Abstract

Decoherence effects associated to the damping of a tunneling two-level system are shown to dominate the tunneling probability at short times in strong coupling regimes in the context of a soluble model. A general decomposition of tunneling rates in dissipative and unitary parts is implemented. Master equation treatments fail to describe the model system correctly when more than a single relaxation time is involved.

1 Introduction

Motion in tunneling phenomena can be seen quite generally as resulting from dispersive effects in the time evolution of spatially localized quantum states which are not energy eigenstates. Since, from this point of view, quantum interference plays a central role in these phenomena, one may ask how are they affected by quantum decoherence processes which occur as a result of coupling to other degrees of freedom. Effects of additional degrees of freedom in tunneling processes have been studied now for a long time and in a variety of contexts [1], but emphasis falls usually on the question of the observable changes on inclusive properties such as tunneling probabilities. However, these questions are often addressed in semi-classical terms, including generalizations of the WKB approach [2], which tend to becloud the dispersive character of the quantum dynamics.

In order to analyze the dispersive dynamics of tunneling we consider in this paper the simple but not unrealistic case of two-level approximations to symmetric, bound, bi-stable systems whose energy spectrum is characterized by a structure of doublets. Each member of one doublet consists of symmetric/antisymmetric superpositions of localized states which
may be seen as coupled by effective tunneling amplitudes. In the two-level approximation
this is conveniently expressed in terms of a spin-1/2 algebra. Dissipation and decoherence
phenomena can be introduced in this description by coupling the two-level system to another
system, possibly with a continuous energy spectrum. A collection of harmonic oscillators is
frequently used in this connection, leading to the “spin-boson” model analyzed by Leggett
and collaborators[3]. There the effects of dissipation on the tunneling rates are studied
independently of explicit control of properties of the tunneling state relating to decoherence
processes. A simpler, soluble model, which allows for a control of this sort, results when
the two-level system is suitably coupled to a generic additional system with continuous
spectrum, as described in detail in section 3 below. In this model the coupled dynamics
can be reduced to the problem of the spreading of a product “doorway state” due to its
coupling to a continuous background also of product states, which allows for a treatment in
terms of the techniques developed long ago by Fano[4] in the context of atomic scattering
theory. While this schematic model is less “realistic” from the point of view of energy-loss
mechanisms, it retains the overall dynamical features of the spin-boson model relating to
cohherence-loss, which is our main concern here. The model allows for the calculation of the
reduced density associated with the two-level system at all times. Model dependences are
indicated by differences in the results obtained in the two cases. We find, in particular, that
transition rates out of a localized initial state can be substantially enhanced by decoherence
in strong coupling regimes.

The use of Master equations for the description of damped two-level systems is well
known[5]. The usual derivation of these equations[6] assume weak-coupling to an harmonic
oscillator reservoir and high temperature, so that their use in strong coupling and zero tem-
perature situations is not warranted. Comparison of the exact model results with solutions
of these Master equations agree for particular forms of the coupling independently of the
overall coupling strength and at zero temperature. In general, however, the perturbative
ingredients of the Master equation derivations appear as limiting factors.

2 Dissipative and unitary tunneling rates.

The quantum state of a two-level subsystem can be generally described in terms of a (time
dependent) hermitian reduced density operator of unit trace $\rho(t)$. The simple two-level
effective Hamiltonian

$$H_\sigma = \frac{\epsilon}{2} (\sigma_3 + \hat{1}_\sigma),$$

where $\hat{1}_\sigma$ stands for the unit $2 \times 2$ matrix, can be understood as describing the tunneling
between the “localized” (“left” and “right”) states

$$|l\rangle \equiv \frac{|+\rangle + |-\rangle}{\sqrt{2}} \quad \text{and} \quad |r\rangle \equiv \frac{|+\rangle - |-\rangle}{\sqrt{2}}$$

where $|\pm\rangle$ are the eigenvectors of the diagonal Pauli matrix $\sigma_3$, and hence also energy eigen-
states. The time dependent density matrix corresponding to the initial condition
\[ \rho(t = 0) = |l\rangle\langle l| \]  

is given in the \(|\pm\rangle\) basis as (with \(\hbar = 1\))

\[ \rho(t) = \frac{1}{2} \begin{pmatrix} 1 & e^{i\epsilon t} \\ e^{-i\epsilon t} & 1 \end{pmatrix} = \rho_2(t). \]  

As is well known, the property of idempotency is equivalent to the purity of the quantum state described by \(\rho(t)\). A tunneling probability \(P(t)\) can be defined as the probability of finding this system in the complementary localized state \(|r\rangle\) at time \(t\), and is readily calculated as

\[ P(t) = \text{Tr} [|r\rangle\langle r|\rho(t)] = \sin^2 \frac{\epsilon t}{2}. \]  

When the two-level subsystem is coupled to additional degrees of freedom its state at time \(t\) is still described by a reduced density matrix which is non-negative, hermitian and of unit trace, but in general not idempotent. In fact, the quantity \(\delta(t) = 1 - \text{Tr}[\rho(t)^2]\) (referred to as the linear entropy or the idempotency defect) is often used as a measure of the decoherence suffered by the two level subsystem through its coupling to the other degrees of freedom.

