-1})\sim\frac{q_0^2}{\hbar}\frac{J(\tilde{\Delta})}{\tilde{\Delta}}\equiv b\ , \tag{6.17}$$

may be much less than one. Then the strength of the interactions between blips and sojourns (S_j,Λ_{jk}, and X_{jk}) given in terms of Q_1 and Q_2 in Eq. (4.21), would typically be small, i.e., of order b. For now we assume that b is indeed small; this will be checked self-consistently using $\tilde{\Delta}^{-1}$, the typical blip and sojourn width that emerges from the calculation. We now work to linear order in b, ignoring in F_n, Eq. (4.19), all the interactions that contribute to $O(b^2)$. When $\varepsilon=0$, both F_3 and F_4 can be replaced by one, since the arguments of the cosines are then proportional to b and only contribute quadratically. Moreover, since the argument of the exponential in F_2 is odd in the blip indices ζ_j, upon summation over these ($\zeta_j=\pm1$) the term linear in b vanishes. Thus to leading order in b only F_1 contributes, and F_n is given by[73]

$$F_n=\prod_{j=1}^{n}\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t_{2j}-t_{2j-1})\right]. \tag{6.18}$$

Equation (6.18) is a reasonable approximation to F_n for typical trajectories which have sojourn and blip widths roughly $\tilde{\Delta}^{-1}$. However, it is *not* of the correct form for those configurations that have blips much narrower than the sojourns separating them. Such configurations are described by the noninteracting-blip approximation in which F_n is given by [see Eq. (4.28)]

$$F_n=\prod_{j=1}^{n}\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t_{2j}-t_{2j-1})\right]\times\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t_{2j}-t_{2j-1})\right]. \tag{6.19}$$

Since Eq. (6.19) has the correct form (by construction) for configurations with narrow blips (say ω_c^{-1}) and reduces to Eq. (6.18) for typical blip widths $\tilde{\Delta}^{-1}$, we expect it to be a reasonable approximation for all possible configurations (provided of course that b is small). With this somewhat heuristic justification for the noninteracting-blip approximation, we now apply it directly to a computation of $P(t)$.

It was shown in Sec. IV that within the noninteracting-blip approximation, with F_n approximated as in Eq. (6.19), the Laplace transform of $P(t)$ could be written in the convenient form [Eq. (4.32)]

$$\tilde{P}(\lambda)=[\lambda+f(\lambda)]^{-1}\ , \tag{6.20}$$

with $f(\lambda)$ given by

$$f(\lambda=\Delta^2\int_0^\infty\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp-\left[\lambda t+\frac{q_0^2}{\pi\hbar}Q_2(t)\right]. \tag{6.21}$$

It is convenient at this stage to absorb the time-independent piece of $Q_2(t)$ into the level splitting Δ. Defining a renormalized level splitting

$$\tilde{\Delta}=\Delta\exp\left[-\frac{q_0^2}{2\pi\hbar}Q_2(t=\infty)\right]=\Delta\exp\left[-\frac{q_0^2}{2\pi\hbar}\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}\right], \tag{6.22}$$

enables us to write $f(\lambda)$ in the form

$$f(\lambda)=\tilde{\Delta}^2\int_0^\infty dt\,e^{-\lambda t}\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[\frac{q_0^2}{\pi\hbar}Q_3(t)\right]. \tag{6.23}$$

Notice that the exponential factor in Eq. (6.22) which relates the renormalized level splitting to Δ is precisely of the Franck-Condon form discussed in Sec. III.C. Since Q_1 and Q_3 approach zero as $t\to\infty$, it is clear that $f(\lambda)$ has a $1/\lambda$ pole [recall that, in the subohmic case, $f(\lambda=0)$ was well defined since $Q_2(t)$ diverged with time]. If we pull this pole out front, then $\tilde{P}(\lambda)$ from Eq. (6.20) can be written as

$$\tilde{P}(\lambda)=\frac{\lambda}{\lambda^2+\tilde{\Delta}^2[1+\lambda\tilde{h}(\lambda)]}\ , \tag{6.24}$$

with $\tilde{h}(\lambda)$ the Laplace transform of $h(t)$ defined by

$$h(t)=\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[\frac{q_0^2}{\pi\hbar}Q_3(t)\right]-1\ . \tag{6.25}$$

To Laplace-invert and determine $P(t)$ it is necessary to locate the poles of $\tilde{P}(\lambda)$. In the absence of damping ($h=0$), these poles are entirely imaginary: $\lambda=\pm i\tilde{\Delta}$. When damping is present and b is small, we expect on physical grounds that these two poles will shift slightly off the imaginary axis, picking up a small negative real part. Setting the denominator of Eq. (6.24) equal to zero and looking for roots near $\pm i\tilde{\Delta}$, we find upon iteration

$$\lambda=\pm i\tilde{\Delta}[1+\lambda h(\lambda)]^{1/2}=\pm i\tilde{\Delta}\left[1\pm\frac{i\tilde{\Delta}}{2}\tilde{h}(\pm i\tilde{\Delta})+\cdots\right]. \tag{6.26}$$

[73] This is clearly similar to the argument used in Sec. V.D and Appendix D.2 in connection with the differences between $P(t)$ and $P^{(0)}(t)$ in the unbiased ohmic case at zero temperature as $\alpha\to0$.

To lowest order in b, the real and imaginary parts of λ are then given by

$$\lambda_I = \pm\tilde{\Delta} , \tag{6.27a}$$

$$\lambda_R = -\frac{\tilde{\Delta}^2}{2}\mathrm{Re}\tilde{h}(\lambda = i\tilde{\Delta}) \equiv -\Gamma_s . \tag{6.27b}$$

It remains to compute the integral for Γ_s,

$$\Gamma_s = \frac{\tilde{\Delta}^2}{2}\int_0^\infty dt \cos(t\tilde{\Delta})h(t) . \tag{6.28}$$

Working to lowest order in b, it is tempting to expand $h(t)$ in Eq. (6.25) in Q_1 and Q_3 to give $h(t) = (q_0^2/\pi\hbar)Q_3(t)$. The integration can then be easily performed by using the original definition of $Q_3(t)$, Eq. (6.16). Upon interchanging the time and frequency integrations, we find

$$\Gamma_s = \frac{q_0^2}{4\hbar}J(\tilde{\Delta}) . \tag{6.29}$$

It can be verified explicitly in this case ($T=0$) that Eq. (6.29) gives the correct answer to lowest order in b, by noting that $h(t)$ can be written as

$$h(t) = \mathrm{Re}\left[\exp\left[\frac{q_0^2}{\pi\hbar}(Q_3 + iQ_1)\right] - 1\right]$$
$$= \mathrm{Re}\sum_{n=1}^{\infty}\frac{(2A_s)^n}{n!}\left[\frac{1}{1-i\omega_c t}\right]^{n(s-1)} . \tag{6.30}$$

Inserting this into Eq. (6.28) and performing the integration demonstrates that the $n=1$ term gives (6.29), and each additional term in the sum contributes to higher orders in b.

Finally we Laplace-invert $\tilde{P}(\lambda)$, which has two poles at $\lambda = -\Gamma_s \pm i\tilde{\Delta}$, to obtain the final result for the superohmic case with $T=0$:

$$P(t) = \cos(\tilde{\Delta}t)\exp(-\Gamma_s t) . \tag{6.31}$$

This describes underdamped coherent oscillations at a frequency $\tilde{\Delta}$, Eq. (6.22), and a damping rate Γ_s, Eq. (6.29). Notice that this result is exactly equivalent to that obtained with the heuristic NMR approach in Sec. III.B, except that the renormalized level splitting $\tilde{\Delta}$ replaces Δ. Although this was anticipated in Sec. III.B, the advantage of the present approach is that $\tilde{\Delta}$ emerges naturally from the calculation and does not have to be put in by hand.

In the light of Eq. (6.29), the requirement that b be small [Eq. (6.17)] is equivalent to the inequality

$$\Gamma_s/\tilde{\Delta} \ll 1 . \tag{6.32}$$

Thus the above approach, and hence $P(t)$ in Eq. (6.31), is only valid when the system is extremely underdamped. We must now check to see under what conditions this is in fact the case. Using the definitions of $\tilde{\Delta}$ and $J(\omega)$, we have

$$\Gamma_s/\tilde{\Delta} \approx A_s(\tilde{\Delta}/\omega_c)^{s-1} \simeq A_s e^{-(s-1)A_s}(\Delta/\omega_c)^{s-1} , \tag{6.33}$$

where A_s, defined in Eq. (6.15), is a dimensionless measure of the coupling strength to the environment. Recall that we are always working in the limit $\Delta \ll \omega_c$ (which was necessary to truncate the original double-well problem into the spin-boson system studied here), so that *no matter how large the coupling A_s is* the inequality (6.32) is satisfied. Thus for superohmic spectral densities ($s>1$), if the system can be reduced to a two-state description, at $T=0$ it will always exhibit *underdamped* coherent oscillations.

We now discuss briefly the cancellation of the unphysical frequency scale ω_c, introduced in truncating the double-well problem into the two-state system. To do so we must argue that $\tilde{\Delta}$ defined in Eq. (6.22) is in fact independent of ω_c. Notice that $\tilde{\Delta}$ is related to Δ by the Franck-Condon factor over the low-frequency oscillators [since $J(\omega)$ defined in (6.1) has an upper cutoff ω_c]. Since Δ is in turn related to the unrenormalized level splitting Δ_0 in the double well by a Franck-Condon factor over the high-frequency ($>\omega_c$) oscillators, the ω_c does indeed cancel out.

We now generalize the discussion of superohmic spectral densities ($s>1$) to include finite temperature. In this case it is convenient to treat $s>2$ and $1<s<2$ separately. For $s>2$, $Q_2(t)$ still approaches a constant as $t\to\infty$, and the $T=0$ analysis just described goes through with only minor modifications. On the other hand, for $1<s<2$, $Q_2(t)$ diverges at long times and more care is needed.

We first consider the case $s>2$ and employ the noninteracting-blip approximation. As in the $T=0$ analysis, although the blips are not dilute, this approximation can be justified when the system is extremely underdamped. We briefly sketch the modification needed to generalize the zero-temperature discussion. Finite temperature enters the general expressions (4.17)—(4.22) for $P(t)$ only through the inclusion of the factor $\coth(\beta\hbar\omega/2)$ in the definition of $Q_2(t)$,

$$Q_2(t) = \int_0^\infty d\omega \frac{J(\omega)}{\omega^2}(1-\cos\omega t)\coth(\beta\hbar\omega/2) . \tag{6.34}$$

For $s>2$, $Q_2(t=\infty)$ is finite, and the renormalized level splitting $\tilde{\Delta}$ in Eq. (6.22) is generalized to read[74]

$$\tilde{\Delta}(\beta) \equiv \Delta \exp\left[-\frac{q_0^2}{2\pi\hbar}\int_0^\infty \frac{d\omega}{\omega^2}J(\omega)\coth(\beta\hbar\omega/2)\right] . \tag{6.35}$$

The only other modification necessary is to include the $\coth(\beta\hbar\omega/2)$ factor in $Q_3(t)$, the finite-time piece of $Q_2(t)$, defined in Eq. (6.16). With this change the damping rate Γ_s in Eq. (6.29) is now given by

$$\Gamma_s(\beta) = \frac{q_0^2}{4\hbar}J(\tilde{\Delta})\coth[\beta\hbar\tilde{\Delta}(\beta)/2] . \tag{6.36}$$

Since the rest of the $T=0$ analysis goes through unchanged, the final results for spectral densities with $s>2$

[74] Actually, for consistency we should neglect the difference between $\tilde{\Delta}(\beta)$ and $\tilde{\Delta}(0)$, since this is a correction of relative order $(k_B T/\hbar\omega_c)^{s-1}$, and similar terms have already been dropped in going from the two-well to the two-state system; see Sec. II.

is simply

$$P(t)=\cos[\tilde{\Delta}(\beta)t]\exp[-\Gamma_s(\beta)t]\ , \tag{6.37}$$

with $\tilde{\Delta}(\beta)$ and $\Gamma_s(\beta)$ defined above. Thus for $s>2$ even at finite temperature the system exhibits underdamped coherent oscillations. It is easy to check that when $\Delta \ll \omega_c$, $\Gamma_s(\beta) \ll \tilde{\Delta}(\beta)$ for all temperatures less than $\hbar\omega_c/k_B$, implying that this underdamped behavior persists up to the largest temperatures of interest. Once again Eq. (6.37) confirms the expected behavior for $P(t)$ discussed in Sec. III.B.

When $1<s<2$ the generalization to finite temperature is not so simple, since $Q_2(t)$ now diverges with time,

$$\frac{q_0^2}{\pi\hbar}Q_2(t)\sim A_s(k_BT/\hbar\omega_c)(\omega_c t)^{2-s},\quad t\to\infty\ . \tag{6.38}$$

However, at large enough temperatures we expect that the blip lengths will be sufficiently suppressed by F_1 in Eq. (4.20a) that the blips will once again form a dilute gas. Under these conditions the analysis of the subohmic case will apply, and $P(t)$ will exhibit overdamped exponential relaxation. In particular, $f(\lambda)$, which enters into the noninteracting-blip approximation [Eqs. (6.20) and (6.21)], has a well-defined series expansion about $\lambda=0$,

$$f(\lambda)=f_0+\lambda f_1+\cdots\ . \tag{6.39}$$

If $|f_1| \ll 1$, the Laplace inversion for $P(t)$ is straightforward, giving pure exponential relaxation

$$P(t)=\exp(-\Gamma_s t)\ , \tag{6.40}$$

with a decay rate

$$\Gamma_s=f(\lambda=0)$$
$$=\Delta^2\int_0^\infty dt\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ . \tag{6.41}$$

This result is equivalent to Fermi's golden rule [see Sec. III.D, Eqs. (3.37) and (3.38)] and, as discussed in the subohmic case, is valid so long as $|f_1| \ll 1$. Using the long-time behavior of $Q_2(t)$ in Eq. (6.38), we find that this requirement is equivalent to

$$T \gg T^* \equiv A_s^{-1}k^{-1}\hbar\omega_c(\tilde{\Delta}/\omega_c)^{2-s}\quad (1<s<2)\ , \tag{6.42}$$

with $\tilde{\Delta}$ the renormalized level splitting defined in Eq. (6.22). Notice that T can satisfy this inequality and still be much smaller than $\hbar\omega_c/k$ as required. Finally, evaluating the integral for Γ_s asymptotically in the limit $kT \ll \hbar\omega_c$, we find

$$\Gamma_s=\left[\frac{(2-s)\sin(\pi s/2)}{2\beta_s\Gamma(s-1)\sin\pi(s-1)}\right]^{1/(2-s)}$$
$$\times\Gamma\left[\frac{3-s}{2-s}\right]\frac{\tilde{\Delta}^2}{\tilde{\omega}}\left[\frac{\hbar\tilde{\omega}}{kT}\right]^{1/(2-s)}\ . \tag{6.43}$$

For $1<s<2$, the system's behavior crosses over from underdamped coherent oscillations to overdamped exponential relaxation as the temperature is raised above T^*. This is analogous to the behavior found for ohmic spectral densities with $\alpha<\frac{1}{2}$ (see Secs. V.C and V.F). It is interesting to observe that, as in the ohmic case with $\alpha<\frac{1}{2}$, in the overdamped regime the relaxation rate is a *decreasing* function of temperature. As the temperature is raised, the environment destroys more of the quantum coherence necessary for tunneling between the two wells, thus reducing the decay rate.

Finally it is instructive to compare our calculation with a frequently used method in chemical physics or polaron theory (cf. Mahan, 1980, p. 528), which is based on a modified golden rule argument. As discussed in Sec. III.D, the golden rule approach assumes that the linear short-time decrease in $P(t)$ may be exponentiated to give an incoherent exponential relaxation $P(t)=\exp(-\Gamma_{\rm FGR}t)$ at all times. The presence of a sufficiently strong environment coupling is supposed to completely destroy any coherence effects. The results obtained above, however, demonstrate that for a system that can be reduced to a two-state (or tight-binding) description, when $J(\omega)\sim\omega^s$ with $s>2$ the behavior is in fact a damped *oscillation at* all relevant temperatures and arbitrarily strong coupling. The inadequacy, in this case, of a description by an exponential decay is easily seen from Eq. (6.13), generalized to finite T. It is only when $f(\lambda=0)$ is finite that $P(t)$ relaxes incoherently with the golden rule rate $\Gamma_{\rm FGR}=f(\lambda=0)$. However, for $s>2$, $f(\lambda=0)$ does not exist, and a $1/\lambda$ pole has to be separated off, which leads to the oscillatory structure (6.31) or (6.37). The divergence of the rate $f(\lambda=0)$ reflects the inadequacy of the golden rule approach in producing this oscillatory behavior. It has been common practice (Holstein, 1959) to circumvent this divergence by subtracting (with, we believe, no justification) an infinite term ("the diagonal processes") from $f(\lambda=0)$ and by assuming that the system relaxes exponentially with a modified—and now finite—golden rule rate

$$\hat{\Gamma}_{\rm FGR}=\tilde{\Delta}^2\int_0^\infty dt\,h(t) \tag{6.44}$$

with $h(t)$ as defined in Eq. (6.25). Comparing this with our result (6.28) for the damping rate Γ_s of the *oscillation,* we see that, up to a factor of 2, $\tilde{\Gamma}_{\rm FGR}$ turns out to be the lowest-order term in a formal expansion of Γ_s in powers of $\tilde{\Delta}$. The modified golden rule rate thus at best only describes the decay of the *envelope* of $P(t)$ to lowest order in $\tilde{\Delta}$.

Equation (6.44) has been used to obtain the well-known T^7 law for the diffusion constant in Holstein's small polaron model (Flynn and Stoneham, 1970). By changing the integration variable t to $t+(i/2)\hbar\beta$ one finds

$$\tilde{\Gamma}_{\rm FGR}=\tilde{\Delta}^2\int_0^\infty dt\left[\exp\left[\frac{q_0^2}{\pi\hbar}\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}\frac{\cos\omega t}{\sinh(\beta\hbar\omega/2)}\right]-1\right]\ . \tag{6.45}$$

Expanding in powers of the interaction, it is easy to see that the linear term (i.e., the "one-phonon process") vanishes if $s>3$.[75] Thus, contrary to Γ_s, the lowest-order contribution usually comes from the second-order term and is given by

$$\tilde{\Gamma}_{\rm FGR}^{(2)} \sim \tilde{\Delta}^2 \int_0^\infty d\omega \frac{J^2(\omega)}{\omega^4 \sinh^2(\beta\hbar\omega/2)} , \tag{6.46}$$

which behaves as T^{2s-3} for small temperatures. In particular, taking $s=5$ gives the well-known T^7 law. To obtain the diffusion constant D from the two-state relaxation rate Γ, it is crucial to assume that the transfer from site to site is completely incoherent so that D in a periodic lattice is simply given by $D=\Gamma a^2$, a being the lattice constant. However, our results imply that for $s>2$ this assumption is inappropriate, since coherence between two adjacent sites is *not* destroyed completely on the relevant time scales.[76]

VII. THE BIASED CASE

In this section we generalize the discussion of the behavior of $P(t)$ to include a bias ε between the two wells. As in Sec. VI we shall consider general spectral densities of the form (6.1). Once again the objective here is to extract the behavior of $P(t)$ from the formally exact expression derived in Sec. IV, Eq. (4.20). This section is organized as follows. In subsection VII.A we generalize the noninteracting-blip approximation, introduced in Sec. IV.C, to include a nonzero bias, which reduces the calculation of $P(t)$ to the performance of Laplace transforms. By studying the long-time behavior that follows, i.e., $\lim_{t\to\infty} P(t)$, we demonstrate that this approximation cannot be trusted (when $\varepsilon\neq 0$) in the underdamped regimes where the system performs coherent oscillations. The heuristic justification offered in Sec. VI, in the underdamped regime when $\varepsilon=0$, is shown to break down in the presence of a nonzero bias. The noninteracting-blip approximation nevertheless can still be justified when the parameters are such that the system exhibits overdamped exponential relaxation, as it will whenever the bias ε is large enough. A general expression is then derived for $P(t)$ in the overdamped regime. In Sec. IV.B, this is used to compute the specific behavior for subohmic, ohmic, and superohmic spectral densities.

