

A Soluble Random-Matrix Model for Relaxation in Quantum Systems

Pier A. Mello,^{1,4} Pedro Pereyra,² and Narendra Kumar³

Received July 14, 1987; revision received January 11, 1988

We study the relaxation of a degenerate two-level system interacting with a heat bath, assuming a random-matrix model for the system-bath interaction. For times larger than the duration of a collision and smaller than the Poincaré recurrence time, the survival probability of still finding the system at time t in the same state in which it was prepared at $t=0$ is exactly calculated.

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

1. INTRODUCTION

The study of relaxation phenomena in quantum mechanical systems is of central importance in statistical mechanics, and various models have been presented in the literature for that purpose.

A model which has frequently been employed in relaxation studies is that of a two-level system interacting with a heat bath. The literature on the subject is very extensive (see, for instance, Refs. 1–7 and references contained therein), since several systems of physical interest can be modeled in that simple way: for example, applications have been found in studies of spin-lattice relaxation,⁽¹⁾ paraelectric resonance relaxation,⁽²⁾ phenomena associated with the so-called molecular polaron,⁽³⁾ and the effect of tunneling friction⁽⁴⁾ in the stabilization of optical isomers.⁽⁵⁾ For a discussion,

¹ Instituto de Física, Universidad Nacional Autónoma de México, 01000 México D.F., México.

² Departamento de Ciencias Básicas, Universidad Autónoma Metropolitana-Azcapotzalco, 02200 México D.F., México.

³ Department of Physics, Indian Institute of Science, Bangalore 560012, India.

⁴ Also at Departamento de Física, UAM-Iztapalapa, and Fellow of the Sistema Nacional de Investigadores.

from a very general point of view, of the physics of a system (both classical and quantum mechanical) interacting with a reservoir, the reader may consult Ref. 8 and references contained therein.

In relaxation problems, the process is frequently found to be insensitive to the details of the interaction, only a few “gross properties,” such as the diffusion coefficient in the Brownian motion problem, 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⁽⁹⁾ 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. Various considerations on this “ergodic problem” can also be found in Ref. 9.

The purpose of the present paper is to implement the philosophy of the previous paragraph in the study of the relaxation of a two-level system with a bath. The system is assumed to have no dynamics of its own, so that, if it were isolated, its two energy levels would be degenerate. We expect to be able to relax this assumption in the future. The bath has a Hamiltonian H_B , and the system–bath interaction \mathcal{V} is written as

$$\mathcal{V} = V\sigma_x \quad (1.1)$$

where V depends only on the bath variables and the Pauli matrix σ_x on those of the system. It is the interaction V that is treated by means of a *random-matrix model*.⁽⁹⁾ The total Hamiltonian of the problem is given by

$$H = H_B + \mathcal{V} \quad (1.2)$$

Suppose that at $t=0$ we prepare the system in an eigenstate, $|1\rangle$ say, of the Pauli matrix σ_z , while the bath is in thermal equilibrium. Since \mathcal{V} can cause transitions between the two eigenstates of σ_z , the problem that we pose is that of calculating the probability of still finding the system in state $|1\rangle$ at time t .

We shall be able to show that the model just described can be solved *exactly* when the time t satisfies the inequalities

$$t_{\text{coll}} \ll t \ll t_P \quad (1.3)$$

where t_{coll} and t_P are 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. 10 to describe relaxation phenomena in nuclear physics, essentially consists in writing the above survival probability as a series expansion in powers of the interaction, averaging term by term and then summing up the full series.

Assumptions on a phenomenological, random, time-dependent interaction are sometimes made in relaxation studies.⁽¹¹⁻¹⁵⁾ 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 notice, incidentally, that the randomness assumed for such a time-dependent interaction has an entirely different origin from the one considered in the present paper, 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 model outlined above; in particular, we discuss in detail the random-matrix ensemble that we propose for the system-bath interaction. The survival probability is written in that section as a series in powers of the interaction. Some representative terms of that series are evaluated in detail in Section 3; a graphical representation for them is given, which is highly advantageous for the evaluation of the most general term. The series can be summed, giving the final result (3.24) for the survival probability. Some features of the result are discussed in Section 4. Finally, Section 5 gives the conclusions of this investigation.

2. THE MODEL

As was outlined in the Introduction, the Hilbert space of the system consists of two states, which we designate by $|\alpha\rangle$, $\alpha = \pm 1$, assuming that they are eigenstates of the Pauli matrix σ_z ; i.e.,

$$\sigma_z |\alpha\rangle = \alpha |\alpha\rangle, \quad \alpha = \pm 1 \quad (2.1)$$

In addition, we denote by $|a\rangle$ a complete set of states of the bath, assuming that they are eigenstates of the bath Hamiltonian H_B , with energy ε_a ; i.e.,

$$(\varepsilon_a - H_B) |a\rangle = 0 \quad (2.2)$$

We shall denote by $\rho(\varepsilon)$ the density of bath states. The states $|\alpha a\rangle$ form a complete set for the system-bath combination, which is assumed to be governed by the Hamiltonian (1.2).

At $t=0$ the system is in state $|\alpha=1\rangle$, while the bath is in thermal equilibrium, described by the canonical ensemble

$$p_i = e^{-\beta \epsilon_i} / Z \quad (2.3)$$

where Z is the bath partition function.