A most convenient way of representing such a reduced density matrix makes use of its eigenvalues and eigenvectors

\[ \rho(t)|t, k\rangle = p_k(t)|t, k\rangle, \quad k = 1, 2; \quad \langle t, k|t, k'\rangle = \delta_{kk'}, \quad 0 \leq p_k(t) \leq 1 \]

in terms of which one can write

\[ \rho(t) = \sum_k |t, k\rangle p_k(t)\langle t, k|. \]  

It should be noted that in general both the eigenvectors and the eigenvalues in (4) are time-dependent. While the eigenvectors evolve unitarily (as they define a time-dependent orthonormal basis in the quantum phase-space of the two-level subsystem) the time-dependence of the eigenvalues \(p_k(t)\) reveal the change in time of the coherence properties of the state of the two-level subsystem. The idempotency defect is in fact given in terms of the eigenvalues \(p_k(t)\) as

\[ \delta = 1 - \sum_k p_k(t)^2 = 2p_1(t)(1 - p_1(t)) \]  

where use has been made of the unit trace property of \(\rho(t)\). In the case of eq. (2), it can be easily checked that \(p_1 = 1\) and \(p_2 = 0\) at all times, so that \(\delta \equiv 0\). Assuming that the reduced density is that which evolves from the initial condition (1), the tunneling probability is now given by

\[ P(t) = \sum_k p_k(t)|\langle r|t, k|\rangle|^2. \]
In view of what has been said concerning the time-dependence of the ingredients of this expression, it is immediately clear that the tunneling rate

\[ R(t) \equiv \dot{P}(t) = \sum_k \dot{p}_k(t)|\langle r|t,k \rangle|^2 + \sum_k p_k(t) \frac{d}{dt}|\langle r|t,k \rangle|^2 \]

splits into two contributions which can be unambiguously ascribed to changes in the coherence properties of the state of the subsystem and to its unitary evolution, respectively:

\[ R_d(t) \equiv \sum_k \dot{p}_k(t)|\langle r|t,k \rangle|^2 = (2|\langle r|t,1 \rangle|^2 - 1)\dot{p}_1(t) \tag{6} \]

and

\[ R_u(t) \equiv \sum_k p_k(t) \frac{d}{dt}|\langle r|t,k \rangle|^2 = (2p_1(t) - 1)\frac{d}{dt}|\langle r|t,1 \rangle|^2. \tag{7} \]

The last forms of \( R_u \) and \( R_d \) make use of the unit trace of \( \rho \) and also of the normalization of \( |r\rangle \). In the case of the purely unitary time evolution under the simple two-level Hamiltonian \( H_{\sigma} \) one has of course \( R_d(t) \equiv 0 \) and \( R_u(t) = R(t) = (\epsilon/2) \sin \epsilon t \). This decomposition of transition rates in dissipative and unitary parts can be simply extended to cases involving reduced densities of larger dimensionality, as indicated in Appendix A.

3 Two-level tunneling with coupling to a continuum.

A simple model allowing for decoherence effects in the two-level tunneling processes is one in which the two-level subsystem described by the Hamiltonian \( H_{\sigma} \) is coupled to an additional "nondescript" set of degrees of freedom (which will be identified by means of a subscript \( b \)) to which is associated an energy spectrum containing one discrete state represented by a normalized state vector \( |0_b\rangle \) in addition to a continuum of states \( |\eta\rangle \), normalized in energy as \( \langle \eta|\eta'\rangle = \delta(\eta - \eta') \). The model is characterized further by the Hamiltonian

\[ H = \frac{\epsilon}{2}(\sigma_3 + \hat{1}_\sigma) \otimes \hat{1}_b + \left( |0_b\rangle e_0\langle 0_b| + \int_{\eta_0}^{\eta} d\eta \langle \eta|\eta\rangle \right) \otimes \hat{1}_\sigma \\
+ \frac{1}{2} \int_{\eta_0}^{\eta} d\eta \ [g(\eta)|\eta\rangle\sigma_-|0_b\rangle + g^*(\eta)|0_b\rangle\sigma_+\langle \eta|] \\
+ \frac{1}{2} \int_{\eta_0}^{\eta} d\eta \ [g'(\eta)|\eta\rangle\sigma_+|0_b\rangle + g'^*(\eta)|0_b\rangle\sigma_-\langle \eta|] \tag{8} \]

where \( g(\eta) \) and \( g'(\eta) \) are coupling matrix elements \( \langle -\eta|\hat{g} + 0_b \rangle \) and \( \langle +\eta|\hat{g}' - 0_b \rangle \) respectively, possibly dependent on \( \eta \). In the special case \( g(\eta) = g'(\eta) \) the coupling terms reduce to

\[ \sigma_x \int_{\eta_0}^{\eta} d\eta \ [\eta]g(\eta)|0_b\rangle + |0_b\rangle g^*(\eta)\langle \eta|] \]
which resembles in its structure the coupling term of the spin-boson model\[3].

A basis in the quantum phase-space of the composite system described by equation (8) can be constructed as \( \{ |s_0 \rangle, \{ |s\eta \rangle \} \) \( s = +, - \), \( \eta_0 \leq \eta \leq \bar{\eta} \), and the adopted structure of the coupling terms shows that the subspaces spanned by the two sets of basis vectors \( \{ |+0 \rangle, \{ |\eta \rangle \} \) and \( \{ |-0 \rangle, \{ |+\eta \rangle \} \) are closed under the action of \( H \). Different choices for the model parameters \( \epsilon, e_0 \), the span of the continuum band \( \eta_0 \) to \( \bar{\eta} \) and the \( \eta \)-dependence of the coupling functions \( g \) and \( g' \) allow for a considerable variety of dynamical regimes. Closest to the situation described by the spin-boson model is that in which \( e_0 = \eta_0 = 0 \) with \( g(\eta) = g^*(\eta) = g'(\eta) \). Some aspects of the relationship of these two models are briefly discussed in Appendix B. The particular version of the model which will be used in the following sections differs from this, however. A manifest feature of this version is the assumption that one has

\[ \eta_0 \ll e_0 \quad \text{and} \quad e_0 + \epsilon \ll \bar{\eta} \]

so that the two product states \( | \pm 0 \rangle \), with eigen-energies \( e_0 \) and \( e_0 + \epsilon \) fall well within a sufficiently wide continuum band of product states \( \{ \pm \eta \} \). This feature will in fact allow for the continuum spreading of the states \( |+0 \rangle \) and \( |-0 \rangle \) through their coupling with states \( |-\eta \rangle \) and \( |+\eta \rangle \) respectively with spreading widths appreciably larger than the doublet splitting \( \epsilon \), a situation which will be seen to characterize strong damping regimes. Furthermore, since these two spreadings are dynamically independent, as they take place in different invariant subspaces of \( H \), there will be in general two distinct relaxation times associated with the damped two-level subsystem.

