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Random-Matrix Model for Dissipative Two-Level Systems

Pedro Pereyra[1]

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Assuming a random-matrix model for the system–bath interaction and using a series expansion for the evolution operator, we studied the relaxation of a non-degenerate two-level system. For times larger than the duration of a collision and smaller than the Poincaré recurrence time, we calculate the survival probability of still finding the system, at time t, in the same state in which it was prepared at $t=0$. For a fixed initial state of the bath, we obtain an exponential transition rate, but when we average over initial states we may get a mixture of decay constants that could distroy the exponential behavior of the transition rate.

KEY WORDS: Quantum relaxation processes; random-matrix theory.

1. INTRODUCTION

One can easily find many physical and chemical systems whose dynamics can be studied by means of two-state models[1–7] where, for a realistic description, an interaction with the environment (heat bath, radiation field, etc.) should be considered. It turns out that the time evolution of two-level systems is substantially modified by such an interaction. Some real systems are intrinsically two-state systems, i.e., they possess a discrete degree of freedom that can take only two values (spin-1/2 particles, photon polarization, etc.). Other systems possess a continuous degree of freedom q, whose dynamics can be described by using a potential energy function $V(q)$ with two separate minima (paraelectric resonance relaxation, stabilization of handed molecules, molecular polarons, tunneling, etc.). Although a complete solution for the dissipative two-level systems seems rather difficult, there is an increasing interest in these problems and significant

[1] Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, 02200 Mexico, D.F., Mexico.

822/65/3-4-23

progress has been achieved. It is usual to consider Hamiltonians with the structure

$$H = H_S + H_E + H_I \tag{1}$$

where H_S describes the isolated two-state system, H_E describes the environment, and H_I the system–environment interaction. One of the well-known Hamiltonians of this kind that has been extensively studied in the literature is the "spin-boson" Hamiltonian[4]

$$H = -\frac{1}{2}\hbar\Delta_0\sigma_x + \frac{1}{2}\varepsilon\sigma_z + \sum_\alpha \left(\frac{1}{2}m_\alpha\omega_\alpha x_\alpha^2 + \frac{p_\alpha^2}{2m_\alpha}\right) + \frac{1}{2}q_0\sigma_z\sum_\alpha C_\alpha x_\alpha \tag{2}$$

Here the isolated two-state system is completely described by the first two terms. The set of harmonic oscillators in the third term represents the bath and the last term represents the system–bath interaction. The physical meaning of the first two terms can be found with the help of a potential energy function $V(q)$ with two separate minima. Legget *et al.* discuss this case and show that the double-well system is effectively described by the Hamiltonian in Eq. (2) if the barrier height V_0 is large compared to $\hbar\omega_R$ and $\hbar\omega_L$ (where ω_R and ω_L are the classical small-oscillation frequencies in the right and left well, respectively) and the bias ("detuning") ε between the ground states is small compared to ω_R and ω_L. When the basis is chosen so that the eigenstate $|\psi_R\rangle$ ($|\psi_L\rangle$) of σ_z with eigenvalue $+1$ (-1) corresponds to the system localized in the right (left) well, the term $(1/2)\,\varepsilon\sigma_x$ represents the difference in the ground-state energies, while the term $(1/2)\,\hbar\Delta_0\sigma_x$ describes the tunneling between the wells. For many cases of practical interest, one can just consider that $\varepsilon = 0$. An alternative interpretation for the first two terms in Eq. (2) is that they represent a particle of spin 1/2 in the magnetic field $H = -\varepsilon\hat{\mathbf{k}} + \hbar\Delta_0\hat{\mathbf{i}}$. One of the quantities that has been calculated by Legget *et al.* is the expectation value of σ_z as a function of t.

Another well-known Hamiltonian is the "rotating-wave" Hamiltonian used in quantum optics to describe the rate process of a two-state atom interacting with a radiation field. In a fictitious spin-1/2 representation, the rotating-wave Hamiltonian is obtained as an approximation of the so-called "dressed-atom" Hamiltonian of the form[6]

$$H = \frac{1}{2}\omega_0\sigma_z + \omega_L\sum_\alpha a_\alpha^+ a_\alpha + \frac{\lambda}{2}\sigma_x\sum_\alpha (a_\alpha + a_\alpha^+) \tag{3}$$

There is no difference at all between (2), with $\varepsilon = 0$, and (3) if in the last case the basis is chosen so that the eigenstates $|\varphi_R\rangle$ ($|\varphi_L\rangle$) of σ_x with eigenvalues $+1$ (-1) correspond to the system localized in the right (left) well. However, if the basis is chosen so that the eigenstates $|1\rangle$ ($|-1\rangle$) of σ_z correspond to the system localized in the right (left) well, the quantity $\langle\sigma_z\rangle_{r\omega}$ calculated with the rotating-wave Hamiltonian does not have the same physical meaning as $\langle\sigma_z\rangle_{sb}$ calculated using the spin-boson Hamiltonian. While $\langle\sigma_z\rangle_{sb}$ is associated with the tunneling process, $\langle\sigma_z\rangle_{r\omega}$ is related to the spin-flip process induced by the interaction with the bath.

In the relaxation problems, the process is frequently found to be insensitive to the details of the interaction, only a few "gross properties" being relevant for its description. This feature is not new in many-body problems, and has often been explicitly described by constructing a collection or ensemble of interactions[7] and calculating an ensemble average of the quantity of interest: if that quantity does not vary appreciably across the ensemble, it can be reasonably represented by its average; if that were not the case, one could certainly calculate the fluctuations of the given quantity across the ensemble. This philosophy has been implemented in the study of the relaxation of a degenerate two-level system interacting with a bath.[8] The purpose of the present paper is to extend the calculations of ref. 8 to the case where one also has a Hamiltonian term associated with the two-level system. The total Hamiltonian of the problem is given as

$$H = \frac{1}{2}\Delta_0\sigma_z + H_B + \sigma_x V \tag{4}$$

The first term describes the dynamics of the isolated two-level system and can be interpreted as the energy of a spin-1/2 particle in the magnetic field $H = (1/2)\Delta_0\hat{\mathbf{k}}$. The third term represents the system–bath interaction, where V depends only on the bath variables, and H_B is the bath Hamiltonian.

