Two-electron localization in a quantum dot molecule driven by a cosine squared field*

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We investigate the dynamics of two interacting electrons confined in a quantum dot molecule under the influence of cosine squared electric fields. The conditions for two-electron localization in the same quantum dot are analytically derived within the frame of the Floquet formalism. The analytical results are compared to numerical results obtained from the solution of the time-dependent Schödinger equation.

Keywords: dynamic localization, Floquet state, Bessel function

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1. Introduction

In recent years, the quantum mechanical control of the dynamics of two-electron quantum dot structures has been the subject of several investigations.[1–7] Most of these studies have concentrated on the dynamic localization effect and on the generation of entangled states of two electrons.[2] In particular, it has been shown that localization in a two-electron quantum dot molecule (QDM) can be achieved by applying an alternating current (AC) electric field[3,4] or by applying an AC–DC driving field.[5,6] The localization conditions involve ratios of the Rabi frequency of the field–matter interaction to the angular frequency of the external driving field corresponding to zeros of an ordinary Bessel function of order determined by the DC field and the effective Coulomb interaction between the two electrons.[7]

For an AC field with amplitude modulation, the driving field is regarded as a bichromatic AC field for which the two components have the same amplitude but different frequencies. However, according to the conditions for the dynamic localization of bichromatic AC electric field,[1] the ratios of the amplitude and frequency are roots of Bessel functions of the first kind, and once the frequencies are different, the corresponding amplitudes should be different. There are some special characters for the AC field with amplitude modulation, compared with the bichromatic AC field. As a special case of amplitude modulation field, we study the dynamic behavior of two electrons in a quantum dot molecule under the influence of a cosine squared external electric field in the present paper. The conditions that we derive using a perturbation analysis for the localization of the two electrons are also numerically tested for the quantum dot structure.

The paper is organized as follows. In the following section we introduce the model for the two-electron quantum dot molecule. Then, in Section 3, we derive analytical conditions for two-electron localization in a quantum dot molecule under a cosine squared electric field. In addition, we present numerical results that verify these conditions. Finally, in Section 4, we conclude this study with a summary of our findings.

2. Theoretical model for the two-electron quantum dot molecule

For the description of the two-electron QDM under study, we apply the Hubbard model.[8] In this model, each quantum dot of the QDM is regarded as a point, and the Hamiltonian of electron in the QDM can be written as

$$H(t) = \sum_{\sigma,i=1,2} e_i(t) d^{\dagger}_{i\sigma} d_{i\sigma} + W \sum_{\sigma} \left(d^{\dagger}_{1\sigma} d_{2\sigma} + d^{\dagger}_{2\sigma} d_{1\sigma} \right) + U_1 \sum_{i} n_{i\uparrow} n_{i\downarrow} + U_2 \sum_{\sigma_1,\sigma_2} n_{1\sigma_1} n_{2\sigma_2}. \quad (1)$$

Here $d^{\dagger}_{i\sigma}$ and $d_{i\sigma}$ are creation and annihilation operators of an electron with spin σ on the i-th dot, $i = 1$ or 2. When the external electric field has a cosine squared form $E(t) = V\cos^2(\omega t)$, the energy levels become $e_i(t) = (-1)^{i+1}\left(V\cos^2(\omega t)\right)/2$, where V and ω are the amplitude and frequency of the driving field. W describes the coupling between two dots, and U_1 and U_2 denote the intradot and interdot Coulomb interactions, respectively.

In real space, the two-electron 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 dot and n electrons at the second dot. The values 1 and $\bar{1}$ indicate the spin-up and spin-down states, respectively. On replacing the basis states $|1,\bar{1}\rangle$ and $|\bar{1},1\rangle$ with $\left(|1,\bar{1}\rangle - |\bar{1},1\rangle\right)/\sqrt{2}$ and $\left(|1,\bar{1}\rangle + |\bar{1},1\rangle\right)/\sqrt{2}$, the

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Hamiltonian of the system takes on the matrix form

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

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

$$H_1(t)=\begin{bmatrix} 2e_1(t)+U_1 & \sqrt{2}W & 0 \\ \sqrt{2}W & U_2 & \sqrt{2}W \\ 0 & \sqrt{2}W & 2e_2(t)+U_1 \end{bmatrix}. \tag{3}$$

There is no mixing between the two subspaces due to there being no spin-flip terms in Eq. (1). Obviously the basis vectors $|1,1\rangle$, $|\bar{1},\bar{1}\rangle$, and $\left(|1,\bar{1}\rangle+|\bar{1},1\rangle\right)/\sqrt{2}$ are the eigenvectors of the Hamiltonian and constitute the trivial triplet subspace, in which the electron number in each dot is invariably one, and the time-dependent term does not influence this characteristics.