The survival probability $P(t)$, i.e., the probability that at time t we still find the system in state $|1\rangle$, regardless of the state of the bath, is given by ($\hbar=1$)

$$P(t) = \sum_{ia} |\langle 1a | e^{-iHt} | 1i \rangle|^2 p_i \quad (2.4)$$

The transition probability $P_{1 \rightarrow -1}$ is given by $1 - P$.

The evolution operator $\exp(-iHt)$ for the full Hamiltonian (1.2) can be expanded in a power series of the interaction \mathcal{V} of (1.1) as

$$e^{-iHt} = e^{-iH_B t} \sum_{n=0}^{\infty} (-i)^n \int_0^t dt_n \cdots \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \mathcal{V}(t_n) \cdots \mathcal{V}(t_2) \mathcal{V}(t_1) \quad (2.5)$$

where $\mathcal{V}(t)$ is the operator \mathcal{V} expressed in the interaction representation; i.e.,

$$\mathcal{V}(t) = e^{iH_B t} \mathcal{V} e^{-iH_B t} = e^{iH_B t} V e^{-iH_B t} \sigma_x \quad (2.6)$$

We recall that V is a Hermitian operator. Substituting (2.6) in (2.5), and this in the expression (2.4) for the survival probability $P(t)$, we observe that only the terms containing even powers of σ_x survive. Using also the Schrödinger equation (2.2) for H_B , we have

$$\begin{aligned} P(t) &= \sum_i p_i \sum_{p,q=0}^{\infty} (-)^{p+q} \sum_{\substack{a_1 \cdots a_{2p-1} \\ a, b_{2q-1} \cdots b_1}} [V_{ia_1} V_{a_1 a_2} \cdots V_{a_{2p-1} a} V_{ab_{2q-1}} \cdots V_{b_{2q-1} b_1} V_{b_1 i}] \\ &\quad \times \int_0^t dt_{2p} \cdots \int_0^{t_2} dt_1 \int_0^t dt'_{2q} \cdots \int_0^{t'_2} dt'_1 \\ &\quad \times \exp i[(\epsilon_i - \epsilon_{a_1})t_1 + (\epsilon_{a_1} - \epsilon_{a_2})t_2 + \cdots + (\epsilon_{a_{2p-1}} - \epsilon_a)t_{2p} \\ &\quad + (\epsilon_a - \epsilon_{b_{2q-1}})t'_{2q} + \cdots + (\epsilon_{b_2} - \epsilon_{b_1})t'_2 + (\epsilon_{b_1} - \epsilon_i)t'_1] \\ &= \sum_i p_i \sum_{p,q=0}^{\infty} P_i^{(p,q)}(t) \end{aligned} \quad (2.7)$$

which expresses our result as a sum of contributions coming from the various initial states i and the values taken by the variables p and q ; the (pq) 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), an extension (used in Ref. 10), to be defined below, of the standard GOE.⁽⁹⁾

The matrix elements V_{ab} of the operator V , in the basis defined by (2.2), are assumed to form a *real symmetric* matrix and, aside from the symmetry requirement, they are considered as *statistically independent Gaussian variables* with zero mean and covariance given by

$$\langle V_{ab} V_{cd} \rangle = v^2(\varepsilon_{ab})(\delta_{ad}\delta_{bc} + \delta_{ac}\delta_{bd}) w_{\Delta(\varepsilon_{ab})}(\varepsilon_a - \varepsilon_b) \quad (2.8)$$

where the angular brackets denote an ensemble average. In other words, the only nonzero covariance is that of V_{ab} with itself, or with V_{ba} . The quantity $\varepsilon_{ab} \equiv (\varepsilon_a + \varepsilon_b)/2$ is the centroid of the two energies $\varepsilon_a, \varepsilon_b$. The weight factor $w_{\Delta(\varepsilon_{ab})}(\varepsilon_a - \varepsilon_b)$ is assumed to have the property

$$w_{\Delta(\varepsilon_{ab})}(\varepsilon_a - \varepsilon_b) \approx \begin{cases} 1, & |\varepsilon_a - \varepsilon_b| \lesssim \Delta(\varepsilon_{ab}) \\ 0, & |\varepsilon_a - \varepsilon_b| > \Delta(\varepsilon_{ab}) \end{cases} \quad (2.9)$$

thus indicating that the interaction V connects eigenstates of H_B within an energy interval $\sim \Delta$. The quantity

$$t_{\text{coll}} \sim 1/\Delta \quad (2.10)$$

which has dimensions of time ($\hbar=1$), is a time associated with one application of the interaction, and has been interpreted as the duration of a collision.⁽¹⁰⁾ As an example, in the simple problem of potential scattering in one dimension, it can be easily verified that t_{coll} is on the order of the time taken by the centroid of a wave packet to travel across the potential.

We shall always assume that Δ contains many bath levels, and we shall allow for the possibility of a slow dependence of Δ on the bath energy. A slow dependence on ε_a of the strength of interaction v^2 and of the density ρ may also occur.

