Coherence destruction of tunneling in a quantum-dot molecule with bias*

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This paper studies the constraint conditions for coherence destruction in tunneling by using perturbation theory and numerical simulation for an AC-field with bias and Coulomb interaction between electrons in a quantum dot molecule. Such conditions can be described by using the roots of a Bessel function $J_n(x)$, where n is determined by both the bias and the Coulomb interactions, and x is the ratio of the amplitude to the frequency of the AC-field. Under such conditions, a coherent suppression of tunneling occurs between localized electronic states, which results from the dynamical localization phenomenon. All the conditions are verified with numerical simulations.

Keywords: dynamic localization, Floquet state, constraint conditions

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1. Introduction

The coherent control of quantum dynamics of electrons by a periodically oscillating external field has been one of the subjects of considerable interest both in nanoscale solid state physics,[1] and in molecular physics under laser fields.[2] The coherent manipulation of entangled quantum states[3] has become a fascinating prospect in that it is an important component of the swiftly developing field of quantum computation. Controlling the time evolution of quantum states and engineering entanglement between quantum particles are two of the major tasks required for quantum information processing. Although the majority of experimental demonstrations of entanglement distribution have so far employed photons, future practical implementations of quantum computers will almost certainly be based on condensed matter systems. Efforts in this direction include controlling electronic charge or spin degrees of freedom in coupled quantum dots.[4]

Since Grossmann[5] first noted that an electron in a symmetric double-well potential can be localized in one of the wells when the system is driven by an AC field, which was termed dynamical localization (DL), analytical and numerical work subsequent to that of Holthaus[6,7] showed that for high frequencies, this localization occurs when the ratio of the field strength to the frequency is a root of the Bessel function J_0. When the ionic and covalent bonding of the electronic states in the quantum-dot molecule (QDM) was observed in the microwave spectrum,[8] The DL phenomenon in the two-electron QDMs had also been studied.[9,10] In the QDM, the repulsive Coulomb interaction between the electrons cannot be ignored, and can enhance the degree of localization to a larger extent in comparison with the non-interacting case.[11] The localization of the interacting electrons depends on both the external AC field and the Coulomb interaction between the electrons, but the restrictive conditions have not been clearly explained in the coupled quantum-dot system.[12−14] Controlling the dynamics by means of the effect known as coherent destruction of tunneling (CDT),[15] Creffield demonstrated a novel ratchetlike effect that enables particles to be coherently manipulated and steered without requiring local control.[16] Lehmann *et al.* has also found that CDT is stable against a static bias in open quantum dots that are attached to leads.[17]

In this paper, we illustrate how the CDT condition results in the conditions for dynamical localization in an AC driven two-electron QDM using a

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perturbation analysis and numerical simulations.

2. Model and method

We consider two coupled quantum dots under the action of a periodic field. We assume that each quantum dot of the QDM can be replaced by a single site. The Hamiltonian within Hubbard model of the system can be written as

$$\begin{aligned} H(t) = & \sum_{\sigma,i=1,2} \varepsilon_i(t) d_{i\sigma}^{\dagger} d_{i\sigma} \\ & + W \sum_{\sigma} \left(d_{1\sigma}^{+} d_{2\sigma} + d_{2\sigma}^{+} d_{1\sigma} \right) \\ & + U_1 \sum_{i} n_{i\uparrow} n_{i\downarrow} + U_2 \sum_{\sigma_1,\sigma_2} n_{1\sigma_1} n_{2\sigma_2}, \quad (1) \end{aligned}$$

where $d_{i\sigma}^{\dagger}$ ($d_{i\sigma}$) creates (destroys) an electron with spin σ on the i-th dot. The energy levels on the dots become $\varepsilon_i(t) = (-1)^{i+1} (F_0 + V\cos(\omega t))/2$, where F_0 and V are the amplitude of the DC and AC voltages, and ω is the driving frequency with period $T = 2\pi/\omega$. The parameter W describes the transition between the two dots, U_1 and U_2 are the on-site and inter-site Coulomb interactions, respectively.