We will focus our attention on the singlet subspace consisting of $|2,0\rangle$, $\left(|1,\bar{1}\rangle-|\bar{1},1\rangle\right)/\sqrt{2}$, $|0,2\rangle$. The Hamiltonian $H_1(t)$ in the singlet subspace with a constant energy shift of U_2 can be written as

$$H_1'(t)=\begin{bmatrix} 2e_1(t)+\kappa & \sqrt{2}W & 0 \\ \sqrt{2}W & 0 & \sqrt{2}W \\ 0 & \sqrt{2}W & 2e_2(t)+\kappa \end{bmatrix}, \tag{4}$$

where $\kappa=U_1-U_2$ is the effective Coulomb interaction. In the absence of a time-dependent term, the eigenvalues and eigenvectors of the Hamiltonian H_1' can be exactly solved. When the time-dependent term is involved, the time periodicity of the Hamiltonian H_1' enables us to describe the quantum evolution process in terms of Floquet theory.[9]

Given an initial state of the system $|\psi(0)\rangle$, its time evolution can be expressed in terms of Floquet states as follows:

$$\psi(t)=\sum_{\alpha=1,2,3}\exp(-\mathrm{i}\varepsilon_\alpha t)\,|u_\alpha(t)\rangle\,\langle u_\alpha(0)|\,\psi(0)\rangle, \tag{5}$$

where ε_α and $|u_\alpha(0)\rangle$ are quasienergies and the corresponding initial Floquet states. They are obtained by diagonalizing the one-period propagator $U(T,0)$ of Hamiltonian H_1', which is determined by integrating the following time-dependent Schrödinger equation ($\hbar=1$) from $t=0$ to $t=T$,

$$\mathrm{i}\frac{\partial}{\partial t}U(t,0)=H_1'(t)\,U(t,0). \tag{6}$$

The propagator $U(t,0)$ satisfies the initial condition $U(0,0)=I_{3\times 3}$, and can be obtained using the equation

$$U(t,0)=\sum_{\alpha=1,2,3}\exp(-\mathrm{i}\varepsilon_\alpha t)\,|u_\alpha(t)\rangle\,\langle u_\alpha(0)|. \tag{7}$$

We can get the Floquet state $|u_\alpha(t)\rangle$ at arbitrary time $t\in[0,T]$ by first calculating $U(T,0)$.

To investigate the dynamic localization of the system, we define $P(t)$ as the occupation probability at time t of the initial state $|\psi(0)\rangle$.[10] Using Eq. (5), we get

$$\begin{aligned} P(t) &= |\langle\psi(0)|\,\psi(t)\rangle|^2 \\ &= \left|\sum_{\alpha,\beta} c_\alpha^* c_\beta \exp[-\mathrm{i}(\varepsilon_\beta-\varepsilon_\alpha)t]\,\langle u_\alpha(0)|\,u_\beta(t)\rangle\right|^2. \end{aligned} \tag{8}$$

At the quasi-energy level crossing points, i.e., $\varepsilon_\beta=\varepsilon_\alpha$, dynamic localization occurs with $P(t)\approx 1$. The degeneracy of the quasi-energies can be used to identify dynamic localization in a quantum system under the action of a periodic field. As a result, the Floquet spectrum method is very useful in the study of the dynamic localization. However, this method still has a shortcoming in that a crossing or avoided crossing is only a necessary condition, not a sufficient condition for localization. To solve this problem, Jiang *et al*. developed the long-time averaged occupation probability (LAOP) method.[11] It has been shown that the LAOP provides both the necessary and sufficient condition for dynamical localization. The LAOP method has therefore been used in this paper.