Suppose that at $t < 0$ we prepare the system in an eigenstate of σ_z, say $|1\rangle$, while the bath is in thermal equilibrium, and that at $t = 0$ we switch on the interaction. Since $\sigma_x V$ induces transitions between the two eigenstates of σ_z, the system will evolve according to the Hamiltonian in Eq. (4); we therefore pose the problem of calculating the probability of still finding the system in state $|1\rangle$ at time $t > 0$. We shall be able to show that, for $\beta\Delta_0 \ll 1$, this problem can be solved, when the time t satisfies the inequalities

$$t_{\text{coll}} \ll t \ll t_p \tag{5}$$

t_{coll} and t_p being times on the order of the duration of a collision (to be distinguished from the time between collisions!) and of the Poincaré recurrence time, respectively. The procedure, inspired by the one followed in ref. 9 to describe relaxation phenomena in nuclear physics, essentially consists in writing the above-mentioned probability as a series expansion in powers of the interaction, averaging term by term and then summing up the full series. It turns out that for a fixed initial state of the bath, the sum converges into an exponential function. As will be seen later, this exponential behavior for the transition rate would be, in general, destroyed when we average over the initial states.

The evolution of quantum systems to statistical equilibrium has also been studied from the point of view of the theory of transport equations.[10,11] A master equation for the probability of finding the system in a state or groups of stationary states of the unperturbed part of the Hamiltonian was derived by van Hove.[11] In his approach, the perturbative part is responsible for the dissipative behavior. Although we are not concerned with a perturbative procedure and from our calculation we do not obtain a differential equation for the just mentioned probability, we should point out that there are some similarities between our procedure and the one followed by van Hove. We also work in the interaction representation and make use of an expansion for the evolution operator. A useful and common assumption is the high density of levels. The special properties introduced by van Hove for the matrix elements of the perturbative term are, in some sense, equivalent to the statistical properties introduced through our random-matrix model.

Assumptions on a phenomenological, random, time-dependent interaction are sometimes made in relaxations studies.[12–16] In the present paper such assumptions are not needed, because we work with the full, time-independent Hamiltonian, and any time dependence should come out as a consequence of the model. We remark, incidentally, that the randomness assumed for such a time-dependent interaction has an entirely different origin from the one considered in the present article, since in standard statistical mechanical problems it is taken for granted that there exists *one* total Hamiltonian for the full problem, and not an ensemble of Hamiltonians as we consider here.

The paper is organized as follows. In Section 2 we define with more precision the random-matrix model outlined above and we write the survival probability as a power series. In order to illustrate the calculation procedure, in Section 3 we evaluate in detail some representative terms for which we also give a graphical interpretation, which becomes advantageous for the evaluation of the most general term. The full series is summed up, giving rise to the astonishingly simple final result of Eq. (43) for the

survival probability. Some features of our results are discussed in Section 4 and conclusions are given in Section 5.

2. THE SURVIVAL PROBABILITY AND THE RANDOM-MATRIX MODEL

Before we discuss the assumptions on the random interaction, let us introduce the notation and write out the physical quantity that we are going to calculate. The eigenstate of σ_z with eigenvalue α is denoted by $|\alpha\rangle$, i.e.,

$$\sigma_z |\alpha\rangle = \alpha |\alpha\rangle, \qquad \alpha = \pm 1 \tag{6}$$

We denote by $|a\rangle$ the eigenstate of the bath Hamiltonian with eigenvalue ε_a, i.e.,

$$H_B |a\rangle = \varepsilon_a |a\rangle \tag{7}$$

The states $|a\alpha\rangle$ form a complete set of states for the system–bath combination, which we assume is governed by the Hamiltonian

$$H = \frac{1}{2} \Delta_0 \sigma_z + H_B + \sigma_x V \tag{8}$$

Let us consider that at $t < 0$ the system is held in the state $|1\rangle$ and the bath is in thermal equilibrium, described by the canonical ensemble

$$p_{a_i} = \frac{1}{Z} e^{-\beta \varepsilon_{a_i}} \tag{9}$$

where Z is the bath partition function. At $t = 0$ the system–bath interaction is switched on, inducing transitions between the two eigenstates of σ_z. The probability $P_{1 \to 1}(t)$ that at a time $t > 0$ we still find the system in the state $|1\rangle$, regardless of the state of the bath, is given by ($\hbar = 1$)

$$P_{1 \to 1}(t) = \sum_{a_i, a} p_{a_i} |\langle 1a| e^{-iHt} |1a_i\rangle|^2 \tag{10}$$

As mentioned before, we are going to simulate the complicated system–bath interaction by introducing an ensemble of interactions and calculating the ensemble average of our quantity of interest, i.e., the ensemble average of $P_{1 \to 1}(t)$. For this pourpose we will first write out

the survival probability as a series in powers of the interaction H_I. In the interaction representation we expand the evolution operator as

$$e^{-iHt} = e^{-iH_0 t} \sum_{n=0} (-i)^n \int_0^t dt_n\, H_I(t_n) \times \int_0^{t_n} dt_{n-1}\, H_I(t_{n-1}) \cdots \int_0^{t_2} dt_1\, H_I(t_1) \tag{11}$$

where H_0 represents the first two terms of Eq. (4) and

$$\begin{aligned} H_I(t) &= e^{iH_0 t} H_I e^{-iH_0 t} \\ &= e^{iH_B t} V e^{-iH_B t} (\sigma_x \cos \Delta_0 t - \sigma_y \sin \Delta_0 t) \\ &= \sum_{b_j, b_{j+1}} |b_j\rangle\, e^{i\varepsilon_{b_j} t} \langle b_j|\, V\, |b_{j+1}\rangle\, e^{-i\varepsilon_{b_{j+1}} t} \langle b_{j+1}| \\ &\quad \times (\sigma_x \cos \Delta_0 t - \sigma_y \sin \Delta_0 t) \end{aligned} \tag{12}$$

