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Localization of two-level systems subject to external fields

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Abstract

The necessary conditions for the localization of a quantum particle in a two-level system subject to periodic oscillations of the height (energy splitting) and the width (tunnelling matrix) of a potential barrier were found. The former field is supposed to have a simple cosine form while the latter has the form of asymmetric pulses or a train of delta-functions.

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Tunnelling and localization in a two-level system (TLS) have been the subject of much investigation since such a system serves as a model for many problems in physics, chemistry and biology. Interest in this problem has quickened after the counter-intuitive discovery by Grossmann *et al* [1] of particle localization in TLS under a properly chosen periodic acting field (coherent destruction of tunnelling; see the recent comprehensive review [2]). The Hamiltonian of a TLS can be expressed in terms of the Pauli matrices σ_i $(i = x, y, z)$ as

$$H = [\Delta + g(t)]\,\sigma_z + [\Delta_0 + f(t)]\,\sigma_x \tag{1}$$

where Δ is the TLS asymmetry and Δ_0 is the tunnelling amplitude. The modulation of the TLS parameters could arise from an (in addition to the dc-field Δ_0) ac-field $f(t)$ changing the width of a potential barrier. The time-dependent field $g(t)$ may come from an ac-field modulation of the energy splitting Δ.

The criteria of localization of a particle in a TLS have been obtained for different special cases of equation (1). When $\Delta_0 = g = 0$, and $f(t) = V_0 \sin(\omega t)$, the localization occurs when $z \equiv \frac{2V_0}{\omega}$ are zeros of the Laguerre polynomial $L_n(z)$ which in the semiclassical limit reduces for high frequencies to the zeroth-order Bessel function $J_0(z)$ [2]. When both dc-field Δ_0 and ac-field $f(t) = V_0 \sin(\omega t)$ are present there are two criteria [3], namely $\frac{2\Delta_0}{\omega}$ has to be an integer, $\frac{2\Delta_0}{\omega} = n$, and $\frac{2V_0}{\omega}$ have to be zeros of the nth-order Bessel function J_n. The corresponding criteria have also been obtained for the cases when $\Delta_0 = g = 0$, and $f(t)$ has the form of symmetric pulses [4] and a train of delta-functions [5]. The random fields have been the subject of some recent research [6, 7].

Some additional progress had been achieved recently by Klinger and Gitterman [8]. If the TLS is subjected to an additional classical field $g(t) = W_0 \cos(\Omega t)$, with $f(t) = 0$, the equation of motion takes the form of the Mathieu equation. However, as was shown in [8], using the appropriate unitary transformation of the Hamiltonian (1) one can eliminate the field $g(t)$ ('dressing effect') which results in replacing the bare tunnelling amplitude Δ_0 with the renormalized one, $\tilde{\Delta}_0$, namely

$$\Delta_0 \to \tilde{\Delta}_0 = \Delta_0 J_0\left(\frac{W_0}{\hbar\Omega}\right)\exp(-a) \tag{2}$$

where a is the overlap integral for thermal-equilibrium photon states with displaced centres. In that case the Hamiltonian (1) takes the following form:

$$H = \Delta\sigma_z + \left[\tilde{\Delta}_0 + f(t)\right]\sigma_x. \tag{3}$$

In this note we use a unified way to establish the number and the form of criteria of localization in the presence of two periodic fields $g(t)$ and $f(t)$ where the latter may have a form of asymmetric or symmetric pulses, or the train of delta-functions.

We consider the TLS system with an external field $f(t)$ while the second field $g(t)$ is either absent (the Hamiltonian (1) with $g(t) = 0$) or has been taken into account by the renormalization procedure (the Hamiltonian (3)).

We assume that the function $f(t)$ in equation (1) or (3) is a pulse of the form

$$f(t) = \begin{cases} A & \text{if} \quad 0 \leqslant t < T_1 \\ -B & \text{if} \quad T_1 \leqslant t < T \end{cases} \tag{4}$$

and $f(t+T) = f(t)$.