In Eq. (1), there are no spin-flip terms. For the two-electron QDM,[10] the real-space two-particle basis vectors are $|1,1\rangle$, $|\bar{1},\bar{1}\rangle$, $|1,\bar{1}\rangle$, $|\bar{1},1\rangle$, $|0,2\rangle$, $|2,0\rangle$, where $|m,n\rangle$ denotes the state of m electrons at the first site and n electrons at the second site. The values 1 and $\bar{1}$ indicate the spin-up and spin-down states, respectively. On replacing $|1,\bar{1}\rangle$ and $|\bar{1},1\rangle$ with $(|1,\bar{1}\rangle - |\bar{1},1\rangle)/\sqrt{2}$ and $(|1,\bar{1}\rangle + |\bar{1},1\rangle)/\sqrt{2}$ respectively, the Hamiltonian of the system in the triplet subspace and the singlet subspace takes on the matrix form

$$H(t) = \begin{bmatrix} U_2 I_{3\times 3} & 0 \\ 0 & H_1(t) \end{bmatrix}. \quad (2)$$

Here, $I_{3\times 3}$ is a 3×3 unit matrix and $H_1(t)$ is given by

$$H_1(t) = \begin{bmatrix} 2\varepsilon_1(t) + U_1 & \sqrt{2}W & 0 \\ \sqrt{2}W & U_2 & \sqrt{2}W \\ 0 & \sqrt{2}W & 2\varepsilon_2(t) + U_1 \end{bmatrix}. \quad (3)$$

There is no mixing between the two subspaces due to no spin-flip terms. Because the triplet states are trivial ones and constant occupation number 1 on each dot, we will focus our attention only on the singlet subspace consisting of $|2,0\rangle$, $(|1,\bar{1}\rangle + |\bar{1},1\rangle)/\sqrt{2}$, $|0,2\rangle$. The Hamiltonian $H_1(t)$ in the singlet subspace with a constant energy shift U_2 is written as

$$H_1'(t) = \begin{bmatrix} 2\varepsilon_1(t) + \kappa & \sqrt{2}W & 0 \\ \sqrt{2}W & 0 & \sqrt{2}W \\ 0 & \sqrt{2}W & 2\varepsilon_2(t) + \kappa \end{bmatrix}, \quad (4)$$

where $\kappa = U_1 - U_2$.

Because $H_1'(t)$ has the property of time periodicity, we can describe the quantum evolution of the system in terms of the Floquet formalism.[14] The solution of the time-dependent Schrödinger equation ($\hbar = 1$)

$$\mathrm{i}\frac{\partial}{\partial t}\psi(t) = H_1'(t)\,\psi(t) \quad (5)$$

is written as

$$\psi(t) = \sum_{\alpha} c_\alpha \exp[-\mathrm{i}\,\varepsilon_\alpha t]\,|u_\alpha(t)\rangle, \quad (6)$$

where $|u_\alpha(t)\rangle$ is a function with the same periodicity as the external AC-field and is called a Floquet state. The variable ε_α is termed the quasi-energy. The Floquet state $|u_\alpha(t)\rangle$ can be obtained from the Floquet equation

$$\left(H_1'(t) - \mathrm{i}\frac{\partial}{\partial t}\right)|u_\alpha(t)\rangle = \varepsilon_\alpha\,|u_\alpha(t)\rangle. \quad (7)$$

The coefficients c_α in Eq. (6) are determined by the initial conditions

$$c_\alpha = \langle u_\alpha(0)|\,\psi(0)\rangle, \quad (8)$$

where $|\psi(0)\rangle$ and $|u_\alpha(0)\rangle$ are the initial state of the system and the Floquet state respectively. The initial Floquet state $|u_\alpha(0)\rangle$ and the quasi-energy ε_α can be obtained by integrating numerically from zero to T the equation

$$\mathrm{i}\frac{\partial}{\partial t}U(t,0) = H_1'(t)\,U(t,0), \quad (9)$$

and diagonalizing $U(T,0) = S\exp(-\mathrm{i}\,D)S^{\dagger}$, where S is a unitary matrix.