A. Noninteracting-blip approximation

The noninteracting-blip approximation was introduced in Sec. IV.C as a means for simplifying the formally exact expression for $P(t)$, Eqs. (4.17)—(4.22). We use the same simplifying assumptions here, i.e., points (1) and (2) in Sec. IV.C., keeping $\varepsilon\neq 0$. Then, within the noninteracting-blip approximation, F_n in Eq. (4.19) takes the form

$$F_n = F_1 F_2 F_3 F_4(\zeta_j) , \tag{7.1}$$

with

$$F_1 = \prod_{j=1}^{n} \exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t_{2j}-t_{2j-1}) \right] , \tag{7.2a}$$

$$F_2 = 1 , \tag{7.2b}$$

$$F_3 = \prod_{j=2}^{n} \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t_{2j}-t_{2j-1}) \right] , \tag{7.2c}$$

and

$$F_4 = \cos\left[\zeta_1 \frac{q_0^2}{\pi\hbar} Q_1(t_2-t_1) - \frac{\varepsilon}{\hbar} \sum_{j=1}^{n} \zeta_j (t_{2j}-t_{2j-1}) \right] . \tag{7.2d}$$

Notice that ε only enters into the term F_4. The sign convention is such that a positive (negative) value of ε corresponds to preparing the particle initially in the unstable (stable) well. In contrast to the unbiased case [Eq. (4.28)], F_n still depends on the blip indices ζ_j. However, the sum over ζ_j in Eq. (4.18) can now easily be performed, giving

$$2^{-n} \sum_{\{\zeta_j\}} F_4(\zeta_j) = \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t_2-t_1) - \frac{\varepsilon}{\hbar}(t_2-t_1 \right] \times \prod_{j=2}^{n} \cos\left[\frac{\varepsilon}{\hbar}(t_{2j}-t_{2j-1}) \right] . \tag{7.3}$$

Then $P(t)$ in Eq. (4.17) is given by

$$P(t) = \sum_{n=0}^{\infty} (-1)^n \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{n-1} \cdots \int_0^{t_2} dt_1 \left[\prod_{j=1}^{n} g(t_{2j}-t_{2j-1}) + h(t_2-t_1) \prod_{j=2}^{n} g(t_{2j}-t_{2j-1}) \right] , \tag{7.4}$$

with the functions $g(t)$ and $h(t)$ defined by

$$g(t) = \Delta^2 \cos(\varepsilon t/\hbar) \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t) \right] \exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t) \right] , \tag{7.5a}$$

$$h(t) = \Delta^2 \sin(\varepsilon t/\hbar) \sin\left[\frac{q_0^2}{\pi\hbar} Q_1(t) \right] \exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t) \right] . \tag{7.5b}$$

The spectral density $J(\omega)$ enters via $Q_1(t)$ and $Q_2(t)$, which are defined in Eq. (4.22). Upon Laplace transforming with respect to time, as in the $\varepsilon=0$ case [see Eqs. (4.31) and (4.32)], we obtain the final result for $\tilde{P}(\lambda)$ within the noninteracting-blip approximation,

$$\tilde{P}(\lambda) = [1 - h(\lambda)/\lambda][\lambda + g(\lambda)]^{-1} . \tag{7.6}$$

[75] For $s=3$ the integral is proportional to T (see Teichler and Seeger, 1981), whereas for $s<3$ the expansion is divergent.

[76] An incoherent relaxation for $s>2$ can only occur if there is a finite bias that is large compared to the tunneling matrix element. See Sec. VII.B below.

Here $g(\lambda)$ and $h(\lambda)$ are, respectively, Laplace transforms of $g(t)$ and $h(t)$. As $\varepsilon \to 0$, Eq. (7.6) reduces to the unbiased expression (4.32).

Before computing $P(t)$ for particular spectral densities, it is useful to examine the long-time behavior of $P(t)$ within the noninteracting-blip approximation. From this we can see some of the shortcomings of the approximation, which occur when $\varepsilon \neq 0$. To be specific, we study the pole of $\tilde{P}(\lambda)$ at $\lambda = 0$, which upon Laplace inversion gives us directly $P(t \to \infty)$, as all other singularities of $\tilde{P}(\lambda)$ have nonzero negative real parts. Since both

$$g_0 \equiv \lim_{\lambda \to 0} g(\lambda) \tag{7.7a}$$

and

$$h_0 \equiv \lim_{\lambda \to 0} h(\lambda) , \tag{7.7b}$$

have well-defined limits (for $\lambda \to 0$ with $\mathrm{Re}\lambda \geq 0$), the pole at $\lambda = 0$ is a simple one. Hence, upon Laplace inversion of $\tilde{P}(\lambda)$, we have $P(t = \infty) = -h_0/g_0$. We show in Appendix E that, for *arbitrary* spectral densities $J(\omega)$, the ratio h_0/g_0 is in fact equal to $\tanh(\varepsilon/2k_BT)$, so that

$$P(t = \infty) = -\frac{h_0}{g_0} = -\tanh(\varepsilon/2k_BT) . \tag{7.8}$$

This result demonstrates that as $T \to 0$ the noninteracting-blip approximation predicts a symmetry breaking for all spectral densities. That is, an infinitesimal bias ε is predicted to localize the particle in one well. However, for both superohmic spectral densities ($s > 1$) and the ohmic spectral density ($s = 1$) with $\alpha < 1$, arguments given in Sec. III.C indicate that the symmetry is actually *not* broken. This can also be inferred in a more rigorous fashion by observing that the partition function of the spin-boson Hamiltonian (at $T = 0$), written as a path integral, is equivalent to the partition function of a classical one-dimensional Ising model with long-range interactions (see Sec. III.E and Chakravarty, 1982). For $J \sim \omega^s$ these interactions fall off as $r^{-\sigma}$ with $\sigma = s + 1$. It is known that when $\sigma > 2$ the classical Ising model is never spontaneously magnetized. For $\sigma = 2$ it is generally believed to be magnetized only when $\alpha > 1$ (Ruelle, 1969; Anderson *et al.*, 1970). Accepting these conclusions, it is apparent that, for spectral densities with $s > 1$ and $s = 1$ with $\alpha < 1$, when $T = 0$ and ε is small but nonzero, the noninteracting-blip approximation (which predicts a symmetry breaking) gives qualitatively incorrect behavior for $P(t)$ at long times. This is in marked contrast with the $\varepsilon = 0$ results of the previous sections, where the noninteracting-blip approximation is "qualitatively" correct, in the sense that the correct value of $P(t)$ is obtained at $t \to \infty$. Perhaps this is not surprising, since it is precisely in these regimes that (at $\varepsilon = 0$) the blips do *not* actually form a dilute gas.

Recall, however, that in Sec. VI.B (with $\varepsilon = 0$) we were able to justify the noninteracting-blip approximation for $s > 1$ at $T = 0$, even though the blips were *not* in fact dilute. Where does the reasoning used here break down when $\varepsilon \neq 0$? Recall that for $s > 1$ we argued that the interactions between blips and sojourns, X_{jk} and Λ_{jk} in Eq. (4.20), were very weak, and thus it was possible to work to linear order in these. Doing so we found that F_n in Eq. (4.17) reduced to a form essentially equivalent to the noninteracting-blip approximation, Eq. (4.28). For the biased system, however, this is no longer the case. The difficulty comes in treating F_4 [Eq. (4.20d)] linearly in X_{j0}. The linear term has the form

$$F_4 \simeq \cos\left[\frac{\varepsilon}{\hbar}\sum_{j=1}^{n}\zeta_j(t_{2j}-t_{2j-1})\right] + \left[\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}\zeta_j X_{j0}\right]\sin\left[\sum_{j=1}^{n}\zeta_j\frac{\varepsilon}{\hbar}(t_{2j}-t_{2j-1})\right] , \tag{7.9}$$

which is entirely nontrivial and gives for F_4 something quite different from the noninteracting-blip approximation, Eq. (7.2d). Thus we conclude that, for $T = 0$ and ε small but nonzero, when the parameters are such that the unbiased ($\varepsilon = 0$) system is underdamped, the noninteracting-blip approximation gives qualitatively incorrect long-time behavior for $P(t)$.

The noninteracting-blip approximation can, however, still be justified when the system exhibits overdamped relaxation (as it always will for large enough bias, see Sec. VII.B). In particular, suppose that $g(\lambda)$ and $h(\lambda)$ in Eq. (7.6) have well-defined expansions about zero,

$$g(\lambda) = g_0 + \lambda g_1 + \cdots , \tag{7.10a}$$

$$h(\lambda) = h_0 + \lambda h_1 + \cdots , \tag{7.10b}$$

with $h_1, g_1 \ll 1$. Then, within the noninteracting-blip approximation, $\tilde{P}(\lambda)$ in Eq. (7.6) can be Laplace inverted to give

$$P(t) = -\tanh(\varepsilon/2k_BT) + [1 + \tanh(\varepsilon/2k_BT)]e^{-\Gamma t} , \tag{7.11a}$$

with

$$\Gamma = g_0 = \Delta^2 \lim_{\lambda \to 0} \int_0^\infty dt\, e^{-\lambda t}\cos(\varepsilon t/\hbar)\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right] \times \exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right] , \tag{7.11b}$$

where we have used Eq. (7.8) relating h_0/g_0 to $\tanh(\varepsilon/2k_BT)$. Notice that Eq. (7.11) describes simple overdamped exponential relaxation of the quantity $P(t) - P(\infty)$.

It is precisely under the condition $g_1 \ll 1$ that we can in fact justify the noninteracting-blip approximation. To see this we first remark that, if the typical blip widths are much smaller than the widths of a typical blip-sojourn pair (i.e., the blips really form a dilute gas), then, since the interacting between blips decay to zero at long times, the

noninteracting-blip approximation should be valid. As in Sec. VI, the average blip width t_b can be estimated by taking the first moment of $g(t)$ in Eq. (7.5a),

$$t_b \simeq g_1/g_0 \ , \tag{7.12}$$

with g_1 and g_0 defined in Eq. (7.10a). Since $g(t)$ oscillates with a factor $\cos(\varepsilon t/\hbar)$, the typical blip width is expected to decrease with increasing bias. The typical width of a blip *and* its neighboring sojourn, on the other hand, can be obtained by observing that for a given time t the dominant term in the expansion of $e^{-\Gamma t}$ in Eq. (7.11a) has $n \simeq g_0 t$ powers of g_0. Since n is proportional to the number of blips, a blip-sojourn pair has a typical width $t/n \simeq g_0^{-1}$. The blips will form a dilute gas when $t_b \ll g_0^{-1}$ or

$$g_1 \ll 1 \ . \tag{7.13}$$

Thus when Eq. (7.13) is satisfied the noninteracting-blip approximation is expected to be valid, and the system should exhibit overdamped exponential relaxation as described by Eq. (7.11).

Before applying the general result (7.11) to specific spectral densities, it is instructive to compare it to the Fermi's golden rule result for $P(t)$, Eqs. (3.37) and (3.38). The results differ only in the convergence factor $e^{-\lambda t}$ in (7.11b), which is absent in the expression for the golden rule decay rate. For ohmic or subohmic spectral densities, where $Q_2(t)$ diverges with time, this difference is moot, since the $\lambda \to 0$ limit can be taken under the integral sign. For superohmic $J(\omega)$, on the other hand, the integral for the golden rule decay rate, Eq. (3.38), is divergent at long times. However, due to the convergence factor, Eq. (7.11b) still gives a well defined and finite decay rate [see Eq. (7.23) below]. In addition to yielding finite decay rates for $s>1$, the noninteracting-blip approach described above has provided us with a simple criterion, (7.13), for the validity of the result (7.11).

$$\Gamma = \Delta^2 \int_0^\infty dt \cos(\varepsilon t/\hbar) \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t)\right] \exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t)\right] \ . \tag{7.14}$$

Using Eqs. (6.9) and (6.11) for $Q_1(t)$ and $Q_2(t)$, we can find this integral asymptotically for T, $\varepsilon \to 0$. For $k_B T \ll \varepsilon \ll \beta_s^{1/1-s}(\hbar\tilde{\omega})$ we find

$$\Gamma = \Gamma(T=0)\left\{1 + \left[2\beta_s \Gamma(s+1)\zeta(s+1)[2\beta_s\Gamma(s)]^{2/s}\left[\frac{\hbar\tilde{\omega}}{\varepsilon}\right]^{2/s}\right]\left[\frac{k_B T}{\hbar\tilde{\omega}}\right]^{1+s} + \cdots\right\} \tag{7.15a}$$

with the zero-temperature decay rate given by

$$\Gamma(T=0) = \frac{(B\Delta)^2}{4\tilde{\omega}}\left[\frac{2\pi[2\beta_s\Gamma(s)]^{1/2}}{s}\right]^{1/2}\left[\frac{\hbar\tilde{\omega}}{\varepsilon}\right]^{(1+s)/2s} \exp\left[-\frac{s}{1-s}[2\beta_s\Gamma(s)]^{1/s}\left[\frac{\hbar\tilde{\omega}}{\varepsilon}\right]^{(1-s)/s}\right] \tag{7.15b}$$

and with B defined in Eq. (6.13). Notice that the zero-temperature decay rate vanishes with an essential singularity as $\varepsilon \to 0$. In the limit T, $\varepsilon \to 0$ the particle remains in the well in which it was initially prepared. At finite temperatures the rate is enhanced by a factor varying as T^{1+s}.

Next we consider the ohmic spectral density (Fisher and Dorsey, 1985; Grabert and Weiss, 1985). When $T=0$, $Q_2(t)$ still diverges as $t \to \infty$, but now only logarithmically [see Eq. (5.4)],

$$\frac{q_0^2}{\pi\hbar} Q_2(t) = \alpha \ln(1+\omega_c^2 t^2) \ . \tag{7.16}$$

B. Results in the overdamped regime

In this subsection we apply the general result for $P(t)$ in the overdamped regime [Eq. (7.11)] to specific spectral densities of the form (6.1); i.e., subohmic ($0<s<1$), ohmic ($s=1$), and superohmic ($s>1$). For each we use Eq. (7.13) to deduce under what conditions the noninteracting-blip approximation is valid, and compute the corresponding overdamped decay rate Γ.

We consider first subohmic spectral densities, $0<s<1$. In this case $Q_2(t)$, defined in Eq. (4.22), diverges with time as $\beta_s(\tilde{\omega}t)^{1-s}$, so that $g(t)$ in Eq. (7.5a) decays rapidly as $t \to \infty$. Using this fact, it is straightforward to show that the validity criterion (7.13) is satisfied (at all T and ε) when $\Delta \ll \beta_s^{1/(1-s)}\tilde{\omega}$. Thus for sufficiently small Δ the noninteracting-blip approximation is valid, and the system exhibits overdamped relaxation as described by Eqs. (7.11). Since $Q_2(t)$ diverges algebraically with time, the limit $\lambda \to 0$ in Eq. (7.11b) can be taken directly, and the decay rate is given simply by the integral

For $\alpha > 1$ this is fast enough that even when ε, $T \to 0$, g_1 in Eq. (7.10a) is finite and of order $(\Delta/\omega_c)^2$. Since this is much less than unity by assumption, the noninteracting-blip approximation is valid for arbitrary temperatures and bias. Equation (7.11a) then shows that for $\alpha > 1$, $\langle \sigma_z(t) \rangle$ relaxes at long times to $-\tanh(\varepsilon/2k_B t)$. If we define a susceptibility to the external biasing field ε, $\chi_0 = \frac{1}{2}\partial\langle\sigma_z\rangle/\partial\varepsilon$, we see that the zero-field susceptibility obeys a Curie-Weiss law, $\chi_0 \sim 1/T$. Recall from Sec. III.E that the spin-boson Hamiltonian for ohmic spectral densities was analogous in many ways to the Kondo problem; specifically, $\alpha > 1$ corresponds to the ferromagnetic Kondo problem, which is known to obey a Curie-Weiss

law, so the above result is not surprising.

When $\alpha<1$, $Q_2(t)$ in Eq. (7.16) grows sufficiently slowly with time that g_1 diverges as T and $\varepsilon\to 0$. In this case one can show, by using Eq. (5.4) for $Q_1(t)$ and $Q_2(t)$ and asymptotically expanding $g(\lambda)$, that the validity criterion (7.13) gives roughly

$$\varepsilon \gg \Delta_r \equiv \Delta(\Delta/\omega_c)^{\alpha/1-\alpha} , \tag{7.17a}$$

when $T=0$ and (as obtained in Sec. V)

$$T \gg \alpha^{-1}\Delta_r , \tag{7.17b}$$

when $\varepsilon=0$. Thus, for sufficiently large bias or temperature, the system exhibits the overdamped behavior (7.11) even when $\alpha<1$. The coherent oscillations present in $P(t)$ for $\alpha<\frac{1}{2}$ and $\varepsilon=T=0$ (analyzed in detail in Sec. V.D) have been completely suppressed.

Let us evaluate the overdamped decay rate for the ohmic rate. With Q_1 and Q_2 from Eq. (5.4), we perform the integration (7.14) asymptotically for $k_BT,\ \varepsilon \ll \hbar\omega_c$ giving (Fisher and Dorsey, 1985; Grabert and Weiss, 1985)

$$\Gamma=\frac{\Delta^2}{2\omega_c}\left[\frac{2\pi k_BT}{\hbar\omega_c}\right]^{2\alpha-1}\frac{\cosh(\varepsilon/2k_BT)}{\Gamma(2\alpha)} \times |\,\Gamma(\alpha+i\varepsilon/2\pi k_BT)\,|^2 . \tag{7.18}$$

For $\varepsilon\to 0$ this reduces to the unbiased decay rate (5.30). When $k_BT \ll |\,\varepsilon\,|$, Eq. (7.18) gives

$$\Gamma=\Gamma(T=0)\left[1+\frac{\pi^2}{3}\alpha(2\alpha-1)(2\alpha-2)(k_BT/\varepsilon)^2+\cdots\right], \tag{7.19}$$

with

$$\Gamma(T=0)=\frac{\pi}{2}\frac{\Delta^2}{\omega_c}\frac{(\varepsilon/\hbar\omega_c)^{2\alpha-1}}{\Gamma(2\alpha)} . \tag{7.20}$$

When $\alpha>1$ the zero-temperature decay rate vanishes as a power law for $\varepsilon\to 0$, in contrast to the subohmic case. The finite temperature enhancement to the decay rate varies as T^2.

Lastly we turn to superohmic spectral densities, $s>1$. For simplicity we discuss only the zero-temperature case. Since $Q_2(t)$ now has a finite limit as $t\to\infty$ [see Eq. (6.14)], so that $g(t)$ does not decay to zero, care must be used in obtaining the asymptotic expansion for $g(\lambda)$ [Eq. (7.10a)]. As in the unbiased analysis of Sec. VI we first absorb the time-independent piece of $Q_2(t)$ into a renormalized level splitting $\tilde{\Delta}$,

$$\Delta=\Delta\exp\left[-\frac{q_0^2}{\pi\hbar}\int_0^\infty d\omega\frac{J(\omega)}{\omega^2}\right], \tag{7.21}$$

giving from Eq. (7.5a)

$$g(\lambda)=\tilde{\Delta}^2\int_0^\infty dt\, e^{-\lambda t}\cos(\varepsilon t/\hbar)\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right] \times\exp\left[\frac{q_0^2}{\pi\hbar}Q_3(t)\right], \tag{7.22}$$

with $Q_3(t)$ defined in Eq. (6.14b). This can conveniently be cast in the form

$$g(\lambda)=\tilde{\Delta}^2\int_0^\infty dt\, e^{-\lambda t}\cos(\varepsilon t/\hbar)\left[\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[\frac{q_0^2}{\pi\hbar}Q_3(t)\right]-1\right]+\frac{\tilde{\Delta}^2\lambda}{\lambda^2+(\varepsilon/\hbar)^2} . \tag{7.23}$$

Since the integrand in Eq. (7.23) now decays to zero as $t\to\infty$, to obtain the decay rate $\Gamma=g_0$ we can simply set $\lambda=0$. Using $Q_1(t)$ and $Q_2(t)$ from Eq. (6.14), we then find that to lowest order in $q_0^2J(\varepsilon/\hbar)/\varepsilon$ the decay rate is given by

$$\Gamma=\left[\frac{\hbar\tilde{\Delta}}{\varepsilon}\right]^2\frac{q_0^2}{2\hbar}J(\varepsilon/\hbar) . \tag{7.24}$$

From Eq. (7.23) it is straightforward to demonstrate that the coefficient of the linear term in $g(\lambda)$, g_1, is at most of order $(\hbar\tilde{\Delta}/\varepsilon)^2$. Thus the validity criterion (7.13) requires that the bias energy ε be large compared to $\hbar\tilde{\Delta}$. When this is satisfied, the system exhibits overdamped relaxation as described by Eq. (7.11), with decay rate (7.24). The coherent oscillations that were present in the unbiased case (Sec. VI.B) are completely suppressed when ε is large enough. The above result for $P(t)$ is equivalent to that obtained from the heuristic discussion in Sec. III.B, except that the renormalized level splitting $\tilde{\Delta}$ enters rather than Δ.

We believe that the results just obtained for the superohmic and $\alpha<1$ ohmic cases are correct "in the limit $\hbar\tilde{\Delta}/\varepsilon\to 0$," in the sense that the absolute corrections to the form of $P(t)$ given by Eq. (7.11) are[77] of order $(\hbar\tilde{\Delta}/\varepsilon)^2$ for all t. (Note that in the limit $t\to\infty$ the *relative* corrections are also of this order, since the value of $P(\infty)$ predicted by Eq. (7.11), namely, $(-\tanh\beta\varepsilon/2)$, must be corrected to $[-(\varepsilon/E)\tanh\beta E/2]$ in the weak-damping case.) It should, however, be pointed out that for fairly short times the *deviation* of $P(t)$ from unity is in general not given correctly by Eq. (7.11). In fact, it is intuitively obvious (see Sec. III.B) that, in a weakly damped two-state system with a small but finite value of $\hbar\tilde{\Delta}/\varepsilon$, the quantity $P(t)$ will have an oscillatory component with a frequency $E=(\varepsilon^2+\hbar^2\tilde{\Delta}^2)^{1/2}$ and an amplitude of order $(\hbar\Delta/\varepsilon)^2$, and that at times short compared to the inverse of $(q_0^2/2\hbar)J(\varepsilon/\hbar)$ this term will actually be much larger than the correction to unity predicted by Eq.

[77] This statement must, as always, be understood in an asymptotic sense; see Sec. V.B.

(7.11). This term nowhere appears in the analysis of this subsection. In fact, if we think in terms of the approximate eigenstates of the weakly damped system, which are nearly localized in the lower and upper wells, respectively, but have a small probability, $\sim(\hbar\tilde{\Delta}/\varepsilon)^2$, of overlap into the "wrong" well, it appears that the method of the present section takes the overlap into account only to the extent that it provides a decay mechanism.

VIII. CONCLUSIONS

This has been a long and no doubt at times tedious paper. For the benefit of those readers, if any there be, who have struggled through it this far, let us try to summarize what we think we have achieved.