Because of σ_x and σ_y in (12), only the even-order terms contribute to (11). Thus, the survival probability takes the form

$$\begin{aligned} P_{1\to 1}(t) &= \sum_{a_i} p_{a_i} \sum_{p,q=0} (-)^{p+q} \int_0^t dt_{2p} \\ &\quad \times \int_0^{t_{2p}} dt_{2p-1} \cdots \int_0^{t_2} dt_1 \int_0^t dt'_{2q} \cdots \int_0^{t'_2} dt'_1 \\ &\quad \times \sum_{\substack{a, b_1, b_2, \ldots, b_{2p-1} \\ b'_1, b'_2, \ldots, b'_{2q-1}}} V_{a_i b_1} V_{b_1 b_2} \cdots V_{b_{2p-1} a} V_{a b'_{2q-1}} \cdots V_{b'_2 b'_1} V_{b'_1 a_i} \\ &\quad \times \exp\{i[(\varepsilon_{a_i} - \varepsilon_{b_1})\, t_1 + \cdots + (\varepsilon_{b_{2p-1}} - \varepsilon_a)\, t_{2p} \\ &\quad + (\varepsilon_a - \varepsilon_{b'_{2q-1}})\, t'_{2q} + \cdots + (\varepsilon_{b'_1} - \varepsilon_{a_i})\, t'_1]\} \\ &\quad \times \exp\{-i\Delta_0[t_1 - t_2 + t_3 - \cdots - t_{2p} + t'_{2q} - t'_{2q-1} + \cdots + t'_2 - t'_1]\} \\ &= \sum_{a_i} p_{a_i} \sum_{p,q} P_{1\to 1}^{(p,q)}(t, a_i) \end{aligned} \tag{13}$$

which depends on the matrix elements of the system–bath interaction and expresses the survival probability as a sum of contributions coming from the various initial states a_i and the values taken by the variables p and q; the (p, q) term is of order $2p + 2q$.

We shall now be more specific about the random-matrix model assumed for V. We propose a *local* GOE (Gaussian orthogonal ensemble),[8] an extension (used in ref. 9) of the standard GOE.[7] The matrix

elements V_{ab} of the operator V, in the basis defined by (7), are assumed to form a *real symmetric* matrix and to be considered as *statistically independent Gaussian variables* with zero mean and covariance given by

$$\langle V_{ab} V_{cd} \rangle = v_a^2(\varepsilon_{ab})(\delta_{ad}\delta_{bc} + \delta_{ac}\delta_{bd})\, \omega_{\Delta_a}(\varepsilon_a - \varepsilon_b) \tag{14}$$

the angular brackets denoting an ensemble average. The only nonzero covariance is that of V_{ab} with itself, or with V_{ba}. This property represents here what the special properties for the matrix elements of the perturbative term represent in the calculation of van Hove. The quantity $\varepsilon_{ab} = (\varepsilon_a + \varepsilon_b)/2$ is the centroid of the two energies ε_a and ε_b. The weight factor $\omega_{\Delta_a}(\varepsilon_a - \varepsilon_b)$ is assumed to be a Lorentzian function of width Δ_a, thus indicating that the interaction V connects eigenstates of H_B within an energy interval $\sim \Delta_a$. We can thus visualize the matrix $\|V_{ab}\|$ as having appreciable elements inside a band of variable width $2\Delta_a$ along the diagonal. The quantity

$$t_{\text{coll}} \sim \frac{1}{\Delta_a} \tag{15}$$

is a time associated with one application of the interaction, and has been interpreted as the duration of a collision.[8,9]

In the limit of a large bath with a high density of levels, we shall always assume that Δ_a contains many bath levels, and we shall allow for the possibility of a slow dependence of Δ_a on the bath energy ε_a. A slow dependence on ε_a of the strength of the interaction v_a^2 and of the density ρ may also occur.

We shall frequently encounter in what follows the quantity $\langle V_{ab}^2 \rangle \rho(\varepsilon_b)$, where $\rho(\varepsilon)$ denotes the density of bath states. Using (14) and defining the quantity

$$\Gamma_a = 4\pi v_a^2 \rho(\varepsilon_a) \tag{16}$$

we write $\langle V_{ab}^2 \rangle \rho(\varepsilon_b)$ as

$$\langle V_{ab}^2 \rangle \rho(\varepsilon_b) = \Gamma_a \omega_{\Delta_a} \tag{17}$$

If as we said before, the dependence on the energy of v_a^2, ρ, and Δ_a is so slow that the quantities can be taken essentially constant inside the interval where ω_{Δ_a} is nonzero; we can then write $\Gamma_a \approx \Gamma_b \approx \Gamma$ and $\Delta_a \approx \Delta_b \approx \Delta$. This will be useful later. This assumption of slow dependence on the energy leads us to consider the significance of the implicit approximation. To first order of the transferred energy we have

$$\ln \rho(\varepsilon_a) \simeq \ln \rho(\varepsilon_b) + \frac{\partial \ln \rho(\varepsilon_b)}{\partial \varepsilon_a} (\varepsilon_a - \varepsilon_b)$$

Considering that, for almost constant total energy, $\varepsilon_a - \varepsilon_b \simeq \Delta_0$, the approximation $\ln \rho(\varepsilon_a) \simeq \ln \rho(\varepsilon_b)$ will hold if $\beta\Delta_0 \ll 1$.

Once we have defined the random matrix model, the next task is to calculate the ensemble average of the survival probability $P(t)$ of Eq. (13), which can then be written as a sum over the various a_i, p, q contributions as

$$\langle P_{1\to 1}(t)\rangle = \sum_{a_i} p_{a_i} \sum_{p,q=0}^{\infty} \langle P_{1\to 1}^{(p,q)}(t, a_i)\rangle$$

$$\equiv \sum_{a_i} p_{a_i} \langle P_{1\to 1}^{a_i}(t)\rangle \tag{18}$$

where each contribution satisfies the relation

$$\langle P_{1\to 1}^{(p,q)}(t, a_i)\rangle = \langle P_{1\to 1}^{(q,p)}(t, a_i)\rangle^* \tag{19}$$

In the next section we calculate the ensemble average of the different (p, q) terms. For fixed initial bath state we will be able to sum the whole series and so obtain an astonishingly simple functional form for the quantity $\langle P_{1\to 1}^{a_i}(t)\rangle$, which is just the survival probability for a given initial state. To obtain the final result, we will calculate the average over the initial states of the bath.