Thus the population $P(t)$ of the initial state $|\psi(0)\rangle$ at time t is

$$\begin{aligned} P(t) &= |\langle\psi(0)|\,\psi(t)\rangle|^2 \\ &= \left|\sum_{\alpha,\beta} c_\alpha^* c_\beta \exp[-\mathrm{i}\,\varepsilon_\beta t]\,\langle u_\alpha(0)|\,u_\beta(t)\rangle\right|^2. \quad (10) \end{aligned}$$

Note that the population is determined by the initial state, the quasi-energies ε_β and the Floquet states

$|u_\beta(t)\rangle$. If the quasi-energies $\{\varepsilon_\alpha\}$ are confined to the first Brillouin zone, another index l in $\{\varepsilon_{\alpha,l}\}$ counts that 'how many photons' have to be subtracted from the eigenenergy $\{E_\alpha\}$ in order to arrive at the first Brillouin zone when the external AC-field is switched off adiabatically, i.e. $V \to 0$. The relation between the Floquet states and the corresponding stationary eigenstates $\{\varphi_\alpha\}$[18] is

$$|u_{\alpha,l}(t)\rangle \to \left|u^0_{\alpha,l}(t)\right\rangle = \varphi_\alpha \exp\left(\mathrm{i}\, l\omega t\right). \tag{11}$$

The quasi-energies can cross as the amplitudes of the external driven field vary. At the crossing points, resonant tunneling and the CDT phenomenon occur.[19] So the degeneracy of quasi-energies can be used to inspect the occurrence of CDT phenomenon in our system. As the parameters in $H_1'(t)$ vary, the quasi-energies can cross each other and the exact crossing points indicate the presence of CDT.

3. Analytic results

The quasi-energies are usually difficult to calculate analytically and numerical methods must be employed. When the driving field dominates the dynamics, the Hamiltonian Eq. (4) can be divided into two parts

$$\begin{aligned} H_1 &= H_a + H_t \\ &= \begin{pmatrix} F_0 + V\cos(\omega t) + \kappa & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -F_0 - V\cos(\omega t) + \kappa \end{pmatrix} + \begin{pmatrix} 0 & \sqrt{2}W & 0 \\ \sqrt{2}W & 0 & \sqrt{2}W \\ 0 & \sqrt{2}W & 0 \end{pmatrix}, \end{aligned} \tag{12}$$

where H_a contains all the interaction terms and is solved exactly, H_t contains all tunneling components and acts as a perturbation.[6] The interaction terms H_a are diagonal and it is straightforward to obtain an orthogonal set of eigenvectors for Eq. (7)

$$\begin{cases} |u_1(t)\rangle = \left(\exp\left[-\mathrm{i}\, t\,(\kappa + F_0 - \varepsilon_1) - \mathrm{i}\,\dfrac{V}{\omega}\sin(\omega t)\right], 0, 0\right), \\ |u_2(t)\rangle = \left(0, \exp\left[\mathrm{i}\, t\varepsilon_2\right], 0\right), \\ |u_3(t)\rangle = \left(0, 0, \exp\left[-\mathrm{i}\, t\,(\kappa - F_0 - \varepsilon_3) + \mathrm{i}\,\dfrac{V}{\omega}\sin(\omega t)\right]\right). \end{cases} \tag{13}$$

Imposing T-periodic boundary conditions $u_\alpha(t+T) = u_\alpha(t)$ reveals the corresponding eigenvalues to be $\varepsilon_1 = \kappa + F_0$, $\varepsilon_2 = 0$, $\varepsilon_3 = \kappa - F_0$. Therefore, the solutions of H_a are:

$$\begin{cases} \psi_1(t) = \left(\exp\left[-\mathrm{i}\, t\,(\kappa + F_0) - \mathrm{i}\,\dfrac{V}{\omega}\sin(\omega t)\right], 0, 0\right), \\ \psi_2(t) = (0, 1, 0), \\ \psi_3(t) = \left(0, 0, \exp\left[-\mathrm{i}\, t\,(\kappa - F_0) + \mathrm{i}\,\dfrac{V}{\omega}\sin(\omega t)\right]\right). \end{cases} \tag{14}$$

These are stationary states in real space, and do not involve resonant tunneling.