First, given as always the WKB condition ($\Delta_0 \ll \omega_0$) and the condition to be strongly in the quantum limit ($kT \ll \hbar\omega_0$: see Sec. II for definitions),[78] we believe we have given, in Sec. II and Appendix A, a quite general and precise prescription for converting the problem of a system moving between two nearly degenerate potential wells while interacting dissipatively with its environment into the standard spin-boson (dissipative two-state) problem. This prescription works whether or not the potential has any particular symmetry and whatever the spectrum of the dissipative interaction, and allows in principle not merely an order-of-magnitude but an exact calculation of the parameters of the relevant two-state problem in terms of those of the extended system (see Dorsey *et al.*, 1985).

Second, we have shown (Secs. V and VI) that the qualitative behavior of the unbiased dissipative two-state system depends quite crucially on the frequency dependence of the dissipative coupling, $J(\omega)$. In particular, if $J(\omega)$ scales as ω^s for frequencies less than, or of order of, the bare tunneling frequency, then we can distinguish four different cases. (1) For $s \geq 2$ we get weakly damped oscillations at all temperatures. (2) For $1 < s < 2$ we get weakly damped oscillations at zero temperature, but a crossover to overdamped behavior as the temperature is raised. (3) For $0 < s < 1$ the system is localized at zero temperature: at finite temperature it relaxes incoherently at a rate proportional to $\exp-(\text{const}\, T^{s-1})$. (4) Finally, in the "marginal" case of ohmic dissipation ($s=1$), the behavior depends qualitatively on the dimensionless dissipation parameter α as well as on T: for $\alpha > 1$, and also for (roughly) $\alpha kT \gg \hbar\Delta_r$, we get incoherent relaxation with a rate proportional to $T^{2\alpha-1}$; for $\alpha < \frac{1}{2}$ and $\alpha kT \lesssim \hbar\Delta_r$ we get oscillations whose Q factor can vary from infinity to zero depending on the precise position in the (α, T) parameter space *plus* an incoherent background; and for $\frac{1}{2} < \alpha < 1$ the behavior is most likely an incoherent relaxation with an α-dependent rate of order Δ_r^{-1}.

Third, we have examined (in Sec. VII) the effect of a finite bias on the dynamics and shown that, even in those cases where the unbiased system shows coherent oscillations, a sufficient bias will suppress them. In particular, this is true for the ohmic and superohmic cases ($s \geq 1$) whenever the bias ε is large compared to the renormalized tunneling frequency $\tilde{\Delta}$ (or Δ_r), even at zero temperature, and the system then relaxes from the upper to the lower well as one would expect from simple perturbation theory.

Fourth, for the special case of ohmic dissipation and $\alpha \leq \frac{1}{2}$, we have been able to obtain (Sec. V and Appendix D) a number of *exact* results. In particular, we have been able to show that "in the limit $\omega_c \to \infty$," in the sense of that phrase precisely defined in Sec. V, the quantity $P(t)$ depends only on α and the renormalized tunneling frequency Δ_r, and is given rigorously by the function defined by Eq. (5.40). We have carried out an approximate computation taking into account "nearest-neighbor" interactions only, with the results given in Table II, and believe that for most practical purposes, in particular for study of the macroscopic quantum coherence phenomenon, the resulting expression for $P(t)$ is an excellent approximation to its true value. We believe that the basis for the results just stated is sufficiently firm that the problem of ohmic dissipation with $\alpha \leq \frac{1}{2}$ can now safely be used, if desired, as a test-bed for approximate theories, whether analytical or numerical, of the general two-state problem (cf. Silbey and Harris, 1984).

A general, and initially unexpected, conclusion from the work of this paper is that in almost all regions of the parameter space of the dissipative two-state system the behavior of $P(t)$ is qualitatively well described by the approximation (4.34) [with Eq. (4.33)] to the exact expression (4.10), that is, by what we have called the "noninteracting-blip approximation." We believe that this conclusion holds for "not too long" times in the sense defined in Sec. III, i.e., for times that, while they can be long compared to the characteristic time scale τ, are small compared to $\tau \ln\omega_c\tau$: it may or may not hold as well for even longer times. This is demonstrated rigorously[79] in Sec. V for the unbiased ohmic case with $\alpha \leq \frac{1}{2}$, and we believe it to be extremely plausible in the more general case, with, however, two exceptions. (1) The case of ($\alpha < 1$) ohmic or superohmic dissipation with a finite but small bias, $0 < \varepsilon \lesssim \tilde{\Delta}$ (or Δ_r). (2) In the ohmic case, the very small region of the parameter space specified by $\frac{1}{2} < \alpha < 1$, $kT \lesssim \hbar\Delta_r$. In the first case we are inclined to suspect that there is a relatively simple modification of the noninteracting-blip approximation that will give the physically correct results. The second case is more problematic and may well display, in the real-time domain, all the complexities familiar from studies of the thermodynamics of the Kondo problem (see Sec. III.E).

[78] Also the "two-state" condition $\varepsilon \ll \hbar\omega_0$.

[79] However, note the remarks in Sec. V.D: if t is large compared to Δ_r^{-1}, even though small compared to $\Delta_r^{-1}\ln\omega_c/\Delta_r$, the noninteracting-blip approximation may give a qualitatively incorrect picture, since the higher terms in Eq. (5.48) overwhelm the first one.

One may wonder what is the physics underlying the noninteracting-blip approximation. As we have developed it in Sec. IV.C, probably the most natural way of putting it is that every time the system, as it were, jumps into an off-diagonal element of the density matrix, it forgets about the last time it did so; that is, we neglect the environment-generated correlations between the different episodes in which the system finds itself in a linear superposition of the two states. This is perhaps not very appealing from an intuitive point of view. However, in a very recent report Aslangul *et al.* (1986) make the illuminating observation that it is possible to obtain the expression for $P(t)$ that follows from the noninteracting-blip approximation in what at first sight is a quite different way: one first carries out the familiar unitary transformation (3.28), so that the Hamiltonian is transformed to Eq. (3.30); next one writes down equations of motion for the spin components and decouples them by replacing quantities like $e^{-i\hat{\Omega}(t)}e^{i\hat{\Omega}(t')}$ by their expectation values for the uncoupled oscillators; and finally one iterates the resulting equation. The final result is just our Eq. (4.29). The second and third steps in this argument are clearly parallel[80] to the technique sketched at the end of Sec. III.B and known in the chemical physics literature as "relaxation theory," which assumes in some sense that the system does not perturb the environment very much; thus the noninteracting-blip approximation could be regarded as equivalent to the assumption that the *process of tunneling* (*not* the system-environment interaction) does not disturb the environment too strongly [see also Zwerger (1983a, 1983b)]. While this approach to the derivation of Eq. (4.29) is perhaps intuitively more appealing than the functional-integral method used in Sec. IV, the advantage of the latter is that it allows us to discuss rather simply the *justification* for Eq. (4.29) and put more or less rigorous bounds on the corrections to it—a goal which, we emphasize, is a major point of this paper.

In comparing the results of this paper with those in the existing literature, it should be carefully borne in mind that, while we have indicated how our general formulas can be used to obtain expressions for the correlation function $C(t)$ [Eq. (3.7)], the explicit results given in this paper are for the quantity $P(t)$ defined in Sec. III.A. By contrast, most of the papers in the literature either calculate $C(t)$ or some related linear-response quantity, or work out formulas for $\langle\sigma_z(t)\rangle$ without explicit specification of the boundary conditions on the environment at $t=0$. Thus we would not necessarily expect the formulas obtained to be identical (although it would be surprising if the qualitative features, e.g., oscillation versus incoherent relaxation, should turn out to be different according to which quantity is calculated).[81] Partly for this reason, and partly simply owing to shortage of space and time, we shall not attempt here a detailed comparison with the work of others (with one exception specified in the next paragraph). However, we should of course remark that a number of features of our results for specific regions of the parameter space have been obtained in the existing literature, by arguments of the kind sketched in Sec. III or related ones.[82] What has been lacking is a unified technique that would give each of these (qualitatively very different) results in that region (and *only* in that region) of the parameter space where it is actually valid, while delineating clearly the boundaries between the various regions. This we hope to have supplied in this paper; in addition, we have filled in a number of regions (e.g., the subohmic case, the superohmic case with $1<s<2$, and the ohmic case with $\alpha<\frac{1}{2}$ but not $\ll 1$), which, at least until very recently, had received little or no discussion.

There is one set of results in the literature with which it is particularly illuminating to compare (some of) the conclusions of this paper. In a series of papers, Pfeifer (1983a, 1983b, and earlier references cited therein) has considered the problem of a chiral molecule interacting with the radiation field. If one makes the so-called dipole approximation, the resulting Hamiltonian is precisely of the "spin-boson" form; if, moreover, the dipole matrix element does not vanish (as is the normal case), then the form of $J(\omega)$ is what we have called ohmic. At first sight the results obtained by Pfeifer appear to resemble ours closely: he finds, like us, that a sufficiently strong interaction with the environment can break the symmetry and "localize" the system (i.e., give the molecule in question a definite chirality). On closer inspection, however, the resemblance dissolves: if we understand his conclusions correctly, Pfeifer finds that at zero temperature the symmetry is always broken, at least partially, whenever the parameters satisfy the inequality (in our notation)

$$\Delta \leq \frac{q_0^2}{4\pi}\int \frac{J(\omega)}{\omega}d\omega\ , \tag{8.1}$$

whereas it remains unbroken when Eq. (8.1) is violated. This conclusion does not agree with those of this paper for any value of s: we find that the symmetric is always broken for $s<1$ and never broken for $s>1$, while for $s=1$ we find that the localization transition occurs at $\alpha=1$ rather than the much smaller value $\alpha\sim\Delta/\omega_c$ which would follow from Eq. (8.1). Since for realistic chiral

[80]We would emphasize, however, that the derivation of Eq. (4.29) given by Aslangul *et al.* (and sketched above) is *not* equivalent to "relaxation theory" as that term has been traditionally understood in the literature (see, for example, Nitzan and Silbey, 1974), which indeed gives quite different results.

[81]Moreover, as remarked in Sec. IV.C, to the extent that both $P(t)$ and $C(t)$ can be calculated by the noninteracting-blip approximation they should be identical for $\omega_c t \gg 1$.

[82]However, for the reasons given in footnote (14) of Garg (1985), we are unable to concur with the claim of Silbey and Harris (1984) that the conclusions of their simple variational calculation agree "in almost all details" with those of Charkavarty and Leggett (1984) (or even with the noninteracting-blip approximation to the latter).

molecules the quantity α is certainly very small compared to 1 (but quite possibly large compared to Δ/ω_c), our conclusions about the effect of the radiation field on such systems even within the dipole approximation would be qualitatively quite different from Pfeifer's. As for his results on the Hamiltonian obtained by the "rotating-wave" approximation (see Sec. I), we believe that they are correct but, for the reasons given in Sec. I, irrelevant to the spin-boson problem.

As remarked earlier, this paper is essentially about a problem in applied mathematics, namely, the dynamics of the model specified by the Hamiltonian (3.1). The question of precisely which physical systems found in nature are well described by this model, and what is the appropriate form of $J(\omega)$ if they are, is one which there is no space to discuss here (except in the sense in which it is treated in Sec. II). A proper discussion would need to take into account the physics specific to each case and would probably double the length of this paper. We hope, nevertheless, that (with the caution expressed in the penultimate paragraph of the Introduction) our results may help to provide theoretical orientation for work on the many two-state systems that occur in solid-state physics, in chemistry, and elsewhere.

Finally, it is worth noting that the problem we have studied in this paper is probably the simplest example of a quantum-mechanical problem that has simultaneously the features of being in the extreme nonclassical limit (see Leggett and Garg, 1985)[83] and being extremely sensitive to dissipation. It is therefore a crucial test-bed for quantum-mechanical many-body theory and would be important as a model problem even if it had no experimental realizations.

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[83]The (exactly soluble) problem of the quantum damped harmonic oscillator, by contrast, corresponds to the extreme semiclassical limit.

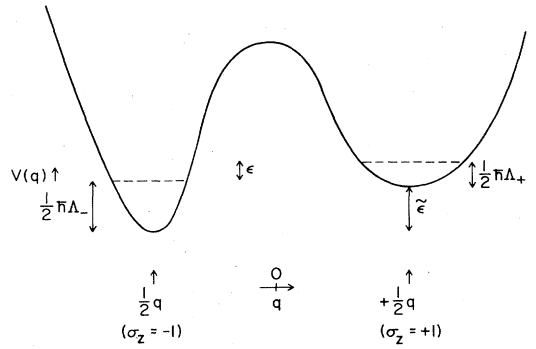

FIG. 9. The biased double-well system.

APPENDIX A: PARTITION FUNCTION FOR AN ASYMMETRIC TWO-WELL SYSTEM

In this appendix we consider a system whose Lagrangian, including its interaction with its environment, is given by Eq. (2.1), with the special choice[84] $F_j(q)=qC_j$, and with a low-frequency cutoff on the environmental spectrum. That is, the Lagrangian is

$$L(q,\dot{q};\{x_j,\dot{x}_j\})=\tfrac{1}{2}M\dot{q}^2-V(q)+\tfrac{1}{2}\sum_j m_j(\dot{x}_j^2-\omega_j^2x_j^2) -q\sum_j C_jx_j-q^2\sum_j C_j^2/2m_j\omega_j^2 , \quad \text{(A1)}$$

where for notational convenience we have omitted the tildes on M and V in Eq. (2.1), and where the coupling to the environment satisfies the constraint

$$J'(\omega)\equiv\frac{\pi}{2}\sum_j (C_j^2/m_j\omega_j)\delta(\omega-\omega_j) =J_0(\omega)(1-e^{-\omega/\omega_c}) \quad \text{(A2)}$$

with the lower cutoff arbitrarily chosen as described in Sec. II. The important feature of the problem (see Fig. 9) is that $V(q)$ has two local minima, which occur at points that, by a suitable choice of the origin of q, we denote $\pm\frac{1}{2}q_0$. The quantity $[V(\frac{1}{2}q_0)-V(-\frac{1}{2}q_0)]$ will be denoted $\tilde{\epsilon}$. The (undamped) classical small-oscillation frequencies around these two minima will be called ω_+ and ω_-, respectively, and the order of magnitude of the actual lowest characteristic frequency of classical motion will be denoted $\omega_{\rm cl}$; thus, for weak damping, we have $\omega_{\rm cl}\sim\omega_+,\omega_-$, while for strong damping (in the ohmic case) we have $\omega_{\rm cl}\sim M\omega_+^2/\eta$, $M\omega_-^2/\eta$, where η is the friction coefficient (we assume, for notational convenience

[84]The generalization to other forms of $F_j(q)$ introduces no new features at this stage; see Sec. II.

only, that ω_+ and ω_- are of the same order of magnitude). The renormalized tunneling frequency, to be calculated below, will be called Δ; it is assumed[85] that by an appropriate choice of ω_c we can ensure that $\Delta \ll \omega_c \ll \omega_{\rm cl}$, i.e., that the classical one-instanton action $S_{\rm cl}$ calculated below is large compared to $\hbar$.

We shall consider the system described above in the limit that the quantities $\hbar\Delta$, $\tilde{\varepsilon}$, and $k_B T$ (and ε, see below) are all small[86] compared to $\hbar\omega_c$ (and hence *a fortiori* to $\hbar\omega_{\rm cl}$) but may have any magnitude relative to one another. What we shall show is that under these conditions (a) the partition function of the system is identical to that of the "biased" two-level system described by the Hamiltonian (1.1), with, however, $\varepsilon \neq \tilde{\varepsilon}$ in general; (b) there is a unique prescription for calculating, from the Lagrangian (A1), the parameters of the two-level problem; and (c) to leading order in the small quantities Δ/ω_c, etc., the parameters Δ, ε, and $k_B T/\hbar$ are independent. [The importance of the last result is that it means that the predictions of a calculation based on the spin-boson Hamiltonian (1.4) are in principle accessible to experimental test; see below.] Although most if not all the ingredients of the calculation to be undertaken below are by now well known, we are not aware of any existing reference where it is explicitly written down,[87] and in view of the importance of obtaining a firm conceptual basis for the spin-boson Hamiltonian we feel that it is worth giving here.

The partition function $Z(\beta)$ may be written in terms of the (unnormalized) system reduced density matrix $\rho(q,q':\beta)$ in the form

$$Z(\beta) = \int \rho(q,q:\beta)dq \ , \tag{A3}$$

where $\rho(q,q':\beta)$ is defined as

$$\rho(q,q':\beta) \equiv \sum_n \int \prod_i dx_i \Psi_n(q,\{x_i\})\Psi_n(q',\{x_i\})\exp -\beta E_n \ , \tag{A4}$$

in which n labels the energy eigenstates of the whole "universe" (system-plus-environment). We express $\rho(q,q:\beta)$ as a path integral and integrate out the environmental degrees of freedom in the standard way (see, for example, Caldeira and Leggett, 1983, Sec. 4), obtaining thereby

$$\rho(q,q:\beta) = \int_{q(0)=q}^{q(\beta\hbar)=q} Dq(\tau)\exp -S_{\rm eff}[q(\tau)]/\hbar \ , \tag{A5}$$

where the effective action $S_{\rm eff}$ is given by

$$S_{\rm eff}[q(\tau)] = \int_0^{\beta\hbar} d\tau [\tfrac{1}{2}M\dot{q}^2 + V(q)] + \tfrac{1}{2}\int_0^{\beta\hbar} d\tau \int_{-\infty}^{\infty} d\tau' \alpha(\tau-\tau') \times [q(\tau)-q(\tau')]^2 \tag{A6}$$

with $\alpha(\tau-\tau')$ given by Eq. (2.7). To make sense of the last term in Eq. (A6) we need, strictly speaking, to specify that $q(\tau)$ is to be continued outside the range $0 \leq \tau \leq \beta\hbar$ by the prescription $q(\tau+\beta\hbar) \equiv q(\tau)$; however, since $\alpha(\tau-\tau')$ falls off as $t^{-2(n+1)}$ for $t \gg \omega_c^{-1}$ (see Sec. II), i.e., faster than t^{-2}, it is clear that the effect of this condition is negligible for $\beta\hbar\omega_c \gg 1$, and we shall ignore it in what follows, assuming that both integrals in the last term of (A6) can be taken from 0 to $\beta\hbar$. Note that in writing Eq. (A5) we have dropped a multiplicative term corresponding to $K_0(T)$ of Eq. (4.23) of Caldeira and Leggett (1983), on the grounds that for $\beta\hbar\omega_c \gg 1$ it is negligibly different from $\exp -\beta\sum_j \hbar\omega_j/2$, and hence only shifts the zero of total energy.

We can evaluate $\rho(q,q)$ in the standard way by finding the classical paths (or near-classical paths; see below) in the "inverted" potential $V_i(q) \equiv -V(q)$; those paths give the exponential factor in $\rho(q,q)$, and the small fluctuations around them give the prefactor. We immediately note one simplifying feature: $\rho(q,q)$ is large only near the local minima $\pm\frac{1}{2}q_0$ of the potential $V(q)$ [maxima of $V_i(q)$]. In fact, it is appreciable only for $|q \mp \frac{1}{2}q_0| \lesssim q_{zp}^{\pm}$, where $q_{zp}^{+}(q_{zp}^{-})$ is the zero-point uncertainty in position of a particle of mass M moving in the harmonic potential which approximates $V(q)$ near $\pm\frac{1}{2}q_0$. Since it follows from the formula to be derived below for the tunneling matrix element Δ, together with the results of Caldeira and Leggett (1983, Sec. 5), that within logarithmic corrections the quantity $\Delta/\omega_{\rm cl}$ is of order $\exp -\lambda q_0^2/q_{zp}^2$, $\lambda \sim 1$, it is clear that to within corrections of relative order $\Delta/\omega_{\rm cl}$ the potential in the regions that make an appreciable contribution to the partition function can be approximated by its harmonic form. Moreover, for q in one of these regions and $\beta\hbar\omega_{\rm cl} \gg 1$, the overwhelming majority of (near-) classical paths that start from q at "time" zero and return there at "time" $\beta\hbar$ are paths in which the system starts out in the direction of the nearby[88] maximum

[85] In view of the results of Caldeira and Leggett (1983) and Leggett (1984b), it is clear that in the case of "normal" dissipation a sufficient condition for this assumption to hold is the inequality $V_0 \gg \hbar\omega_{\rm cl}$, where V_0 is a typical barrier height (it is implicitly assumed here that the barrier shape is not too pathological). Thus the condition may well be fulfilled for a heavily damped system, even though it was not for the corresponding undamped one. For the (unusual) case of "anomalous" dissipation, special care is necessary; see Leggett (1984b), Sec. 3A.

[86] It actually turns out that a sufficient condition for the validity of the results of this section is $\varepsilon \ll \hbar\omega_{\rm cl}$ (with no restriction on $\tilde{\varepsilon}$). The regime $\hbar\omega_c \ll \varepsilon \ll \hbar\omega_{\rm cl}$, while formally covered by these results, is, however, not very interesting, since we must have $\Delta/\omega_c \ll 1$, and so in this regime would have $\hbar\Delta/\varepsilon \ll 1$, a limit in which the spin-boson problem fails to show its full generality.

[87] We are not even aware of any such complete calculation for an undamped system for the case in which ω_+ and ω_- are different (though see Zinn-Justin, 1983, Sec. 3).

