Tunneling control by high-frequency driving

Ilya Vorobeichik and Nimrod Moiseyev
Department of Chemistry and Minerva Center for Non Linear Physics, Technion–Israel Institute of Technology, Haifa 32000, Israel

(Received 24 July 1998)

The second-order perturbation theory in the framework of the Kramers-Henneberger oscillating frame representation of the Hamiltonian [H. A. Kramers, *Quantum Mechanics* (North-Holland, Amsterdam, 1956); W. C. Henneberger, Phys. Rev. Lett. **21**, 838 (1968)] is used to study the tunneling process in a periodically driven double-well potential. The eigenstates of the Floquet Hamiltonian are efficiently approximated when a field frequency is larger than a classical frequency of the time-averaged Hamiltonian. The conditions for coherent enhancement and suppression of tunneling are obtained when the standard perturbation theory fails. It is shown that the enhancement and suppression of tunneling is due to field-induced coupling between states of a one-period averaged effective potential. [S1050-2947(99)00103-1]

PACS number(s): 42.50.Hz, 03.65.−w, 73.40.Gk, 12.38.Bx

Interest in tunable short-wavelength sources has stimulated numerous experimental and theoretical investigations of photoinduced dynamics in strong laser fields [1,2]. The physical phenomena in strong laser fields are very different from weak fields, which implies that one cannot use perturbation theory around the field-free Hamiltonian in photoinduced processes in strong fields. The proof that the radius of convergence of perturbation expansions in ac and dc fields is zero [3] supports this hypothesis. However, in the limit of high-frequency driving, the Kramers-Henneberger (KH) oscillating frame representation [4] can be used for an effective description of physical systems in strong laser fields [1,2]. We show that high-frequency second-order perturbation theory based on the KH frame representation can be used for control of tunneling enhancement and suppression in periodically driven double-well potentials.

The Hamiltonian of a one-dimensional system (chosen as a model) driven by the periodic field is given by

$$H(x,t)=\frac{p_x^2}{2m}+V(x)+Sx\,\sin(\omega t), \tag{1}$$

where S and ω are the amplitude and the frequency of the driving. The solution of the Schrödinger equation is expanded in the basis set of eigenfunctions of the Floquet Hamiltonian

$$\left(-i\hbar\frac{\partial}{\partial t'}+H(x,t')\right)\Phi_n(x,t')=\mathcal{E}_n\Phi_n(x,t'), \tag{2}$$

where t' serves as an additional coordinate in the generalized Hilbert space [5,6] of square-integrable functions, which are defined on the domain $-\infty<x<+\infty$ and $0<t'<T$. $T=2\pi/\omega$ is the period of the driving, and $\Phi_n(x,t)=\Phi_n(x,t+T)$ and $\mathcal{E}_n$ are the quasistationary Floquet states and the quasienergies, respectively.

The oscillating frame representation of Eq. (1) is obtained by two successive unitary transformations, wherein a pure time-dependent term (which physically is not important since it yields only an overall phase factor) is dropped (see, e.g., Ref. [11]). The KH oscillating frame Hamiltonian is given by

$$\tilde{H}(x,t)=\frac{p_x^2}{2m}+V(x+\alpha_0\,\sin(\omega t)), \tag{3}$$

where $\alpha_0=S/m\omega^2$. In this representation, the quasienergies are all shifted by the same amount (known as ''the ponderomotive energy'') $\mathcal{E}_n=E_n+S^2/4m\omega^2$, where

$$\left(-i\hbar\frac{\partial}{\partial t'}+\tilde{H}(x,t')\right)\tilde{\Phi}_n(x,t')=E_n\tilde{\Phi}_n(x,t'). \tag{4}$$

Since we are interested only in quasienergy differences, the spectrum of the Floquet Hamiltonian in Eq. (4) is sufficient.