We can thus visualize the matrix $\|V_{ab}\|$ as having appreciable elements inside a band of variable width 2Δ along the diagonal, as schematically represented in Fig. 1.

We shall frequently encounter in what follows the quantity $\langle V_{ab}^2 \rangle \rho(\varepsilon_b)$ which, from (2.8), we write as

$$\langle V_{a \neq b}^2 \rangle \rho(\varepsilon_b) = v^2(\varepsilon_{ab}) \rho(\varepsilon_b) w_{\Delta(\varepsilon_{ab})}(\varepsilon_a - \varepsilon_b) \quad (2.11)$$

The above dependence on energy of v^2 , ρ and Δ will be assumed to be so slow that these three quantities can be taken essentially constant inside

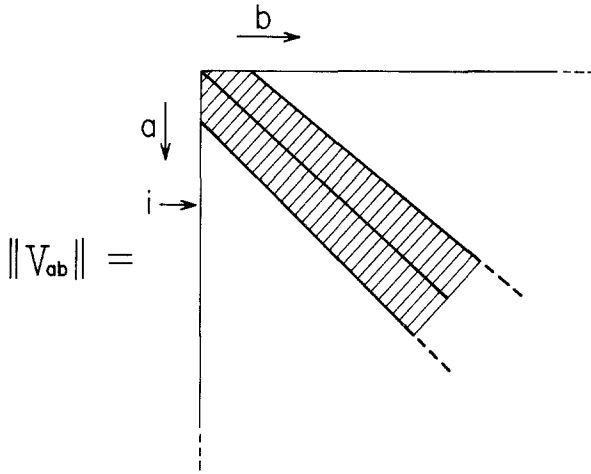


Fig. 1. Schematic representation of the structure of the interaction matrix $\|V_{ab}\|$ with the local GOE used in Eq. (2.8). Also indicated is a typical state i such that the full energy interval $\varepsilon_i \pm \Delta_i$ to which it is connected by the interaction is not cut out by the lower bound of the bath spectrum.

the interval where (2.11) is nonzero; we can then write $v^2(\varepsilon_{ab}) \approx v^2(\varepsilon_a) \approx v^2(\varepsilon_b)$, and similarly for ρ and Δ . We then write

$$\begin{aligned} \langle V_{a \neq b}^2 \rangle \rho(\varepsilon_b) &\approx v^2(\varepsilon_a) \rho(\varepsilon_a) w_{\Delta_a}(\varepsilon_a - \varepsilon_b) \\ &\equiv u^2(\varepsilon_a) w_{\Delta_a}(\varepsilon_a - \varepsilon_b) \end{aligned} \quad (2.12)$$

where $\Delta_a \equiv \Delta(\varepsilon_a)$.

We close this section by indicating that our goal is now the calculation of the ensemble average of the survival probability $P(t)$ of Eq. (2.7), which can then be written as a sum over the various i, p, q contributions as

$$\langle P(t) \rangle = \sum_i p_i \sum_{p,q=0}^{\infty} \langle P_i^{(p,q)}(t) \rangle = \sum_i p_i \langle P_i(t) \rangle \quad (2.13)$$

where each contribution satisfies the relation

$$\langle P_i^{(p,q)}(t) \rangle = \langle P_i^{(q,p)}(t) \rangle^* \quad (2.14)$$

This program will be carried out in the next section.

3. CALCULATION OF THE SURVIVAL PROBABILITY

We first calculate in detail some representative terms in the expansion (2.13). It will then be easy to infer the general rules and apply them to the calculation of the survival probability.

3.1. Some Particular Terms in the Expansion (2.13)

1. The term $p = 0, q = 0$ just gives 1.
2. The term $p = 1, q = 0$ is given by [see (2.7)]

$$\langle P_i^{(1,0)}(t) \rangle = - \int_0^t dt_2 \int_0^{t_2} dt_1 \left[\sum_a \langle V_{ia}^2 \rangle e^{i(\varepsilon_i - \varepsilon_a)(t_1 - t_2)} \right] \quad (3.1)$$

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

$$Dt \ll 1 \quad (3.2a)$$

where D is the mean level spacing. This can be looked on as a large-volume limit. If $1/D$ is interpreted as the Poincaré recurrence time t_P , we thus need

$$t \ll t_P \quad (3.2b)$$

which is certainly satisfied. We shall neglect the fact that for the single term $i = a$, $\langle V_{ia}^2 \rangle$ is twice as big as for an off-diagonal term [see Eq. (2.8)]; it can be easily checked that the relative error that we make is of the order of $t/\rho(\varepsilon_i) \sim t/t_P(i)$, which is negligible. We thus use (2.12) to write

$$\begin{aligned} \sum_a \langle V_{ia}^2 \rangle e^{i(\varepsilon_i - \varepsilon_a)\tau} &= u^2(\varepsilon_i) \int_0^\infty w_{\Delta_i}(\varepsilon_i - \varepsilon_a) e^{i(\varepsilon_i - \varepsilon_a)\tau} d\varepsilon_a \\ &= u^2(\varepsilon_i) \int w_{\Delta_i}(x) e^{-ix\tau} dx \equiv u^2(\varepsilon_i) \tilde{w}_i(\tau) \end{aligned} \quad (3.3)$$

We shall consider initial bath states i like the one indicated in Fig. 1, such that the full energy interval $\varepsilon_i \pm \Delta_i$ 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_i satisfy this condition. If the structure of the matrix V were as indicated in Fig. 1, our analysis would thus be valid above a certain minimum temperature T_0 (depending on the specific structure of the matrix), in order to avoid any “threshold effect.” We shall see that above T_0 the result does not depend on the specific value of Δ_i .

