

Coherence and Decoherence in Tunneling between Quantum Dots

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Coupled quantum dots are an example of the ubiquitous quantum double potential well. In a typical transport experiment, each quantum dot is also coupled to a continuum of states. Our approach takes this into account by using a Green's function formalism to solve the full system. The time-dependent solution is then explored in different limiting cases. In general, a combination of coherent and incoherent behavior is observed. In the case that the coupling of each dot to the macroscopic world is equal, however, the time evolution is purely coherent.

The double-well potential is one of the simplest and best understood problems in modern quantum mechanics. Its utility is likewise unparalleled. Potential applications of double-well devices have been noted in Refs. [1–5]. For such devices to be useful, an understanding of the processes which couple the microscopic device to the macroscopic environment is paramount. That is to say, the decoherence processes of such systems must be well understood. To this end, we consider a simple exactly solvable model of two coupled quantum dots. An excellent review of related systems and some approximate solutions are given in Ref. [6].

Each dot is coupled to an environment (a triple-barrier system) as in Fig. 1. The environment consists of a continuum of states, as would be appropriate for a macroscopic lead. Only one state in each quantum dot is considered, which amounts to the assumption that the tunneling parameters connecting our two states to any neglected state are much less than the energy differences with that state.

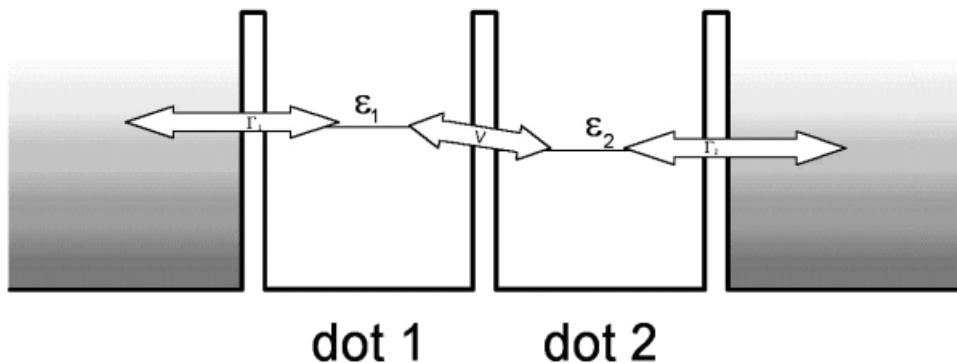


Fig. 1. Schematic diagram of the problem

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The Hamiltonian of the system can be written as the sum of two terms, $H = H_0 + H_c$. The first term, H_0 , represents the dynamics of the simple two-state system,

$$H_0 = \varepsilon_1 d_1^\dagger d_1 + \varepsilon_2 d_2^\dagger d_2 + V(d_1^\dagger d_2 + d_2^\dagger d_1) \doteq \begin{pmatrix} \varepsilon_1 & V \\ V & \varepsilon_2 \end{pmatrix}, \quad (1)$$

where d_i^\dagger creates an electron in dot i , and the other symbols are defined in Fig. 1. V may be chosen real and positive without loss of generality. The second term, H_c , reflects the coupling of each dot to its respective lead,

$$H_c = \sum_{i=1}^2 \sum_k (V_{ki} c_{ki}^\dagger d_i + V_{ki}^* d_i^\dagger c_{ki} + \varepsilon_{ki} c_{ki}^\dagger c_{ki}), \quad (2)$$

where the sum on k runs over the states in the continuum adjoining dot i , c_{ki}^\dagger creates an electron in the k -th state of the continuum adjoining dot i , ε_{ki} is the energy of the k -th state of the appropriate continuum, and V_{ki} is the tunneling parameter from the dot to the continuum. Throughout the paper, we use units with $\hbar = 1$.

In the following, we adopt a Green's function approach which parallels that taken in Ref. [7]. The retarded Green's function is defined by

$$G_{ij}(t) = -i\Theta(t) \langle \{d_i(t), d_j^\dagger(0)\} \rangle, \quad (3)$$

where $\Theta(t)$ is the well known step function, $\{, \}$ denotes the anticommutator, and $\langle \rangle$ denotes the quantum mechanical and thermodynamic average. The retarded Green's function is the sum of the amplitude for an electron to propagate forward in time and that for a hole to propagate backward in time. As such, it is a purely dynamical quantity, independent of the occupancies of the energy levels of the system.