Using the (t,t') method [7], in which t' acts as an additional coordinate, a time-independent perturbative expansion can be applied to Eq. (4). Following the work of Gavrila [1], a one-period time-averaged Hamiltonian is chosen as the zeroth-order one:

$$H_0(x)=\frac{p_x^2}{2m}+\mathcal{V}_0(x), \tag{5}$$

where

$$\mathcal{V}_0(x)=\frac{1}{T}\int_0^T V(x+\alpha_0\,\sin(\omega t'))dt'. \tag{6}$$

The zeroth-order contribution to the spectrum of the Floquet Hamiltonian is then field strength dependent and is given by

$$\left(-i\hbar\frac{\partial}{\partial t'}+H_0(x)\right)\Psi_{k,m}^{(0)}(x,t')=E_{k,m}^{(0)}\Psi_{k,m}^{(0)}(x,t'), \tag{7}$$

where $E_{k,m}^{(0)}=E_k^{(0)}+\hbar\omega m$ $(k=1,2,\ldots;\ m=0,\pm1,\pm2,\ldots)$,

$$\Psi_{k,m}^{(0)}(x,t')=\phi_k^{(0)}(x)\exp(i\omega m t'), \tag{8}$$

and

$$H_0(x)\phi_k^{(0)}(x)=E_k^{(0)}\phi_k^{(0)}(x). \tag{9}$$

The perturbation $V(x,t')$ is defined as

$$V(x,t')=\sum_{n\neq 0}\mathcal{V}_n(x)\exp(i\omega nt'), \tag{10}$$

where $\mathcal{V}_n(x)$ is the nth Fourier component of the potential in the oscillating frame representation. The first-order correction to the eigenvalues vanishes,

$$E_k^{(1)}=\langle\langle\Psi_{k,m}^{(0)}(x,t')|V(x,t')|\Psi_{k,m}^{(0)}(x,t')\rangle\rangle=0, \tag{11}$$

and the second-order correction quasienergy term is given by

$$E_k^{(2)}=\sum_{n\neq 0}\sum_{k'}\frac{|\langle\phi_k^{(0)}(x)|\mathcal{V}_n(x)|\phi_{k'}^{(0)}(x)\rangle|^2}{E_k^{(0)}-E_{k'}^{(0)}+\hbar\omega n}. \tag{12}$$

Since we consider a time-periodic potential, Eq. (12) obtained by the (t,t') method is equivalent to Eq. (103) of Ref. [1], p. 465, which was developed by Gavrila using the Green's function of the Floquet Hamiltonian. The difference is that the (t,t') method can be extended to the nonperiodic Hamiltonians provided the laser pulse duration is much larger than one optical cycle.

One should expect this perturbation expansion to hold when the frequency of the field is larger than a classical frequency of the particle Ω in the time-averaged potential. It can be exemplified for the case of a periodically driven harmonic oscillator [8]. In this case, the potential in the KH frame is given by

$$V(x,t)=\frac{m\Omega^2}{2}[x^2+\alpha_0^2\sin^2(\omega t)]+\left(\frac{\Omega}{\omega}\right)^2 Sx\sin(\omega t). \tag{13}$$

The first term in Eq. (13) is the harmonic oscillator with a time-periodic (always positive) energy shift. It can be time averaged, resulting in the effective zeroth-order rise of the energy levels. The second term is a small perturbation provided $\omega\gg\Omega$. Therefore, for sufficiently large field frequency one can use the perturbation expansion for much stronger fields than in standard perturbation theory.

Tunneling in the presence of the external periodic field has been investigated extensively in recent years [9–16]. It was demonstrated [10,11,15,16] that the coherent enhancement and suppression of tunneling is based on a dynamical symmetry of the Floquet Hamiltonian ($x\to -x$, $t\to t+T/2$) and is associated with exact and avoided crossings of quasienergies. It was also shown [11,15,16] that the completeness of tunneling in the presence of the driving is preserved when two Floquet states, associated with the lowest almost degenerate pair of states in the double-well potential [which we denote by $\psi_1(x)$, $\psi_2(x)$], dominate the expansion of the solution of the time-dependent Schrödinger equation. In this case, one can show that the tunneling rate is determined by the splitting of a pair of Floquet states, i.e.,