General state vectors in each of the invariant subspaces of \( H \) can be written as

\[
\begin{align*}
|\psi_a \rangle &= a_0 | +0 \rangle + \int_{\eta_0}^{\bar{\eta}} d\eta A(\eta) | -\eta \rangle \\
|\psi_b \rangle &= b_0 | -0 \rangle + \int_{\eta_0}^{\bar{\eta}} d\eta B(\eta) | +\eta \rangle.
\end{align*}
\]

In terms of these expansions, the eigenvalue problem for \( H \)

\[
(E - H) |\psi_{a,b}^{(E)} \rangle = 0
\]

can be reduced to two independent pairs of coupled equations with similar structure for the expansion coefficients

\[
\begin{align*}
(E - \epsilon - e_0) a_0^{(E)} &= \int_{\eta_0}^{\bar{\eta}} d\eta g^*(\eta) A^{(E)}(\eta), \\
(E - \eta) A^{(E)}(\eta) &= g(\eta) a_0^{(E)}
\end{align*}
\]  

and

5
\((E - e_0)b_0^{(E)} = \int_{\eta_0}^{\bar{\eta}} d\eta \ g^*(\eta)B^{(E)}(\eta),\)

\((E - \epsilon - \eta)B^{(E)}(\eta) = g'(\eta)b_0^{(E)}.\)  \((10)\)

The solutions of these coupled equations has been given long ago by Fano\(^4\) and van Kampen\(^7\). In the case of eqs. \((9)\) one has

\(|a_0^{(E)}|^2 = \frac{|g(E)|^2}{[E - \epsilon - e_0 - F(E)]^2 + \pi^2|g(E)|^4} \quad (11)\)

with \(F(E)\) given by the principal value integral

\[ F(E) = \mathcal{P} \int_{\eta_0}^{\bar{\eta}} d\eta \ \frac{|g(\eta)|^2}{E - \eta}. \quad (12)\]

The continuum coefficients are

\[ A^{(E)}(\eta) = \left[ \mathcal{P} \frac{E - \eta + z(E)\delta(E - \eta)}{E - \eta} \right] g(\eta)a_0^{(E)} \quad (13)\]

with

\[ z(E) = \frac{E - \epsilon - e_0 - F(E)}{|g(E)|^2}. \]

The value of the amplitude \(a_0^{(E)}\) involves a phasing convention which is subsequently carried over to the \(A^{(E)}(\eta)\) through equation \((13)\). The solution of eqs. \((10)\) is of course completely analogous and does not have to be given explicitly here.

Strictly speaking, when the integration limits of the continuum variable \(\eta\) are finite, the spectrum of \(H\) may include discrete states outside the continuum range, subject to the \(\eta\)-dependence of the coupling parameters \(g(\eta)\). Whenever needed, the discrete eigenvalues of \(H\) can be obtained (e.g. in the case of eqs. \((9)\) as solutions \(E_d < \eta_0\) or \(E_d > \bar{\eta}\) of the dispersion equation

\[ E - \epsilon - e_0 = \int_{\eta_0}^{\bar{\eta}} d\eta \ \frac{|g(\eta)|^2}{E - \eta}. \]

In this case eq. \((13)\) is replaced by

\[ A^{(E_d)}(\eta) = \frac{g(\eta)}{E_d - \eta} \]

and \(a_0^{(E)}\) is determined from the normalization condition (up to an arbitrary phase factor) as
\[ |a_0^{(E_d)}|^2 = \left(1 - \left(\frac{dF(E)}{dE}\right)_{E=E_d}\right)^{-1}. \]

The low-energy discrete solutions are specially relevant for comparison of this model with other models of the damping mechanism, such as the many-oscillators model (see Appendix B).

### 3.1 Time evolution of a localized initial condition.

Using the stationary states of \( H \) as determined above one can write the time evolution of the localized initial state

\[ |t = 0\rangle = \frac{|+\rangle + |-\rangle}{\sqrt{2}} \otimes |0_b\rangle = |l\rangle \otimes |0_b\rangle. \quad (14) \]

Note that in the absence of coupling, \( g(\eta) = g'(\eta) = 0 \), the time evolution reduces to that found in section 2. In general, the component states \(|+ 0_b\rangle\) and \(|- 0_b\rangle\) can be written in terms of the stationary states determined from the solutions of eqs. (9) and (10), so that

\[ |t\rangle = e^{-iHt}|t = 0\rangle = \frac{e^{-iHt}}{\sqrt{2}} \left( \sum_{E_d} a_0^{(E_d)} |\psi_a^{(E_d)}\rangle + \int_{\eta_0}^{\eta} dE \ a_0^{(E)*} |\psi_a^{(E)}\rangle \right) \]

\[ + \sum_{E_d} b_0^{(E_d)} |\psi_b^{(E_d)}\rangle + \int_{\eta_0}^{\eta} dE \ b_0^{(E)*} |\psi_a^{(E)}\rangle \right) \]

When the continuum range extends over a sufficiently broad energy interval on both sides of \( e_0 \) the discrete state amplitudes \( a_0^{(E_d)} \) and \( b_0^{(E_d)} \) become very small and can be neglected. In what follows we assume this to be the case in order to avoid unessential complications. By re-expressing the stationary states in terms of the factorized bases, forming the total density \( |t\rangle\langle t| \) and taking its trace over the \( b \)-states one obtains for the reduced density of the two level system at time \( t \)

\[ \rho(t) = \begin{pmatrix} \rho_{++}(t) & \rho_{+-}(t) \\ \rho_{-+}^{\ast}(t) & 1 - \rho_{++}(t) \end{pmatrix} \]

with

\[ \rho_{++}(t) = \frac{1}{2} \left( 1 + \left| \int_{\eta_0}^{\eta} dE \ |a_0^{(E)}|^2 e^{-iEt}\right|^2 - \left| \int_{\eta_0}^{\eta} dE \ |b_0^{(E)}|^2 e^{-iEt}\right|^2 \right) \quad (15) \]

and
\[
\rho_{+-}(t) = \frac{1}{2} \left( \int_{\eta_0}^{\eta} dE |a_0^{(E)}|^2 e^{-iEt} \int_{\eta_0}^{\eta} dE' |b_0^{(E')}|^2 e^{-iE't} + \int_{\eta_0}^{\eta} dE \int_{\eta_0}^{\eta} dE' b_0^{(E')}*a_0^{(E)} e^{-i(E-E')t} \int_{\eta_0}^{\eta} d\eta B^{(E)}(\eta) A^{(E')}*(\eta) \right). \tag{16}
\]