[88] For q between the two maxima of $V_i(q)$ there is of course another class of paths, in which the system just moves to the distant maximum. However, it is easy to see that for the important values of q the corresponding contribution to $\rho(q,q)$ is suppressed by a factor $\sim \exp -2S_{\rm cl}/\hbar \sim (\Delta/\omega_{\rm cl})^2$ relative to that of the paths described above.

of $V_i(q)$ with just enough kinetic energy to reach it, sits there and at the other maximum for long periods with occasional transits between them, and finally rolls off so as to return to q, with finite kinetic energy, at time $\beta\hbar$. The classical action along this type of path (we take q near $+\frac{1}{2}q_0$ for definiteness) differs from that along the related path for $\rho(q_0/2,q_0/2)$ only by the small pieces occurring near the end point, which for $\beta\hbar\omega_c \gg 1$, $\Delta/\omega_c \ll 1$ are essentially identical to the pieces that would occur were we to calculate $\rho(q,q)$ for a single-well harmonic potential with minimum at $\frac{1}{2}q_0$. Furthermore, the prefactor is identical in the two cases, since the expression that determines the eigenvalues of the spectrum of small fluctuations (see below) is *everywhere* identical, in this approximation, for the paths determining $\rho(q,q)$ and $\rho(q_0/2,q_0/2)$. Thus we reach the physically rather obvious conclusion that the ratio $\rho(q,q)/\rho(q_0/2,q_0/2)$ for those values of q near $\frac{1}{2}q_0$ which contribute appreciably to the partition function of the two-well system is identical, in the limit $\Delta/\omega_{\rm cl}\to 0$, to the value it would have for a particle moving, with the relevant damping, in a single harmonic well centered at $\frac{1}{2}q_0$ and with the same value of $V''(\frac{1}{2}q_0)$ as the real potential. The form of $\rho(q,q)$ for a damped harmonic oscillator may be obtained in any number of ways, in particular by a path-integral method (see Caldeira and Leggett, 1983, Appendix B). It is proportional to $\exp -q^2/q_{zp}^2$, where q is now measured from the potential minimum and the zero-point spread q_{zp} is given by Eq. (B9) of this reference, with $\beta\to\infty$. In the limit of interest to us ($\beta\hbar\omega_c \gg 1$, $\beta\hbar\omega_{\rm cl} \gg 1$), the definition (A5) of $\rho(q,q)$ shows that it is normalized, for the damped oscillator, by $\int \rho(q,q)dq = \exp -\beta E_0$, where E_0 is the ground-state energy of the oscillator-plus-environment (with the quantity $\sum_j \hbar\omega_j/2$ subtracted). Thus, if for the two-well problem we denote $\rho(q_0/2,q_0/2)$ by ρ_+ and $\rho(-q_0/2-q_0/2)$ by ρ_-, then apart from an overall numerical constant[89] we have

$$Z(\beta) = \{(q_{zp}^+)\rho_+ + (q_{zp}^-)\rho_-\} \ . \tag{A7}$$

Thus from now on it is adequate to consider only those paths that start and terminate at the local maxima $\pm\frac{1}{2}q_0$ of $V_i(q)$.

Let us choose for definiteness the deeper well to be the one occurring at $+q_0/2$ (i.e., redraw Fig. 9, so that $\tilde{\varepsilon}<0$) and consider the possible paths that start and end there; for subsequent convenience we consider a general time interval T, not necessarily equal to $\beta\hbar$, between the start and finish. As usual, the paths are of two types. First, there is the "trivial" path, $q(\tau) = +q_0/2$ for all τ. If we choose the zero of energy (for the moment) to lie halfway between the minima $V(q_0/2)$ and $V(-q_0/2)$, then from our definition of the bias $\tilde{\varepsilon}$ the action along the above classical path is $+\frac{1}{2}\tilde{\varepsilon}T/\hbar$. To calculate the small fluctuations around this path we introduce the quantity $\Pi(\omega) \equiv -M^{-1}[\alpha(\omega-\alpha(0)]$, where $\alpha(\omega)$ is the Fourier (not Laplace) transform of $\alpha(\tau-\tau')$. $\Pi(\omega)$ is related to $J'(\omega)$ by Eq. (2.19) of Leggett (1984b); note in particular that for an ohmic spectrum with low-frequency cutoff ω_c we have $\Pi(\omega) \cong 2\gamma\,|\,\omega\,|$, $(\gamma \equiv \eta/2M)$ for $\omega \gg \omega_c$. Using Eq. (B4) of Caldeira and Leggett (1983) or its generalization, we see that the contribution of the small fluctuations around the classical path to ρ_+ is the multiplicative factor

$$C_+(T) = \text{const} \prod_{n=0}^{\infty} \{M[\omega_+^2 + \omega_n^2 + \Pi(\omega_n)]\}^{-1/2} \ , \qquad \omega_n \equiv n\pi/T \ . \tag{A8}$$

(A quantity C_- is defined by a similar expression with $\omega_+ \to \omega_-$.) The question of the value of the constant in Eq. (A8) is somewhat delicate; it is a function of the precise definition of the functional integrals over q and the x_i in the expression [Eq. (4.12) of Caldeira and Leggett (1983)] which, after integration out of the x_i, led to Eq. (A5) above. For a set of harmonic oscillators coupled together by a linear coordinate-coordinate coupling it may be shown explicitly that there is a unique choice of the definition, which depends only on the oscillator masses and not on their frequencies or couplings, that guarantees that the ground-state wave function is normalized apart from a factor $\exp -E_0T/\hbar$. Thus, with the linear coupling described by Eq. (A1), it follows that we can always choose the definition so that $\rho(q,q)$ is normalized for *both* the damped harmonic oscillators, i.e., that centered at $+\frac{1}{2}q_0$ and that at $-\frac{1}{2}q_0$, apart from a similar T-dependent factor that will in general be different for the two oscillators. Equivalently, we can choose the constant in Eq. (A8) in such a way that for $\omega_{\rm cl}T \gg 1$ we have (apart from a common numerical factor of order unity, see above)

$$C_+(T) = (q_{zp}^+)^{-1}\exp -\Lambda_+ T \ ,$$
$$C_-(T) = (q_{zp}^-)\exp -\Lambda_- T \ , \tag{A9}$$

where C_- is the corresponding contribution of the small fluctuations for the oscillator at $-\frac{1}{2}q_0$, and Λ_+, Λ_- are defined by

$$\Lambda_{+,-}(T) \equiv \text{const} \left[+ \tfrac{1}{2} \sum_n \ln[\omega_{+,-}^2 + \omega_n^2 + \Pi(\omega_n)] \right] , \qquad \omega_n \equiv n\pi/T \ , \tag{A10}$$

where the constant is such as to guarantee the result (A9). Evidently Eq. (A10) diverges at the high-frequency end, and in contrast to the undamped case this divergence is not eliminated, in the ohmic or superohmic cases, by subtracting of the corresponding expression for a free particle, until we take account of the high-frequency cutoff on

[89] Strictly speaking, in the ensuing arguments $q_{zp}^{\pm}$ should be everywhere replaced by $(\rho_{\pm}^{(0)})^{-1}$, where $\rho_{\pm}^{(0)}$ denotes the probability density at $\pm q_0/2$ of the appropriate damped harmonic oscillator centered at this point. This differs from $q_{zp}^{\pm}$ by the numerical factor $\pi^{1/2}$. Since $q_{zp}^{\pm}$ will cancel out of the final answer anyway, we do not write this factor explicitly to avoid cluttering up the formulas.

$J(\omega)$ [hence on $\Pi(\omega)$]. This simply reflects the fact that the energy shift of the "universe" ground state due to the system-oscillator coupling is ultraviolet divergent in these cases, as can easily be seen from second-order perturbation theory.[90] However, in the present context what is important is not the absolute values $\Lambda_{+,-}$ but the *difference* $\delta\Lambda \equiv \Lambda_+ - \Lambda_-$. This is given by

$$\delta\Lambda = \frac{1}{2\pi}\int_0^\infty d\omega \ln\left[\frac{\omega_+^2+\omega^2+\Pi(\omega)}{\omega_-^2+\omega^2+\Pi(\omega)}\right] \tag{A11}$$

and is ultraviolet convergent for any form of $\Pi(\omega)$ [recall that $\Pi(\omega)$ is, by Eq. (2.19) of Leggett (1984b), always positive]. For the special case of no dissipation [$\Pi(\omega)\equiv 0$] the quantity $\delta\Lambda$ is simply $(\omega_+ - \omega_-)/2$, as we should expect, since it is simply $\hbar^{-1}$ times the difference in zero-point energies of the two oscillators. In the case of ohmic dissipation with damping constant $\gamma \equiv \eta/2M$, we can evaluate $\delta\Lambda$ explicitly for all γ. The result is

$$\delta\Lambda = \tfrac{1}{2}[\omega_+ f(\alpha_+) - \omega_- f(\alpha_-)] , \tag{A12}$$

where $\alpha_{+,-} \equiv \gamma/\omega_{+,-}$ and $f(\alpha)$ is the function defined by Eq. (B29) of Caldeira and Leggett (1983). For strong damping $\delta\Lambda$ is of order $(\omega_+^2 - \omega_-^2)/2\gamma$ to within logarithmic factors.

Putting together the results of the above few paragraphs, we see that if we could confine ourselves to the "trivial" paths discussed there, i.e., if we could neglect transits between the two wells, then the partition function would be given by

$$\begin{aligned} Z(\beta) &= (q_{zp}^+)\rho_+ + (q_{zp}^-)\rho_- \\ &= (q_{zp}^+)\exp(-\tfrac{1}{2}\tilde{\varepsilon}T/\hbar)C_+(T) + (q_{zp}^-)\exp(+\tfrac{1}{2}\tilde{\varepsilon}T/\hbar)C_-(T) \\ &= \exp\left[-\frac{1}{2}\frac{\tilde{\varepsilon}}{\hbar} - \Lambda_+\right]T + \exp\left[+\frac{1}{2}\frac{\tilde{\varepsilon}}{\hbar} - \Lambda_-\right]T \quad (T \equiv \beta\hbar) . \end{aligned} \tag{A13}$$

By a suitable redefinition of the zero of energy we can reduce this to the form

$$Z(\beta) = \cosh(\beta\varepsilon/2), \quad \varepsilon \equiv \tilde{\varepsilon} + \hbar\delta\Lambda . \tag{A14}$$

Thus the partition function is equivalent to that of a two-state system in which the states are each localized within one of the wells: the energy splitting ε is the difference $\tilde{\varepsilon}$ in the potential minima plus the difference in zero-point energies, as we should have expected intuitively.

We now turn to the second important class of paths, namely, the "tunneling" paths in which the system moves, at intervals long compared to $\omega_{\rm cl}^{-1}$, from one well to the other. In the special case of a totally symmetric double well ($\varepsilon = \tilde{\varepsilon} = 0$), the calculation of these paths to the partition function is straightforward and proceeds in the usual way (cf., for example, Coleman, 1979; Olive *et al.*, 1979); there is a classical path (the so-called instanton) that takes the system from $+\frac{1}{2}q_0$ at $\tau = -\infty$ to $-\frac{1}{2}q_0$ at $\tau = +\infty$, with $q(\tau)$ appreciably different from these values only for a time of order $\omega_{\rm cl}^{-1}$, and we simply assume that for $\beta\hbar\omega_{\rm cl} \gg 1$ we can approximate the total path by a sequence of such paths and their inverses, calculating the action on each instanton segment as if it were the only one in an infinite time range. The fact that we have a low-frequency cutoff on the environment spectrum guarantees that the single-instanton action $S_{\rm cl}$ remains finite, though in the ohmic and subohmic cases $S_{\rm cl}$ has an important dependence on ω_c (see Sec. II).

For the general case (ε and/or $\tilde{\varepsilon} \neq 0$) the situation is somewhat more complicated. In the first place, for $\tilde{\varepsilon} \neq 0$ there is no classical path that brings the system from rest at $+\frac{1}{2}q_0$ to rest at $-\frac{1}{2}q_0$. To deal with this complication we note that there is nothing particularly sacrosanct about paths that solve the classical equation of motion; the only advantage of using them as, as it were, the first approximation to the physically important paths is that the contribution of the fluctuations around them has a particularly simple form. In the present problem there is no reason why we should not use, as our first approximation, a "near-classical" path, i.e., one that satisfies the classical equation of motion for most but not all of the time. A convenient choice of such a path is given by the following prescription. Suppose that $+\frac{1}{2}q_0$ is the deeper minimum: then, in the *inverted* potential, a system rolling off the corresponding maximum with zero initial kinetic energy would reach the lower maximum at $-\frac{1}{2}q_0$ with sufficient energy ($-\tilde{\varepsilon}$) to overshoot it. Imagine, however, that we add to the lower peak an extra harmonic piece, as indicated in Fig. 10, equal to

$$[\tilde{\varepsilon} - \tfrac{1}{2}M\omega_-^2(q + \tfrac{1}{2}q_0)^2]\theta(\Delta q - |\, q + q_0/2\,|) ,$$

where $\Delta q \equiv [2(-\tilde{\varepsilon})\hbar/M\omega_-^2]^{1/2}$. Then the system, moving classically[91] in the new potential, would come to rest exactly at the point $-q_0/2$, and moreover the function $q(\tau)$ and its first two derivatives would be finite along the classical path in question. We take this classical path [call it $q_{\rm ncl}(\tau)$] as the zero-order "near-classical" path for the *actual* potential, evaluate the action along it, and con-

[90] In computing the energy shift it is essential to include the effect of the "counterterm" (the last term) in Eq. (A1).

[91] In the actual calculation of the classical path we must of course include the nonlocal term in the equation of motion which arises from the last term in the effective action (A6).

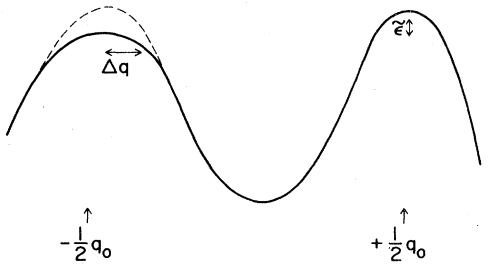

FIG. 10. Fictitious potential used to construct the "near-classical" path for $\tilde{\varepsilon}\neq 0$.

sider the small fluctuations around it. If we write $q(\tau)\equiv q_{\rm ncl}(\tau)+\delta q(\tau)$, where $\delta q(-\infty)=\delta q(\infty)=0$, then the "fluctuation" term in the action $\delta S\equiv S_{\rm eff}[q(\tau)]-S_{\rm eff}[q_{\rm ncl}(\tau)]$ contains as usual a term $\delta S^{(2)}$ that is quadratic in $\delta q(\tau)$, but also a term $\delta S^{(1)}$ linear in it, which on using the equation of motion of $q_{\rm ncl}(\tau)$ takes the form

$$\delta S^{(1)}=\int M\omega_-^2 Z_{\rm ncl}(\tau)\delta q(\tau)\theta[\Delta q-Z_{\rm ncl}(\tau)]d\tau\ , \tag{A15}$$

where for brevity we have defined $Z_{\rm ncl}(\tau)\equiv q_{\rm ncl}(\tau)+q_0/2$. Since $\delta S^{(2)}$ has the standard form, bilinear in $\delta q(\tau)$ and $\delta\dot{q}(\tau)$, we can define the corresponding normalized eigenvectors $q_n(\tau)$ and eigenvalues λ_n in the usual way. Were it not for the term $\delta S^{(1)}$, the small fluctuations [other than the "zero mode" $q_0(\tau)=\text{const}\,dq_{\rm ncl}(\tau)/d\tau$, for which see below] would give the standard factor $D_0'\equiv\prod_{n>0}\lambda_n^{-1/2}$ (where D_0' actually depends in general on the position of the bounce center; see below). The effect of the term $\delta S^{(1)}$ is to multiply this expression by the extra factor

$$F\equiv\exp\sum_{n>0}C_n^2\lambda_n^{-1}\hbar^{-1}\ , \tag{A16}$$

where C_n is given by

$$C_n\equiv(M\omega_-^2)^2\int Z_{\rm ncl}(\tau)q_n(\tau)\theta[\Delta q-Z_{\rm ncl}(\tau)]d\tau\ . \tag{A17}$$

Note that the contribution of the projection C_0 of $\delta q(\tau)$ on the zero mode gives no contribution to F. In fact, the total contribution of the zero mode to the functional integral is the same as it would be if the path $q_{\rm ncl}(\tau)$ were truly classical, that is, $(B^*/2\pi\hbar)^{1/2}T$ where B^* is the integral of twice the kinetic energy along the path [see erratum to Caldeira and Leggett (1983)], and T is the total time allowed for it.

We must finally take into account the fact that, when evaluating the complete partition function, we must not overcount the contribution of the small fluctuations around the long pieces of the path where $q(\tau)$ is nearly stationary at the values $\pm\frac{1}{2}q_0$. To ensure this we divide the result obtained so far by the quantity $C_+(t_1)C_-(T-t_1)$, where $C_{+,-}(t)$ was defined in Eq. (A8). It is convenient also to multiply and divide by a factor $(q_{zp}^+q_{zp}^-)^{1/2}$ and thus to write the total multiplicative factor associated with a single-instanton event in the functional integral in the form

$$I_0=\frac{\Delta}{2}(q_{zp}^+q_{zp}^-)^{1/2}\ , \tag{A18}$$

where the quantity Δ, which will be subsequently identified as $(2/\hbar$ times) the "bare" tunneling matrix element for the two-state problem, is given by

$$\Delta=\left[\frac{2D_0'(t_1)}{(q_{zp}^+q_{zp}^-)^{1/2}C_+(t_1)C_-(T-t_1)}\right]\times F\left[\frac{B^*}{2\pi\hbar}\right]^{1/2}\exp-S_{\rm cl}/\hbar\ . \tag{A19}$$

Here $D_0'(t_1)$ is defined as

$$D_0'(t_1)=\prod_{n=1}^{\infty}\lambda_n^{-1/2}(t_1)\ , \tag{A20}$$

where λ_n are the eigenvalues of the bilinear form representing the correction to the action from the small fluctuations around the (near)-classical instanton path for an instanton centered at time t_1 (the "zero mode" corresponding to a rigid time translation of the instanton is omitted in the product); $C_+(t_1)$ and $C_-(T-t_1)$ are defined as in Eq. (A8); F is the expression (A16); B^* is the time integral of twice the kinetic energy over the instanton path $q_{\rm ncl}(\tau)$; and $S_{\rm cl}$ is the action evaluated along this path. The expression for an "anti-instanton" (classical path going from $-\frac{1}{2}q_0$ to $+\frac{1}{2}q_0$) is obtained from Eq. (A19) by the substitution $C_+\rightleftarrows C_-$ [the (near)-classical path is the time-reversed version of the instanton, and hence $S_{\rm cl}, F, B^*$ are unchanged and $D_0'(t_1)$ is changed only in a trivial way; see below].

A number of features of Eq. (A19) should be noted. First, it is clear from Eq. (A19) that the quantity in large parentheses, and hence the whole expression (A19), has the dimensions of frequency, as it should. Second, although the quantities D_0', C_+, and C_- individually depend on the value of t_1, it is clear intuitively that the combination in large parentheses must be independent of t_1, and thus Δ is also independent of the time at which the instanton occurs. By the same argument, the factor for an anti-instanton is identical to Δ. Third, if we compare two forms of potential $V(q)$, one of which gives $\varepsilon=0$ and the other a finite value of ε small compared to $\hbar\omega_{\rm cl}$, it is clear that the difference in the action $S_{\rm cl}$ evaluated along the (near)-classical path in the two cases can be at most of order $\varepsilon/\hbar\omega_{\rm cl}$. The other factors in Eq. (A19) similarly depend on ε only to this order.[92] Thus, in the limit of interest to us ($\Delta/\omega_{\rm cl}$, $k_BT/\hbar\omega_{\rm cl}$, $\varepsilon/\hbar\omega_{\rm cl}$ all very small compared to unity), it is consistent to treat Δ, ε, and $k_BT/\hbar$ as independent parameters whose relative magnitudes can be varied at will by suitable adjustments of the experimental conditions.

[92]Note that it is irrelevant to this conclusion whether $\tilde{\varepsilon}$ is comparable to $\hbar\omega_c$ or even $\hbar\omega_{\rm cl}$ (as in realistic cases it might well be).

The actual evaluation of Eq. (A19) for a particular form of $V(q)$ and of $J(\omega)$ may of course be far from trivial: compare Caldeira and Leggett (1983, Sec. 5 and Appendix D) and Chang and Chakravarty (1984), where the analogous calculations are done for the case of tunneling out of a metastable well. The important point for our purposes is that Δ (a) is in principle defined, by (A19), uniquely in terms of the parameters of the original two-well problem, and (b) depends on the low-frequency cutoff ω_c. The implications of point (b) are discussed in Sec. II.