Under these conditions, $\tilde{w}_i(\tau)$ of Eq. (3.3) is real, symmetric in τ , appreciable only inside the interval $1/\Delta_i$ of the variable τ , and has the property

$$\int_{-\infty}^{\infty} \tilde{w}_i(\tau) d\tau = 2\pi w_{\Delta_i}(0) = 2\pi \quad (3.4)$$

We recall that $\tilde{w}_i(\tau)$ has to be used inside the time integral of Eq. (3.1); therefore, for time intervals much larger than $1/\Delta_i$ [which was interpreted in (2.10) as the duration of a collision], we essentially get the same result if we replace $\tilde{w}_i(\tau)$ by $2\pi\delta(\tau)$. This approximation is independent of the strength v^2 of the interaction appearing in (2.11) and depends only on the quantity Δ . It may be useful to work out a simple example to check the approximation. Suppose that

$$w_{\Delta}(x) = e^{-x^2/2\Delta^2}$$

Then

$$\tilde{w}_{\Delta}(\tau) = (2\pi\Delta^2)^{1/2} e^{-\Delta^2\tau^2/2}$$

We can evaluate exactly the integral that will be relevant for (3.1) as

$$\begin{aligned} \int_0^t dt_2 \int_0^{t_2} dt_1 \tilde{w}(t_1 - t_2) &= \pi t \operatorname{erf}\left(\frac{t\Delta}{\sqrt{2}}\right) - (2\pi)^{1/2} \Delta \int_0^t e^{-\Delta^2 x^2/2} dx \\ &\approx \pi t \end{aligned}$$

if $t\Delta \gg 1$. This is indeed the same result that we would obtain by replacing $\tilde{w}(\tau) \rightarrow 2\pi\delta(\tau)$ and realizing that the t_1 integration goes only up to t_2 , thus covering “half of the δ -function” and giving rise to a factor 1/2.

We thus write (3.3) as

$$\sum_a \langle V_{ia}^2 \rangle e^{i(\varepsilon_i - \varepsilon_a)\tau} = \frac{1}{2} \Gamma(\varepsilon_i) \delta(\tau) \quad (3.5)$$

where, for later convenience, we have defined

$$\Gamma(\varepsilon) \equiv 4\pi u^2(\varepsilon) \quad (3.6)$$

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

$$t_{\text{coll}} \ll t \ll t_{\text{P}} \quad (3.7)$$

We thus get, for the (1, 0) term of (3.1)

$$\langle P_i^{(1,0)}(t) \rangle = -\frac{\Gamma(\varepsilon_i)/2}{2} t \quad (3.8)$$

In preparation for the analysis of the more complicated terms, it will be useful to introduce a graphical representation for the term we have just calculated. In Fig. 2 and the following ones, we indicate two time intervals,

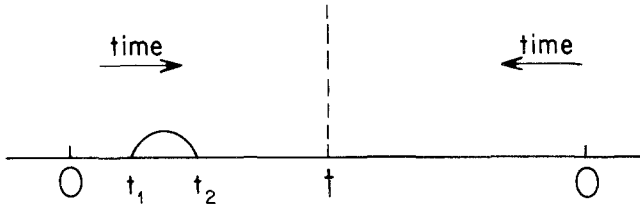


Fig. 2. Graphical representation of the $p = 1, q = 0$ term of Eq. (3.1).

from 0 to t , which should contain, respectively, the $2p$ and $2q$ ordered time variables of Eq. (2.7). In the present $(1, 0)$ case, Eq. (3.1) just contains t_1 and t_2 , which are indicated in Fig. 2. The line joining them, to be called a *contraction*, indicates the ensemble average of the two corresponding V 's [remember that in Eq. (2.5) every t_i has a $\mathcal{V}(t_i)$ associated with it]. It is clear that our result (3.8) can be written at once from the diagram, following the rules:

- (a) Assign to the contraction a factor $\Gamma(\varepsilon_i)/2$.
- (b) Assign to the contraction an extra factor $1/2$ [whose origin is explained above Eq. (3.5)].
- (c) The two times t_1 and t_2 are reduced to a single one [due to the δ -function (3.5)], to be integrated from 0 to t ; that integration gives a factor t .

Finally, we see from Eq. (2.14) that the $p = 0, q = 1$ term gives the same contribution (3.8), so that to *first order* we have

$$P_i(t) = 1 - \Gamma(\varepsilon_i)(t/2) + \dots \tag{3.9}$$

and

$$P_{i,1 \rightarrow -1} = \Gamma(\varepsilon_i)(t/2) + \dots \tag{3.10}$$

Result (3.10) coincides with that obtained from the “golden rule” of quantum mechanics,⁽¹⁶⁾ where a restriction on time similar to (3.7) also appears, the role of \mathcal{A} being played by the energy interval over which V_{ia}^2 varies appreciably. The structure of the matrix V indicated in Fig. 1 is not required to obtain the golden rule, though; however, it 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 will be calculated using a well-known theorem of statistics^(9,10): 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. 3. We shall need the relation

$$\langle V_{ab} V_{bc} \rangle = \langle V_{ab}^2 \rangle \delta_{ac} \tag{3.11}$$

which is a consequence of the basic assumption (2.8).