The last term of eq. (16) is the only one in which the continuum amplitudes \(A^{(E')}(\eta)\) and \(B^{(E)}(\eta)\) intervene explicitly. This term describes a re-correlation of components of the state of the two-level system in the single continuum subspace of system \(b\), to which they couple through \(g(\eta)\) and \(g'(\eta)\). In fact, a simple variant of the model that avoids this re-correlation process can be devised by adding a second continuum \{\(\zeta\}\} orthogonal to the first, i.e. \(\langle \eta | \zeta \rangle \equiv 0\), to which the component \(|-0_b\rangle\) is coupled through \(g'(\zeta)\). It is easy to see that the resulting expressions for \(\rho_{++}\) and \(\rho_{+-}\) are in this case identical to eqs. (15) and (16) except for the absence of the last term in the latter.

The tunneling probability at time \(t\) of the two-level subsystem, from the initial state \(|l\rangle\) to the complementarily localized state \(|r\rangle\), defined in terms of the reduced density matrix \(\rho(t)\) as in eq. (3), is generally given as

\[
P(t) = \text{Tr} [\langle r | r | \rho(t) \rangle] = \frac{1}{2} (1 - 2 \text{Re} \rho_{+-}) \tag{17}
\]

and the idempotency defect (5) of the reduced density is

\[
\delta(t) = 2 \left[ \rho_{++}(t) (1 - \rho_{++}(t)) - |\rho_{+-}(t)|^2 \right] = 2 \det \rho(t). \tag{18}
\]

### 3.2 Special case: single relaxation time.

An interesting particular case is that in which \(g'(\eta) \equiv 0\), so that \(|-0_b\rangle\) is a stationary state of \(H\) while \(|+0_b\rangle\) is spread through its coupling to the \(|-\eta\rangle\) continuum. In this case the reduced density matrix elements are simply given in terms of the spectral distribution \(|a_0^{(E)}|^2\), eq. (11), of the state \(|+0_b\rangle\) as

\[
\rho_{++}(t) \rightarrow \frac{1}{2} \left| \int_{\eta_0}^{\eta} dE |a_0^{(E)}|^2 e^{-iEt} \right|^2, \quad g'(\eta) \equiv 0 \tag{19}
\]

and

\[
\rho_{+-}(t) \rightarrow \frac{1}{2} \int_{\eta_0}^{\eta} dE |a_0^{(E)}|^2 e^{-i(E-E_0)t}, \quad g'(\eta) \equiv 0. \tag{20}
\]

These expressions can be immediately evaluated in closed form when the matrix elements \(g(\eta)\) are independent of \(\eta\), and the energy shift \(F(E)\), eq. (12) is slowly energy dependent over an interval of the order of \(\pi |g|^2\) in the neighborhood of \(E = \epsilon + e_0\). This will in fact be the case when the continuum range extends over sufficiently broad intervals both above and below this energy. Equation (11) is then well approximated by the Breit-Wigner form
\[ |a_0^{(E)}|^2 \rightarrow \frac{|g|^2}{(E - e_R)^2 + \pi^2 g^2} = \frac{1}{2\pi} \frac{\Gamma}{(E - e_R)^2 - \pi^2} \]

where \( e_R - \epsilon - e_0 - F(e_R) = 0 \) and \( \Gamma = 2\pi|g|^2 \) is the usual width parameter of the Breit-Wigner distribution, given in Golden Rule form. Note that for large \( \bar{\eta} - e_0 \simeq e_0 - \eta_0 \) one has \( F(e_R) \simeq F(e_0) \simeq 0 \) so that \( e_R - e_0 \simeq \epsilon \). Extending the integration limits to \( \pm \infty \) one obtains by simple contour integrations

\[ \rho_{++}(t) = \frac{1}{2} e^{-\Gamma t} \quad \text{and} \quad \rho_{+-}(t) = \frac{1}{2} e^{-i(e_R-e_0)t-\frac{\pi}{2}} \]  

so that

\[ P(t) = \frac{1}{2} \left( 1 - e^{-\frac{\pi}{2}} \cos(e_R - e_0)t \right). \]  

It should be kept in mind that the model assumptions allow \( \Gamma > \epsilon \), in which case the initial time-dependence of \( P(t) \) is dominated by the decaying exponential factor. The decoherence process undergone by the reduced density as measured by the idempotency defect \( \delta(t) \) is given by

\[ \delta(t) = \frac{1}{2} e^{-\Gamma t} \left( 1 - e^{-\Gamma t} \right) \]

so that the tunneling and the decoherence rates

\[ \dot{P}(t) = \frac{e^{-\frac{\pi}{2}}}{2} \left( \frac{\Gamma}{2} \cos(e_R - e_0)t + (e_R - e_0) \sin(e_R - e_0)t \right) \]

and

\[ \dot{\delta}(t) = \frac{\Gamma}{2} e^{-\Gamma t} \left( 2e^{-\Gamma t} - 1 \right) \]