3. Localization conditions and numerical results

Numerical methods are usually employed to calculate the quasi-energies. When the difference between the two types of Coulomb interaction, κ, is much larger than the tunneling coefficient, W, the Hamiltonian equation (4) can be divided into two parts H_a and H_t

$$\begin{aligned} H_1' = &\begin{pmatrix} V\cos^2(\omega t)+\kappa & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -V\cos^2(\omega t)+\kappa \end{pmatrix} \\ &+\begin{pmatrix} 0 & \sqrt{2}W & 0 \\ \sqrt{2}W & 0 & \sqrt{2}W \\ 0 & \sqrt{2}W & 0 \end{pmatrix}. \end{aligned} \tag{9}$$

In the interaction term H_a, all the interaction terms are diagonal, and it is straightforward to obtain an exact, orthogonal set of eigenvectors for Eq. (6). We rewrite the driving electric field $E(t)=V\cos^2(\omega t)$ as $E(t)=\frac{V}{2}(1+\cos(2\omega t))$. The three eigenvectors are then

$$\begin{cases} |u_1(t)\rangle = \left(\exp\left[-\mathrm{i}t\left(\kappa+\dfrac{V}{2}-\varepsilon_1\right)\right.\right. \\ \qquad\qquad \left.\left.-\mathrm{i}\dfrac{V}{4\omega}\sin(2\omega t)\right],0,0\right), \\ |u_2(t)\rangle = (0,\exp[\mathrm{i}t\varepsilon_2],0), \\ |u_3(t)\rangle = \left(0,0,\exp\left[-\mathrm{i}t\left(\kappa-\dfrac{V}{2}-\varepsilon_3\right)\right.\right. \\ \qquad\qquad \left.\left.+\mathrm{i}\dfrac{V}{4\omega}\sin(2\omega t)\right]\right). \end{cases} \tag{10}$$

Using the T-periodic boundary condition $u_\alpha(t+T)=u_\alpha(t)$, we can get the eigenvalues $\varepsilon_1=\kappa+V/2$, $\varepsilon_2=0$, and $\varepsilon_3=$

$\kappa - V/2$, and the corresponding eigenvectors,

$$\begin{cases} \psi_1(t) = \left(\exp\left[-\mathrm{i}t\left(\kappa+\dfrac{V}{2}\right)\right.\right. \\ \qquad \left.\left.-\mathrm{i}\dfrac{V}{4\omega}\sin(2\omega t)\right],0,0\right), \\ \psi_2(t) = (0,1,0), \\ \psi_3(t) = \left(0,0,\exp\left[-\mathrm{i}t\left(\kappa-\dfrac{V}{2}\right)\right.\right. \\ \qquad \left.\left.+\mathrm{i}\dfrac{V}{4\omega}\sin(2\omega t)\right]\right). \end{cases} \tag{11}$$

These are stationary states in real space, and the number of electrons in each dot never changes with time.

When the tunneling perturbation H_t is taken into account, the number of electrons on each dot might change due to resonant tunneling.[12] The tunneling probability is determined by the elements of matrix H_t,

$$\begin{aligned} (H_\mathrm{t})_{i,j} &= \langle\langle \psi_i(t)|H_\mathrm{t}|\psi_j(t)\rangle\rangle \\ &= \frac{1}{T}\int_0^T \mathrm{d}t\,\langle\psi_i(t)|H_\mathrm{t}|\psi_j(t)\rangle, \end{aligned} \tag{12}$$

where $\langle\langle\cdots\rangle\rangle$ denotes the inner product for the three eigenvectors $|\psi_i(t)\rangle$, which are T-periodic functions.[13,14] By using the well-known identity

$$\exp[-\mathrm{i}\beta\sin\omega t] = \sum_{\mathrm{m}=-\infty}^{\infty} \mathrm{J_m}(\beta)\exp[-\mathrm{i}m\omega t], \tag{13}$$

to rewrite the eigenvectors $|\psi_i(t)\rangle$, we can straightforwardly obtain the elements of matrix H_t in the form of the Bessel function of the first kind,

$$H_\mathrm{t} = \sqrt{2}W\begin{bmatrix} 0 & \mathrm{J}_{-n}(V/4\omega) & 0 \\ \mathrm{J}_{-n}(V/4\omega) & 0 & \mathrm{J}_n(V/4\omega) \\ 0 & \mathrm{J}_n(V/4\omega) & 0 \end{bmatrix}, \tag{14}$$

with $\kappa - V/2 = -2n\omega$.