3. THE ENSEMBLE AVERAGE OF THE SURVIVAL PROBABILITY

As an illustration, we calculate in detail some representative terms in the expansion (18). It will then be easy to infer the general values and apply them to the calculation of the survival probability.

3.1. Some Particular Terms in the Expansion (18)

1. *The term* $(p=0, q=0)$. In this case we just have

$$\langle P_{1\to 1}^{(0,0)}(t)\rangle = 1 \tag{20}$$

2. *The term* $(p=1, q=0)$. From (13) we have

$$\langle P_{1\to 1}^{(1,0)}(t, a_i)\rangle = \int_0^t dt_2 \int_0^{t_2} dt_1$$

$$\times \left\{ \exp[i\Delta_0(t_2 - t_1)] \sum_{b_1} \langle V_{a_i,b_1}^2 \rangle \exp[i(\varepsilon_{b_1} - \varepsilon_{a_i})(t_2 - t_1)] \right\} \tag{21}$$

We now concentrate on the calculation of the quantity in wavy brackets, which, as we shall see, appears systematically in the more complicated terms. The sum over b_1 can be replaced by an integral if the exponential varies only negligibly from one level ε_{b_1} to the next; for this to happen, one needs times such that

$$Dt \ll 1 \tag{22a}$$

where D is the mean level spacing. If $1/D$ is interpreted as the Poincaré recurrence time t_p, we thus need

$$t \ll t_p \tag{22b}$$

which is certainly satisfied. We shall neglect the fact that for the single term $a_i = b_1$, $\langle V^2_{a_i b_1} \rangle$ is twice as big as for an off-diagonal term [see Eq. (14)]; it can be easily checked that the relative error that we make is of the order of $t/\rho(\varepsilon_i) \sim t/t_p$, which is negligible. We thus use (17) and the comment made right after that equation to write ($\tau \equiv t_2 - t_1$)

$$\begin{aligned} &\sum_{b_1} \langle V^2_{a_i, b_1} \rangle \exp[i(\varepsilon_{b_1} - \varepsilon_{a_i})\tau] \\ &\quad = v^2_{a_i} \rho(\varepsilon_{a_i}) \int_0^\infty \omega_\Delta(\varepsilon_{a_i} - \varepsilon_{b_1}) \exp[i(\varepsilon_{b_1} - \varepsilon_{a_i})\tau] \, d\varepsilon_{b_1} \\ &\quad = \frac{\Gamma_{a_i}}{4\pi} \int \omega_\Delta(x) \exp(ix\tau) \, dx \equiv \frac{\Gamma_{a_i}}{4\pi} \tilde{\omega}(\tau) \end{aligned} \tag{23}$$

We shall consider initial bath states a_i such that the full energy interval $\varepsilon_{a_i} \pm \Delta$, to which they are connected by the interaction, is not cut out by the lower bound of the spectrum; for a given temperature, we shall assume that the relevant ε_{a_i} fulfill this condition; our analysis would thus be valid above a certain minimum temperature T_0 (depending on the specific structure of the matrix V), in order to avoid any "threshold effect." At variance with the degenerate case of ref. 8, we shall see that above T_0 the result does depend on Δ. Under these conditions, $\tilde{\omega}(\tau)$ of Eq. (23) is real, symmetric in τ, appreciable only inside the interval $\Delta\tau \sim 1/\Delta$, and has the property

$$\int_{-\infty}^{\infty} \tilde{\omega}(\tau) \, d\tau = \pi\omega(0) \tag{24}$$

We recall that $\tilde{\omega}(\tau)$ has to be used inside the time integral of Eq. (21). Therefore, for times much larger than $1/\Delta$ [which was interpreted in

Eq. (15) as the duration of a collision], $\tilde{\omega}(\tau)$ behaves like a δ-function and we can write

$$\exp(\mp i\Delta_0\tau)\sum_{b_1}\langle V^2_{a_i,b_1}\rangle \exp[i(\varepsilon_{a_i}-\varepsilon_a)\tau] = \frac{\Delta}{\Delta \pm i\Delta_0}\,\Gamma(\varepsilon_{a_i})\,\delta(\tau) \tag{25}$$

To summarize, the times involved in the problem are assumed to fulfill the inequalities

$$t_{\text{coll}} \ll t \ll t_p \tag{26}$$

We thus get, for the (1, 0) term of (21), the expression

$$\langle P^{(1,0)}_{1\to 1}(t, a_i)\rangle = -\frac{\Gamma_{a_i}}{2}\frac{t\Delta}{2(\Delta - i\Delta_0)} \tag{27}$$

the last factor 1/2 arising from the fact that the t_1 integration in (21) goes only up to t_2, thus covering "half of the δ-function."

In preparation for the analysis of the more complicated terms, we use, as in ref. 8, a graphical representation for the term we have just calculated. In Fig. 1 and the following ones, we have indicated two time intervals, from 0 to t, which should contain, respectively, the $2p$ and $2q$ ordered time variables of Eq. (13). In the present case, Eq. (21) just contains t_1 and t_2, which have been indicated in Fig. 1. The line joining them, to be called a *contraction*, indicates the ensemble average of the two corresponding V's [remember that in Eq. (11) every t_i has an $H_I(t_i)$ associated with it]. It is clear that our result (27) can be written at once from the diagram, by following the rules:

(a) Assign to the contraction a factor $\Gamma_{a_i}/2$.

(b) Assign to the contraction an extra factor 1/2, whose origin is explained right after Eq. (27).