are both proportional to the damping width \( \Gamma \), related to the single relaxation time \( \tau_d \) defined as \( \tau_d = 1/\Gamma \). Moreover, \( \dot{P}(t) \) contains the period of unitary evolution \( \tau_u \equiv 2\pi/(e_R - e_0) \simeq 2\pi/\epsilon \) as an additional, independent time scale. In the strong coupling regime \( \tau_d \ll \tau_u \) eq. (22) shows dominance of coherence loss effects in \( P(t) \) for times \( t < \tau_d \) leading eventually to saturation at \( P = 1/2 \). The sorting of dissipative and unitary contributions to the tunneling rate \( \dot{P}(t) \) is achieved through the calculation of the rates \( R_d(t) \) and \( R_u(t) \) introduced in section 2. As shown in eqs. (3) and (4), this involves the time dependence of the eigenvalues and eigenvectors of the reduced density. The relevant ingredients can be expressed in a straightforward way in terms of the reduced density matrix elements \( \rho_{++}(t) \) and \( \rho_{+-}(t) \). Since the resulting expressions are lengthy and not particularly illuminating they will not be given here. Numerical results illustrating these features, obtained using the matrix elements given in eq. (21), are shown in figs. 1 and 2 respectively for the weak and strong coupling regimes. The figures show \( P(t), \delta(t) \) and the tunneling rates \( \dot{P}(t), R_d(t) \) and \( R_u(t) \). The correlation of \( \delta(t) \) with \( R_d(t) \) and the dominance of the latter over \( R_u(t) \) in the strong coupling regime are clearly seen.
3.3 General case: two relaxation times.

When both \( g(\eta) \) and \( g'(\eta) \) are different from zero the matrix elements of the reduced densities are given by the complete expressions (15) and (16). Using the tunneling initial condition of subsection 3.1 and under the assumptions used in subsection 3.2 the first of these can be evaluated to yield

\[
\rho_{++}(t) = \frac{1}{2} \left( 1 + e^{-\Gamma t} - e^{-\Gamma' t} \right)
\]  

(24)

where \( \Gamma' \), defined as the width parameter \( \Gamma' = 2\pi |g'|^2 \) \((g' \text{ having been assumed to be independent of } \eta)\) of the distribution

\[
|b_0^{(E)}|^2 = \frac{1}{2\pi} \frac{\Gamma'}{(E - e_R')^2 + \frac{\Gamma'^2}{4}},
\]

introduces an additional time scale in the evolution of the composite system. As for \( \rho_{+-} \) one gets, from eq. (16), using eq. (13) and the methods of ref. [4]

\[
\rho_{+-}(t) = \frac{1}{2} \left[ e^{-i(e_R - e_R')t - \frac{\Gamma + \Gamma'}{2} t} + 2\sqrt{\Gamma\Gamma'} e^{i(e_R - e_R')t} \left( 1 - e^{-\frac{\Gamma + \Gamma'}{2} t} \right) \right]
\]

(25)

where the last term is due to the re-correlation processes mentioned in subsection 3.1. Note that under conditions in which the shift functions \( F(e_R) \) and \( F'(e_R') \) are small one has \( e_R - e_R' \simeq \epsilon \). This will be assumed to be the case from here on in order to save notation.

The tunneling probability is given by eq. (17) as

\[
P(t) = \frac{1}{2} - \frac{\cos \epsilon t}{2} \left[ \frac{2\sqrt{\Gamma\Gamma'}}{\Gamma + \Gamma'} + e^{-\frac{\Gamma + \Gamma'}{2} t} \left( 1 - \frac{2\sqrt{\Gamma\Gamma'}}{\Gamma + \Gamma'} \right) \right]
\]

(26)

which shows that the re-correlation processes give rise to steady state oscillations of \( P(t) \) after the transient associated with the decaying exponential has died down. The amplitude of the steady-state oscillations depends on the damping widths \( \Gamma \) and \( \Gamma' \), however, and is maximum when \( \Gamma = \Gamma' \), in which case the transient actually cancels out and the undamped form of \( P(t) \), eq. (3), is recovered.

This last result does not imply, however, that there is no decoherence when \( \Gamma = \Gamma' \). The general expression for \( \delta(t) \) obtained from eq. (18) can be written as

\[
\delta(t) = \frac{1}{2} \left( 1 + e^{-\Gamma t} - e^{-\Gamma' t} \right) \left( 1 - e^{-\Gamma t} + e^{-\Gamma' t} \right) - \frac{1}{2} e^{-(\Gamma + \Gamma') t} - \frac{2\sqrt{\Gamma\Gamma'}}{\Gamma + \Gamma'} \left( 1 - e^{-\frac{\Gamma + \Gamma'}{2} t} \right) \left[ e^{-\frac{\Gamma + \Gamma'}{2} t} \cos \epsilon t + \frac{\sqrt{\Gamma\Gamma'}}{\Gamma + \Gamma'} \left( 1 - e^{-\frac{\Gamma + \Gamma'}{2} t} \right) \right]
\]

and reduces, when \( \Gamma = \Gamma' \), to

\[
\delta(t) \xrightarrow{\Gamma=\Gamma'} 2e^{-\Gamma t} \left( 1 - e^{-\Gamma t} \right) \sin^2 \epsilon t
\]
which vanishes only asymptotically, as $t \to \infty$. In the general case $\Gamma \neq \Gamma'$ with $\Gamma, \Gamma' \neq 0$, one has the asymptotic limit

$$
\lim_{t \to \infty} \delta(t) = \frac{1}{2} - \frac{2\Gamma \Gamma'}{(\Gamma + \Gamma')^2}.
$$

The restriction $\Gamma, \Gamma' \neq 0$ is necessary since the limit $t \to \infty$ does not commute with the limit $\Gamma' \to 0$. If the alternate version of the model with two orthogonal continua is used, all terms involving factors $\sqrt{\Gamma \Gamma' / (\Gamma + \Gamma')}$ are absent, both in $P(t)$ and in $\delta(t)$. In this case the two-level system decoheres maximally when $t \to \infty$ as two orthogonal components of the two-level subsystem become correlated to orthogonal continuum wave packets.

The dissipative and unitary tunneling rates $R_d$ and $R_u$ can also be obtained from the reduced density in a straightforward way. A typical result for moderately strong coupling is shown in fig. 3.