When the tunneling perturbation H_t is considered, resonant tunneling may occur if the quasi-energies of H_a match (i.e. are degenerate). The tunneling probability is determined by the perturbing operator H_t,

$$(H_t)_{i,j} = \langle\langle \psi_i(t)|H_t|\psi_j(t)\rangle\rangle = \frac{1}{T}\int_0^T \mathrm{d}t\, \langle\psi_i(t)|H_t|\psi_j(t)\rangle, \tag{15}$$

where $\langle\langle\cdots\rangle\rangle$ denotes the inner product in an extended Hilbert space of T-periodic functions.[12,13]

The tunneling probability changes with parameters of the driving field for certain Coulomb interaction κ. For the case $\kappa \neq n\omega$, the quasi-energy crossings of H_a occur between two levels. The variation of the quasi-energies of H_a as a function of the bias F_0 is shown in Figs. 1(a) and 1(c).

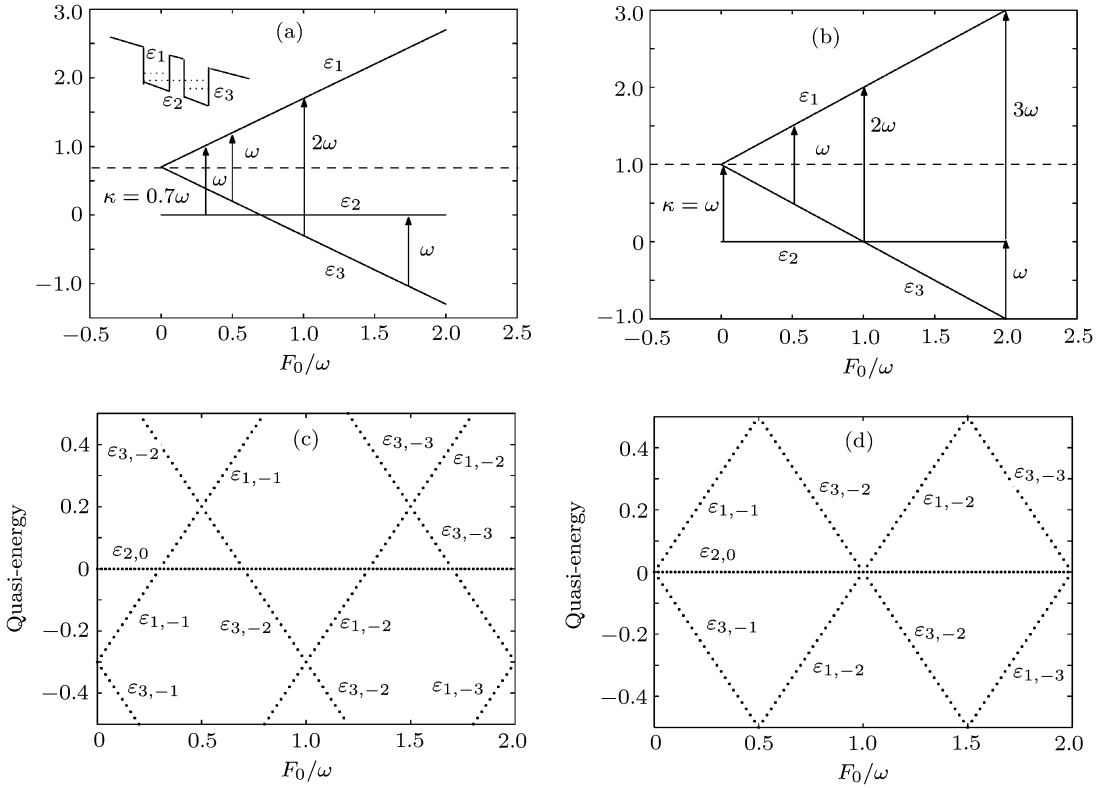


Fig. 1. The variation of the quasi-energies of H_a as a function of the bias with different Coulomb interactions: (a) $\kappa = 0.7\omega$; (b) $\kappa = \omega$. Figures (c) and (d) show the corresponding quasi-energy spectra in the first Brillouin zone.