As the basic wavefunction we use those localized in the 'right' and 'left' wells, and the wavefunction $\Psi(t)$ corresponding to the Hamiltonian (1) is described on this basis by the amplitudes

$$C(t) \equiv \begin{pmatrix} c_l(t) \\ c_r(t) \end{pmatrix}.$$

Our aim now is to find the time-propagation 2×2 matrix $U(t, t_0)$ on a single period of (4), $U(T, 0) \equiv U$ defined as

$$C(T) = UC(0). \tag{5}$$

Using the commutation relation for the Pauli matrices σ_i one can find [4] the following equation of motion for the amplitude $C(t)$:

$$\frac{\mathrm{d}C(t)}{\mathrm{d}t} = \begin{pmatrix} -\mathrm{i}[\Delta_0 + f(t)] & -\mathrm{i}\Delta \\ -\mathrm{i}\Delta & \mathrm{i}[\Delta_0 + f(t)] \end{pmatrix} C(t). \tag{6}$$

Two first-order differential equations (6) with constant coefficients can easily be solved, which define the propagation matrix $U_1(t)$ for $0 \leqslant t < T_1$ as

$$C(t) = U_1(t,0)C(0) = \begin{Bmatrix} [\cos(\omega_1 t) - \mathrm{i}\alpha_1 \sin(\omega_1 t)] & -\mathrm{i}\beta_1 \sin(\omega_1 t) \\ -\mathrm{i}\beta_1 \sin(\omega_1 t) & [\cos(\omega_1 t) + \mathrm{i}\alpha_1 \sin(\omega_1 t)] \end{Bmatrix} C(0) \tag{7}$$

where

$$\omega_1 = \sqrt{\Delta^2 + (\Delta_0 + A)^2} \qquad \alpha_1 = \frac{\Delta_0 + A}{\omega_1} \qquad \beta_1 = \frac{\Delta}{\omega_1}. \tag{8}$$

Equations (7) define $c_l(T_1)$ and $c_r(T_1)$ which serve as initial conditions for $T_1 \leqslant t < T$ in equations which differ from (7) in replacing A by $-B$, i.e.

$$\begin{aligned} C(t) &= U_2(t, T_1)C(T_1) \\ &= \begin{Bmatrix} \{\cos[\omega_2(t - T_1)] - \mathrm{i}\alpha_2 \sin[\omega_2(t - T_1)]\} & -\mathrm{i}\beta_1 \sin[\omega_2(t - T_1)] \\ -\mathrm{i}\beta_1 \sin[\omega_2(t - T_1)] & \{\cos[\omega_2(t - T_1)] + \mathrm{i}\alpha_2 \sin[\omega_2(t - T_1)]\} \end{Bmatrix} C(T_1) \end{aligned} \tag{9}$$

with

$$\omega_2 = \sqrt{\Delta^2 + (\Delta_0 - B)^2} \qquad \alpha_2 = \frac{\Delta_0 - B}{\omega_2} \qquad \beta_2 = \frac{\Delta}{\omega_2}. \tag{10}$$

A single-period propagation matrix U is equal to the product of $U_2(T, T_1)$ and $U_1(T_1, 0)$, defined in equations (7) and (9), and turns out to be equal to

$$U = \begin{Bmatrix} a - \mathrm{i}b & c - \mathrm{i}d \\ -c - \mathrm{i}d & a + \mathrm{i}b \end{Bmatrix} \tag{11}$$

where

$$\begin{aligned} a &= \cos(\omega_1 T_1)\cos[\omega_2(T - T_1)] - (\alpha_1\alpha_2 + \beta_1\beta_2)\sin(\omega_1 T_1)\sin[\omega_2(T - T_1)] \\ b &= \alpha_2 \sin[\omega_2(T - T_1)]\cos(\omega_1 T_1) + \alpha_1 \sin(\omega_1 T_1)\cos[\omega_2(T - T_1)] \\ c &= (\alpha_1\beta_2 - \alpha_2\beta_1)\sin(\omega_1 T_1)\sin[\omega_2(T - T_1)] \\ d &= \beta_1 \sin(\omega_1 T_1)\cos[\omega_2(T - T_1)] + \beta_2 \sin[\omega_2(T - T_1)]\cos(\omega_1 T_1)\,. \end{aligned} \tag{12}$$