3.4 Interpretation of model results.

In spite of the schematic character of the model, the features emerging from its analysis underline relevant aspects which should be kept in mind in the study of more realistic cases. As shown explicitly e.g. in the general equation (17), the coherence properties directly relevant for localization are, in the representation used there, contained in the real part of the matrix element $\rho_{+-}$. The harmonic time dependence of this quantity in the absence of any external entanglements is modified when these effects are turned on by making $g$ and $g'$ (or, equivalently, $\Gamma$ and $\Gamma'$) different from zero, as can be read from the time dependent term of equation (26). In the case considered in section 3.2 ($\Gamma \neq 0$, $\Gamma' = 0$) the harmonic oscillations are damped by the effects of the external coupling, leading, in the strong coupling limit, to tunneling rates dominated by the associated relaxation times, rather than by the oscillation period. When also $\Gamma' \neq 0$, on the other hand, a new undamped oscillatory term arises due to contributions to $\text{Re} \rho_{+-}$ coming from continuum components, an effect which has been referred to as a re-correlation process in section 3.3. The amplitude of the damped component is at the same time reduced, leading to its complete cancellation in the limiting case $\Gamma = \Gamma' \neq 0$.

It is important to stress that the coherence properties bearing on the purity of the complete tunneling state, which can be measured in a basis-independent way in terms of the determinant of the reduced density matrix (see equation (18)), involve other dynamic quantities besides the localization-specific correlation part $\text{Re} \rho_{+-}$, and therefore in general correlate poorly with the tunneling probability $P(t)$. In particular, when $\Gamma = \Gamma' \neq 0$ the transient decoherence undergone by the tunneling state has no effect on the tunneling probability, since the localization-specific coherence properties remain the same as in the absence of the external couplings due to the re-correlation process. The decomposition of the tunneling rate $\dot{P}(t)$ into dissipative and unitary parts $R_d(t)$ and $R_u(t)$ can thus be seen as expressing the dependence of the time rate of change of the localization-specific correlation part $\text{Re} \rho_{+-}$ in terms of contributions associated to the (unitary) time evolution of the
eigenvectors and from the (non-unitary) time evolution of the eigenvalues of the reduced density which describes the tunneling state. Only the latter contributions relate to the overall decoherence of the tunneling state.

4 Master equation results.

The dissipative dynamics of the reduced density matrix of a two-level system is often described in terms of a master equation valid in a weak-coupling regime, derived [6] under the assumption of linear coupling to a reservoir of harmonic oscillators, which is subsequently eliminated from the description under the assumption of the validity of a Born-Markov approximation. In addition, one assumes in the derivation that correlation functions involving reservoir degrees of freedom can be meaningfully evaluated for all times using the initial state of the reservoir, usually taken to be a thermal equilibrium state. The usual form of the master equation [5] is obtained assuming that the coupling to the reservoir is given by

\[ H_{\text{int}} = \sum_k \left( g_k b_k^\dagger \sigma_- + g_k^* b_k \sigma_+ \right) \]

where \( b_k, b_k^\dagger \) are the lowering and rising operators for the \( k \)-th bath oscillator. This coupling term is similar to the term involving \( g(\eta) \) in eq. (8) if one associates the ground state of the reservoir with the discrete state \( |0_b\rangle \) of the model. The resulting form of the equation is then, in the limit of zero temperature,

\[ \dot{\rho}(t) = -i \frac{\epsilon}{2} [\sigma_3, \rho(t)] + \frac{\gamma}{2} (2\sigma_- \rho(t) \sigma_+ - \sigma_+ \sigma_- \rho(t) - \rho(t) \sigma_+ \sigma_-) \]

where \( \gamma \) is a damping coefficient related to \( H_{\text{int}} \) and to the distribution of reservoir frequencies.

The solution of this equation satisfying the initial condition

\[ \rho_{++}(0) = \rho_{+-}(0) = \frac{1}{2} \]

is

\[ \rho_{++}(t) = \frac{1}{2} e^{-\gamma t} \quad \text{and} \quad \rho_{+-}(t) = \frac{1}{2} e^{i\epsilon t - \frac{\gamma}{2} t} \]

which reproduces the result (21), with the correspondence \( \gamma \leftrightarrow \Gamma \), up to details related to the shift function \( F(E) \) in that case. It should be kept in mind, however, that the derivation of the master equation is limited to weak coupling regimes due to the Born-Markov approximation.

One may next try and include effects analogous to those produced by the coupling term involving \( g'(\eta) \) in the model Hamiltonian (8) by adding a new term to \( H_{\text{int}} \) in the derivation of the master equation. Thus, using now

\[ H_{\text{int}} \rightarrow \sum_k \left( g_k b_k^\dagger \sigma_- + g_k^* b_k \sigma_+ \right) + \sum_k \left( g'_k b_k^\dagger \sigma_+ + g'_k^* b_k \sigma_- \right) \]
we obtain, following the standard derivation procedure [6], the modified master equation

$$\dot{\rho}(t) = -i\frac{\epsilon}{2} [\sigma_3, \rho(t)] + \frac{\gamma}{2} (2\sigma_-\rho(t)\sigma_+ - \sigma_+\sigma_-\rho(t) - \rho(t)\sigma_+\sigma_-)$$

$$+ \frac{\gamma'}{2} (2\sigma_+\rho(t)\sigma_- - \sigma_-\sigma_+\rho(t) - \rho(t)\sigma_-\sigma_+) + \frac{\sqrt{\gamma\gamma'}}{\gamma} (2\sigma_+\rho(t)\sigma_+ + 2\sigma_-\rho(t)\sigma_-)$$