Note that resonant tunneling may occur between $\psi_1(t)$ and $\psi_3(t)$ with absorption of m photons when the bias satisfies the condition $\epsilon_1 - \epsilon_3 = m\omega$, i.e., $F_0 = m\omega/2$, where the system can be described by an effective two-level approximation.[11,20] The reduced perturbing operator H'_t has the following form in the subspaces $\psi_1(t)$ and $\psi_3(t)$,

$$H'_t = \Gamma(W,\kappa)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{16}$$

where $\Gamma(W,\kappa)$ is a function of the tunneling W and Coulomb interaction κ. Using the well-known identity

$$\exp[-\mathrm{i}\,\beta\sin\omega t] = \sum_{m=-\infty}^{\infty} \mathrm{J}_m(\beta)\exp[-\mathrm{i}\,m\omega t] \tag{17}$$

to rewrite the form of $|\psi_i(t)\rangle$, $(i = 1, 3)$, we can straightforwardly obtain

$$H'_t = \Gamma(W,\kappa)\mathrm{J}_m\,(2V/\omega)\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{18}$$

which implies that resonant tunneling between $|\psi_1(t)\rangle$ and $|\psi_3(t)\rangle$ is forbidden if the AC-field satisfies $\mathrm{J}_m\,(2V/\omega) = 0$. Therefore, the constraint conditions for CDT are

$$\mathrm{J}_m\,(2V/\omega) = 0, \quad \text{with} \quad 2F_0 = m\omega, \tag{19}$$

which can be viewed as the dynamics of a single particle with charge $2e$.[21]

Similarly, resonant tunneling between $\psi_1(t)$ and $\psi_2(t)$ may occur when the bias satisfies $\epsilon_1 - \epsilon_2 = F_0 + \kappa = m\omega$, i.e., $F_0 = m\omega - \kappa$, which yields $F_0 = 0.3\omega, 1.3\omega, \ldots$ for the case of Figs. 1(a) and 1(c). According to H_t in Eq. (12), the tunneling probability is determined by $\mathrm{J}_m\,(V/\omega)$. When $\mathrm{J}_m\,(V/\omega) = 0$, CDT occurs. Therefore, the constraint condition for CDT is

$$\mathrm{J}_m\,(V/\omega) = 0, \quad \text{with} \quad F_0 + \kappa = m\omega. \tag{20}$$

And the resonant tunneling between $\psi_2(t)$ and $\psi_3(t)$ occurs when $\epsilon_2 - \epsilon_3 = F_0 - \kappa = m\omega$, i.e., $F_0 = m\omega + \kappa$, which is $F_0 = \kappa = 0.7\omega, 1.7\omega, \ldots$ for the case of Figs. 1(a) and 1(c). The constraint condition for CDT is therefore

$$\mathrm{J}_m\,(V/\omega) = 0, \quad \text{with} \quad F_0 - \kappa = m\omega. \tag{21}$$

The constraint conditions (19)–(21) describe CDT among the three states $|\psi_1\,(t)\rangle$, $|\psi_2\,(t)\rangle$, and

$|\psi_3(t)\rangle$. In fact, the constraint conditions (20) and (21) describe the roles of both the Coulomb interactions and the bias in resonant quantum tunneling. When $F_0 = \kappa - m\omega$ or $F_0 = m\omega - \kappa$, one of the two electrons can tunnel between the two quantum dots while absorbing (or emitting) m photons. If the ratio of the amplitude V to the frequency of the external AC-field is one of the roots of the Bessel function $\mathrm{J}_m(V/\omega)$, CDT occurs. The constraint condition (19) describes the situation in which both electrons simultaneously tunnel between the quantum dots, i.e. with entanglement of the two electrons. The Coulomb interaction does not change after tunneling. Thus resonant tunneling between the localized states $|\psi_3(t)\rangle$ and $|\psi_1(t)\rangle$ can be treated as a single particle with effective charge $2e$ by using two-level approximations.[21,22]