Using (3.11), we can write diagram A as

$$\begin{aligned} \langle P_i^{(1,1)A}(t) \rangle &= \int_0^t dt_2 \int_0^{t_2} dt_1 \int_0^{t_1} dt'_2 \int_0^{t'_2} dt'_1 \left[\sum_{a_1} \langle V_{ia_1}^2 \rangle e^{i(\varepsilon_i - \varepsilon_{a_1})(t_1 - t_2)} \right] \\ &\times \left[\sum_{b_1} \langle V_{ib_1}^2 \rangle e^{i(\varepsilon_i - \varepsilon_{b_1})(t'_2 - t'_1)} \right] \end{aligned} \tag{3.12}$$

which shows that the basic block of Eq. (3.5) makes its appearance again. We thus apply to each contraction the rules found above, to write

$$\langle P_i^{(1,1)A}(t) \rangle = \left(\frac{\Gamma(\varepsilon_i)/2}{2} t \right)^2 \tag{3.13}$$

Diagram B involves *cross contractions*, i.e., contractions that cross the dashed line. Using (3.11), one can see that the block (3.5) occurs again.

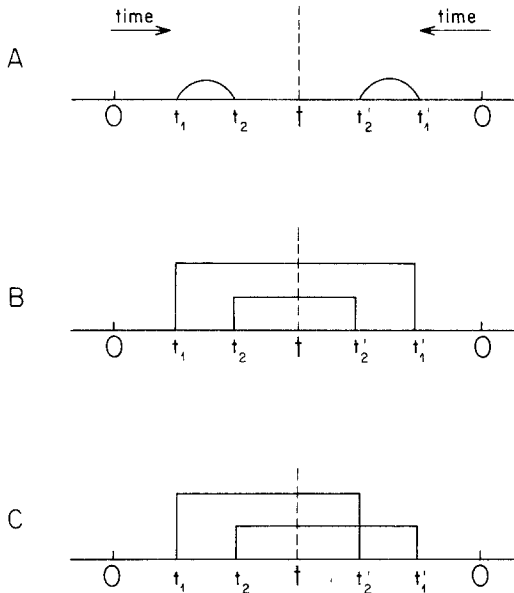


Fig. 3. The three diagrams arising from the $p=1, q=1$ term in the expansion of Eqs. (2.7) and (2.13).

This will be a common feature of all the remaining terms! Rule (a) above Eq. (3.9) is valid for any contraction, but rule (b) is clearly needed only for non-cross-contractions. The equivalent of rule (c) is now the following: due to the δ -functions of (3.5), $t'_1 = t_1$ 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 $t^2/2!$. The result is thus

$$\langle P_i^{(1,1)B}(t) \rangle = [F(\varepsilon_i)/2]^2 t^2/2! \tag{3.14}$$

Diagram C involves the special feature of *crossing lines*, which, due to the basic assumption (2.8), kill one summation, in contrast with diagrams A and B; its contribution can be easily seen to be of order $t/\rho(\varepsilon_i) = t/t_P(i)$, relative to A or B, and hence negligible. The fact that *contractions with intersecting lines are negligible* is a well known rule.^(9,10)

4. The term (4, 0) gives rise to the three diagrams of Fig. 4.

For diagram A we apply rules (a) and (b) and then realize that we are left with two ordered times to be integrated from 0 to t , giving $t^2/2!$. The result is then

$$\langle P_i^{(2,0)A}(t) \rangle = \frac{[F(\varepsilon_i)/2]^2 t^2}{2^2 \cdot 2!} \tag{3.15}$$

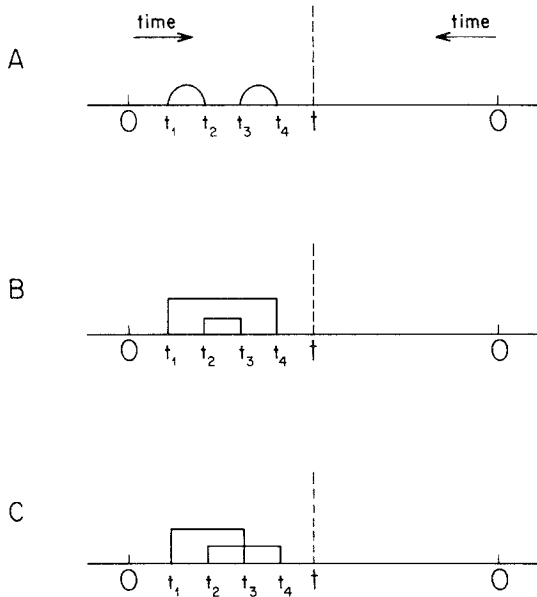


Fig. 4. The three diagrams arising from the (4, 0) term in the expansion (2.7), (2.13).

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.