(28)

where \(\gamma'\) is the constant analogous to \(\gamma\) but related to the new terms added to \(H_{\text{int}}\). The solution of this equation satisfying the same initial condition (27) is

$$\rho_{++}(t) = \frac{1}{2} e^{-\gamma' t} + \frac{\gamma'}{\gamma + \gamma'} \left(1 - e^{-(\gamma + \gamma') t}\right)$$

and

$$\rho_{+\pm}(t) = \frac{e^{-(\gamma + \gamma') t}}{2\sqrt{\epsilon^2 - \gamma\gamma'}} \left[ \sqrt{\gamma\gamma'} - i\epsilon \sin \left(2\sqrt{\epsilon^2 - \gamma\gamma'} t \right) + \sqrt{\epsilon^2 - \gamma\gamma'} \cos \left(2\sqrt{\epsilon^2 - \gamma\gamma'} t \right) \right]$$

which is different from the corresponding results obtained in subsection 3.3. In particular, the model result for \(\rho_{++}(t)\), eq. (24), involves two relaxation times associated to the damping widths \(\Gamma\) and \(\Gamma'\) appearing in the difference of separate exponentials, while the master equation result involves just one “effective” relaxation time appearing in a single exponential involving the sum \(\gamma + \gamma'\). The relation between these two results can be revealed by expanding both solutions to first order in the damping parameters. One obtains, from the master equation result,

$$\rho_{++}(t) \to \frac{1}{2} - \frac{\gamma}{2} t + \frac{\gamma'}{2} t$$

which is identical to what one obtains from eq. (24) with the replacements \(\gamma \leftrightarrow \Gamma\) and \(\gamma' \leftrightarrow \Gamma'\). The expansion of the master equation result for \(\rho_{+\pm}(t)\) coincides likewise with the expansion of eq. (23). These facts can be understood by recalling that a Born-Markov approximation is involved in the derivation of the master equation. The Born approximation implies a truncation of an expansion in the couplings, producing a result which is subsequently “exponentiated” to all orders through the Markov assumption. As a result of this there is no general guarantee for results of the master equation which go beyond the order of the truncation involved in the Born approximation. In particular, the dynamics leading to two different relaxation times is not properly accounted for. Note, in this connection, that when \(\gamma = \gamma'\) (i.e. when the two relaxation times coincide) the master equation result reproduces the model result up to a small shift of the bare frequency \(\epsilon\), if one restricts oneself to weak coupling regimes.

It may be argued that the master equation (28) is derived on the assumption of a reservoir of harmonic oscillators, which differs from the dynamical assumptions of the model defined by the Hamiltonian (8). However, the same master equation also follows from this Hamiltonian, with the usual (in fact, even somewhat weaker) derivation assumptions, establishing, in particular, the correspondence \(\gamma \leftrightarrow \Gamma\) and \(\gamma' \leftrightarrow \Gamma'\). The Born approximation has to be performed in the same way in both cases, indicating again that it is at the root of the discussed discrepancies.
5 Concluding remarks.

The main general conclusion to be drawn from the analysis of the model described by the Hamiltonian (8) with localized initial condition (14) is that a clear distinction should be made between coherence properties relating a) to localization in the tunneling degree of freedom and b) to the degree of quantum purity of the reduced density (4) describing the quantum state of the tunneling system, as measured e.g. by the linear entropy (5). Coherence properties of class a) are carried by the real part of off-diagonal matrix element $\rho_{+-}(t)$ in the basis which diagonalizes $H_\sigma$ or, equivalently, by the diagonal matrix elements in the localized basis $\{|r\rangle, |l\rangle\}$, e.g. $\rho_{rr}(t) = 1/2 - \text{Re}\rho_{+-} = P(t)$. Coherence properties of class b), on the other hand, are carried by the eigenvalues of the reduced density, and involve therefore other dynamic quantities in addition to that which is relevant for class a).

The contribution of decoherence processes undergone by the reduced density to the coherence properties of class a) can be isolated through the general decomposition of the tunneling rate $\dot{P}(t)$ into dissipative and unitary parts, eqs. (7) and (6). Results for the damped two-level model show that the dissipative component contributes most at times short on the scale of the bare frequency $\epsilon$. The enhanced initial tunneling rate in the strong coupling case with no re-correlation effects (see fig. 2) is dominated by the dissipative component, and can thus be interpreted in terms of a large effect of the coherence loss of the tunneling state also on the localization-specific correlation properties of the initial state of the two-level subsystem.

Comparison of the exact solution of the model with master equation results derived in the usual way from the model Hamiltonian indicates that master equations appear to be inadequate to deal with situations involving more than a single relaxation time. This difficulty can be ascribed to the Born approximation involved in the derivation of these equations.

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Appendix A.

A general reduced density matrix can always be written in terms of its time dependent natural orbitals $|n(t)\rangle$ and associated eigenvalues $p_n(t)$ as

$$\rho(t) = \sum_n |n(t)\rangle p_n(t) \langle n(t)|.$$  

The probability that the state thus described is found in a given (time independent) subspace defined in terms of a projector

$$\mathcal{P} \equiv \sum_k |b_k\rangle \langle b_k|,$$  

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where the \( |b_k\rangle \) constitute an orthonormal set of state vectors, is given by

\[
P(t) = \text{Tr} [\rho(t)P].
\]

The vectors \( |b_k\rangle \) can be expanded in the natural orbitals of \( \rho(t) \) as \( |b_k\rangle = \sum_n \beta_n^{(k)}(t)|n(t)\rangle \) so that \( P(t) \) is expressed as

\[
P(t) = \sum_n p_n(t) \sum_k |\beta_n^{(k)}|^2.
\]

Derivation with respect to time then gives dissipative and unitary contributions proportional to \( \dot{p}_n \) and \( \dot{\beta}_n^{(k)} \) respectively.

**Appendix B.**

In view of the widespread use of coordinate coupling to a collection of harmonic oscillators in order to introduce damping effects on the dynamics of simple quantum-mechanical systems (including two-level systems), and since the results obtained in this way seem to be at variance with those of the continuum model for the damping as used in section \( \S \) this Appendix deals briefly with a comparison of features of the two models. Instead of the implementation which minimizes “threshold” effects adopted in that section, the case \( e_0 \simeq \eta_0 \simeq 0 \) with \( g(\eta) = g^*(\eta) = g'(\eta) \) of the continuum model will be considered, together with with the “zero bias” spin-boson model \( \S \).