In the special case of $\kappa = n\omega$, all three quasi-energies of H_a are degenerate, as shown in Figs. 1(b) and 1(d). Thus the three states can support resonant tunneling if the bias satisfies $F_0 = m\omega$. In such a case the two-level approximation is not usable, but we can obtain the tunneling probability determined by

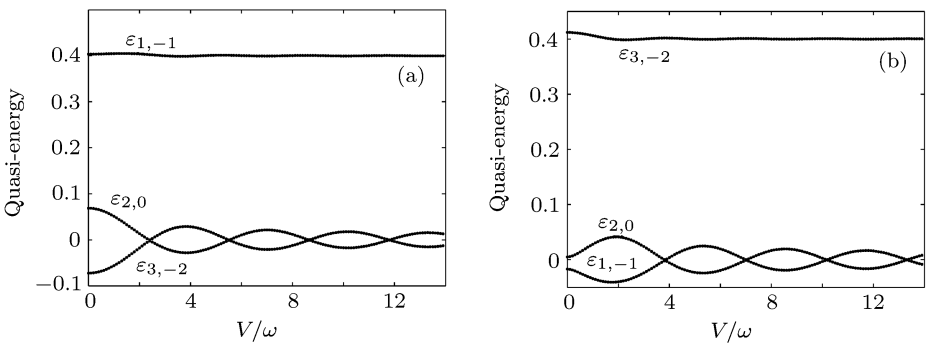
$$H_t = \sqrt{2}W \begin{bmatrix} 0 & \mathrm{J}_{-n-m}(V/\omega) & 0 \\ \mathrm{J}_{-n-m}(V/\omega) & 0 & \mathrm{J}_{n-m}(V/\omega) \\ 0 & \mathrm{J}_{n-m}(V/\omega) & 0 \end{bmatrix}. \tag{22}$$

We know that there is no amplitude of the external AC-field that simultaneously satisfies both $\mathrm{J}_{-n-m}(V/\omega) = 0$ and $\mathrm{J}_{n-m}(V/\omega) = 0$ except for the cases $m = 0$ or $n = 0$. The cases of both $m = 0$ (the pure external AC-field driven system) and $n = 0$ (the single electron system) have been investigated in previous work.[12,13,22]

4. Numerical simulation

In order to verify the above constraint conditions, we used the numerical solution of differential equation (7) to determine $P_{\min}$, the minimum value of the probabilities $P(t) = |\langle\psi(0)|\psi(t)\rangle|^2$ which describe the population evolution of the initial state $|\psi(0)\rangle$. This enables us to quantify the degree to which the biased AC-field brings about CDT. Figure 2 demonstrates that the above analytical results are in the excellent agreement with the numerical simulation for $W = 0.05\omega$, $\kappa = 0.7\omega$. Figures 2(a) and 2(b) are the quasi-energies with amplitude of the AC field respectively for $F_0 = m\omega + \kappa = 0 + 0.7\omega$ and $F_0 = m\omega - \kappa = \omega - 0.7\omega = 0.3\omega$. The CDT occurs for the initial state $|0,2\rangle$ in Fig. 2(c) and the initial state $|2,0\rangle$ in Fig. 2(d). Such examples also illustrates that the constraint condition for CDT depends on the initial state. Figures 2(e) and 2(f) illustrate that the conditions for CDT depend on the initial state and the parameter of driven electric field.