The final stage of the calculation of the partition function $Z(\beta)$ is now straightforward. We consider all those paths that start from, say, $+\frac{1}{2}q_0$ and include n instantons and n anti-instantons. If we choose the zero of energy to lie at the point

$$\tfrac{1}{2}[V(\tfrac{1}{2}q_0)+V(-\tfrac{1}{2}q_0)+\tfrac{1}{2}\hbar(\Lambda_+ +\Lambda_-)] ,$$

then a time interval dt spent in the $+$ well (the lower one) will have associated with it a factor $\exp(-\tilde{\varepsilon}/2)dt/\hbar$ from the classical action and, according to Eq. (A9), a factor $(q_{zp}^+)^{-1}\exp(-\delta\Lambda)dt$ from the harmonic fluctuations around the classical (trivial) path. Thus the total factor associated with this interval is $(q_{zp}^+)^{-1}\exp(\varepsilon/2)dt/\hbar$, where ε is $\tilde{\varepsilon}+\hbar\delta\Lambda$. The corresponding factor for the $-q_0/2$ well is $(q_{zp}^-)^{-1}\exp(-\varepsilon/2)dt/\hbar$. According to Eq. (A19), each instanton or anti-instanton is associated with a factor $(\Delta/2)(q_{zp}^+ q_{zp}^-)^{-1/2}$. Thus, in the expression for ρ_+, all the factors of $(q_{zp}^-)^{-1}$ cancel, as do all the factors of $(q_{zp}^+)^{-1}$ except for the last, which is in turn canceled by the factor q_{zp}^+ in the expression (A3) for $Z(\beta)$. A similar remark applies to paths that start at and return to $-q_0/2$. We finally obtain for $Z(\beta)$

$$Z(\beta)=\sum_{n=0}^{\infty} S_n(\beta)(\Delta/2)^{2n} , \tag{A21}$$

where the coefficients $S_n(\beta)$ are defined by

$$S_0(\beta)=2\cosh(\beta\varepsilon/2) , \tag{A22}$$

$$S_n(\beta)=\tfrac{1}{2}[S_n(\beta:\varepsilon)+S_n(\beta:-\varepsilon)]\equiv S_n(\beta:\varepsilon), \quad n>0$$

where

$$S_n(\beta:\varepsilon)\equiv 2\int_0^{\beta\hbar} dt_{2n}\int_0^{t_{2n}} dt_{2n-1}\cdots\int_0^{t_2} dt_1 \exp\frac{\varepsilon}{2\hbar}\left[\sum_{j=0}^{n}(t_{2j+1}-t_{2j})-\sum_{j=0}^{n-1}(t_{2j+2}-t_{2j+1})\right] \tag{A23}$$

($t_{2n+1}\equiv\beta\hbar, t_0\equiv 0$).

It remains for us to show that the series (A21) is identical to the partition function of a two-level system with bias ε and tunneling matrix element $\Delta\hbar/2$, that is, to the expression

$$Z(\beta)=2\cosh\frac{\beta}{2}(\varepsilon^2+\hbar^2\Delta^2)^{1/2} . \tag{A24}$$

To demonstrate this we simply write the recurrence relation

$$S_n(\beta:\varepsilon)=\int_0^{\beta\hbar} dt'\int_0^{t'} dt \exp\frac{\varepsilon}{2\hbar}(\beta h-2t'+t) \times S_{n-1}(t\hbar^{-1}:\varepsilon) , \tag{A25}$$

derive from it the relation

$$\frac{d^2S_n(\beta:\varepsilon)}{d(\beta\hbar)^2}=\left[\frac{\varepsilon}{2\hbar}\right]^2 S_n(\beta)+S_{n-1}(\beta) , \tag{A26}$$

and apply Eq. (A26) to the series (A21), obtaining

$$\frac{d^2Z(\beta:\varepsilon)}{d(\beta\hbar)^2}=\tfrac{1}{4}(\hbar^{-2}\varepsilon^2+\Delta^2)Z(\beta) . \tag{A27}$$

Since $Z(0)$ is clearly 2 and $(dZ/d\beta)_{\beta=0}$ equally clearly zero, the unique solution of Eq. (A27) is of the form (A24). This completes our proof.

We finally add a brief note on the generalization to the case of a general $F_j(q)$ in the original Lagrangian (2.1). If the range of the functions $F_j(q)$ is large compared to the zero-point spreads $q_{zp}^{\pm}$ [which, of course, in the strongly damped case must themselves be determined self-consistently, taking account of the form of $F_j(q)$], then the generalization is entirely straightforward; in this case the situation in the harmonic regions ($|q\pm q_0/2|\lesssim q_{zp}^{\pm}$) is identical to that discussed above,[93] the only difference being that C_j is replaced (for the purpose of obtaining the oscillator characteristics only; see Sec. II) by $(\partial F_j/\partial q)_{q=\pm 1/2q_0}$. The only effect of the different form of $F_j(q)$ is then to modify the expressions for the parameters of the two-state system as detailed at the end of Sec. II.

The case in which $F_j(q)$ has a range comparable to, or shorter than, $q_{zp}^{\pm}$ is more troublesome. In this case the probability density distribution for the relevant isolated damped harmonic oscillator is not in general Gaussian, and a number of the results we have used above fail. We would regard it as improbable in the extreme that these differences change the qualitative features of the results obtained here. At worst they are likely to give us a more cumbersome expression for the "bare" tunneling matrix element that enters the two-state problem. At the time of writing we have not worked out the appropriate theory in detail.

[93] With one exception: If the damping of the oscillators at $\pm\frac{1}{2}q_0$ is different, then the expression for $\delta\Lambda$ [Eq. (A11) above] has to be modified, with $\Pi(\omega)$ replaced by $\Pi_+(\omega)[\Pi_-(\omega)]$ in the numerator (denominator). The quantity $\delta\Lambda$ may then depend on the high-frequency behavior of the environment, not just on its behavior for $\omega\lesssim\omega_{cl}$.

APPENDIX B: ALTERNATIVE DERIVATIONS OF EQS. (4.1) AND (4.17)

1. Relation between $P^{(1)}(t)$ and $P^{(2)}(t)$

In this part of this appendix we shall show that the quantities $P^{(1)}(t)$ and $P^{(2)}(t)$ defined in Sec. III are identical for a system coupled to a bath of oscillators with arbitrary spectral density. We do this by calculating $P^{(1)}(t)$ in exact analogy with the calculation of $P^{(2)}(t)$ in Sec. IV and showing that we recover Eq. (4.1).

Let us recall that the influence functional $F[x(\tau),y(\tau')]$ used in Sec. IV is a product of single-oscillator functionals. For each such oscillator, whose coordinates we denote here by X and Y, this is defined by

$$F[x,y]=\int DX\int DY\int DX_i dY_i dX_f \rho_i(X_i,Y_i)\exp\frac{i}{\hbar}[S_0(X)-S_0(Y)+S_1(X,x)-S_1(Y,y)]\ . \tag{B1}$$

Here, S_0 is the action for the oscillator trajectory $X(\tau)$ in the absence of interactions, and S_1 is the action arising from these interactions; ρ_i is the initial density matrix of the oscillator at time t_0, and it is understood that $Y_f=X_f$. The result (4.5) is then true for *any* t_0 and t, provided ρ_i is the thermal equilibrium density matrix [which we denote here by $\rho_{\rm Th}(X_i,Y_i)$] for an oscillator *whose mean position is given by* $\langle X\rangle=0$.

The probability $\tilde{p}(x_f{:}t)$ that a system which was at $x=x_i$ at $t=0$ will be found to have a location x_f at a later time t, given that the environment was in equilibrium with the system at $t=0$, is defined in analogy with $p(x_f{:}t)$ of Eq. (4.1),

$$\tilde{p}(x_f{:}t)=\int Dx\int Dy\, A[x]A^*[y]\tilde{F}[x,y]\ , \tag{B2}$$

where $\tilde{F}$ is again a product of single-oscillator functionals such as (B1), with the difference that now $t_0=0$, and ρ_i describes an oscillator in equilibrium under the action of a steady force $-Cx_i$,[94] so that

$$\rho_i(X_i,Y_i)=\rho_{\rm Th}(\tilde{X}_i,\tilde{Y}_i)\ , \tag{B3}$$

with

$$\begin{matrix}\tilde{X}_i\\ \tilde{Y}_i\end{matrix}=\begin{matrix}X_i\\ Y_i\end{matrix}+\frac{Cx_i}{m\omega^2}\ . \tag{B4}$$

It is now straightforward to show that

$$S_0(X)+S_1(X,x)=S_0(\tilde{X})+S_1(\tilde{X},\tilde{x})+S_2(x)\ , \tag{B5}$$

where

$$\tilde{x}=x-x_i\ , \tag{B6}$$

$$S_2(x)=\frac{C^2}{m\omega^2}x_i\int_0^t[x(\tau)-\tfrac{1}{2}x_i]d\tau\ , \tag{B7}$$

and X and $\tilde{X}$ are related by the same shift as in (B4). It follows that

$$\tilde{F}[x,y]=\exp\frac{i}{\hbar}[S_2(x)-S_2(y)]F[\tilde{x},\tilde{y}]\ . \tag{B8}$$

Multiplying the $\tilde{F}$'s for all oscillators, and using Eqs. (3.2) and (4.6a) of $J(\omega)$ and L_1 in Eq. (4.5) for F, we get for the full influence functional

$$\tilde{F}[x,y]=\exp\left[\frac{2i}{\pi\hbar}\left[x_i\int_0^t d\tau[x(\tau)-y(\tau)]L_3(\tau)\right]\right]\times F[x,y]_{t_0=0}\ , \tag{B9}$$

with

$$L_3(\tau)=\int_0^\infty\frac{J(\omega)}{\omega}\cos\omega\tau\, d\omega\ . \tag{B10}$$

We have explicitly indicated in Eq. (B9) that in using Eq. (4.5) to evaluate the influence functional pertaining to $P^{(1)}(t)$ we are to set $t_0=0$, as opposed to taking $t_0\to\infty$ for $P^{(2)}(t)$. Note, however, that as a consequence of the constraints (4.2),

$$F[x,y]_{t_0\to\infty}=F[x,y]_{t_0=0}\exp\frac{2i}{\pi\hbar}\left[x_i\int_0^t d\tau[x(\tau)-y(\tau)]\tilde{L}_3(\tau)\right]\ , \tag{B11}$$

where

$$\tilde{L}_3(\tau)=\lim_{t_0\to\infty}\int_{t_0}^0 ds\int_0^\infty d\omega\, J(\omega)\sin\omega(\tau-s)\ . \tag{B12}$$

It is easy to show that if $J(\omega)/\omega$ is integrable near $\omega=0$,[95] then the contribution from t_0 vanishes in the limit, and $\tilde{L}_3(\tau)=L_3(\tau)$. Therefore,

$$F[x,y]_{t_0\to-\infty}=\tilde{F}[x,y]\ , \tag{B13}$$

which proves the equivalence of $\tilde{p}(x_f{:}t)$ and $p(x_f{:}t)$, and *a fortiori* of $P^{(1)}(t)$ and $P^{(2)}(t)$.

[94] The constant C is the coupling constant C_i appearing in Eq. (2.1) for the oscillator in question.

[95] This condition covers all the spectral densities of interest. In fact, if it is not satisfied, the problem is "pathological."

2. Alternative derivation[96] of Eq. (4.17)

It is convenient for the present purpose to write the Hamiltonian $\hat{H}$ in the second-quantized notation

$$\hat{H}=-\tfrac{1}{2}\hbar\Delta\sigma_x+\tfrac{1}{2}\varepsilon\sigma_z+\sum_\alpha\hbar\omega_\alpha(a_\alpha^\dagger a_\alpha+\tfrac{1}{2}) +\tfrac{1}{2}q_0\sigma_z\sum_\alpha f_\alpha(a_\alpha+a_\alpha^\dagger)\,, \tag{B14}$$

where $f_\alpha=(\hbar/2m_\alpha\omega_\alpha)^{1/2}C_\alpha$. Given this Hamiltonian we ask the following question: Suppose that at time t_i the spin is definitely known to be in a given state, say $\uparrow$, and the environment is in its thermal equilibrium state. Then what is the probability $W_\uparrow$ that at time $t_f>t_i$ the spin is in the same state $\uparrow$, but with the environment in any other possible state? $W_\uparrow$ is then given by

$$W_\uparrow=\sum_{n,m}\frac{e^{-\beta E_n}}{Z_{\rm env}}\,|\,G^{(\uparrow)}_{m,n}(t_f,t_i)\,|^2\,. \tag{B15}$$

Here E_n are the energy levels of the environment and Z_{env} is the partition function. $G^{(\uparrow)}_{mn}(t_f,t_i)$ is the probability amplitude for the transition in which at t_i the environment is in state n and the spin $\uparrow$, and as t_f the spin is $\uparrow$ but the environment is any possible state m. A sum over all possible final states of the environment is denoted by a sum over m. We now calculate $W_\uparrow$ using standard time-ordered perturbation theory. The method followed here is discussed in detail by Chang and Chakravarty (1985). For convenience let us write

$$\hat{H}=\hat{H}_0+\hat{H}_I\,, \tag{B16}$$

where

$$H_0=\tfrac{1}{2}\varepsilon\sigma_z+H_e+\sigma_z H_c \tag{B17}$$

and

$$\hat{H}_I=-\frac{\hbar}{2}\Delta\sigma_x\,. \tag{B18}$$

The environment Hamiltonian H_e is given by

$$H_e=\sum_\alpha\hbar\omega_\alpha(a_\alpha^\dagger a_\alpha+\tfrac{1}{2}) \tag{B19}$$

and the coupling term H_c is given by

$$H_c=\tfrac{1}{2}q_0\sum_\alpha f_\alpha(a_\alpha^\dagger+a_\alpha)\,.$$

Therefore

$$G^{(\uparrow)}_{mn}(t_f,t_i)=\left\langle m\uparrow\left|e^{iH_0(t_f-t_i)/\hbar}T\exp\left[-\frac{i}{\hbar}\int_{t_i}^{t_f}\hat{V}(t)dt\right]\right|n\uparrow\right\rangle\,. \tag{B20}$$

The operator $\hat{V}(t)=-(\hbar/2)\Delta e^{iH_0t/\hbar}\sigma_x e^{-iH_0t/\hbar}$. Thus

$$G^{(\uparrow)}_{mn}(t_f,t_i)=\sum_{n=0}^{\infty}\left[-\frac{i}{\hbar}\right]^n\int_{t_i}^{t_f}dt_1\int_{t_i}^{t_1}dt_2\cdots\int_{t_i}^{t_{n-1}}dt_n\langle m\uparrow|e^{-iH_0(t_f-t_i)/\hbar}\hat{V}(t_1)\hat{V}(t_2)\cdots\hat{V}(t_n)|n\uparrow\rangle\,. \tag{B21}$$

Now, noticing that $\hat{H}_0$ is diagonal in the spin space, it is possible to write

$$W_\uparrow=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\int_{t_i}^{t_1}dt_2\cdots\int_{t_i}^{t_{2i-1}}\int_{t_i}^{t_f}ds_1\cdots\int_{t_i}^{s_{2j-1}}ds_{2j} \times\left[\sum_{m,n}\frac{e^{-\beta E_n}}{Z_{\rm env}}\langle n|(e^{iH_{0+}s_{2j}/\hbar}e^{-iH_{0-}s_{2j}/\hbar})\cdots(e^{iH_{0-}s_1/\hbar}e^{-iH_{0+}s_1/\hbar})|m\rangle \times\langle m|(e^{iH_{0+}t_1/\hbar}e^{-iH_{0-}t_1/\hbar})\cdots(e^{iH_{0-}t_{2i}/\hbar}e^{-iH_{0+}t_{2i}/\hbar})|n\rangle\right]\,, \tag{B22}$$

where

$$H_{0\pm}=\pm\frac{\varepsilon}{2}+H_e\pm H_c\,. \tag{B23}$$

The sum over the intermediate states $|\,m\,\rangle$ can be carried out, resulting in

$$W_\uparrow=\frac{1}{Z_{\rm env}}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\cdots\int_{t_i}^{t_{2i-1}}dt_{2i}\int_{t_i}^{t_f}ds_1\cdots\int_{t_i}^{s_{2j-1}}ds_{2j}\sum_n e^{-\beta E_n}\langle n|\cdots|n\rangle\,, \tag{B24}$$

[96]This derivation is included mainly because, following the appearance of the paper of Chakravarty and Leggett (1984), a number of papers by other authors have characterized the functional-integral derivation used in it and here as "very complicated," or words to that effect.

where the integrand is

$$\sum_n e^{-\beta E_n}\langle n \mid \cdots \mid n\rangle = \mathrm{Tr}[e^{-\beta H_e}(e^{iH_{0+}s_{2j}/\hbar}e^{-iH_{0-}s_{2j}/\hbar})\cdots(e^{iH_{0-}s_1/\hbar}e^{-iH_{0+}s_1/\hbar}) \times (e^{iH_{0+}t_1/\hbar}e^{-iH_{0-}t_i/\hbar})\cdots(e^{iH_{0-}t_{2i}/\hbar}e^{-iH_{0+}t_{2i}/\hbar})] \,. \tag{B25}$$

Here the exponential factors do not commute with each other. We now order the operators on the contour C_δ (δ infinitesimal), as shown in Fig. 11. Let us also define

$$\zeta(z)=\zeta_+(z)=\sum_{m=1}^{2i}(-1)^{m+1}[\theta(z-t_m)-\theta(z-t_{m+1})] \tag{B26}$$

when z is measured along segment I (θ is the usual step function), and

$$\zeta(z)=\zeta_-(z)=\sum_{n=1}^{2j}(-1)^{n+1}[\theta(z-s_n)-\theta(z-s_{n+1})] \tag{B27}$$

when z is in segment II. Finally, we set $\zeta(z)=0$ for z in segment III. For $W_\uparrow$ we then have

$$W_\uparrow=\frac{1}{Z_{\mathrm{env}}}\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\cdots\int_{t_i}^{t_{2i-1}}dt_{2i}\int_{t_i}^{t_f}ds_1\cdots\int_{t_i}^{s_{2j-1}}ds_{2j} \times\left[\exp\left[-\frac{i\varepsilon}{2\hbar}\int_{C_\delta}dz\zeta(z)\right]\right]\mathrm{Tr}\left[T_{C_\delta}\exp -i/\hbar\int_{C_\delta}dz[H_e(z)+\zeta(z)H_c(z)]\right] . \tag{B28}$$

If we define

$$Z_\lambda=\mathrm{Tr}\left[T_{C_\delta}\exp\left[-\frac{i}{\hbar}\int_{C_\delta}dz[H_e(z)+\lambda\zeta(z)H_c(z)\right]\right] , \tag{B29}$$

then it follows that

$$W_\uparrow=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\cdots\int_{t_i}^{t_{2i-1}}dt_{2i}\int_{t_i}^{t_f}ds_1\cdots\int_{t_i}^{s_{2j-1}}ds_{2j} \times\exp\left[-\frac{i\varepsilon}{2\hbar}\int_{C_\delta}dz\,\zeta(z)\right]\exp\left[-\int_0^1 d\lambda\int_{C_\delta}dz\,\zeta(z)\langle H_c(z)\rangle_\lambda\right] , \tag{B30}$$

where

$$Z_\lambda\langle A(z)\rangle_\lambda=i\,\mathrm{Tr}\left[T_{C_\delta}\exp\left[-\frac{i}{\hbar}\int_{C_\delta}dz'[H_e(z')+\lambda\zeta(z')H_c(z')]\right]A(z)\right] . \tag{B31}$$

Using the equation of motion for $\langle a_\alpha(s)\rangle_\lambda$ it is quite straightforward to evaluate $\langle H_c(z)\rangle_\lambda$; the details can be found in the paper by Chang and Chakravarty (1985). The final answer for $W_\uparrow$ can be written in the form

$$W_\uparrow=\sum_{i=0}^{\infty}\sum_{j=0}^{\infty}(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\int_{t_i}^{t_1}dt_2\cdots\int_{t_i}^{t_{2i-1}}dt_{2i} \times\int_{t_i}^{t_f}ds_1\int_{t_i}^{s_1}ds_2\cdots\int_{t_i}^{s_{2i-1}}ds_{2i}\exp\left[-\frac{i\varepsilon}{2\hbar}\int_{t_i}^{t_f}dt'[\zeta_+(t')-\zeta_-(t')]+\frac{\varphi}{h}\right] , \tag{B32}$$

where

$$\frac{\varphi}{\hbar}=-\int_{t_i}^{t_f}ds\int_{t_i}^{s}ds'[\zeta_+(s)\zeta_+(s')K_1(s-s')+\zeta_-(s)\zeta_-(s')K_1^*(s-s')] +\int_{t_i}^{t_f}ds\int_{t_i}^{t_f}ds'\zeta_-(s)\zeta_+(s')K_1(s-s')-\int_{t_i}^{t_f}ds\int_{t_i}^{t_f}ds'[\zeta_+(s)-\zeta_-(s)][\zeta_+(s')-\zeta_-(s')]K_2(s-s') . \tag{B33}$$

The expressions K_1 and K_2 are given by

$$K_1(s-s')=\frac{q_0^2}{4}\sum_\alpha\frac{C_\alpha^2}{2m_\alpha\omega_\alpha\hbar}e^{-i\omega_\alpha(s-s')}\equiv\left[\frac{q_0^2}{\pi\hbar}\right]\frac{1}{4}\int_0^\infty d\omega\,J(\omega)[\cos\omega(s-s')-i\sin\omega(s-s')] \tag{B34}$$

and

$$K_2(s-s')=\frac{q_0^2}{4}\sum_\alpha \frac{C_\alpha^2}{2m_\alpha\omega_\alpha\hbar}\frac{1}{(e^{\beta\hbar\omega_\alpha}-1)}e^{-i\omega_\alpha(s-s')}$$
$$\equiv\left[\frac{q_0^2}{\pi\hbar}\right]\frac{1}{4}\int_0^\infty d\omega J(\omega)[\cos\omega(s-s')-i\sin\omega(s-s')]\frac{1}{e^{\beta\hbar\omega}-1}\ . \tag{B35}$$

It is not difficult to rewrite $\varphi/\hbar$ in the form

$$\frac{\varphi}{\hbar}=i\left[\frac{q_0^2}{\pi\hbar}\right]\int_{t_i}^{t_f}ds\int_{t_i}^{s}ds'\left[\frac{\zeta_+(s)-\zeta_-(s)}{2}\right]\left[\frac{\zeta_+(s')+\zeta_-(s')}{2}\right]L_1(s-s')$$
$$-\frac{q_0^2}{\pi\hbar}\int_{t_i}^{t_f}ds\int_{t_i}^{s}ds'\left[\frac{\zeta_+(s)-\zeta_-(s)}{2}\right]\left[\frac{\zeta_+(s')-\zeta_-(s')}{2}\right]L_2(s-s')\ , \tag{B36}$$

where, as defined in Sec. IV,

$$L_1(s-s')\equiv\int_0^\infty J(\omega)\sin\omega(s-s')d\omega \tag{B37}$$

and

$$L_2(s-s')\equiv\int_0^\infty J(\omega)\cos\omega(s-s')\coth(\beta\hbar\omega/2)d\omega\ . \tag{B38}$$

A moment's reflection will convince the reader that ξ and χ as defined in Sec. IV are nothing but

$$\xi(s)=\left[\frac{\zeta_+(s)-\zeta_-(s)}{2}\right] \tag{B39}$$

and

$$\chi(s)=\left[\frac{\zeta_+(s)+\zeta_-(s)}{2}\right]\ . \tag{B40}$$

We can therefore write the probability $W_\uparrow$

$$W_\uparrow=\sum_{i=0}^\infty\sum_{j=0}^\infty(-1)^{i+j}\left[\frac{\Delta}{2}\right]^{2i+2j}\int_{t_i}^{t_f}dt_1\int_{t_i}^{t_1}dt_2\cdots\int_{t_i}^{t_{2i-1}}dt_{2i}$$
$$\times\int_{t_i}^{t_f}ds_1\int_{t_i}^{s_1}ds_2\cdots\int_{t_1}^{s_{2j-1}}ds_{2j}\exp\left[-\frac{i\varepsilon}{h}\int_{t_i}^{t_f}dt'\xi(t')\right]$$
$$\times\exp\left[i\left[\frac{q_0^2}{\pi\hbar}\right]\int_{t_i}^{t_f}d\tau\int_{t_i}^{\tau}ds[L_1(\tau-s)\xi(\tau)\chi(s)+iL_2(\tau-s)\xi(\tau)\xi(s)]\right]\ . \tag{B41}$$

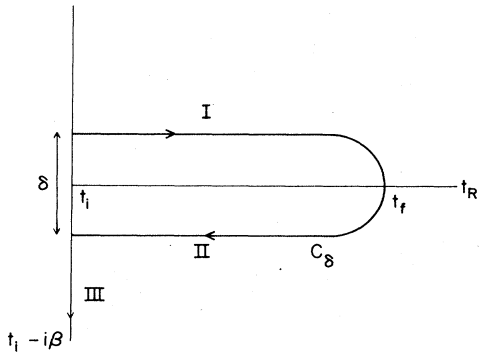

FIG. 11. Contour for the evaluation of Eq. (B25).