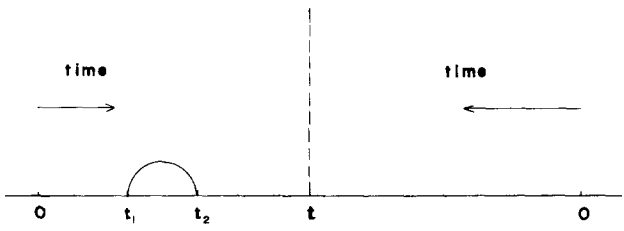

Fig. 1. Graphical representation of the $(p = 1,\ q = 0) = (1, 0)$ term of Eq. (21).

(c) The two times t_1 and t_2 are reduced to a single one [due to the δ-function (25)], to be integrated from 0 to t; that integration gives a factor $t\Delta/(\Delta - i\Delta_0)$.

Finally, we see from Eq. (19) that the $(p=0,\ q=1)$ term gives a contribution which is the complex conjugate of (27), so that, to *first order*, *we have*

$$\langle P^{a_i}_{1\to 1}(t)\rangle = 1 - \frac{\Gamma_{a_i}}{2}\frac{\Delta^2 t}{\Delta^2+\Delta_0^2} + \cdots \tag{28}$$

and

$$\langle P^{a_i}_{1\to -1}(t)\rangle = \frac{\Gamma_{a_i}}{2}\frac{\Delta^2 t}{\Delta^2+\Delta_0^2} + \cdots \tag{29}$$

Result (29) coincides with that obtained from the "golden rule" of quantum mechanics,[17] where a restriction on time similar to (26) also appears, the role of Δ being played by the energy interval over which $V^2_{a_i a}$ varies appreciably. The structure of the matrix V, which is not required to obtain the golden rule, turns out to be very useful in the evaluation of the higher-order terms of the series, as we shall see.

3. *The higher-order terms.* These terms will be calculated using a well-known theorem of statistics[7–9]: in order to calculate the average of a product of zero-centered Gaussian variables, one contracts those variables in pairs and sums over all possible pair-contraction patterns.

As an example, the (1, 1) term involves the three diagrams shown in Fig. 2. We shall need the relation

$$\langle V_{ab} V_{bc}\rangle = \langle V^2_{ab}\rangle \delta_{ac} \tag{30}$$

which is a consequence of the basic assumption (14).

Using (30), we can write diagram A as

$$\begin{aligned}
&\langle P^{(1,1)}_{1\to 1}(t, a_i)\rangle_A \\
&\quad = \int_0^t dt_2 \int_0^{t_2} dt_1 \int_0^t dt'_2 \int_0^{t'_2} dt'_1 \\
&\qquad \times \left\{ \exp[i\Delta_0(t_2 - t_1)] \sum_{b_1} \langle V^2_{a_i, b_1}\rangle \exp[i(\varepsilon_{b_1} - \varepsilon_{a_i})(t_2 - t_1)] \right\} \\
&\qquad \times \left\{ \exp[-i\Delta_0(t'_2 - t'_1)] \sum_{b'_1} \langle V^2_{a_i b'_1}\rangle \exp[-i(\varepsilon_{b'_1} - \varepsilon_{a_i})(t'_2 - t'_1)] \right\}
\end{aligned} \tag{31}$$

which shows that the basic block of Eq. (25) makes its appearance again. We thus apply to each contraction the rules found above to write

$$\langle P_{1\to 1}^{(1,1)}(t, a_i)\rangle_A = \left(\frac{\Gamma_{a_i}}{2}\right)^2 \frac{\Delta^2 t^2}{2^2}\left(\frac{1}{\Delta + i\Delta_0}\right)\left(\frac{1}{\Delta - i\Delta_0}\right) \tag{32}$$

Diagram B involves *cross contractions*, i.e., contractions that cross the dashed line. Using (30), one can see that the block (25) occurs again. This will be a common feature of all the remaining terms! Rules (a) and (b) above are valid for any contraction. The rule (c) is now the following: due to the δ-functions of (24), $t_1' = t_1$ and $t_2' = t_2$, so that we have *two ordered times*, t_1 and t_2, to be integrated from 0 to t, giving

$$(t^2/2)[(\Delta/(\Delta + i\Delta_0)) + (\Delta/(\Delta - i\Delta_0))]^2$$

The result is thus

$$\langle P_{1\to 1}^{(1,1)}(t, a_i)\rangle_B = \left(\frac{\Gamma_{a_i}}{2}\right)^2 \frac{\Delta^2 t^2}{2^2 \cdot 2}\left(\frac{2\Delta}{\Delta^2 + \Delta_0^2}\right)^2 \tag{33}$$

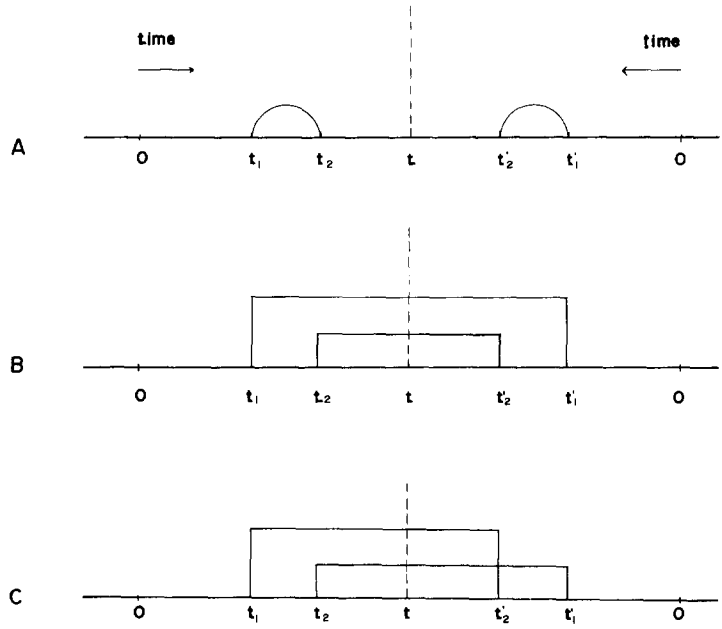

Fig. 2. The three diagrams arising from the $(p = 1,\ q = 1) = (1, 1)$ term in the expansion of Eqs. (13) and (18).