$$\omega_{tun}\simeq\frac{\Delta}{\hbar}, \tag{14}$$

where $\Delta=|E_2-E_1|$. For the field-free case E_2 and E_1 are energies of the first two almost degenerate states [$\psi_1(x)$, $\psi_2(x)$] and the tunneling rate is associated with the unperturbed energy splitting Δ_0. When the field is turned on, the quasienergy splitting grows and the tunneling rate is enhanced. In addition, exact crossings between the quasienergy doublet occur and then the tunneling is suppressed [12,13]. A further tunneling enhancement is obtained when a singlet-doublet crossing takes place. Then one of Floquet states of the doublet interacts with the third state and an avoided crossing between quasienergies of Floquet states with the same symmetry occurs. In this case a three-state dynamics is obtained [15]. However, exactly at the avoided crossing point, the complete oscillations of the tunneling probability are preserved and the tunneling rate is again proportional to the splitting between the two quasienergies of the doublet [Eq. (14)]. The latter grows significantly due to the interaction between one of the doublet states with the third state, and the tunneling is further enhanced. Therefore, if one can efficiently approximate the quasienergies splitting, one could predict the tunneling enhancement and suppression.

In the low-driving-frequency limit, i.e., when $\omega\ll\Omega$, a two-level system approximation can be used to calculate the quasienergy splitting. In this case [12,13,17]

$$\Delta=\Delta_0 J_0\left(\frac{2S\langle\psi_1|x|\psi_2\rangle}{\hbar\omega}\right), \tag{15}$$

where J_0 is the zeroth-order Bessel function. This model can efficiently account for the tunneling suppression, but is unable to predict the tunneling enhancement.

We show that using high-frequency (HF) second-order perturbation theory one can calculate the tunneling splitting and explain the coherent tunneling enhancement and suppression in the high-frequency–strong-field limit. We consider a double-well potential in the form

$$V(x)=-D(e^{-a(x-x_1)^2}+e^{-a(x-x_2)^2}), \tag{16}$$

where the ionization energy $D=2$, $x_1=-x_2=10$, and $a=0.015$ (atomic units are used throughout). This potential supports six doublets of states with energy below the top of the barrier and therefore corresponds to a semiclassical regime.

From Eqs. (7), (11), and (12) one obtains that in the framework of second-order perturbation theory the tunneling splitting is given by

$$\Delta=\Delta^{(0)}+\Delta^{(2)}, \tag{17}$$

where

$$\Delta^{(0)}=|E_2^{(0)}-E_1^{(0)}| \tag{18}$$

is the zeroth-order term that is due to the change in energy levels in the one-period averaged effective potential (7) and

$$\Delta^{(2)}=|E_2^{(2)}-E_1^{(2)}| \tag{19}$$

is the second-order correction term that is due to the field-induced coupling between states (12). The zeroth-order approximation can be used to estimate the classical frequency Ω in the effective averaged double-well potential [11] and to find the range of α_0 values for which the complete tunneling will still be relevant. The conditions for that are problem dependent and in our example studied, for $\alpha_0>7$ the one-period averaged effective potential is no longer a double-