The integrals can now easily be ordered according to blips and sojourns. We finally note that $P(t)$ used in the text is related to $W_\uparrow(t)$ by the relation $[1+P(t)/2]=W_\uparrow(t)$.

APPENDIX C: MAPPING TO THE TOULOUSE HAMILTONIAN FOR $\alpha=\frac{1}{2}$

In this appendix we shall sketch how the dynamics of the spin-boson problem for $\alpha=\frac{1}{2}$ can be directly mapped onto the dynamics of the Toulouse Hamiltonian (Toulouse, 1969). The mapping is an approximate one that relies on neglect of terms "of order ω_c^{-1}" (to be made more precise later on). Consider then the Toulouse Hamiltonian consisting of spinless fermions which can hybridize with a local "d level" situated at the Fermi energy. The hybridization matrix element is in general energy dependent. This energy dependence will be, as usual, tak-

en to be smooth and insignificant. It will be assumed that the fermions hybridize with the local level only within a bandwidth. Explicitly the Toulouse Hamiltonian H_T is given by[97]

$$H_T=\sum_k \varepsilon_k c_k^\dagger c_k + V\sum_k (d^\dagger c_k + c_k^\dagger d)\ . \tag{C1}$$

Here $c_k^\dagger$ is the creation operator of the spinless fermions and $d^\dagger$ that of the local level. To simplify the arithmetic we have already assumed V to be energy independent throughout the bandwidth centered around the Fermi level, in accord with our assumption of its smooth and insignificant variation.

We wish to solve the following problem: Given that at time $t=-\infty$ the "environment" (i.e., the fermions) was in its thermal equilibrium state, and that for all times $t\le 0$ the system (i.e., the d level) is known to have occupation $n_d=1$, what is its occupation $\langle n_d(t)\rangle$ at a later (positive) time t? The quantity discussed in the text is $P(t)\equiv 2\langle n_d(t)\rangle -1$. Thus

$$\langle n_d(t)\rangle = \sum_{n,m}\frac{e^{-\beta E_n}}{Z_{\rm env}}\,|\,G_{mn}(t;n_d=1)\,|^2\ , \tag{C2}$$

where E_n are the energy eigenvalues of the environment and $Z_{\rm env}$ its partition function. $G_{mn}(t;n_d=1)$ is the probability amplitude that the environment is originally in the state n and the occupation of the d level is equal to one, while at a later time t the environment is in a state m but n_d is still unity. As in Appendix B.2 it is easy to show, using the usual time-ordered perturbation theory, that

$$\begin{aligned}\langle n_d(t)\rangle = \sum_{l,l'=0}^{\infty}(-1)^{l+l'}V^{2l+2l'}\int_0^t dt_1\cdots\int_0^{t_{2l-1}}dt_{2l}\int_0^t ds_1\cdots\int_0^{s_{2l-1}}ds_{2l}\\ \times\frac{1}{Z_{\rm env}}{\rm Tr}\left[e^{-\beta H_0}\left(\sum_{k_{2l'}}c_{k_{2l'}}(s_{2l})\right)\left(\sum_{k_{2l'-1}}c^\dagger_{k_{2l'-1}}(s_{2l'-1})\right)\cdots\left(\sum_{k'_1}c^\dagger_{k'_1}(s_1)\right)\right.\\ \left.\times\left(\sum_{k_1}c_{k_1}(t_1)\right)\cdots\left(\sum_{k_{2l-1}}c_{k_{2l-1}}(t_{2l-1})\right)\left(\sum_{k_{2l}}c^\dagger_{k_{2l}}(t_{2l})\right)\right]\ ,\end{aligned} \tag{C3}$$

where

$$c_k(t)=e^{-i\varepsilon_k t/\hbar}c_k,\quad c_k^\dagger(t)=e^{i\varepsilon_k t/\hbar}c_k^\dagger\ . \tag{C4}$$

In order to carry out further calculations it is convenient to separate out all the time dependences and write

$$\begin{aligned}\langle n_d(t)\rangle = \sum_{l,l'=0}^{\infty}(-1)^{l+l'}V^{2l+2l'}\sum_{k'_1,k'_2\cdots k'_{2l}}\sum_{k_1,k_2\cdots k_{2l}}\int_0^t dt_1\cdots\int_0^{t_{2l-1}}dt_{2l}\int_0^t ds_1\cdots\int_0^{s_{2l-1}}ds_{2l}\\ \times\exp-\frac{i}{\hbar}[\varepsilon_{k'_{2l}}s_{2l'}-\varepsilon_{k'_{2l-1}}s_{2l'-1}+\cdots-\varepsilon_{k'_1}s_1]\exp-\frac{i}{\hbar}[\varepsilon_{k_1}t_1-\cdots+\varepsilon_{k_{2l-1}}t_{2l-1}-\varepsilon_{k_{2l}}t_{2l}]\end{aligned} \tag{C5}$$

$$\times\frac{1}{Z_{\rm env}}{\rm Tr}\left[e^{-\beta H_0}c_{k_{2l'}}c^\dagger_{k_{2l'-1}}c_{k_{2l'-2}}\cdots c_{k'_2}c^\dagger_{k'_1}c_{k_1}c^\dagger_{k_1}\cdots c_{k_{2l-1}}c^\dagger_{k_{2l}}\right]\ , \tag{C6}$$

where H_0 is the free-fermion Hamiltonian $\sum_k \varepsilon_k c_k^\dagger c_k$. The calculation of the trace is standard [see, for example, Fetter and Walecka (1971), pp. 237–241] and gives rise to pairwise contractions, i.e.,

$$\begin{aligned}\frac{1}{Z_{\rm env}}{\rm Tr}\left[e^{-\beta H_0}c_{k_{2l'}}c^\dagger_{k_{2l'-1}}c_{k_{2l'-2}}\cdots c_{k_2}c^\dagger_{k'_1}c_{k_1}c^\dagger_{k_2}\cdots c_{k_{2l-1}}c^\dagger_{k_{2l}}\right]\\ =\dot{c}_{k_{2l'}}\dot{c}^{\dagger\cdot}_{k_{2l'-1}}\ddot{c}_{k_{2l'-2}}\cdots\dddot{c}_{k_{2l}}+\dot{c}_{k_{2l'}}\dot{c}^{\dagger\cdot\cdot}_{k_{2l'-1}}\dot{c}_{k_{2l'-2}}\cdots\dddot{c}^{\dagger}_{k_{2l}}+\cdots\ ,\end{aligned} \tag{C7}$$

where the only nonzero contractions are

$$\dot{c}^{\dagger\cdot}_k\dot{c}_k=\frac{1}{1+e^{\beta\varepsilon_k}}=n(\varepsilon_k) \tag{C8}$$

and

$$\dot{c}_k\dot{c}^{\dagger\cdot}_k=\frac{1}{1+e^{-\beta\varepsilon_k}}=1-n(\varepsilon_k)\ . \tag{C9}$$

[97] See Eq. (3.87); as in Sec. V.B we set $L=1$ for convenience.

Further analysis requires us to evaluate expressions of the form $\sum_k [1-n(\varepsilon_k)]e^{i\varepsilon_k t}$ and $\sum_k n(\varepsilon_k)e^{i\varepsilon_k t}$ (it is irrelevant whether t is greater or less than zero). With a given cutoff prescription these are easy to evaluate for any arbitrary temperature. However, our ability to put the resulting expression for $\langle n_d(t)\rangle$ in the form corresponding to $[1+P(t)]/2$ of the spin-boson Hamiltonian depends crucially on keeping terms only of leading order in $\omega_c t$. For example, consider $T=0$. Then with the choice of a smooth cutoff

$$\sum_k [1-n(\varepsilon_k)]e^{i\varepsilon_k t} = \int_{-\infty}^{+\infty} \rho(\varepsilon)e^{i\varepsilon t}e^{-|\varepsilon|/\omega_c}[1-n(\varepsilon)] = \frac{\rho_0\omega_c}{(1-i\omega_c t)} \tag{C10}$$

and similarly

$$\sum_k n(\varepsilon_k)e^{i\varepsilon_k t} = \frac{\rho_0\omega_c}{(1+i\omega_c t)} , \tag{C11}$$

where we have assumed that the density of states $\rho(\varepsilon)$ varies insignificantly and can be replaced by its value $\rho(0)$ at the Fermi surface taken to be the zero of the energy. With these expressions it can be verified that the resulting expression for $\langle n_d(t)\rangle$ cannot be matched exactly to the spin-boson problem unless only terms of the leading order in $\omega_c t$ are kept. Thus if we are interested only in the long-time limit it is more convenient immediately to take the limit $|\omega_c t| \to \infty$ in the above expressions and regularize the short-time behavior at the very end. This has the advantage that, apart from the factors of i, both of the above expressions are equally simple. We show here only the zero-temperature result:

$$\langle n_d(t)\rangle = \sum_{l,l'} (-1)^{l+l'}(V^2\rho_0\omega_c)^{l+l'} \int_0^t dt_1 \cdots \int_0^{t_{2l-1}} dt_{2l} \int_0^t ds_1 \cdots \int_0^{s_{2l-1}} ds_{2l} e^{A(t_1,\cdots t_{2l},s_1\cdots s_{2l})} , \tag{C12}$$

where

$$A(t_1,\cdots t_{2l},s_1\cdots s_{2l}) = \sum_{i<j} (-1)^{i+j}\ln[1+i\omega_c(t_i-t_j)] + \sum_{i<j} (-1)^{i+j}\ln[1-i\omega_c(s_i-s_j)]$$
$$- \sum_{i=1}^{2l}\sum_{j=1}^{2l'} (-1)^{i+j}\ln[1+i\omega_c(s_j-t_i)] . \tag{C13}$$

Here, as stated above, we have regularized the short-time behavior at the end by replacing $\pm i\omega_c(t_i-t_j)$ by $1\pm i\omega_c(t_i-t_j)$. Any results that depend on time scales of the order of the cutoff cannot be obtained correctly. It is now a matter of redefinition to put the above expression in terms of blips and sojourns. The interesting point to note here is that the expression for $\langle n_d(t)\rangle$ gives the same result for $\tilde{P}(t)$ as the spin-boson case, but with $\alpha=\frac{1}{2}$ and $\Delta^2=(4\rho_0\omega_c V^2)$, in complete agreement with the bosonization transcription in Sec. III.E [see Eqs. (3.74) and (3.75)].

APPENDIX D: THE CASE OF OHMIC DISSIPATION FOR $T=0$, $\varepsilon=0$, AND $0\le\alpha\le\frac{1}{2}$

1. Justification of Eq. (5.40)

The formula for $P(t)$ that follows from Eqs. (4.17)—(4.20) with the insertion of (5.4) in the limit $T\to 0$ is [cf. Eqs. (5.35)—(5.37); see Fig. 12 for definitions of the quantities appearing in Eqs. (D3)—(D6) below]

$$P(t) = \sum_{n=0}^{\infty} (-1)^n \Delta^{2n} K_n(t) , \tag{D1}$$

$$K_n(t) \equiv 2^{-n} \sum_{\{\xi_j=\pm 1\}} \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1} \cdots \int_0^{t_2} dt_1 F_1\{t_m\}F_2\{t_m,\xi_i\}F_3\{t_m,\xi_i\} , \tag{D2}$$

$$F_1\{t_m\} \equiv \prod_{j=1}^{n} (1+b_j^2)^{-\alpha} , \tag{D3a}$$

$$F_2\{t_m,\xi_i\} \equiv \prod_{k=1}^{n}\prod_{j=k+1}^{n} \frac{[1+(b_j+u_{jk})^2][1+(b_k+u_{jk})^2]^{\alpha\xi_j\xi_k}}{[1+(b_j+b_k+u_{jk})^2][1+u_{jk}^2]} , \tag{D3b}$$

$$F_3\{t_m,\xi_i\} \equiv \prod_{k=0}^{n-1} \cos\left[2\alpha \sum_{j=k+1}^{n} \xi_j X_{jk}\right] , \tag{D3c}$$

where we have combined the terms F_3 and F_4 in Eqs. (4.20c) and (4.20d) for simplicity of notation, where the quantities b_j and s_j denote, respectively, the length of the jth blip and the jth sojourn in units of ω_c^{-1}, and where the quantity u_{jk} is defined, as in Sec. V, by

$$u_{jk} \equiv s_k + \sum_{l=k+1}^{j-1} (b_l+s_l) . \tag{D4}$$

The quantity X_{jk} appearing in Eq. (D3c) is given by Eq. (5.10), that is,

$$X_{jk} \equiv \tan^{-1}\left[\frac{b_j s_k (b_j + s_k + 2y_{jk})}{[1+y_{jk}(y_{jk}+s_k)][1+(y_{jk}+b_j)(y_{jk}+b_j+s_k)]+s_k^2}\right], \tag{D5}$$

$$y_{jk} \equiv u_{jk} - s_k \equiv \sum_{l=k+1}^{j-1} (b_l + s_l) . \tag{D6}$$

Our purpose here is to demonstrate that "to order ω_c^{-1}" (see below) it is adequate to replace F_1, F_2, and F_3 by the simpler expressions

$$F_1' = \prod_{j=1}^{n} b_j^{-2\alpha} , \tag{D7a}$$

$$F_2' \equiv \prod_{k=1}^{n} \prod_{j=k+1}^{n} \frac{(b_j+u_{jk})(b_k+u_{jk})^{2\alpha\zeta_j\zeta_k}}{(b_j+b_k+u_{jk})u_{jk}} , \tag{D7b}$$

$$F_3' \equiv \prod_{k=0}^{n-1} \cos\pi\alpha \equiv (\cos\pi\alpha)^n . \tag{D7c}$$

We start by proving, for $0 \le \alpha \le \frac{1}{2}$, two general theorems that are essential to the subsequent derivation: (1) The influence functional (when summed over the $\{\eta_j\}$) is never negative; (2) F_2 is bounded above by the expression $\prod_{k=1}^{n}[f(\alpha)(b_k+s_k)/s_k)]^{2\alpha}$, where $f(\alpha)$ is finite and independent of n. These two theorems are not too easy to extract directly from Eqs. (D1)—(D7), but they follow very simply if we go back to the original formula (4.7) for the influence functional and note that for the ohmic case we have

$$L_1(\tau-s) = \frac{2\eta\omega_c^3(\tau-s)}{[1+\omega_c^2(\tau-s)^2]^2} \ge 0 , \tag{D8a}$$

$$L_2(\tau-s) = \eta\omega_c^2\left[\frac{1-\omega_c^2(\tau-s)^2}{[1+\omega_c^2(\tau-s)^2]^2}\right] . \tag{D8b}$$

Theorem (1) now follows from the fact that an upper limit on the contribution to the (magnitude of the) phase of the influence functional from the interaction of a given blip with all succeeding sojourns (which is just $2\alpha\sum_{j=k+1}^{n}\zeta_j X_{jk}$) is given by the expression

$$(q_0^2/\pi\hbar)\int_0^\infty dt \int_0^t dt' L_1(t') = \pi\alpha . \tag{D9}$$

Thus the factor F_3, Eq. (D3c), is not only positive but is bounded below by $(\cos\pi\alpha)^n$, and, trivially, above by unity. Theorem (2) follows from the fact that for any set of $\{\zeta_j\}$ an upper bound on the quantity F_2 is clearly given, from Eq. (4.7), by the expression

$$\prod_{k=1}^{n} \exp\left[+q_0^2/\pi\hbar \int^{(k)} d\tau \int ds \, |L_2(\tau-s)|\right] ,$$

where the notation $\int^{(k)}$ indicates that s runs over the kth blip and τ runs from t_{2k+1} to infinity. This expression may in turn be verified to be bounded above by $\prod_{k=1}^{n}[f(\alpha)(b_k+s_k)/s_k]^{2\alpha}$, where $f(\alpha)$ can, for example, be chosen to be $2^{-2\alpha}e^{2\alpha}$.

The next step in the argument may be easier to follow if we temporarily assume that $F_1'F_2'$ is an upper bound on F_1F_2. In that case it follows at once that an upper bound on $K_n(t)$ is given by $(\sec\pi\alpha)^n$ times the value of $K_n(t)$ that would be obtained from the replacements (D7). As we have seen in Sec. V, the latter is equal to $\Delta^{-2n}(\Delta_{\rm eff}t)^{2n(1-\alpha)}\Gamma^{-1}[2n(1-\alpha)+1]$ times a dimensionless factor, arising from the interblip interactions, which is rigorously bounded above, for all $\alpha \le \frac{1}{2}$, by 2^n. It is clear, therefore, that for any finite value ν of the time *measured in units of* $\Delta_{\rm eff}^{-1}$, we can neglect all terms in the series (D1) for $P(t)$ that correspond to values of n much larger than $\nu^{2(1-\alpha)}\sec\pi\alpha$. This result (which could, of course, be formulated quite rigorously) is crucial to our proof (to prove the same result with time measured in units of the "bare" inverse frequency Δ^{-1} would, of course, be trivial, but totally uninformative).

In fact, we have been unable to prove that $F_1'F_2'$ is an upper bound on F_1F_2. However, the conclusion of the last paragraph still follows, with a minor modification, from theorem 2 above, since this guarantees us that F_2 is bounded above by a constant which, apart from the numerical factor $2^{-2\alpha}e^{2\alpha}$ in $R(\alpha)$, is the same as that shown below [Eq. (D34)] to occur in the bound for $r_n(\alpha)$, i.e., for F_2'. Since F_1 clearly *is* bounded above by F_1', the only difference is that $\nu^{2(1-\alpha)}\sec\pi\alpha$ in the argument of the last paragraph is multiplied by the n-independent constant $2^{-2\alpha}e^{2\alpha}$. The general conclusion is clearly not affected.

The proof of the legitimacy of the replacements (D7) now proceeds in three stages. In the first stage we put an upper bound on the contribution to the coefficients $K_n(t)$ of "short" blip-sojourn pairs, that is, those with length of order ω_c^{-1} or less. To be specific, let us consider the contribution of paths containing m pairs of blips and immediately subsequent sojourns (b_l, s_l) such that $b_l + s_l \le \mu$. We rearrange the integrand F_1, F_2, F_3 into three new factors G_1, G_2, G_3 as

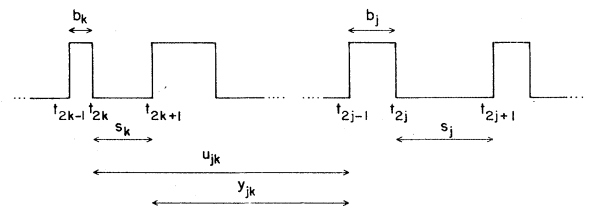

FIG. 12. Definitions of the quantities occurring in Eqs. (D3)—(D6) (this is Fig. 5, repeated here for convenience).

$$G_1 \equiv \prod_j{}' (1+b_j^2)^{-\alpha} \prod_k{}' \prod_{j>k}{}' Z_{jk}^{\alpha\zeta_j\zeta_k} \prod_k{}' \cos\left[2\alpha \sum_{l=k+1}^{n} \zeta_l X_{lk}\right], \tag{D10a}$$

$$G_2 \equiv \prod_j{}'' (1+b_j^2)^{-\alpha} \prod_k{}'' \prod_{j>k}{}'' Z_{jk}^{\alpha\zeta_j\zeta_k} \prod_k{}'' \cos\left[2\alpha \sum_{l=k+1}^{n}{}'' \zeta_l X_{lk}\right], \tag{D10b}$$

$$G_3 \equiv \prod_j{}' \prod_k{}'' Z_{jk}^{\alpha\zeta_j\zeta_k} \prod_k{}'' \left[\frac{\cos\left[2\alpha \sum_{l=k+1}^{n} \zeta_l X_{kl}\right]}{\cos\left[2\alpha \sum_{l=k+1}^{n}{}'' \zeta_l X_{kl}\right]}\right], \tag{D10c}$$

where the single prime denotes a product or sum over pairs with $b_l + s_l \le \mu$ and the double prime the complementary product or sum, and Z_{jk} is the quantity in square brackets in Eq. (D3b). Note that in the definition of G_3, Eq. (D10c), there is no restriction $j > k$.