This shows that the rule (c) assigns a factor $(\Delta/(\Delta - i\Delta_0))$ or $(\Delta/(\Delta + i\Delta_0))$ for each non-cross-contraction, depending upon whether it contracts t_i with t_{i+1} or t_1' with t_{i+1}', and a factor $[(\Delta/(\Delta + i\Delta_0)) + (\Delta/(\Delta - i\Delta_0))]$ for each cross-contraction.

Diagram C involves the special feature of *crossing lines, which,* due to the basic assumption (14), kill one summation, in comparison with diagrams A and B; its contribution can be easily seen to be of order $t/\rho(\varepsilon_{a_i}) \sim t/t_p$, relative to A or B, and hence negligible. The fact that *contractions with crossing lines are negligible* is a well-known rule.[7-9]

4. *The term* (2, 0). This term gives rise to the three diagrams of Fig. 3. For diagram A we apply rules (a) and (b) above and then realize that we are left with two ordered times to be integrated from 0 to t, giving $(t^2/2!)(\Delta/(\Delta - i\Delta_0))^2$. The result is then

$$\langle P_{1\to 1}^{(2,0)}(t, a_i)\rangle_A = \left(\frac{\Gamma_{a_i}}{2}\right)^2 \frac{\Delta^2 t^2}{2^2 \cdot 2!}\left(\frac{1}{\Delta - i\Delta_0}\right)^2 \tag{34}$$

Diagram B does not contribute, because the time ordering, in addition to the δ-functions that occur, annihilates the integration domain. We thus find the rule that *non-cross-contractions can only be contiguous.*

Finally, diagram C is negligible because it involves intersecting lines.

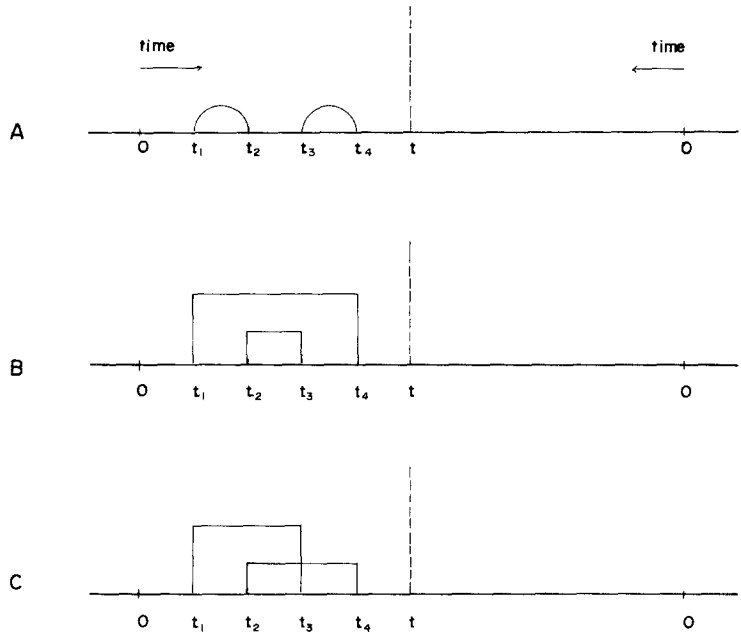

Fig. 3. The three diagrams arising from the (4, 0) term in the expansions (13) and (18).

5. *The term* $(p, 0)$. From the above considerations, the only diagram that contributes to the term $(p, 0)$ contains p contiguous non-cross-contractions, or "bubbles," thus giving

$$\langle P_{1\to 1}^{(p,0)}(t, a_i)\rangle = (-)^p \left(\frac{\Gamma_{a_i}}{2}\right)^p \frac{t^p}{2^p p!} \left(\frac{\Delta}{\Delta - i\Delta_0}\right)^p \tag{35}$$

6. *The term* $(p=2, q=2)$. We consider the two diagrams of Fig. 4, taken from those that contribute to this term.

Diagram A. From rules (a) and (b) above, we have the following contributions:

$$4 \text{ contractions} \Rightarrow \left(\frac{\Gamma_{a_i}}{2}\right)^4 \frac{1}{2^4}$$

The equivalent of rule (c) is now the following: due to the cross contractions we get δ-functions that can be used to eliminate t_1' and t_2', setting them equal to t_3 and t_4, respectively, and bringing them to the LHS of the diagram; we also have $t_3' = t_4'$, which can again be brought to the LHS of the diagram and integrated from t_4 to t. We are left with four ordered times on the LHS, to be integrated from 0 to t, giving

$$\frac{t^4}{4!} \left|\frac{\Delta}{\Delta - i\Delta_0}\right|^2 \left(\frac{\Delta}{\Delta + i\Delta_0} + \frac{\Delta}{\Delta - i\Delta_0}\right)^2$$

We finally have

$$\langle P_{1\to 1}^{(2,2)}(t, a_i)\rangle_A = \left(\frac{\Gamma_{a_i}}{2}\right)^4 \frac{t^4}{2^4 \cdot 4!} \left|\frac{\Delta}{\Delta - i\Delta_0}\right|^2 \left(\frac{2\Delta^2}{\Delta^2 + \Delta_0^2}\right)^2 \tag{36}$$

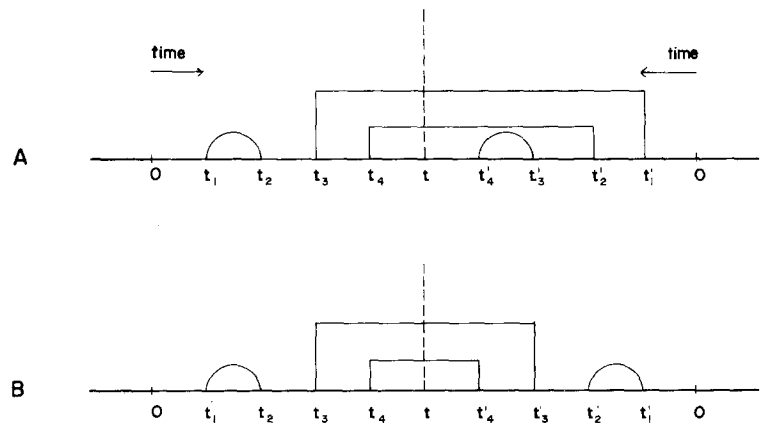

Fig. 4. Two of the diagrams arising from the (2, 2) term in the expansions (13) and (18).