In the special case of $\kappa = n\omega$, the two-level approximation is not usable, all three quasi-energies of H_1' are shown in Fig. 3(a). The three states can support resonant tunneling if the bias satisfies $F_0 = m\omega$. When $\mathrm{J}_{-n-m}(V/\omega) = 0$, both CDT between $\psi_1(t)$ and $\psi_3(t)$ and CDT between $\psi_1(t)$ and $\psi_2(t)$ occur. The initial localized state $\psi_1(t=0) = |2,0\rangle$ will remain in a condition of DL as time evolves, as demonstrated in Fig. 3(b).



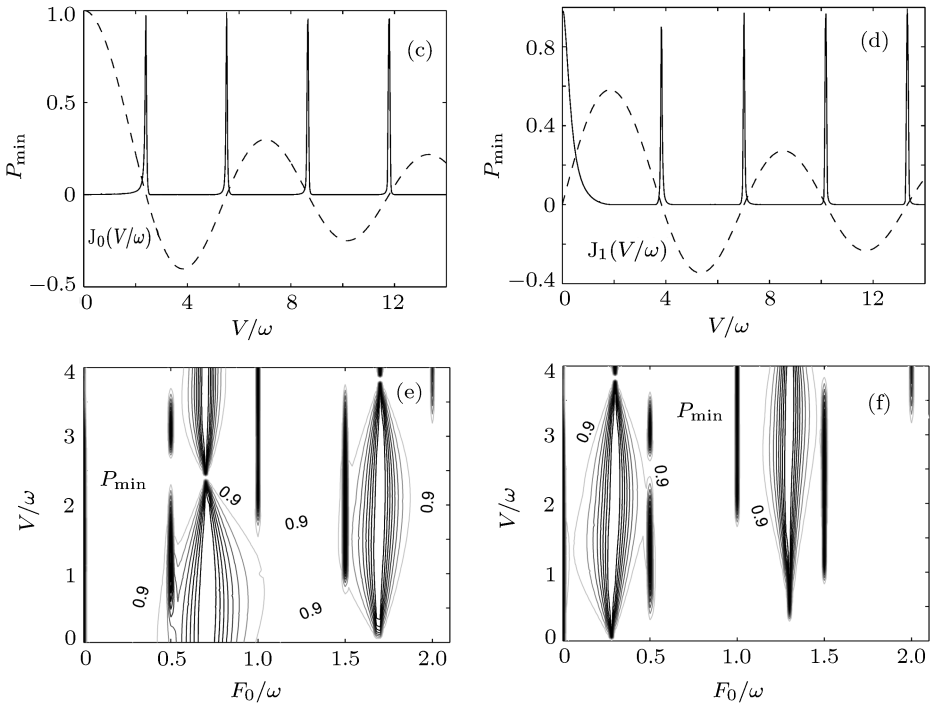


Fig. 2. The variation of the quasi-energies and $P_{\min}$ of an initial state as a function of the amplitude of the external AC-field with $\kappa = 0.7\omega$ and $W = 0.05\omega$. The peak of $P_{\min}$ corresponds to CDT: (a) the quasi-energies with $F_0 = m\omega + \kappa = 0 + 0.7\omega$; (b) the quasi-energies with $F_0 = m\omega - \kappa = \omega - 0.7\omega = 0.3\omega$; (c) $P_{\min}(V/\omega)$ of the initial state $|0, 2\rangle$ with $F_0 = 0.7\omega$ and $J_0(V/\omega)$; (d) $P_{\min}(V/\omega)$ of the initial state $|2, 0\rangle$ with $F_0 = 0.3\omega$ and $J_1(V/\omega)$. Figures (e) and (f) show the contours of $P_{\min}$ as a function of F_0 and V, respectively, for the initial states $|0, 2\rangle$ and $|2, 0\rangle$ near $F_0 = \omega$, which illustrates that the conditions for CDT depend on the initial state. The dark areas denote small $P_{\min}$.

Similarly, when $J_{n-m}(V/\omega) = 0$, both CDT between $\psi_3(t)$ and $\psi_1(t)$ and CDT between $\psi_3(t)$ and $\psi_2(t)$ occur. The initial localized state $\psi_3(t = 0) = |0, 2\rangle$ will also remain in DL, as demonstrated in Fig. 3(c).