It is a simple matter to calculate $G_0(t)$ from H_0 in the Heisenberg picture. From this, one can find the Fourier transform $G_0(E) = \int_{-\infty}^{\infty} dt G_0(t) e^{iEt}$, and finally the inverse

$$G_0^{-1}(E) \doteq \begin{pmatrix} E - \varepsilon_1 + i0^+ & -V \\ -V & E - \varepsilon_2 + i0^+ \end{pmatrix}. \quad (4)$$

The full Green's function can then be obtained from Dyson's equation,

$$G^{-1}(E) = G_0^{-1} - \Sigma. \quad (5)$$

Here Σ is the self-energy due to interactions with the continua,

$$\Sigma \doteq \begin{pmatrix} -i\Gamma_1/2 & 0 \\ 0 & -i\Gamma_2/2 \end{pmatrix}. \quad (6)$$

In the broad-band limit for the continua, the Γ_i are independent of energy, and are [8]

$$\Gamma_i = 2\pi \sum_k |V_{ki}|^2 \delta(E - \varepsilon_{ki}). \quad (7)$$

Application of Dyson's equation and inversion yields the total Green's function of the energy,

$$G(E) \doteq \left[\begin{pmatrix} E - \varepsilon_1 + i\frac{\Gamma_1}{2} \\ E - \varepsilon_2 + i\frac{\Gamma_2}{2} \end{pmatrix} - V^2 \right]^{-1} \begin{pmatrix} E - \varepsilon_2 + i\frac{\Gamma_2}{2} & V \\ V & E - \varepsilon_1 + i\frac{\Gamma_1}{2} \end{pmatrix}. \quad (8)$$

$G(t)$ is then the inverse Fourier transform of $G(E)$.

Consider a single electron initially localized in dot 1 at time $t = 0$. From the first row of $G(t)$, we can determine the probability P_2 for the electron to tunnel to dot 2 and the probability P_1 for the electron to remain at or return to dot 1, as functions of time,

$$P_1(t) = |G_{11}(t)|^2 = \frac{V^2}{|\omega|^2} e^{-\bar{\Gamma}t} \left(\frac{\omega_i + \Gamma'}{\Gamma' - \omega_i} e^{\omega_i t} + \frac{\Gamma' - \omega_i}{\omega_i + \Gamma'} e^{-\omega_i t} + \frac{i\omega_r + \Gamma'}{i\omega_r - \Gamma'} e^{i\omega_r t} + \frac{i\omega_r - \Gamma'}{i\omega_r + \Gamma'} e^{-i\omega_r t} \right), \quad (9)$$

$$P_2(t) = |G_{12}(t)|^2 = \frac{2V^2}{|\omega|^2} e^{-\bar{\Gamma}t} (\cosh \omega_i t - \cos \omega_r t),$$

where

$$\bar{\Gamma} \equiv \frac{\Gamma_1 + \Gamma_2}{2}, \quad \Gamma' \equiv \frac{\Gamma_2 - \Gamma_1}{2}, \quad (11)$$

and

$$\omega \equiv \omega_r + i\omega_i \equiv \sqrt{4V^2 + (\varepsilon_2 - \varepsilon_1 - i\Gamma')^2}. \quad (12)$$

Note that the processes in which a different electron enters a dot from one of the leads, and is annihilated by $d_i(t)$, give a vanishing contribution to $G(t)$ because such processes occur with random phases and average to zero.

Some understanding of the physical meaning of the solution may be arrived at by examining the limiting case of identical quantum dots, i.e. $\varepsilon_1 = \varepsilon_2$. In that case, we have

$$\omega = \sqrt{4V^2 - \Gamma'^2}, \quad (13)$$

where ω must be either purely real or purely imaginary. Working with $P_2(t)$ for algebraic simplicity, we find that if $2V > |\Gamma'|$, ω is purely real, and

$$P_2(t) = \frac{4V^2}{\omega^2} e^{-\bar{\Gamma}t} \sin^2 \frac{\omega t}{2}. \quad (14)$$

In this limit, the solution exhibits the characteristic coherent behavior of Rabi oscillations, as one would expect from a simple two-well problem. The presence of the environment is visible in the exponentially decaying envelope function: electrons leave/enter the two-state system at an overall rate $\bar{\Gamma}$.