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

$$\langle P_i^{(p,0)}(t) \rangle = (-)^p \frac{[\Gamma(\varepsilon_i)/2]^p t^p}{2^p p!} \tag{3.16}$$

6. We consider the two diagrams of Fig. 5, taken from those that contribute to the term $(2, 2)$.

From rules (a) and (b), we have the following contributions for diagram A:

$$\begin{aligned} \text{four contractions} &\Rightarrow [\Gamma(\varepsilon_i)/2]^4 \\ \text{two non-cross-contractions} &\Rightarrow (1/2)^2 \end{aligned}$$

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 $t^4/4!$. We finally have

$$\langle P_i^{(2,2)A}(t) \rangle = \frac{[\Gamma(\varepsilon_i)/2]^4 t^4}{2^2 4!} \tag{3.17}$$

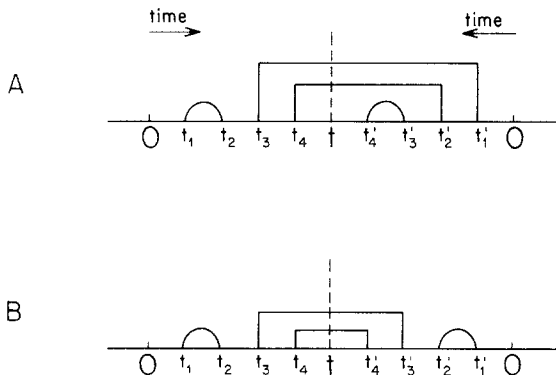


Fig. 5. Two of the diagrams arising from the $(2, 2)$ term in the expansion (2.7), (2.13).

For 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 the 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 $2 \cdot t^4/4!$. The result is then

$$\langle P_i^{(2,2)\text{B}}(t) \rangle = \frac{[\Gamma(\varepsilon_i)/2]^4}{2^2} 2 \cdot \frac{t^4}{4!} \tag{3.18}$$

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 ($2k$).

The structure of the general diagram is illustrated in Fig. 6. 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

$$\sum_{i=1}^{2k+1} n_i + k = p \tag{3.19a}$$

$$\sum_{i=1}^{2k+1} n'_i + k = q \tag{3.19b}$$

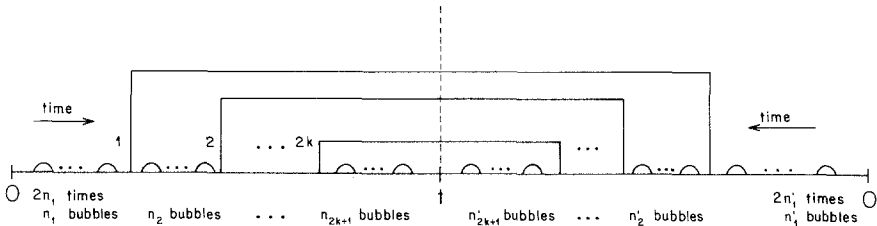


Fig. 6. The general diagram arising from the expansion (2.7), (2.13).

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

1. A factor $(-)^{p+q}$.
2. Each contraction gives a factor $\Gamma(\varepsilon_i)/2 \Rightarrow [\Gamma(\varepsilon_i)/2]^{p+q}$.
3. Each bubble gives a factor $1/2 \Rightarrow (1/2)^{p+q-2k}$.
4. Time integrations. We bring all the times to the lhs. As a result, we have $n_1 + n'_1$ bubbles between 0 and the first cross-contraction, $n_2 + n'_2$ between the first and the second cross-contraction, etc. The number of time variables to be integrated from 0 to t is thus

$$(n_1 + n'_1) + \cdots + (n_{2k+1} + n'_{2k+1}) + 2k = p + q \quad (3.20)$$

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. The $2k$ times associated with the cross-contractions are indeed ordered; between the $(i-1)$ th and the i th cross-contractions we have $n_i + n'_i$ bubbles, of which n_i are ordered among 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 i th 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

$$\frac{t^{p+q}}{(p+q)!} \prod_{i=1}^{2k+1} \binom{n_i + n'_i}{n_i}$$

Collecting the above results and summing over all allowed diagrams, we find the survival probability of Eq. (2.13), before averaging over initial states, as

$$\begin{aligned} \langle P_i(t) \rangle &= \sum_{pqk} (-)^{p+q} \frac{[\Gamma(\varepsilon_i)/2]^{p+q}}{2^{p+q-2k}} \frac{t^{p+q}}{(p+q)!} \\ &\times \sum'_{\{n_i\}\{n'_i\}} \binom{n_1 + n'_1}{n_1} \cdots \binom{n_{2k+1} + n'_{2k+1}}{n_{2k+1}} \end{aligned} \quad (3.21)$$

The prime in the last summation indicates that the restrictions (3.19) have to be enforced.