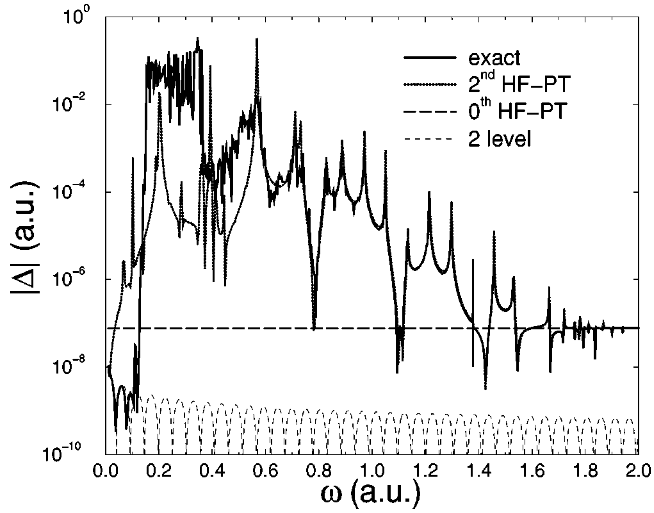

FIG. 1. Quasienergy splitting of two Floquet states that have maximal overlap with the first two unperturbed states in the double-well potential $[\psi_1(x),\ \psi_2(x)]$, as a function of the driving frequency for $\alpha_0=3$. The solid line stands for the numerically exact result calculated by the (t,t') method [7] using 128 Fourier basis functions $[\exp(in2\pi x/L),\ L=120]$, 5 Floquet channels, and $250/\omega$ time steps. The dotted line stands for the quasienergy splitting calculated using second-order high-frequency perturbation theory (HF-PT) in the Kramers-Henneberger oscillating frame representation of the Hamiltonian (17). The long-dashed line stands for the zeroth-order term in the high-frequency perturbation expansion (18). The dashed line stands for the quasienergy tunneling splitting calculated using two-level system approximation (15).

well potential and therefore, for larger values of α_0, many Floquet states will contribute and the tunneling completeness will be lost.

In Fig. 1 the tunneling splitting as a function of the driving frequency calculated using the second-order HF perturbation expansion (17) is compared with the numerically exact solution for $\alpha_0=3$. Since $\alpha_0=S/m\omega^2$ is kept constant, when the frequency of the driving increases, the driving amplitude increases as well. As one can see in Fig. 1, the second-order HF perturbation expansion is an excellent approximation for the tunneling splitting for $\omega>0.8$, which is about 4 times the classical frequency ($\Omega\simeq\Delta_{2-3}^{(0)}\simeq0.2$ for $\alpha_0=3$ in our case studied). For very small driving frequencies, the two-level system approximation (15) is very good and for large frequencies, the zeroth-order splitting associated with the one-period averaged effective potential is obtained. In the range $0.1<\omega<0.6$ both approximations break down. However, the exact numerical calculation shows that in this range of driving frequencies and field amplitudes many Floquet states contribute to the solution of the Schrödinger equation, i.e., the completeness of the tunneling is lost. This is because we consider large driving amplitudes for which close quasienergy states are strongly mixed. The completeness is regained once the driving frequency is close to (or higher than) the top of the barrier energy in the effective potential $E_{SEP}^{(0)}\equiv\mathcal{V}_0(x=0)$. (In our case, $E_{SEP}^{(0)}\simeq0.8$ for $\alpha_0=3$.) For such frequencies, distinct singlet-doublet crossings occur, each time when the driving frequency is in resonance with the energy difference between the lowest doublet of states and other states in the one-period averaged effective potential.