In the case that $\varepsilon_1 = \varepsilon_2$ and $2V < |\Gamma'|$, on the other hand, we find a purely imaginary ω , and

$$P_2(t) = \frac{4V^2}{|\omega|^2} e^{-\bar{\Gamma}t} \sinh^2 \frac{|\omega| t}{2}. \quad (15)$$

The hyperbolic function and the resulting lack of Rabi oscillations demonstrate that interdot tunneling is completely incoherent in this regime.

In the more general case that $\varepsilon_1 \neq \varepsilon_2$, neither the circular nor the hyperbolic functions vanish, giving a combination of both coherent and incoherent behavior. For $\Gamma' = 0$, however, a purely real ω is recovered, and the coherent evolution of Eq. (14) is obeyed with Rabi frequency

$$\omega = \sqrt{4V^2 + (\varepsilon_1 - \varepsilon_2)^2}. \quad (16)$$

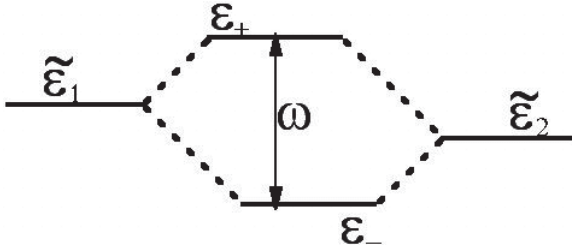


Fig. 2. Hybridization of the complex energy levels $\tilde{\epsilon}_i$ yields resonances ϵ_{\pm} with complex level splitting ω , the nature of which determines the behavior of the system

This somewhat startling result is especially gratifying when viewed in the context of measurement theory: $\Gamma' = 0$ indicates that the coupling of the two-well system to the environment does not distinguish between the dots, and thus the coherence between the dots is in no way destroyed by the macroscopic world.

Additional insight may be gained by examining the poles of the Green's function, which can be interpreted as complex energy levels of the system, or resonances [9]. Defining complex energy levels

$$\tilde{\epsilon}_i = \epsilon_i - i\Gamma_i/2 \quad (17)$$

for each dot by including the local self-energy, the poles of $G(E)$ may be written as

$$\epsilon_{\pm} = \frac{\tilde{\epsilon}_1 + \tilde{\epsilon}_2}{2} \pm \sqrt{\left(\frac{\tilde{\epsilon}_2 - \tilde{\epsilon}_1}{2}\right)^2 + V^2}. \quad (18)$$

This is the standard formula for the hybridization of two energy levels coupled by a matrix element V , except that the energy levels here are complex (see Fig. 2). It can be understood from Dyson's equation that the poles of $G(E)$ should have this form, if the interdot tunneling is taken as the perturbation, rather than the coupling to the environment. Neglecting interdot tunneling, the Green's function is diagonal and consists of two independent Breit-Wigner resonances at $\tilde{\epsilon}_1$ and $\tilde{\epsilon}_2$. The interdot tunneling operator then hybridizes these resonances via Dyson's equation, leading to the poles displayed in Eq. (18). From Eqs. (12) and (18), it is easy to see that the energy difference is

$$\epsilon_+ - \epsilon_- = \omega. \quad (19)$$

Thus ω can be interpreted as the complex level splitting between the hybridized states, corresponding to a complex Rabi frequency: ω_r is the frequency of real Rabi oscillations, while ω_i is the rate of incoherent tunneling.

We have presented an exactly solvable model for the tunneling dynamics of a two-level quantum system coupled to a macroscopic environment, appropriate to describe a double quantum dot connected to conducting leads. Despite its simplicity, this model displays many of the essential features of more complicated models [6]. The tunneling dynamics is determined by the complex Rabi frequency given in Eq. (12). Our results can be interpreted in terms of measurement theory: interdot coherence is suppressed to the degree that the environment can distinguish between the two orbitals.

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