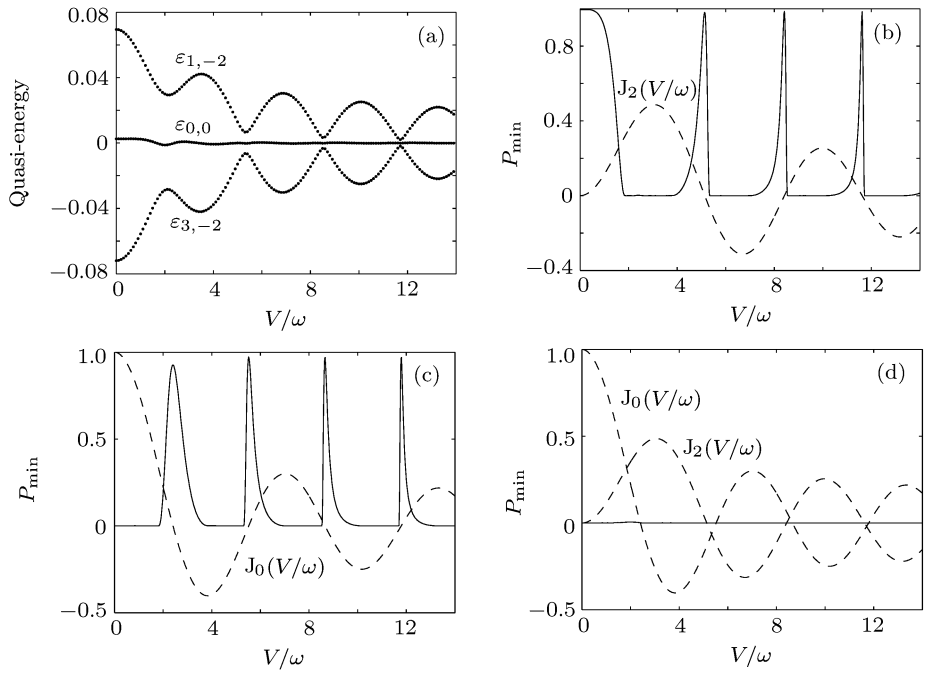


Fig. 3. The quasi-energies and $P_{\min}$ of different initial states as a function of the amplitude of the external AC-field in a special system with $F_0 = \kappa = \omega$ and $W = 0.05\omega$. The peak in $P_{\min}$ corresponds to CDT: (a) the quasi-energy spectrum; (b) $P_{\min}$ of the initial state $|2, 0\rangle$ and the values of $J_m(V/\omega)$ with $m = \kappa + F_0 = 2$; (c) $P_{\min}$ of the initial state $|0, 2\rangle$ and the values of $J_m(V/\omega)$ with $m = \kappa - F_0 = 0$; (d) $P_{\min}$ of the initial state $(|1, \bar{1}\rangle + |\bar{1}, 1\rangle)/\sqrt{2}$, $J_0(V/\omega)$, and the values of $J_2(V/\omega)$.

Then, as demonstrated in Fig. 3(d), CDT between $\psi_2(t)$ and $\psi_1(t)$ and CDT between $\psi_2(t)$ and $\psi_3(t)$ do not occur simultaneously. In other words, the initially delocalized state $\psi_2(t=0) = (|1,\bar{1}\rangle + |\bar{1},1\rangle)/\sqrt{2}$ cannot remain delocalized as time evolves.

5. Conclusion

In summary, we have presented an analytical method for studying CDT in external driven AC-field, biased QDMs containing two interacting electrons. Under CDT conditions a coherent suppression of tunneling between electronic states occurs. Using an analytic approach which is justified in the material under study, we have managed to describe CDT with quantum resonant tunneling. Depending on the value of the Coulomb interaction between the two electrons, the CDT constraint conditions for the AC-field are different. The two-level approximation is not suitable for describing the system if the Coulomb interaction is an integer times the frequency of the AC-field.

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