Using Eq. (19) of Ref. 17, we can evaluate the last sum in Eq. (3.21), with the result

$$\sum'_{\{n_i\}\{n'_i\}} = \binom{p+q}{2k} \binom{p+q-2k}{p-k} \quad (3.22)$$

The remaining sums in (3.21) can also be performed, the result being

$$\langle P_i(t) \rangle = \frac{1}{2}[1 + e^{-\Gamma(\varepsilon_i)t}] \quad (3.23)$$

Averaging over initial states as in (2.13), we finally have

$$\langle P(t) \rangle = \frac{1}{2}[1 + \langle e^{-\Gamma(\varepsilon)t} \rangle_\beta] \quad (3.24)$$

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

$$\langle e^{-\Gamma(\varepsilon)t} \rangle_\beta = \frac{1}{Z} \int_0^\infty e^{-\Gamma(\varepsilon)t} e^{-\beta\varepsilon} \rho(\varepsilon) d\varepsilon \quad (3.25)$$

with Z the bath partition function of Eq. (2.3).

Equation (3.24) 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 (3.23), we get back the first-order result (3.9) provided by the golden rule.

On the other hand, as $t \rightarrow \infty$, the survival probability tends to 1/2, indicating that both states of the system, $\alpha = \pm 1$, become equally populated.

From (3.24) we can calculate the *transition probability* as

$$\langle P_{1 \rightarrow -1}(t) \rangle = \frac{1}{2}[1 - \langle e^{-\Gamma(\varepsilon)t} \rangle_\beta] \quad (4.1)$$

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

$$\Pi(t) \equiv \langle \sigma_z \rangle \quad (4.2)$$

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

$$\Pi(t) = \langle P(t) \rangle - \langle P_{1 \rightarrow -1}(t) \rangle \quad (4.3)$$

Using (3.24) and (4.1), we then find

$$\Pi(t) = \langle e^{-\Gamma(\varepsilon)t} \rangle_\beta \quad (4.4)$$

We now center our discussion on this last quantity.

It is clear from (3.23) that before averaging over initial states we get an exponential decay for the polarization, for any i . However, if $\Gamma(\varepsilon_i)$

depends on ε_i , each initial state contributes with its own decay probability to the average (4.4) and the result is, in general, a *nonexponential* decay law.

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

$$\Gamma(\varepsilon) = \Gamma \quad (4.5)$$

the polarization (4.4) shows the exponential decay

$$\Pi(t) = e^{-\Gamma t} \quad (4.6)$$

For a nonconstant $\Gamma(\varepsilon)$, even a slow energy dependence may be important in distorting the exponential (4.6), since $\Gamma(\varepsilon)$ occurs in the exponent in Eq. (4.4). We write (4.4) as

$$\Pi(t) = \frac{\int \exp[-\Gamma(\varepsilon)t - \beta\varepsilon + \ln \rho(\varepsilon)] d\varepsilon}{\int \exp[-\beta\varepsilon + \ln \rho(\varepsilon)] d\varepsilon} \quad (4.7)$$

and evaluate the two integrals in the saddle-point approximation. The equation for the saddles ε_0 and ε_1 arising from the denominator and numerator, respectively, are

$$\left[\frac{d \ln \rho(\varepsilon)}{d\varepsilon} \right]_{\varepsilon_0} = \beta \quad (4.8a)$$

$$\left[\frac{d \ln \rho(\varepsilon)}{d\varepsilon} \right]_{\varepsilon_1} = \beta + \Gamma'(\varepsilon_1)t \quad (4.8b)$$

Assuming that one gets only one saddle ε_0 and one ε_1 , we have

$$\Pi(t) = e^{-\Gamma(\varepsilon_1)t} \left[\frac{-[d^2 \ln \rho(\varepsilon)/d\varepsilon^2]_{\varepsilon_0}}{[\Gamma''(\varepsilon_1)t - [d^2 \ln \rho(\varepsilon)/d\varepsilon^2]_{\varepsilon_1}]^{1/2}} \right] \frac{\rho(\varepsilon_1)}{\rho(\varepsilon_0)} e^{\beta(\varepsilon_0 - \varepsilon_1)} \quad (4.9)$$

As a check, when $\Gamma(\varepsilon) = \Gamma$, the two saddles are identical and (4.9) reduces to (4.6).

Equation (4.9) gives the general structure of the result: there is an explicit time dependence in the exponential and inside the square root, as well as a dependence on time through the position of the saddle ε_1 , since t appears explicitly in the saddle equation (4.8b). More explicit results can only be obtained with a more specific form for $\Gamma(\varepsilon)$ and $\rho(\varepsilon)$.

5. SUMMARY AND DISCUSSION

The survival probability was written in Eq. (2.7) as a series in powers of the system–bath interaction. We proposed, for the latter, a random-matrix model—a “local GOE”—that allowed the calculation of the ensemble average of every term of the above expansion; the time involved was

requested to be large compared with a time on the order of the duration of a collision and small compared with a recurrence, or Poincaré, time [see inequality (3.7)]. The whole series could actually be summed, giving the final exponential law (3.23) when we fix the initial state of the bath. When we average over initial states, we may get a mixture of decay constants that could destroy the exponential behavior [see Eqs. (3.24), (4.1), (4.4)]. We observe that no restriction was ever imposed on the strength of the interaction, in contrast with the weak coupling assumption sometimes made in the literature.⁽⁶⁾