The factor G_1 is clearly bounded above by unity. G_2 is (nearly) the integrand of $K_{n-m}(t)$; see below. Consider now the factor G_3, which expresses the interactions between the "short" and "long" blips. Since each of the cosine factors is bounded below by $\cos\pi\alpha$ and above by unity, the product of quotients is clearly bounded above[98] by $(\sec\pi\alpha)^{n-m}$. Now consider the double product of $Z_{jk}^{\alpha\zeta_j\zeta_k}$. Clearly we have

$$Z_{jk} \equiv \frac{[1+(b_j+u_{jk})^2]\cdot[1+(b_k+u_{jk})^2]}{[1+(b_j+b_k+u_{jk})^2]\cdot[1+u_{jk}^2]} \le \left[\frac{1+(b_j+u_{jk})^2}{1+u_{jk}^2}\right] \le 1+\frac{2\mu u_{jk}+\mu^2}{1+u_{jk}^2}, \tag{D11}$$

where the last step follows from the observation that b_j is by construction not greater than μ. Consider this expression for fixed j and variable k, recalling that the pair j is by construction "short" and the pair k "long." Quite generally, the above expression is bounded above by $(1+2\mu+\mu^2)$, so the values of k that are the nearest long pairs to j give a factor in the product at most $(1+\mu)^4$. All other values of k correspond to $u_{jk} \ge |l_{jk}|\mu$, where l_{jk} is the ordinal number, counting long pairs only, of the kth blip relative to the jth: Note that l can have either sign. Thus we have for such cases $Z_{jk} \le (1+|l_{jk}|^{-1})^2$. A parallel argument, with u_{jk} in Eq. (D11) replaced by (b_k+u_{jk}), can obviously be constructed for Z_{jk}^{-1}. Thus we have

$$\prod_k{}'' Z_{jk}^{\alpha\zeta_j\zeta_k} \le (1+\mu)^{4\alpha} \prod_k{}'' (1+|l_{jk}|^{-1})^{2\alpha} \le [C(1+\mu)(n-m)]^{4\alpha}, \tag{D12}$$

where the last inequality follows from the facts that $\ln(1+x) \le x$ and that there cannot be more than $n-m$ long blips either to the right or to the left of the jth. In Eq. (D12), C is a calculable numerical constant of order unity, which is independent of n and m. Since the contribution corresponding to each j in the product in G [Eq. (D10c)] is bounded above in this way, we have

$$G_3 \le [C(1+\mu)(n-m)]^{4m\alpha} \sec^{n-m}\pi\alpha \equiv G_3^{\max}. \tag{D13}$$

Consider now the contribution $\delta K_{nm}^{(1)}(\mu)$ to $K_n(t)$, which arises from the region R of phase space corresponding to m blip-sojourn pairs of length $\le\mu$. From Eq. (D13) and the fact that $G_1 \le 1$, we have

$$\delta K_{nm}^{(1)}(\mu) \le G_3^{\max} \int^R dt_{2n} \cdots dt_1 G_2. \tag{D14}$$

The quantity G_2 is clearly everywhere positive. If it were not for the slightly different cosine factor,[99] it would be just the integrand in the expression for $K_{n-m}(t)$; moreover, for any given configuration of the m "short" pairs, the region of integration over the $n-m$ "long" ones is contained in the region of integration for $K_{n-m}(t)$. Since the cosine factor must always lie between $\cos\pi\alpha$ and 1, any error arising from this has already been taken into account by the factor $\sec^{n-m}(\pi\alpha)$ in $G_3^{\max}$. Thus it is clear that the integral over R is bounded above by the phase space available for the m short pairs, which is in turn less than $C_m^n(\frac{1}{2}\mu^2\omega_c^{-2})^m$, times the value of $K_{n-m}(t)$ (here we took into account that μ is the blip length in unity of ω_c^{-1}). Hence, using the upper bound on $K_{n-m}(t)$ already obtained, namely,

$$\sec^{n-m}(\pi\alpha) \times \Delta^{-2(n-m)} (\Delta_{\rm eff} t)^{2(n-m)(1-\alpha)} \Gamma^{-1}[2(n-m)(1-\alpha)+1] \times 2^{n-m},$$

we find that the total error $\delta K_n^{(1)}$ incurred in $K_n(t)$ by neglecting configurations with any blip-sojourn pair shorter than μ is bounded by the inequality

$$\delta K_n^{(1)}(t:\mu) \le \Delta^{-2n} \sum_{m=1}^{n} C_m^n \varphi^{2m}(\mu) \left[\frac{\Delta}{\omega_c}\right]^{2m} (\tilde{\Delta}_{\rm eff} t)^{2(n-m)(1-\alpha)} (n-m)^{4m\alpha} \Gamma^{-1}[2(n-m)(1-\alpha)+1], \tag{D15}$$

[98] This limit is by no means the best we can get on this factor, but it has the virtue of simplicity.

[99] Arising from the fact that in the integrand (D10b) the blip and sojourns that are nearest neighbors are not necessarily contiguous, whereas in the expression for $K_{n-m}(t)$ they always are.

where for conciseness we have defined the quantities

$$\varphi(\mu)\equiv 2^{-1/2}\mu[C(1+\mu)]^{2\alpha}\,, \tag{D16a}$$

$$\tilde{\Delta}_{\rm eff}\equiv(2^{1/2}\sec\pi\alpha)^{1/(1-\alpha)}\Delta_{\rm eff}\,. \tag{D16b}$$

Using the obvious upper bounds $C_m^n\le n^m/m!$, $(n-m)^{4m\alpha}\le n^{4m\alpha}$, $\Gamma^{-1}[2(n-m)(1-\alpha)+1]\le 1$, we find

$$\delta K_n^{(1)}(t:\mu)\le\Delta^{-2n}(\tilde{\Delta}_{\rm eff}t)^{2n(1-\alpha)}[(\exp\lambda^2)-1]\,, \tag{D17}$$

$$\lambda\equiv n^{(1+4\alpha)/2}\varphi(\mu)\left[\frac{\Delta}{\omega_c}\right]\frac{\cos\pi\alpha}{(\Delta_{\rm eff}t)^{1-\alpha}}$$

$$\equiv{\rm const}n^{(1+4\alpha)/2}\varphi(\mu)\cos\pi\alpha(\omega_c t)^{-(1-\alpha)}\,, \tag{D18}$$

where the constant is of order unity and remains finite in the limit $\alpha\to\frac{1}{2}$. In the expression for the error in $P(t)$, the factor Δ^{-2n} is of course canceled [cf. Eq. (D1)].

It is clear that for fixed values of n, μ, $(\Delta_{\rm eff}t)$, and $\alpha(<\frac{1}{2})$, Eq. (D17) (or rather this times Δ^{2n}) can be made as small as we please by choosing Δ/ω_c small enough. Moreover, we already know that for fixed $\Delta_{\rm eff}t$ we can neglect, in the expression for $P(t)$, values of n large compared to $(\Delta_{\rm eff}t)(\sec\pi\alpha)^{1/2-2\alpha}$, so that it follows that for fixed μ and $\Delta_{\rm eff}t$ (and fixed $\alpha<\frac{1}{2}$), the corrections to $P(t)$ from blip-sojourn pairs shorter than μ can be made negligibly small by a suitably small value of Δ/ω_c. Note that it does *not* follow from the above argument that for fixed Δ/ω_c the corrections tend to zero in the limit $\omega_c t\to\infty$; attractive as this conjecture may be, it would need further work to demonstrate it. This concludes the first step of the argument.

The next stage consists in showing that, for the remaining region of the phase space (all blip-sojourn pairs larger than μ) we can (a) approximate the complicated factors $\cos\{2\alpha\sum_{j=k+1}^n\xi_r X_{jk}\}$ for each k by the simpler factors $\cos(2\alpha X_{k,k+1})$, and (b) neglect the 1 by comparison with the b_j's, etc., in the expression F_2, except for nearest-neighbor pairs of blips. Taking the second point first, we see that for $j>k+1$ the quantity u_{jk} [Eq. (D4)] is always greater than μ for the relevant paths, and hence the error in the quantity Z_{jk} [Eq. (D11)] induced by dropping the 1's is easily shown to be less than $2\mu^{-2}$ times the value so obtained, as is the error in Z_{jk}^{-1}. Consequently the relative error in the factor F_2 [Eq. (D3b)] induced by dropping the 1's for all except nearest-neighbor pairs of blips is less than $[\exp(2\alpha n^2\mu^{-2})-1]$.

Similarly, for the cosine terms, we have, using the obvious inequality $|\cos(x+y)-\cos x|\le\sqrt{2}y$, the result

$$\left|\cos2\alpha\sum_{j=k+1}^n\zeta_j X_{jk}-\cos2\alpha X_{k,k+1}\right|\le 2\sqrt{2}\,\alpha\sum_{j=k+2}^n X_{jk}\,. \tag{D19}$$

Now it is straightforward to demonstrate, from Eq. (D5), the inequality $X_{jk}\le 2y_{jk}^{-1}\le 2\mu^{-1}$ for $j\ge k+2$, and hence the absolute error in the kth cosine term induced by dropping all the X_{jk} for $j\ge k+2$, relative to the value so obtained, is bounded above by $2\sqrt{2}\,\alpha(\ln n)\mu^{-1}\sec\pi\alpha$. It follows that the error in F_3, relative to the value as obtained, is bounded above by the expression $\exp[2\sqrt{2}\,\alpha(n\ln n)\sec(\pi\alpha)\mu^{-1}]-1$. It is clear that by taking μ large enough compared to 1 this error may be made as small as we please for any n and any $\alpha<\frac{1}{2}$.

The final step consists in showing that in addition to the above approximations we may (a) drop the 1's in F_1; (b) drop the 1's in the nearest-neighbor terms in F_2 (which are the only ones in which they survive); (c) set all the quantities $\cos(2\alpha X_{k,k+1})$ equal to $\cos\pi\alpha$. The argument proceeds in two stages, in parallel with that given above, except that to justify it we need (a) to show that the contribution of paths with short blips ($<\mu^{-1}$) is negligible; (b) show the same for short sojourns; and (c) combine both results. In view of the fact that the factor $(1+b_j^2)^{-1}Z_{j,j+1}^{\alpha\xi_j\xi_{j+1}}$ is less than 2 for any choice of the ξ_j, the contribution $\delta K_{nm}^{(2)}(\mu)$ from (for example) configurations having m blips shorter than μ to K_n is bounded by an expression similar to (D15):

$$\delta K_{nm}^{(2)}\le 2^m C_m^n(\mu t\omega_c^{-1})^m\sec^{n-m}(\pi\alpha)K_{n-m}(t)\,. \tag{D20}$$

The argument proceeds as above, and we find a result identical to (D17) except that the factors $\varphi(\mu)$ and Δ/ω_c are replaced by $2\mu^{1/2}$ and $\Delta(t/\omega_c)^{1/2}$, respectively, and there is an extra factor of 2^n. Since for $\alpha<\frac{1}{2}$ the quantity $\Delta^2/(\Delta_{\rm eff}\omega_c)$ can be made as small as we please by a suitable choice of Δ/ω_c, the rest of the argument leading to the neglect of short blips goes through as in the blip-plus-sojourn case. Again, similarly to this case, we can obviously show that, in the region of phase space where no blips are shorter than μ, the relative error in the quantity F_1 induced by neglecting the 1 is at most $[\exp(n\alpha\mu^{-2})-1]$, etc.; moreover, the cosine factors are bounded in this region below by $\cos\pi\alpha$ and above by unity.

Finally, we get rid of the short sojourns in a completely similar way, using again the fact that the factor $(1+b_j^2)^{-1}Z_{j,j+1}^{\alpha\xi_j\xi_{j+1}}$ is always less than 2, and bound the error incurred by dropping the 1 in the nearest-neighbor factors for the region corresponding to no short sojourns, exactly as in the blip-plus-sojourn calculation. The outcome of all this is as follows. Given any finite value of $\Delta_{\rm eff}t$, and any value of α less than $\frac{1}{2}$, Δ/ω_c can always be chosen small enough that we can find a dimensionless number μ that will enable us to make as small as we please *both* (a) the error incurred by neglecting all paths with any blips or sojourns of length less than μ [which is in general of order $(\Delta/\omega_c)^\gamma\mu^{\gamma'},\gamma,\gamma'>0$, when this quantity is small; see, for example, Eq. (D17)], and (b) the error incurred in making the approximations (D7) for all other paths, which is of order $\mu^{-\nu}$, $\nu>0$ [see the estimates above and below Eq. (D19)]. However, since the appropriate choice of μ is clearly proportional to a positive power, less than 1 and less than γ/γ', of ω_c/Δ, it is clear from the formula for the integral obtained by the substitutions (D7) that extending the integral (with substituted integrand) back again to cover "short" blips and sojourns

will give a further relative correction which, once again, can be made as small as we please as we take Δ/ω_c to zero. Thus the final conclusion is that, for any given value of $\Delta_{\rm eff}t$ and $\alpha(<\frac{1}{2})$, it is possible to find a value of Δ/ω_c such that the error (absolute or relative[100]) incurred in $P(t)$ in simply making the replacements (D7) and continuing to carry out the integrals over all the phase space can be made less than any specified number. We reemphasize that it is in this sense, and in this sense *only*, that we claim to have established rigorously that Eq. (5.40) is exact "in the limit $\Delta/\omega_c \to 0$."

Finally, it should be carefully noted that the above proof relies heavily not only on the fact that $\cos\pi\alpha$ is finite and positive (which is, of course, always true for $\alpha<\frac{1}{2}$), but also on the fact that the influence function itself is everywhere positive. It therefore fails not only for $\alpha>\frac{1}{2}$ but also (in generalized form), even for $\alpha<\frac{1}{2}$, in the case of a finite bias ε whenever t exceeds $\pi(\frac{1}{2}-\alpha)\varepsilon^{-1}$. The generalization is therefore only of any interest in the case of a very small bias, $\varepsilon \ll (1-2\alpha)\Delta_{\rm eff}$, and even in that case will not necessarily give the long-time behavior correctly (see Sec. VII). Of course, it is conceivable that a much more generally valid proof of the legitimacy of neglecting the difference between Eqs. (D3) and (D7) could be found; at the time of writing we have not investigated this question.

2. Bounds and other relations for the coefficients $\tilde{K}_n(\alpha)$

In this part of this appendix we shall establish the various properties of the coefficients $\tilde{K}_n$ that were referred to in the discussion of interblip correlations in Sec. V.D. It is convenient to introduce the ratio

$$r_n(\alpha)=\tilde{K}_n(\alpha)/\tilde{K}_n^{(0)}(\alpha)\ , \tag{D21}$$

where $\tilde{K}_n^{(0)}$ is the value obtained by neglecting the interblip factor, namely, $1/\Gamma[2n(1-\alpha)+1]$ [see Eq. (5.43)]. We shall show that (i) $\tilde{K}_n(\alpha)-\tilde{K}_n^{(0)}(\alpha)=O(\alpha^2)$ as $\alpha\to 0$; (ii) $1<r_n(\alpha)\le[R(\alpha)]^{n-1}$, where $R(\alpha)$ is a finite n-independent number, for all values of α in the interval $(0,\frac{1}{2})$; (iii) $r_n(\alpha)-1$ vanishes as $(1-2\alpha)$ as $\alpha\to\frac{1}{2}$, and further that corrections to this result that arise from nonnearest-neighbor interblip correlations vanish as $(1-2\alpha)^2$ in the same limit. Unfortunately, we do not have a single argument for all three properties, but the separate arguments are all relatively straightforward.

Equation (5.42) for $\tilde{K}_n(\alpha)$ may be written as

$$\tilde{K}_n(\alpha)=[\Gamma(1-2\alpha)]^{-n}\int_0^1 dz_{2n}\int_0^{z_{2n}} dz_{2n-1}\cdots\int_0^{z_2} dz_1\prod_{j=1}^{n}(z_{2j}-z_{2j-1})^{-2\alpha}\Lambda_n\{z_m\}\ , \tag{D22}$$

where the interblip correlation factor Λ_n is given by

$$\Lambda_n\{z_m\}=2^{-n}\sum_{\{\zeta_j=\pm1\}}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}[P_{jk}\{z_m\}]^{2\alpha\zeta_j\zeta_k}\ , \tag{D23}$$

$$P_{jk}\{z_m\}\equiv(b_j+u_{jk})(b_k+u_{jk})/[u_{jk}(b_j+b_k+u_{jk})]\ , \tag{D24}$$

and where in analogy to the definitions above we have defined

$$b_j\equiv z_{2j}-z_{2j-1},\quad s_j\equiv z_{2j+1}-z_{2j},\quad u_{jk}\equiv z_{2j-1}-z_{2k}\equiv s_k+\sum_{l=k+1}^{j-1}(b_l+s_l)\ . \tag{D25}$$

It is useful to transform the nested integral in Eq. (D22) as follows. Consider the function of the variable z obtained by replacing the upper limit of the z_{2n} integral in Eq. (D22) by z, and Laplace-transform the resulting function with respect to z. A few changes of the orders of integration, as in Sec. IV.C, enable one to see that the Laplace transform is proportional to a simple power of the transform variable, which is easily inverted. Finally setting $z=1$, we get

$$r_n(\alpha)=[\Gamma(1-2\alpha)]^{-n}\int_0^\infty db_1\int_0^\infty ds_1\cdots\int_0^\infty db_n\int_0^\infty ds_n\exp\left[-\sum_{j=1}^{n}(s_j+b_j)\right]\prod_{j=1}^{n}b_j^{-2\alpha}\Lambda_n\ , \tag{D26}$$

where Λ_n continues to be formally defined by Eqs. (D23)—(D25).

To establish property (i) above, we simply expand Eq. (D23) in powers of α:

$$\Lambda_n=2^{-n}\sum_{\{\zeta_j=\pm1\}}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}\{1+2\alpha\zeta_j\zeta_k\ln P_{jk}+2\alpha^2\ln^2 P_{jk}+\cdots\}\ . \tag{D27}$$

The desired result follows when we note that the sum of $\zeta_j\zeta_k$ over all values of the ζ's vanishes, so that Λ_n differs from unity by a term of order α^2.

With regard to property (ii), the lower bound for r_n follows when we view the sum on the ζ's in Eq. (D23) as an arithmetic mean of 2^n quantities. This is bounded below by the geometric mean, which clearly equals unity, as does the resulting lower bound for the integral in Eq. (D26).

[100]The statement about relative error clearly needs slight reformulation when $P(t)$ is very close to a zero. The nature of the reformulation is obvious from the above argument and will not be spelt out here.

To obtain the upper bound on r_n, we define the quantity

$$H_k \equiv \prod_{j=k+1}^{n} P_{jk} \ . \tag{D28}$$

Since

$$P_{jk} = 1 + \{ b_j b_k / [u_{jk}(b_j + b_k + u_{jk})] \} \geq 1 \ , \tag{D29}$$

we have

$$\Lambda_n \leq \prod_{k=1}^{n-1} H_k^{2\alpha} \ . \tag{D30}$$

We now note that if we define $Y_j \equiv b_j + s_j$, we have

$$(b_j + u_{jk})/(b_j + b_k + u_{jk}) \leq (Y_j + u_{jk})/(Y_j + b_k + u_{jk}) \ , \tag{D31}$$

so that

$$H_k \leq \prod_{j=k+1}^{n} \left[\frac{(Y_j + u_{jk})(b_k + u_{jk})}{(Y_j + b_k + u_{jk}) u_{jk}} \right] . \tag{D32}$$

The product on the right is so constructed that each term in it contains two factors (one each in the numerator and denominator), which cancel against two factors in the succeeding term in the product. Thus we get

$$H_k \leq \frac{b_k + s_k}{s_k} \cdot \frac{Y_n + u_{n,k+1}}{Y_n + b_k + u_{n,k+1}} \leq \frac{b_k + s_k}{s_k} \ . \tag{D33}$$

Combining Eqs. (D26), (D30), and (D33), we find

$$r_n(\alpha) \leq [R(\alpha)]^{n-1} \ , \tag{D34}$$

where

$$R(\alpha) = \frac{1}{\Gamma(1-2\alpha)} \int_0^\infty \int_0^\infty e^{-(s+b)} \left[\frac{s+b}{sb} \right]^{2\alpha} ds \, db$$

$$= \frac{\Gamma(1-2\alpha)\Gamma(2-2\alpha)}{\Gamma(2-4\alpha)} \ . \tag{D35}$$

This factor tends to $1 + 2\alpha + O(\alpha^2)$ in the limit $\alpha \to 0$, and to 2 in the limit $\alpha \to \frac{1}{2}$. Thus, as stated in Leggett and Garg (1985), we have a rigorous bound on the corrections to $P(t)$ from interblip correlations:

$$|\delta P(t)| \leq \sum_{n=2}^{\infty} \frac{[R^{n-1}(\alpha) - 1]}{\Gamma[2n(1-\alpha)+1]} (\Delta_{\rm eff} t)^{2n(1-\alpha)} \ . \tag{D36}$$

It is easy to see why $R(\alpha)$ does not approach unity as $\alpha \to \frac{1}{2}$. As argued in Sec. V.D, we expect the contribution to the integral to come entirely from the region $b_j \to 0$ for all j. Although the bound (D33) reduces to the correct value (unity) in this limit, its behavior in the limit $s_j \to 0$ is very different from that of H_k itself, with the result that, in the bound, short sojourns and short blips are equally important. To overcome this difficulty, we return to Eq. (D29) and use the inequality $(1+y)^{2\alpha} \leq 1 + y^{2\alpha}$ for $\alpha \leq \frac{1}{2}$ and $y \geq 0$ to write

$$P_{jk}^{2\alpha} \leq 1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k + u_{jk})} \right]^{2\alpha}$$

$$\leq 1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k)} \right]^{2\alpha} , \tag{D37}$$

which implies

$$\Lambda_n \leq \prod_{j=1}^{n-1} \prod_{j=k+1}^{n} \left[1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k)} \right]^{2\alpha} \right] . \tag{D38}$$

We can thus write the upper bound on the deviation of the ratio r_n from unity as a sum of corrections from various collections of the interblip interactions. It is not difficult to show that the corrections from a single nearest-neighbor term are of order $(1-2\alpha)$. The only other terms of the same order arise from sets of an arbitrary number of *contiguous* nearest-neighbor corrections and are automatically included in $P^{(1)}(t)$. One can also show that the corrections from a single second- or further-neighbor term are of order $(1-2\alpha)^2$, and it is obvious that the inclusion of any other terms (whether or not they arise from nearest neighbors) cannot lower the order. As stated in Sec. V.D, we have therefore proved that the corrections to $P^{(0)}(t)$ vanish as $(1-2\alpha)$ in the limit $\alpha \to \frac{1}{2}$, and the corrections to $P^{(1)}(t)$ vanish as $(1-2\alpha)^2$.