If the transition matrix U is equal to the identity matrix I, $U = \pm I$, a particle comes back to its initial position after a time equal to the period of the external field, i.e. the initially empty state will remain empty (coherent localization). Note that caution is required in the interpretation of the results which means, in fact, 'stroboscopic localization'. Indeed, we have replaced the continuous time in the Hamiltonian (1) by the discrete times nT, which makes the interpretation slightly ambiguous since, in addition to localization, when a particle never visits the second state, a situation may occur where a particle comes back to the initial state after visiting the second state at half periods $n\frac{T}{2}$ [9]. Which of these two scenarios occurs has to be checked by numerical analysis of the equation of motion or by the following consideration. In addition to the necessary condition for localization, $U = \pm I$, the sufficient conditions for localization mean that the probability of staying in an initially chosen well will remain small (less than $\frac{1}{2}$) over one period. To meet the latter requirement, the transition from one well to another has to be comparatively small, which can be achieved by having small off-diagonal terms in the matrices entering equations (7) and (9) compared with the diagonal ones, i.e.

$$\beta_{1,2} < \alpha_{1,2}. \tag{13}$$

As follows from equations (12), the necessary condition for localization, $U = \pm I$, i.e. $a = \pm 1$, $b = c = d = 0$, will be satisfied if

$$T_1\sqrt{\Delta^2 + (\Delta_0 + A)^2} = n\pi \qquad (T - T_1)\sqrt{\Delta^2 + (\Delta_0 - B)^2} = m\pi \tag{14}$$

where n and m are integers. Conditions (14) represent the resonance conditions linking the characteristic times of an external pulse T and T_1 and the characteristic rates of the TLS ω_1 and ω_2 defined in (8) and (10).

Let us consider the different limiting cases of equation (14).

1. There is no tunnelling amplitude in the absence of an external field ($\Delta_0 = 0$), and the external pulse (4) is symmetric ($A = B$, $T_1 = \frac{T}{2}$). Then equation (14) reduces to

$$T = \frac{2\pi m}{\sqrt{\Delta^2 + A^2}} \tag{15}$$

where m is the integer. Hence, the onset of localization requires quite rigid restriction (15) on the amplitude A and duration T of an external pulse.

The result (15) can also be applied to the case when the field-free tunnelling amplitude is non-zero, $\Delta_0 \neq 0$, but there is an additional classical periodic field $g(t) = W_0 \cos(\Omega t)$. Then, the localization takes place if, in addition to condition (15), the amplitude W_0 of the field and its frequency Ω satisfy the condition $J_0\left(\frac{W_0}{\hbar\Omega}\right) = 0$ which, according to (2) means that $\tilde{\Delta}_0 = 0$. Note that the latter condition on the parameters of a classical field is independent of condition (15) of an external pulse.

2. Let us replace the pulse (4) by the delta-function potential. This may be achieved by setting $B = 0$, $A \to \infty$ and $T_1 \to 0$ in such a way that $AT_1 = \text{const} \equiv C$. Then, one gets from (14)

$$T = \frac{\pi m}{\sqrt{\Delta^2 + \Delta_0^2}} \quad \text{and} \quad C = n\pi \tag{16}$$

where m and l are integers. The criterion (16) is also applicable in the presence of an additional periodic field $g(t) = V_0 \cos(\Omega t)$ with the proviso that, according to (2), Δ_0 is replaced by $\tilde{\Delta}_0$. Hence, for the onset of localization one gets (even for $\Delta_0 = 0$) two restrictions (16), separately for the period T and the strength C of the delta-function potential, compared with only one restriction (15) for a pulse potential.

Note that we neglect dissipation assuming that the inverse relaxation time is larger than the characteristic frequencies of our problem. Although dissipation, in general, tends to suppress coherence [10, 11], it turns out [12] that weak dissipation can stabilize the localized state while strong dissipation destroys it. Recently [13] the spin-boson Hamiltonian was studied analytically in connection with the resonance phenomena in the presence of both periodic force and dissipation. The influence of dissipation on the localization of TLS remains to be investigated.

In conclusion, we have extended the necessary criteria for the coherent destruction of tunnelling to TLS with asymmetrically oscillating height and width of the potential barrier.

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