As was remarked in the Introduction, Eq. (1.2) represents the total *time-independent* Hamiltonian. Thus, there is no need in this approach to make assumptions on the correlation time of any time-dependent interaction, as is frequently done in the literature.⁽¹¹⁻¹⁵⁾ Indeed, any time dependence follows as a consequence of the model. For instance, in the interaction representation the wave function $|\Psi\rangle_I$ satisfies the equation

$$i \frac{\partial}{\partial t} |\Psi\rangle_I = \mathcal{V}(t) |\Psi\rangle_I \quad (5.1)$$

where $\mathcal{V}(t)$ is given in Eq. (2.6). The matrix elements of $\mathcal{V}(t)$ are

$$\langle \alpha a | \mathcal{V}(t) | \beta b \rangle = \delta_{\alpha, -\beta} V_{ab} e^{i(\epsilon_a - \epsilon_b)t} \quad (5.2)$$

Since $\|V_{ab}\|$ is a random matrix, (5.2) is a random, time-dependent matrix, whose properties follow from (5.2) and the definition of the ensemble for the V_{ab} . In particular, the time correlation of two matrix elements like (5.2) is periodic.

Our result (3.23) is so simple that a more direct derivation of it would certainly be welcome. A cumulant expansion associated with a random Gaussian operator can be cut if its correlation time is very short⁽¹³⁾; but this is not the case here, as remarked in the previous paragraph, so that we cannot offer this argument as an explanation for (3.23). What seems to be playing a similar role in the present analysis is the inequality $t_{\text{coll}} \ll t$. In any case, the question deserves a closer examination.

We mentioned that our results are valid above a certain minimum temperature if the interaction matrix has the structure shown in Fig. 1. An extension of the analysis to avoid this limitation would be desirable. We also mentioned that the golden rule (which gives the first-order term) is obtained under more general conditions on the structure of the interaction than those used here (however, on approaching threshold one needs longer and longer times for its validity). The structure of V that we do assume permits the evaluation of the expansion to all orders; whether an ensemble average can still be calculated for all the terms under more general conditions is certainly worth investigating.

Our results cannot be *directly* compared with those of the comprehensive study of Ref. 8, for two reasons: (1) In our model Hamiltonian (1.2) the system has no dynamics of its own, whereas in Ref. 8 it does; (2) in the present paper, it is the system–bath interaction that causes transitions between the two relevant states of the system (eigenstates of σ_z), whereas in Ref. 8 such transitions are caused by the system Hamiltonian itself, which is proportional to σ_x . Perhaps there is a closer connection with two related problems (which, in turn, can be related to the spin-boson problem), also discussed in Ref. 8: the Kondo and the Toulouse problems (see, for instance, Ref. 8, Sections III E and VB, respectively), where one considers a “bath” Hamiltonian, and a “system–bath” interaction responsible for causing transitions: indeed, the exponential decay derived in the previous section of the present paper is consistent with the behavior reported in Eq. (5.27) of Ref. 8.

The inclusion of the system Hamiltonian mentioned above is certainly a very important one, which gives rise to a host of very interesting effects.^(1–8) The model Hamiltonian (1.2) studied here thus has to be taken as a starting point, from which we plan to analyze various extensions in the future.

REFERENCES

1. L. T. Muus and P. W. Atkins, eds., *Electron–Spin Relaxation in Liquids* (Plenum Press, New York, 1972).
2. L. M. Sander and H. B. Shore, *Phys. Rev. B* **3**:1472 (1971).
3. N. Rivier and T. J. Coe, *J. Phys. C* **10**:4471 (1977).
4. S. Chakravarty and A. J. Leggett, *Phys. Rev. Lett.* **52**:5 (1984).
5. R. A. Harris and R. Silbey, *J. Chem. Phys.* **78**:7330 (1983).
6. A. Nitzan and R. J. Silbey, *J. Chem. Phys.* **60**:4070 (1974).
7. A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, *Rev. Mod. Phys.* **59**:1 (1980).
8. H. Spohn, *Rev. Mod. Phys.* **53**:569 (1980).
9. T. A. Brody, J. Flores, J. B. French, P. A. Mello, A. Pandey, and S. S. M. Wong, *Rev. Mod. Phys.* **53**:385 (1981).
10. D. Agassi, H. A. Weidenmüller, and G. Mantzouranis, *Phys. Rep.* **22**:145 (1975); D. Agassi, C. M. Ko, and H. A. Weidenmüller, *Ann. Phys. (N.Y.)* **107**:140 (1977); H. A. Weidenmüller, in *Theoretical Methods in Medium-Energy and Heavy-Ion Physics*, K. W. McVoy and W. A. Friedman, eds. (Plenum Press, New York, 1978).
11. P. W. Anderson, *J. Phys. Soc. Japan* **9**:316 (1954).
12. R. Kubo, *J. Phys. Soc. Japan* **17**:1100 (1962).
13. R. F. Fox, *Phys. Rep.* **48**:179 (1978), part II.
14. N. G. van Kampen, *Physica* **74**:215, 239 (1974).
15. R. H. Terwiel, *Physica* **74**:248 (1974).
16. A. Messiah, *Quantum Mechanics*, Vol. II, p. 736 (Wiley, New York, 1966).
17. E. Netto, *Lehrbuch der Kombinatorik*, Chapter 13 (Chelsea, New York, 1927).