In both cases the Hamiltonian can be split as \( H = H_\sigma + H_b + H_{\text{int}} \) with \( H_\sigma = \frac{i}{2} \sigma_3 \) and

\[
H_b = |0_b\rangle e_0 \langle 0_b | + \int_{\eta_0}^{\eta} d\eta |\eta\rangle \eta \langle \eta |, \quad H_{\text{int}} = \sigma_1 \int_{\eta_0}^{\eta} d\eta g(\eta) (|\eta\rangle \langle 0_b | + |0_b\rangle \langle \eta |) \equiv \sigma_1 G
\]

for the continuum model of equation (8) and

\[
H_b = \sum_\alpha \hbar \omega_\alpha a_\alpha^\dagger a_\alpha, \quad H_{\text{int}} = \sigma_1 \sum_\alpha g_\alpha \sqrt{\frac{\hbar}{2m_\alpha \omega_\alpha}} (a_\alpha^\dagger + a_\alpha) \equiv \sigma_1 G.
\]

for the spin-boson model. A useful way of representing these operators uses the spin basis of localized states in which \( \sigma_1 \) is diagonal. The Hamiltonian is then represented in both cases as

\[
H = \begin{pmatrix}
H_b + G & -\frac{i}{2}\epsilon \\
\frac{i}{2}\epsilon & H_b - G
\end{pmatrix}.
\]

The operators \( H_b \pm G \) can be separately diagonalized exactly in the two cases. This solves the problem completely in the extreme adiabatic limit \( \epsilon \to 0 \). In general, matrix elements in the off-diagonal blocks involving \( H_\sigma \) are modified by overlap factors involving eigenstates of
the two operators $H_b \pm G$. Rather than dealing with the full problem, we restrict ourselves to the perturbative effects of $H_b$ for the lowest adiabatic states. These are, in both cases, a degenerate doublet which we denote by $|\phi_0^\pm\rangle$, with energy $E_0$. The secular matrix to be considered is then

$$
\begin{pmatrix}
E_0 & -\frac{i}{2} \epsilon \langle \phi_0^+ | \phi_0^- \rangle \\
\frac{i}{2} \epsilon \langle \phi_0^- | \phi_0^+ \rangle & E_0
\end{pmatrix}.
$$

In the case of the spin-boson model the overlap $\langle \phi_0^+ | \phi_0^- \rangle$ involves oscillator coherent states with opposite displacements which depend, in particular, on the coupling constants $g_\alpha$. The ensuing reduction of the overlap implies the reduction of the splitting of the perturbed states, favoring the slowing down of transition rates out of localized states. In the case of the continuum model, on the other hand, $E_0$ is the root which lies below $\eta_0$ of the dispersion equation

$$E_0 - e_0 = \int_{\eta_0}^{\eta} d\eta \frac{g^2(\eta)}{E_0 - \eta}.
$$

The corresponding unperturbed states can be expanded as

$$|\phi_0^{(\pm)}\rangle = a_0^{(\pm)} |0\rangle + \int_{\eta_0}^{\eta} d\eta A^{(\pm)}(\eta) |\eta\rangle$$

the expansion coefficients being given by

$$|a_0^{(\pm)}|^2 = \frac{1}{1 + \frac{1}{4} \int_{\eta_0}^{\eta} d\eta \frac{g^2(\eta)}{(E_0 - \eta)^2}}$$

and

$$A^{(\pm)}(\eta) = \pm \frac{g(\eta)}{E_0 - \eta} a_0^{(\pm)}.
$$

and the overlap factor is

$$\langle \phi_0^{(+)} | \phi_0^{(-)} \rangle = \frac{1 - \frac{1}{4} \int_{\eta_0}^{\eta} d\eta \frac{g^2(\eta)}{(E_0 - \eta)^2}}{1 + \frac{1}{4} \int_{\eta_0}^{\eta} d\eta \frac{g^2(\eta)}{(E_0 - \eta)^2}}.
$$

The behavior of this object involves the energy dependence of the coupling function $g(\eta)$ and of the solution $E_0$ of the dispersion equation. In the case when $g^2(\eta) = \gamma \eta^s$, with $0 \leq s < 1$ one finds, for fixed $e_0 = \eta_0 = 0$ that $E_0$ approaches minus infinity and $|a_0^{(\pm)}|^2$ approaches unity as the high energy cut-off $\bar{\eta}$ increases. In the same limit the overlap also approaches unity and the transition rate out of the localized states approaches its free value. For values of $\bar{\eta}$ not too large in comparison with $\epsilon$ the overlap is smaller than one, leading to a quenching of this transition rate. These behaviors are supported by exact numerical results.
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Figure captions.

Fig. 1 - Tunneling probability $P(t)$, idempotency defect $\delta(t)$ (top) and tunneling rates $R_d(t)$, $R_u(t)$ and $\dot{P}(t) = R_d(t) + R_u(t)$ (bottom) in the single finite relaxation time, weak-coupling case with parameters $\Gamma = 0.3$ and $\epsilon = 1$. The time scale is defined so that $\bar{t} = 1$.

Fig. 2 - Same as Figure 1 in the single finite relaxation time, strong coupling case with parameters $\Gamma = 3$, $\epsilon = 1$. Note the smaller depth of the time scale in this case.

Fig. 3 - Same as Figure 1 in the case of two finite relaxation times with parameters $\Gamma = 2$, $\Gamma' = .5$, $\epsilon = 1$. 
Figure 1: Tunneling probability $P(t)$, idempotency defect $\delta(t)$ (top) and tunneling rates $R_d(t)$, $R_u(t)$ and $\dot{P}(t) = R_d(t) + R_u(t)$ (bottom) in the single finite relaxation time, weak-coupling case with parameters $\Gamma = 0.3$ and $\epsilon = 1$. The time scale is defined so that $\bar{\hbar} = 1$.

Figure 2: Same as Figure 1 in the of single finite relaxation time, strong coupling case with parameters $\Gamma = 3$, $\epsilon = 1$. Note the smaller depth of the time scale in this case.

Figure 3: Same as Figure 1 in the case of two finite relaxation times, with parameters $\Gamma = 2$, $\Gamma' = .5$, $\epsilon = 1$. 