When the element $(H_\mathrm{t})_{i,j}$ is zero, the tunneling between $|\psi_i(t)\rangle$ and $|\psi_j(t)\rangle$ is forbidden. In other words, the initially delocalized state $\psi_1(0) = |2,0\rangle$ or $\psi_3(0) = |0,2\rangle$ can remain in dynamic localization as time evolves if $\mathrm{J}_n(V/4\omega) = 0$.

In order to verify the above constraint condition, we employed the fourth-order Runge–Kutta algorithm for solving the time-dependent differential equation (7) with the initial condition $|\psi(0)\rangle = |0,2\rangle$. As mentioned above, this initial state corresponds to the localization of an electron pair in the second quantum dot. We regard the dynamic localization phenomenon as occurring if P_min, the minimum value of the probabilities $P(t) = |\langle\psi(0)|\,\psi(t)\rangle|^2$ that describe the population evolution of the initial state $|0,2\rangle$, is larger than 0.5. Figure 1 illustrates the phase diagram of P_min as a function of the amplitude of the driving field, V, and the effective Coulomb interaction, κ, for the case where the tunneling matrix element is $W = 0.15\omega$.

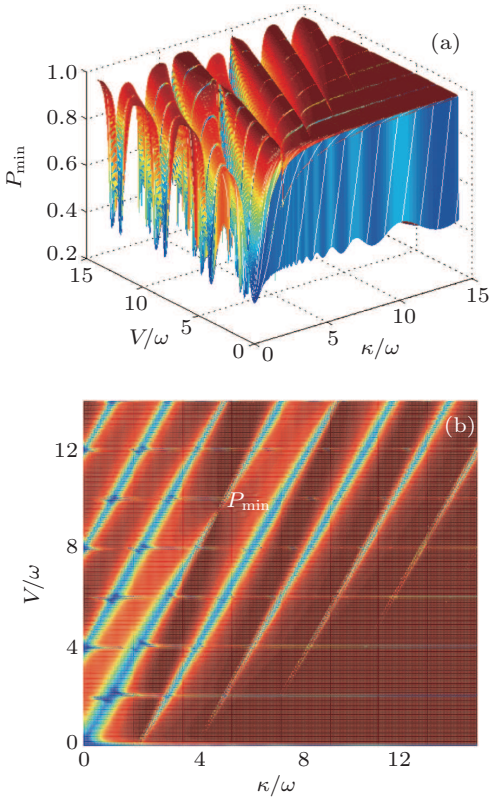


Fig. 1. (color online) Three-dimensional (a) and plane view (b) of the dependence of P_min for the initial state $|0,2\rangle$ less than $500\pi/\omega$ on κ and V, $W = 0.15\omega$.

Note that the phase diagram $P_\mathrm{min}(\kappa, V)$ in Fig. 1 agrees with the above analytical result. In particular, the initial state $|\psi(0)\rangle = |0,2\rangle$ remains localized except in regions near the lines $V = 2\kappa + 4n$, $n = 0, \pm1, \pm2, \ldots$.

For the case $n = 0$, the amplitude of the driving field V and the effective Coulomb interaction κ satisfy the relation $V = 2\kappa$, with $\kappa \geq 0$, which is the diagonal line in Fig. 1(b). Figure 2 shows the population $P(t)$ and minimum P_min of the initial state $|\psi(0)\rangle = |0,2\rangle$ as functions of the amplitude of the driving field V. According to Fig. 2(a), we find that the initial state $|\psi(0)\rangle = |0,2\rangle$ remains localized in the second dot with $\kappa = 4.83\omega$ and $V = 9.88\omega$. Such an amplitude for the driving field satisfies the Bessel function relation $\mathrm{J}_0(V/4\omega) = 0$, as shown in Fig. 2(b). The numerical results thus agree well with the analytical condition Eq. (14) for $n = 0$.