Diagram B. We again use the δ-functions to bring all the times to the LHS. We have two times $t_1 = t_2$ and $t_2' = t_1'$ varying independently (i.e., they are not ordered) from 0 to t_3, and then two ordered times t_3 and t_4, to be integrated from 0 to t. If t_1 and t_1' were ordered, the whole time integral would give $t^4/4!$; however, the two possibilities $t_1 < t_1'$ and $t_1 > t_1'$ give the same contribution, so that we get $2t^4/4!$. The result is then

$$\langle P_{1\to 1}^{(2,2)}(t, a_i)\rangle_A = \left(\frac{\Gamma_{a_i}}{2}\right)^4 \frac{2t^4}{2^4 \cdot 4!} \left|\frac{\Delta}{\Delta - i\Delta_0}\right|^2 \left(\frac{2\Delta^2}{\Delta^2 + \Delta_0^2}\right)^2 \tag{37}$$

3.2. The General Rules. Evaluation of the Survival Probability

We now collect the rules that we have found from the above analysis. First, the qualitative rules:

1. Only contractions with nonintersecting lines contribute.
2. Non-cross-contractions can only be contiguous (bubbles).
3. The number of cross contractions must be even.

The structure of the general diagram is illustrated in Fig. 5. It has the following characteristics:

(a) There are $2p$ times on the LHS and $2q$ on the RHS.

(b) There are $(2p + 2q)/2 = p + q$ contractions. Out of these, $2k$ are cross contractions; there are left $(2p - 2k)/2 = p - k$ bubbles on the LHS and $(2q - 2k)/2 = q - k$ on the RHS.

(c) We have the relations

$$\sum_{i=1}^{2k+1} n_i + k = p \tag{38a}$$

$$\sum_{i=1}^{2k+1} n_i' + k = q \tag{38b}$$

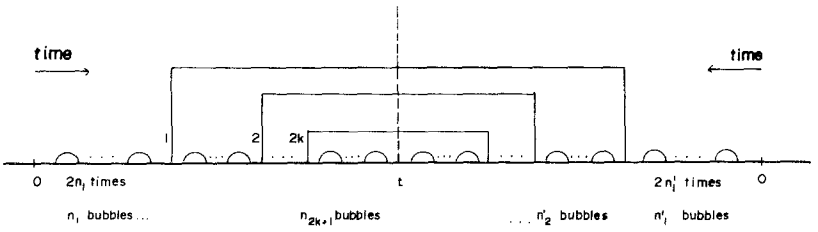

Fig. 5. The general diagram arising from the expansions (13) and (18).

We now have the following numerical contributions to the (p, q) term:

1. A factor $(-)^{p+q}$.
2. Each contraction gives a factor

$$\frac{1}{2}\frac{\Gamma_{a_i}}{2} \Rightarrow \frac{1}{2^{p+q}}\left(\frac{\Gamma_{a_i}}{2}\right)^{p+q}$$

3. Time integrations. Each bubble in the LHS gives a factor $\Delta/(\Delta - i\Delta_0)$, each bubble in the RHS gives a factor $\Delta/(\Delta + i\Delta_0)$, and each cross contraction a factor

$$\left(\frac{\Delta}{\Delta - i\Delta_0}\right) + \left(\frac{\Delta}{\Delta + i\Delta_0}\right)$$
$$\Rightarrow \left(\frac{\Delta}{\Delta + i\Delta_0}\right)^{q-k}\left(\frac{\Delta}{\Delta - i\Delta_0}\right)^{p-k}\left(\frac{2\Delta^2}{\Delta^2 + \Delta_0^2}\right)^{2k}$$

We bring all the times to the LHS. As a result, we have $n_1 + n_1'$ bubbles between 0 and the first cross contractions, $n_2 + n_2'$ between the first and the second cross contractions, etc. The number of time variables to be integrated from 0 to t is thus

$$(n_1 + n_1') + (n_2 + n_2') + \cdots + (n_{2k+1} + n_{2k+1}') + 2k = p + q \qquad (39)$$

If these $p + q$ time variables were *all* ordered, the final time integral from 0 to t would give $t^{p+q}/(p+q)!$. This is not the case, though, because: the $2k$ times associated with the cross contractions are indeed ordered; between the $(i-1)$th and the ith cross contractions we have $n_i + n_i'$ bubbles, of which n_i are ordered aong themselves, n_i' are also ordered among themselves, but the n_i ones can be in any position relative to the n_i' ones: the total number of possibilities for the ith interval is thus the number of permutations of $n_i + n_i'$ objects, disregarding the permutations of n_i and n_i' objects separately; i.e., $(n_i + n_i')!/n_i!\, n_i'!$.

The final result of the time integrations is thus

$$\frac{t^{p+q}}{(p+q)!}\prod_{i=1}^{2k+1}\binom{n_i + n_i'}{n_i}\left(\frac{\Delta}{\Delta - i\Delta_0}\right)^{p-k}$$
$$\times\left(\frac{\Delta}{\Delta + i\Delta_0}\right)^{q-k}\left(\frac{2\Delta^2}{\Delta^2 + \Delta_0^2}\right)^{2k}$$

Collecting the above results and summing over all allowed diagrams, we find the survival probability of Eq. (18), before averaging over initial states, as

$$\langle P_{1\to 1}^{a_i}(t)\rangle = \sum_{p,q,k} (-)^{p+q} \frac{(\Gamma_{a_i}/2)^{p+q}}{2^{p+q}(p+q)!} \left(\frac{\Delta t}{\Delta - i\Delta_0}\right)^{p-k} \times \left(\frac{\Delta t}{\Delta + i\Delta_0}\right)^{q-k} \left(\frac{2t\Delta^2}{\Delta^2+\Delta_0^2}\right)^{2k} \times \sum_{\{n_i\}\{n_i'\}}{}' \binom{n_i+n_1'}{n_2}\binom{n_2+n_2'}{n_2}\cdots\binom{n_{2k+1}+n_{2k+1}'}{n_{2k+1}} \quad (40)$$

The prime in the last summation indicates that the restrictions (38) have to be enforced.