3. Transfer matrix treatment of interblip effects

In the first part of this appendix we have provided a rigorous justification for the approximations (5.40)—(5.42). The resulting formulas are still much too intractable, but we have seen that if we make the further approximation of neglecting the interblip effects, they simplify enormously, and the final answer $P^{(0)}(t)$ [Eq. (5.44)] is quite compact. Having examined, in the second part of this appendix, the precise extent to which this second approximation is valid, we now turn to the question of quantitatively estimating the errors involved in making it. To do this we argue, as in Sec. V.D, that the nearest-neighbor correlations are of primary importance, and so we shall for the moment neglect all others. In other words, we approximate the coefficients $\tilde{K}_n(\alpha)$ in Eq. (5.41) by $\tilde{K}_n^{(1)}(\alpha)$, where

$$\tilde{K}_n^{(1)}(\alpha) = [\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \cdots \int_0^{z_2} dz_1 \prod_{j=1}^{n} (z_{2j} - z_{2j-1})^{-2\alpha}$$

$$\times 2^{-n} \sum_{\{\xi_k = \pm 1\}} \prod_{k=1}^{n-1} \left[\frac{(z_{2k+2} - z_{2k})(z_{2k+1} - z_{2k-1})}{(z_{2k+2} - z_{2k-1})(z_{2k+1} - z_{2k})} \right]^{2\alpha \xi_k \xi_{k+1}} . \tag{D39}$$

As in Sec. V.D, we denote the resulting approximation to $P(t)$ by $P^{(1)}(t)$.

If we now work in units such that $\Delta_{\rm eff}=1$, and Laplace-transform $P^{(1)}(t)$ with respect to time, we get (using a notation like that of Sec. V.F),

$$\tilde{P}^{(1)}(\lambda)=\sum_{n=0}^{\infty}(-1)^n\lambda^{2n(1-\alpha)-1}r_n^{(1)}(\alpha)\ , \tag{D40}$$

$$r_n^{(1)}=[2\Gamma(1-2\alpha)]^{-n}\sum_{\{\xi_j\}}\int_0^\infty db_1\int_0^\infty ds_1\cdots\int_0^\infty db_n\prod_{j=1}^{n}e^{-b_j}b_j^{-2\alpha}\prod_{j=1}^{n-1}e^{-s_j}(P_{j+1,j})^{2\alpha\xi_j\xi_{j+1}}\ , \tag{D41}$$

where P_{jk} is defined in Eq. (D24). Note that we have already performed the integral on s_n. [It is clear that $r_n^{(1)}$ is the approximation to r_n of Eq. (D26) obtained by keeping only nearest-neighbor terms.]

It is now apparent that if we define a transfer operator $\hat{K}$ via the relation

$$\hat{K}[\varphi(b_1,\xi_1)]=\psi(b_2,\xi_2)$$
$$\equiv\frac{1}{2\Gamma(1-2\alpha)}\sum_{\xi_1=\pm1}\int_0^\infty\int_0^\infty db_1ds_1e^{-(b_1+s_1)}b_1^{-2\alpha}\left[\frac{(b_1+s_1)(b_2+s_1)}{s_1(b_1+b_2+s_1)}\right]^{2\alpha\xi_1\xi_2}\varphi(b_1,\xi_1)\ , \tag{D42}$$

a generalized inner product $\psi\circ\varphi$ for any two functions $\psi(b,\xi)$ and $\varphi(b,\xi)$ by

$$\psi\circ\varphi=[2\Gamma(1-2\alpha)]^{-1}\sum_{\xi}\int_0^\infty db\,e^{-b}b^{-2\alpha}\psi(b,\xi)\varphi(b,\xi)\ , \tag{D43}$$

and the unit function

$$u(b,\xi)=1\ , \tag{D44}$$

then the coefficients $r_n^{(1)}$ can be written as

$$r_n^{(1)}(\alpha)=u\circ(\hat{K}^{n-1}u),\quad n\geq2\ . \tag{D45}$$

Note that $u\circ u=1$, so that if we define $\hat{K}^0$ to be the identity operator, this equation holds for $n=1$ as well.

Let us now define a function $\varphi(b,\xi)$ to be *even* if $\varphi(b,+)=\varphi(b,-)$, and *odd* if $\varphi(b,+)=-\varphi(b,-)$. It is easy to see that the subspaces of even and odd functions are invariant under $\hat{K}$, i.e., the action of $\hat{K}$ on an even (odd) function yields another even (odd) function. Since u is even, we can replace $\hat{K}$ by its restriction to the even subspace. The resulting operator is clearly symmetric. (Our numerical work, discussed below, strongly indicates that it is also positive definite, which is to be expected on physical grounds.) Let us denote its eigenvectors and eigenvalues by v_m and e_m, so that

$$\hat{K}v_m(\alpha)=e_m(\alpha)v_m(\alpha)\ . \tag{D46}$$

We choose the eigenfunctions to be normalized ($v_m\circ v_m=1$), and label them so that $e_1\geq e_2\geq e_3\ldots$. If we assume that the v_m's span the even subspace of $\hat{K}$,[101] we can write

$$r_n^{(1)}(\alpha)=\sum_{m=1}^{\infty}e_m^{n-1}(u\circ v_m)^2\ . \tag{D47}$$

[101]The operator $\hat{K}$ clearly possesses odd eigenfunctions as well, which we never need to find, since their projection on u vanishes.

It is now obvious that the sum in Eq. (D40) can be replaced by another sum of functions of λ, each one of which is associated with an eigenfunction of $\hat{K}$. If we define

$$A_m(\alpha)=(u\circ v_m)^2/e_m\ , \tag{D48}$$

then $\tilde{P}^{(1)}(\lambda)$ can be written as

$$\tilde{P}^{(1)}(\lambda)=\lambda^{-1}\left[1-\sum_m A_m\right]+\sum_m A_m(\lambda+e_m\lambda^{2\alpha-1})^{-1}\ . \tag{D49}$$

It remains to invert this equation to obtain $P^{(1)}(t)$. The first term obviously leads to a constant. The second term is seen by comparison with Eqs. (4.32) and (5.59) to be a sum of functions of exactly the same form as $P^{(0)}(t)$, i.e., effectively Mittag-Leffler functions [see Eq. (5.44)], the only difference being that there is a separate frequency associated with each function. The full form of $P^{(1)}(t)$ is thus seen to be (with $\Delta_{\rm eff}$ restored)

$$P^{(1)}(t)=\sum_m A_m(\alpha)\psi(\Delta_m t)+C\ , \tag{D50}$$

$$\Delta_m=\Delta_{\rm eff}[e_m(\alpha)]^{1/(2-2\alpha)}\ , \tag{D51}$$

$$C=1-\sum_m A_m\ . \tag{D52}$$

[The function $\psi(y)$, which is the Mittag-Leffler function apart from a factor $y^{2(1-\alpha)}$, is defined in Eq. (5.44).]

The constant C in Eq. (D50) is a nuisance, since it implies that $P(t)\not\to0$ as $t\to\infty$. On physical grounds this is very unlikely, and, indeed, our numerical work shows that C does vanish to the accuracy of our calculations (a little better than 1%). We do not have a rigorous demonstration of this, however, and a proof (or disproof) would be welcome. For the rest of this appendix, we shall assume that C vanishes.

We have evaluated the first few eigenvalues and eigenvectors of $\hat{K}$ numerically for several values of α. In Table III of the text we show $e_m(\alpha)$ and $A_m(\alpha)$ for $m=1,2$. (Details of our numerical work are given below.) In each

case the $m=2$ corrections amount to no more than a few percent. We do not show the values of e_m and A_m for $m>2$ because the A_m's are always smaller than A_2 by at least an order of magnitude, and so their contribution to $P^{(1)}(t)$ is utterly negligible for "reasonable" times that are not so long that $P(t)$ is negligibly small. Note that the numbers in the table are consistent with the requirement that corrections to $P^{(0)}(t)$ vanish as α^2 and $(1-2\alpha)$ in the limits $\alpha\to 0$ and $\alpha\to\frac{1}{2}$, respectively. In the first limit it is possible to do just a little better. Perturbation theory shows that

$$e_1(\alpha)=1+(\tfrac{2}{3}\pi^2-5)\alpha^2+O(\alpha^3)\ , \tag{D53}$$

which is consistent with the numerical results.

We show below that it is possible to treat further-neighbor interactions similarly and that when this is done the structure of Eq. (D50) continues to be valid except that the A_m and e_m are modified and C is replaced by a polynomial in $\Delta_m t$. Since we have not attempted a numerical evaluation of these quantities when second- or further-neighbor interactions are included, we describe here our numerical calculations for the nearest-neighbor interactions, i.e., for the entries in Table III. We convert the integral eigenvalue equation (D46) into a matrix equation by approximating the b integral using a Gauss-Laguerre quadrature. [This is a Gaussian quadrature based on the associated Laguerre polynomials, which are orthonormal with the inner product (D43). For a general discussion of Gaussian quadrature formulas based on an arbitrary system of orthonormal polynomials see Stoer and Bulirsch (1980) or Davis and Rabinowitz (1975).] The s integral appearing in the definition (D42) of $\hat{K}$ is evaluated by breaking it into two parts, from 0 to a suitable chosen value s_0, and from s_0 to ∞, and the two parts are approximated by a Gauss-Jacobi and yet another Gauss-Laguerre quadrature, respectively. The nodes and weights for all these quadratures are evaluated by using the efficient algorithm of Golub and Welsch (1969). By varying the number of quadrature points we estimate that the entries in Table III are accurate to better than a percent for all values of α, except those for e_2 and A_2, which may be off the mark by a few percent for the larger α values.

We finally note that it is straightforward to generalize the above formalism to take into account interactions up to lth neighbors. (Nearest neighbors correspond to $l=1$.) Using an obvious generalization of the notation, the coefficient $r_n^{(l)}(\alpha)$ is given by an equation identical to Eq. (D41), except that the second product in the integrand is replaced by

$$\prod_{k=1}^{n-1} e^{-s_k} \prod_{j=k+1}^{j_0} (P_{jk})^{2\alpha\xi_j\xi_k}\ , \tag{D54}$$

where $j_0=\max(n,k+l)$. The required generalization of the transfer operator is given by

$$\hat{K}[\varphi(\rho_l,\ldots,\rho_1)]=\psi(\rho_{l+1},\ldots,\rho_2)\equiv\frac{1}{2\Gamma(1-2\alpha)}\int d\rho_l\cdots\int d\rho_1\frac{e^{-(b_1+s_1)}}{b_1^{2\alpha}}\prod_{j=2}^{l+1}(P_{j1})^{2\alpha\xi_1\xi_j}\varphi\ , \tag{D55}$$

where ρ_j stands for the triple of variables $\{b_j,s_j,\zeta_j\}$, and $\int d\rho_j$ denotes an integral from 0 to ∞ with respect to b_j and s_j, and a sum on ζ_j. The inner product (D43) is generalized to

$$\psi\circ\varphi\equiv\frac{r_l^{-1}(\alpha)}{[2\Gamma(1-2\alpha)]^l}\int d\rho_l\cdots\int d\rho_1 e^{-(b_l+s_{l-1}+\cdots+s_1+b_1)}\prod_{j=1}^{l} b_j^{-2\alpha}\prod_{k=1}^{l-1}\prod_{j=k+1}^{l}(P_{jk})^{2\alpha\xi_j\xi_k}\psi\varphi\ . \tag{D56}$$

The factor $r_l^{-1}(\alpha)$ has been inserted here to ensure that the relation

$$u\circ u=1 \tag{D57}$$

continues to hold, where u is the generalized unit function.

It is now plain that if we can find a complete set of eigenvectors $v_m^{(l)}$ and eigenvalues $e_m^{(l)}$ of $\hat{K}$, we can write in analogy with Eqs. (D48)–(D52)

$$A_m^{(l)}(\alpha)=Q_l^{-1}(\alpha)[e_m^{(l)}]^l(v_m^{(l)}\circ u)^2\ , \tag{D58}$$

$$P(t)=\sum_{m=1}^{\infty}A_m^{(l)}\psi(\Delta_m^{(l)}t)+\Delta P^{(l)}(t)\ , \tag{D59}$$

$$\Delta_m^{(l)}=\Delta_{\rm eff}[e_m^{(l)}(\alpha)]^{1/(2-2\alpha)}\ , \tag{D60}$$

where $\Delta P^{(l)}(t)$ is a finite polynomial of the form

$$\Delta P^{(l)}(t)=\sum_{n=0}^{l-1}(-1)^n\left[\tilde{K}_n-\tilde{K}_n^{(0)}\sum_m(e_m^{(l)})^nA_m^{(l)}\right](\Delta_{\rm eff}t)^{2n(1-\alpha)}\ . \tag{D61}$$

We discuss briefly in Sec. V.E the question of whether or not the function $\Delta P^{(l)}(t)$ vanishes identically.

APPENDIX E: ASYMPTOTIC BEHAVIOR OF $P(t)$ IN THE NONINTERACTING-BLIP APPROXIMATION

In this appendix we show that, within the noninteracting-blip approximation, $P(t)$ approaches $-\tanh(\varepsilon/2k_BT)$ as $t\to\infty$, regardless of the spectral density $J(\omega)$. From Sec. VII, Eq. (7.6), we have that within this approximation

$$P(t=\infty)=-h_0/g_0\ , \tag{E1}$$

where g_0 and h_0, defined in Eq. (7.7), are given by

$$g_0=\frac{\Delta^2}{2}\int_{-\infty}^{\infty}dt\cos(\varepsilon t/\hbar)\cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ , \tag{E2}$$

$$h_0=\frac{\Delta^2}{2}\int_{-\infty}^{\infty}dt\sin(\varepsilon t/\hbar)\sin\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]\exp\left[-\frac{q_0^2}{\pi\hbar}Q_2(t)\right]\ . \tag{E3}$$

It is convenient to introduce a function of $G(t)$,

$$\begin{aligned}G(t)&\equiv\frac{q_0^2}{\pi\hbar}[Q_2(t)+iQ_1(t)]\\&=\frac{q_0^2}{\pi\hbar}\int_0^{\infty}d\omega\frac{J(\omega)}{\omega^2}[(1-\cos\omega t)\coth(\beta\hbar\omega/2)+i\sin\omega t]\ ,\end{aligned} \tag{E4}$$

where the second line follows directly from the definitions of Q_1 and Q_2 in Eq. (4.22). One can verify from Eq. (E4) that $G(t)$ satisfies the relations

$$G(t-i\beta\hbar)=G^*(t)=G(-t)\ . \tag{E5}$$

Using Eq. (E5), we can express g_0 in (E2) as an integral over $G(t)$ and

$$g_0=\frac{\Delta^2}{4}\int_{-\infty}^{\infty}dt\,e^{i\varepsilon t/\hbar}[e^{-G(t)}+e^{-G(t-i\beta\hbar)}]\ . \tag{E6}$$

Since $G(t)$ is analytic in the strip $-i\beta\hbar\le\mathrm{Im}\,t\le 0$ [from Eq. (E4)], the integration contour in the second integral in Eq. (E6) can be shifted, giving

$$g_0=\frac{I\Delta^2}{4}(1+e^{-\beta\varepsilon})\ , \tag{E7}$$

with the definition

$$I=\int_{-\infty}^{\infty}dt\exp[i\varepsilon t/\hbar-G(t)]\ . \tag{E8}$$

The same analysis for h_0 gives

$$h_0=\frac{I\Delta^2}{4}(1-e^{-\beta\varepsilon})\ , \tag{E9}$$

so that

$$P(t=\infty)\equiv-h_0/g_0=-\tanh(\varepsilon/2k_BT)\ . \tag{E10}$$

APPENDIX F: SOME LEADS INTO THE LITERATURE OF THE TWO-STATE PROBLEM AND RELATED TOPICS

The number of papers in the literature on the thermodynamics and dynamics of a system described by the Hamiltonian (1.4), or minor variants of it, certainly runs into many hundreds and probably thousands. Within this vast literature different "citation traditions" have grown up, depending on the context in which the problem is considered (quantum optics, chemical physics, polaron theory, etc.). To help the reader gain some idea of the variety of applications of this problem, and the many different lines of approach to it that have been explored, we list below in no particular order a few papers, mostly recent ones, that are both of interest in their own right and give useful references to various areas of the literature, with some indication of the principal emphasis of each. Note that not all of these papers restrict themselves to the limit $\Delta/\omega_c\to 0$ studied in this paper. We also give a few references on related topics, in particular, some relevant to Sec. II and Appendix A of this paper. We emphasize that the papers cited are often not the first, historically, to develop the approach in question, but earlier work can be traced through them.

1. The two-state system—thermodynamics

Carmeli, B., and D. Chandler, 1985, J. Chem. Phys. **82**, 3400 (variational and computational approaches).

Jongeward, G. A., and P. G. Wolynes, 1983, J. Chem. Phys. **79**, 3517 (path-integral methods).

Spohn, H., and R. Dümcke, 1985, J. Stat. Phys. **41**, 389 (rigorous results).

2. The two-state system—dynamics

Aslangul, C., N. Pottier, and D. Saint-James, 1986, J. Phys. (Paris), **47**, 1657 (generalized relaxation theory).

Beck, R., W. Götze, and P. Prelovsek, 1979, Phys. Rev. A **20**, 1140 (mode-coupling approach to ohmic case, but with $\Delta/\omega_c\gg 1$).

Becker, K. W., and J. Keller, 1986, Z. Phys. B **62**, 477 (methods from metal physics).

Behrman, E. C., G. A. Jongeward, and P. G. Wolynes, 1983, J. Chem. Phys. **79**, 6277 (path-integral methods).

Behrman, E. C., G. A. Jongeward, and P. G. Wolynes, 1985, J. Chem. Phys. **83**, 668 (variational and computational methods).

Bialek, W. S., 1983, Ph.D. thesis, University of California, Berkeley (biophysical applications).

de Raedt, B., and H. de Raedt, 1984, Phys. Rev. B **29**, 5325 (computational).

Harris, R. A., and L. Stodolsky, 1981, J. Chem. Phys. **74**, 2145 (Bloch equations, weak coupling approach).

Maleev, S. V., 1980, Zh. Eksp. Teor. Fiz. **79**, 1995 [Sov. Phys. JETP **52**, 1008 (1980)] (diagrammatic techniques).

Silbey, R. A., and R. A. Harris, 1984, J. Chem. Phys. **80**, 2615 (ohmic case, variational methods).

Wagner, M., 1985, J. Phys. A **18**, 1915 (phonon-assisted transport).

3. Related topics

Chandler, D., and P. G. Wolynes, 1981, J. Chem. Phys. **74**, 4078 (path-integral methods for general problem of quantum system in condensed phase).

Graham, R., and M. Höhnerbach, 1984, Z. Phys. B **57**, 233 (approximation schemes for single-mode model).

Hänggi, P., 1986, J. Stat. Phys. **42**, 105 (tunneling out of metastable well—review).

Joos, E., and H. D. Zeh, 1985, Z. Phys. B **59**, 223 (quantum measurement theory).

Kagan, Yu., and N. V. Prokof'ev, 1986, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 434 [JETP Lett. **43**, 558 (1986)] (general considerations on tunneling and coherence in the presence of dissipation).

Klinger, M. I., 1983, Phys. Rep. **94**, 183 (quantum diffusion in solids).

Schmid, A., 1986, Ann. Phys. (N.Y.), in press (many-dimensional WKB problem; cf. H. J. de Vega, B. L. Gervais, and B. Sakita, 1979, Phys. Rev. D **19**, 604).

Zinn-Justin, J., 1983, Nucl. Phys. B **218**, 333 (instanton methods).

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