For the case of $n = 1$, the amplitude of the driving field and the effective Coulomb interaction satisfy the relation $V = 2\kappa + 4$, and $V \geq 4$ with $\kappa \geq 0$, which is the line above the diagonal line in Fig. 1(b). Figure 3 shows the minimum population $P_\mathrm{min}(V)$ of the initial state $|\psi(0)\rangle = |0,2\rangle$. Note that the dynamic localization occurs with the driving field strength V satisfying the relation $\mathrm{J}_1(V/4) = 0$. This demonstrates the excellent agreement between the numerical results and the analytical condition of Eq. (14) for $n = 1$. With increasing n, the amplitude of the driving field V is more important than the effective Coulomb interaction κ. The two electrons can then be viewed as a single particle with charge $2e$.[15]

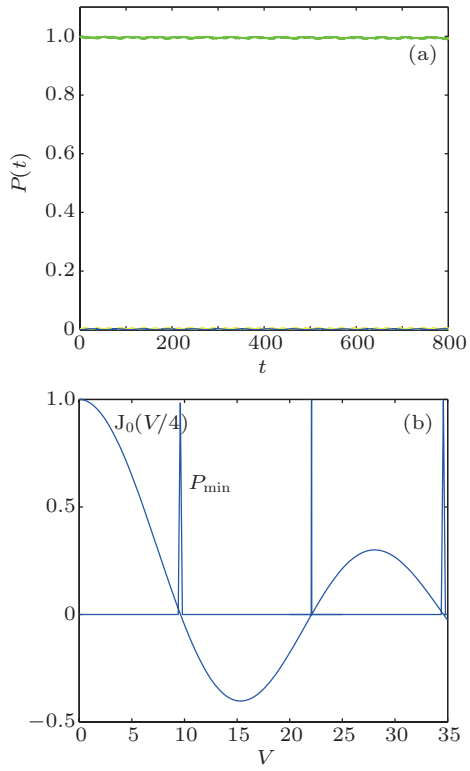


Fig. 2. (color online) (a) The population evolution $P(t)$ of the initial state $|0,2\rangle$ for time less than $266T$, $\kappa = 4.83\omega$, $V = 9.88\omega$, $W = 0.15$, and $\omega = 1$. (b) $J_0(V/4)$ and the minimum $P_{\min}(V)$ less than $1000T$ with $W = 0.15$ for the case of $V = 2\kappa$.

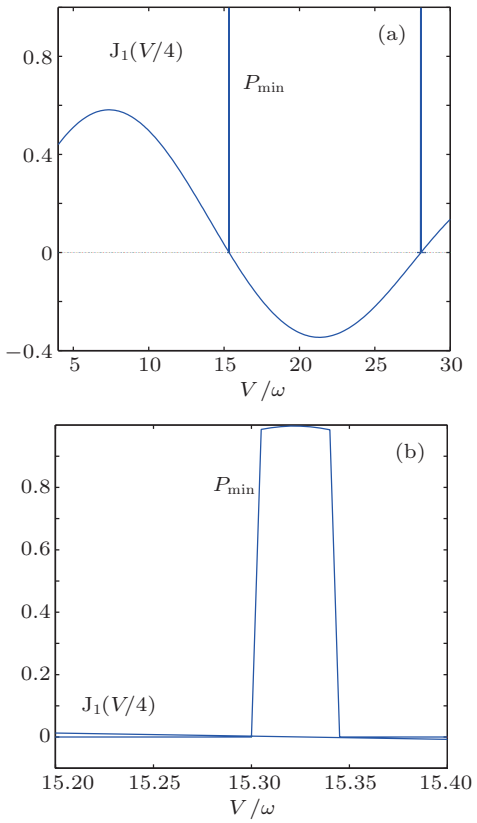


Fig. 3. (color online) (a) The minimum $P_{\min}(V)$ and $J_1(V/4)$ for the case of $V = 2\kappa+4$ with $W = 0.15$ and $\omega = 1$. (b) Detail of $P_{\min}(V)$ and $J_1(V/4)$ near $V = 15.3\omega$.