Using Eq. (19) of ref. 18, we can evaluate the last sum in Eq. (40), with the result

$$\sum_{\{n_i\}\{n_i'\}}{}' = \binom{p+q}{2k}\binom{p+q-2k}{p-k} \quad (41)$$

The remaining sums in (40) can also be performed, obtaining, for a fixed initial state, the following expression:

$$\langle P_{1\to 1}^{a_i}(t)\rangle = \frac{1}{2}\left[1+\exp\left(-\frac{\Gamma_{a_i}\Delta^2}{\Delta^2+\Delta_0^2}t\right)\right] \quad (42)$$

To obtain the final result, we have to average over the initial states as indicated in Eq. (18). In the limit of high density of levels, we finally have

$$\langle P_{1\to 1}(t)\rangle = \frac{1}{2}\left[1+\left\langle \exp\left(-\frac{\Gamma(\varepsilon)\Delta^2}{\Delta^2+\Delta_0^2}t\right)\right\rangle_\beta\right] \quad (43)$$

where $\langle\cdots\rangle_\beta$ indicates the thermal average

$$\left\langle \exp\left(-\frac{\Gamma(\varepsilon)\Delta^2}{\Delta^2+\Delta_0^2}t\right)\right\rangle_\beta = \frac{1}{Z}\int_0^\infty \exp\left(-\frac{\Gamma(\varepsilon)\Delta^2}{\Delta^2+\Delta_0^2}t\right)\exp(-\beta\varepsilon)\,\rho(\varepsilon)\,d\varepsilon \quad (44)$$

Z being the bath partition function of Eq. (8).

Equation (43) is our main result. A discussion of some of its properties is given in the next section.

4. PROPERTIES OF THE SURVIVAL PROBABILITY

We first observe that, if we expand the exponential in (42), we get back the first-order result (28) provided by the golden rule. Although the

precise final functional form of the survival probability is not yet known and will depend on the particular level density assumed for the thermal bath, the large-t limit can be easily calculated. If the level density $\rho(\varepsilon)$ is such that the product

$$\exp\left(-\frac{\Gamma(\varepsilon)\,\Delta^2}{\Delta^2+\Delta_0^2}\,t\right)\exp(-\beta\varepsilon)\,\rho(\varepsilon)$$

is a uniformly bounded function, for all values of t, the limit calculation and the averaging over initial states commute. For a level density $\rho(\varepsilon)$ belonging to this class of functions, we find that, as $t\to\infty$, the survival probability tends to 1/2. This is a sensible result related to the limitation $\beta\Delta_0 \ll 1$. It indicates that both states of the system, $\alpha=\pm 1$, become equally populated.

From (43) we can calculate the *transition probability* as

$$\langle P_{1\to -1}(t)\rangle = \frac{1}{2}\left[1-\left\langle \exp\left(-\frac{\Gamma(\varepsilon)\,\Delta^2}{\Delta^2+\Delta_0^2}\,t\right)\right\rangle_\beta\right] \tag{45}$$

We can also calculate the *polarization* $\pi(t)$, defined as

$$\pi(t)=\langle\sigma_z\rangle \tag{46}$$

where the bracket denotes a quantum mechanical plus an ensemble average. Writing $\sigma_z=|1\rangle\langle 1|-|-1\rangle\langle -1|$, we can express the polarization as

$$\pi(t)=\langle P_{1\to 1}(t)\rangle-\langle P_{1\to -1}(t)\rangle \tag{47}$$

Using (43) and (45), we then find

$$\pi(t)=\left\langle \exp\left(-\frac{\Gamma(\varepsilon)\,\Delta^2}{\Delta^2+\Delta_0^2}\,t\right)\right\rangle_\beta \tag{48}$$

We now center our discussion on this last quantity.

It is clear from (42) that before averaging over initial states we get an exponential decay for the polarization, for any a_i. However, if Γ_{a_i} depends on ε_i each initial state contributes with its own decay probability to the average (48) and the result is, in general, a nonexponential decay law.

Therefore, if $\Gamma(\varepsilon)$ is a constant, independent of ε, i.e.,

$$\Gamma(\varepsilon)=\Gamma \tag{49}$$

the polarization (48) shows the exponential decay

$$\pi(t)=\exp-\left(\frac{\Gamma\Delta^2}{\Delta^2+\Delta_0^2}\,t\right) \tag{50}$$

For a nonconstant $\Gamma(\varepsilon)$, even a slow energy dependence may be important in distorting the exponential (50), since $\Gamma(\varepsilon)$ occurs in the exponent in Eq. (48). More explicit results can be obtained with more specific forms for $\Gamma(\varepsilon)$ and $\rho(\varepsilon)$.

5. SUMMARY AND CONCLUSIONS

We were able to extend the random-matrix model used in ref. 8 to the case where the total Hamiltonian contains a term which describes the two-level-system dynamics. As in ref. 8, we considered a "local GOE" for the system–bath interaction and calculated the ensemble average of the survival probability for times larger than the duration of a collision and smaller than the recurrence or Poincaré time. It was also possible to sum the whole series into a compact functional form. The final result is expressed as an average over the initial states whose level density depends on the particular thermal bath of the problem. As we mentioned before, the survival probability depends both on the width of the weight factor that appears in the definition of the "local GOE" in Eq. (14) and on the parameter Δ_0 related to the strength of the magnetic field around which the spin-1/2 particle is assumed to precess. At the end, the total effect of the additional term in the Hamiltonian is to multiply t by the factor $\Delta^2/(\Delta^2+\Delta_0^2)$. In the particular case of $\Gamma(\varepsilon)$ constant, the survival probability becomes a simple function [see Eq. (50)] and clearly the effect of the factor $\Delta^2/(\Delta^2+\Delta_0^2)$ is to reduce, for a given time t, the probability of a spin-flip process. A number of applications of our result are under investigation.

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