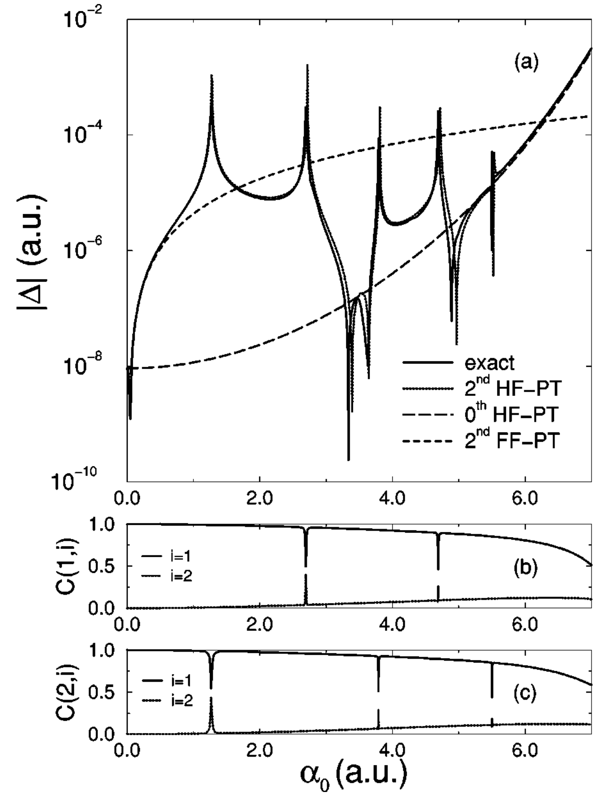

FIG. 2. (a) Quasienergy splitting of two Floquet states that have maximal overlap with the first two unperturbed states in the double-well potential $[\psi_1(x),\ \psi_2(x)]$, as a function of α_0 for the driving frequency $\omega=1.07$. The solid, dotted, and long-dashed lines are defined as in Fig. 1. The dashed line stands for the quasienergy tunneling splitting calculated using second-order perturbation theory with the field-free (FF) Hamiltonian $\mathcal{H}(x,t')=-i\hbar\partial/\partial t'+p_x^2/2m+V(x)$ as the zeroth-order Hamiltonian. (b) Projection of the Floquet states onto the first unperturbed state of the double-well potential $C(1,i)=\int\psi_1(x)\Phi_i(x,0)dx$, as a function of α_0. The solid line $(i=1)$ stands for the maximal projection and the dotted line $(i=2)$ stands for the one before maximal. (c) Same as (b) for the second unperturbed state of the double-well potential $\psi_2(x)$.

In Fig. 2 the tunneling splitting calculated using the second-order HF perturbation expansion (17) as a function of α_0 for $\omega=1.07$ is compared with the numerically exact solution and with the second-order perturbation theory when the field-free Hamiltonian is the zeroth-order one. Again, since the frequency is held fixed, the increase of α_0 means the increase of the driving amplitude. As one can see in Fig. 2, the field-free perturbation theory is able to describe the tunneling splitting only for very small values of α_0 [dashed line in Fig. 2(a)]. However, the second-order perturbation theory based on the oscillating frame representation is a good approximation for all values of α_0. Another important result is that *the second-order correction in the HF perturbation expansion dominates over the zeroth-order one*. The latter becomes important only for large values of α_0 for which the tunneling completeness is lost [see Figs. 2(b) and 2(c)]. Therefore, the tunneling enhancement is a result of a resonant or nonresonant coupling between states in the effective potential (12). For small values of α_0 the tunneling splitting begins to grow approximately as a second power of the driving amplitude due to the *nonresonant coupling of one of the* *doublet states to a third state* and it exhibits additional resonant growth due to singlet-doublet crossings. The crossings occur each time when the difference between energy levels of the one-period averaged effective potential coincides with $\hbar\omega n$. In addition, the exact quasienergy crossings in the doublet occur and then the tunneling is suppressed. The enhancement and suppression are based on the coupling between one of the doublet states to the excited states, while the second state in the doublet remains uncoupled. In the strong-field case, this is possible when the energy of the third state is above the top of the barrier since in this energy region, the difference between adjacent states is much larger than below the top of the barrier. Therefore, although the field is strong, not many Floquet states are mixed and two- or three-state dynamics is obtained. However, one cannot use very high driving frequencies to couple very-high-energy states since their interaction with the states of the lowest doublet is very small. One can show that the zeroth-order behavior of the states above the top of the barrier is different from that of the doublet states. The energy of the low doublet states grows as α_0 grows. This is because they are localized near the minima of the potential wells where the potential is well approximated by an harmonic oscillator. From Eq. (13) one can see that the energy levels of the harmonic oscillator are shifted up in the one-period time-averaged potential. However, the zeroth-order high-energy states are lowered since the double-well potential becomes broader after one-period averaging. Therefore, for certain values of the field amplitude, the zeroth-order energy difference between the lowest doublet of states and high states will be in resonance with the photon energy.

We gratefully acknowledge discussions with Professor P. Hänggi and S. Kohler. This work was supported by the Israel Academy of Sciences and Humanities and by the fund for the promotion of research at the Technion.

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