In the case where $n = -1$, the relation $V = 2\kappa - 4$ with $V \geq 0$ and $\kappa \geq 2$ is the line under the diagonal in Fig. 1(b). Figure 4 shows the minimum value $P_{\min}(V)$ for time less than $1000T$ for the population of the initial state $|0,2\rangle$. Note that dynamic localization occurs when the driving field strength V satisfies the relation $J_{-1}(V/4) = 0$, which again shows the good agreement between the analytic conditions and the numerical results. With decreasing n, the effective Coulomb interaction κ becomes more important than the amplitude of the driving field. The external driving field can then be ignored when $V \ll \kappa$, and the initial state $|0,2\rangle$ remains in the second quantum dot. Dynamic localization occurs when the amplitude of the driving electric field V is comparable to the effective Coulomb interaction κ and satisfies the relation $J_{-n}(V/4) = 0$.

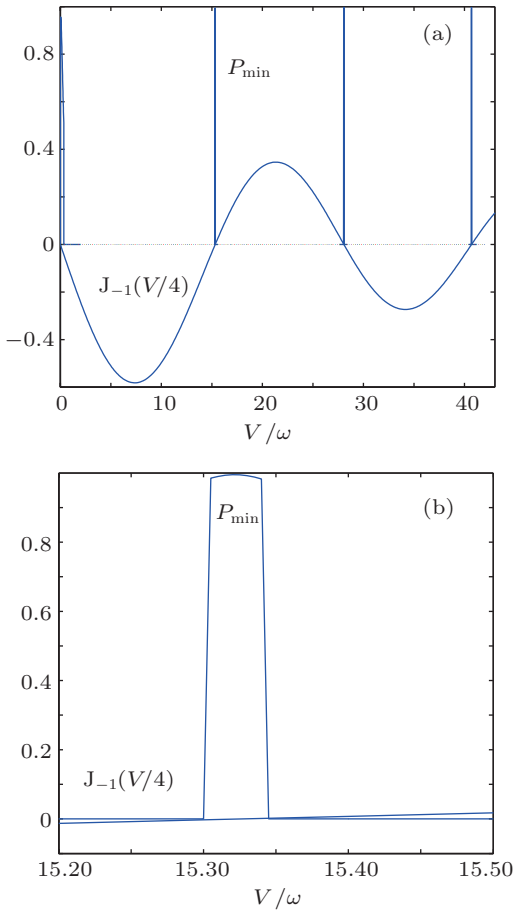


Fig. 4. (color online) (a) The minimum $P_{\min}(V)$ and $J_{1-}(V/4)$ for the case of $V = 2\kappa - 4$ with $W = 0.15$ and $\omega = 1$. (b) Detail of $P_{\min}(V)$ and $J_{-1}(V/4)$ near $V = 15.3\omega$.

As a result, the amplitude of the driving electric field V is relevant to the effective Coulomb interaction κ while dynamic localization is occurring. According to this, the effective Coulomb interaction κ could be worked out with the help of the angular frequency and amplitude of the external driving field. Such a conclusion could not be achieved in the case of an AC–DC driving field $E(t) = E_0 + E\cos(\omega t)$,[5] where E_0 is irrespective to E. As a possible application of the cosine squared driving field, it is probably used to measure the

effective Coulomb interaction between electrons in a quantum dot molecule.[16] Such an experimental method depends sensitively on the parameters of the driving field, thereby giving the attractive possibility of coherently manipulating electronic states in semiconductor nanostructures by means of laser pulses[17] or oscillating gate potentials.

4. Conclusion

In summary, we have presented the effect of a cosine squared driving field on the dynamics of two electrons in a system of two quantum dots. The results are different from those obtained both with a cosine external AC driving field[18,19] and with combined DC–AC fields.[4,7] Using separately the perturbation approximation method and the fourth-order Runge–Kutta algorithm, we have found that resonant tunneling between the localized states $|0,2\rangle$ and $|2,0\rangle$ occurs if the value of the effective Coulomb interaction κ between the two electrons and the strength of the driving field satisfy the relation $V/\omega = 2\kappa/\omega + 4n$. Such resonant tunneling is destroyed if the parameters simultaneously satisfy the relation $\mathrm{J}_{\pm n}(V/4) = 0$. In that case, dynamic localization occurs. The above conclusions imply a possible application of the cosine squared driving field to measure the effective Coulomb interaction between electrons in a quantum dot molecule or in ultrafast electron transfer.

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