Control of Localization and Suppression of Tunneling by Adiabatic Passage

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We show that a field of frequency ω combined with its second harmonic 2ω driving a double-well potential allows us to localize the wave packet by adiabatic passage, starting from the delocalized ground state. The relative phase of the fields allows us to choose the well of localization. We can suppress (and restore) the tunneling subsequently by switching on (and off) abruptly the fields at well-defined times. The mechanism relies on the fact that the dynamics is driven to an eigenstate of the Floquet Hamiltonian which is a localized state.

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Generating and controlling coherent superpositions of states is of great interest, in particular, for the recent developments of quantum computing [1]. Quantum tunneling is a natural example of superpositions of states, which correspond to spatially localized states. An important goal is to achieve the control of driven tunneling (see, e.g., [2] for a review). Practical realizations can be considered in coupled multiquantum dot systems that can be now built experimentally [3]. Enhancement of tunneling by a nonresonant [4,5] or resonant [6] pulse-shaped field, and the coherent destruction of tunneling (CDT) [7–11] by a cw field are well established. The CDT as shown in [7,8] occurs when the field amplitude allows one to preserve the two bare states $|1\rangle$ and $|2\rangle$ as eigenstates of the Floquet Hamiltonian (dressed by the field) and to make the associated quasienergies cross such that the tunneling time between the two states becomes infinite when the field is on. The CDT has been differently obtained in [10,11], when one of the localized states is an eigenstate of the Floquet Hamiltonian, which requires the coupling to an asymmetric excited electronic surface $|e\rangle$ of similar amplitudes: $|\langle e|\mu|1\rangle| \approx |\langle e|\mu|2\rangle|$ with μ the coupling operator. The CDT by two fields of different frequencies has been investigated in [12]. The CDT proposed so far in the literature is only partially controlled in the sense that one does not know the state of the system, i.e., the phase ξ of the stopped superposition $|1\rangle + e^{i\xi}|2\rangle$, since the initial tunneling state is generally unknown. This can be circumvented if one can also control the localization from the initial unlocalized ground state $|1\rangle$. It has been numerically shown in [13] that the localization is possible by the use of a pulse quasiresonant between the two tunneling states, however, under very restrictive conditions of field amplitudes, frequencies, and also absolute phases.

In this Letter we show a novel mechanism based on adiabatic passage that allows us to control the localization (i.e., with the knowledge of the localization time). This process is robust in the sense that it requires the control of the peak field amplitudes and frequencies but not of the absolute phase of the total field, nor of their pulse areas. Using subsequently the fields but suddenly switched on and off, we propose a consistent scheme of control from localization to suppression of tunneling. The mechanism is formulated as the preparation of one of the coherent superpositions $|\pm\rangle = (|1\rangle \pm |2\rangle)/\sqrt{2}$ in a system of two near-degenerate bare states $\{|1\rangle, |2\rangle\}$ of opposite parity. The key elements of the process are (i) the superpositions $|\pm\rangle$ become *eigenstates* of the Floquet Hamiltonian for specific field amplitudes and (ii) the pulse shapes allow us to reach one of the eigenstates from the ground state $|1\rangle$ by adiabatic passage. Adiabatic passage provides thus a technique to prepare the system in a localized state at a well-defined time. More precisely, a field of an appropriate frequency ω combined with its second harmonic 2ω, coupling the states $|1\rangle$ and $|2\rangle$ by a three-photon process (initially near-resonant, detuned by the energy difference δ between the two states), will induce dynamical Stark shifts that will compensate the detuning δ for specific field amplitudes. Adiabatic passage from the initial delocalized state $|1\rangle$ leads thus to one of the localized states whose localization is controlled by the relative phase of the two fields. The dynamics stays localized as long as the field amplitudes stay subsequently constant.

This localized state can then be used for other controlled manipulations such as the controlled switching on and off of the tunneling. In particular, the tunneling effect can start if the fields are switched off suddenly (more precisely, on a time scale T_{off} satisfying $\delta T_{\mathrm{off}} \ll 1$). The tunneling can be suppressed again if the fields are switched on again but suddenly, at a precisely determined time given by the period of the free tunneling. The wave packet can be alternatively redelocalized by adiabatic passage if the fields are switched off adiabatically.

We first introduce an *effective* model to analyze the qualitative aspects of the mechanism, and then we implement the strategy in a complete model with a double-well potential.

The key to be able to localize with the laser field consists first in noticing that the two localized states $|\pm\rangle$ are eigenstates of the Floquet Hamiltonian. This leads then to a strategy to reach them by adiabatic transport. This can be formulated by considering first the effective two-level system (in a resonant approximation)

$$H_{\rm eff}(t) = \hbar\begin{pmatrix} 0 & \Omega(t)e^{i\varphi} \\ \Omega(t)e^{-i\varphi} & \Delta(t) \end{pmatrix} \qquad (1)$$

in the bare basis $\{|1\rangle, |2\rangle\}$, where we assume that the Rabi frequency $\Omega(t)$ and the dynamical detuning (including the relative Stark shift) $\Delta(t)$ are both real such that $\Omega(t) > 0$ and at early times $\Omega(-\infty) = 0$, $\Delta(-\infty) \equiv \delta > 0$, without loss of generality. In the adiabatic limit, the propagator contains on its columns the instantaneous eigenvectors of (1): $|\psi_+\rangle = e^{i\varphi}\cos(\theta/2)|1\rangle + \sin(\theta/2)|2\rangle$, $|\psi_-\rangle = \sin(\theta/2)|1\rangle - e^{-i\varphi}\cos(\theta/2)|2\rangle$, $H_{\rm eff}(t)\psi_\pm = \frac{\hbar}{2}\times[\Delta(t) \pm \sqrt{\Delta^2(t) + 4\Omega^2(t)}]\psi_\pm$. It reads

$$U(t,-\infty) = \begin{pmatrix} e^{-i\eta_-(t)}\sin\frac{\theta(t)}{2} & e^{i[\varphi-\eta_+(t)]}\cos\frac{\theta(t)}{2} \\ -e^{-i[\varphi+\eta_-(t)]}\cos\frac{\theta(t)}{2} & e^{-i\eta_+(t)}\sin\frac{\theta(t)}{2} \end{pmatrix}, \qquad (2)$$

$$\tan\theta(t) = -\frac{2\Omega(t)}{\Delta(t)}, \qquad 0 \le \theta(t) < \pi, \qquad (3)$$

combined with the dynamical phases

$$\eta_\pm(t) = \frac{1}{2}\int_{-\infty}^{t} ds[\Delta(s) \pm \sqrt{\Delta^2(s) + 4\Omega^2(s)}]. \qquad (4)$$

We emphasize that the phases of the eigenvectors have been chosen as usual to satisfy the parallel transport: $\langle\psi_\pm|\partial/\partial t|\psi_\pm\rangle = 0$, leading to a zero geometric phase if one considers a nonclosed trajectory in the parameter space. We can thus generate by adiabatic passage the coherent superposition $|\pm\rangle$ when $\theta = \pi/2$, i.e., for

$$\Omega(t) \gg |\Delta(t)| \qquad (5)$$

and for a controllable phase φ. Starting from either state $|1\rangle$ or $|2\rangle$ [with initially $\theta(-\infty) = \pi$ here], we can generate by adiabatic passage the coherent superposition $|-\rangle$ or $|+\rangle$ (i.e., with θ going from π to $\pi/2$) by choosing the phase as $\varphi = 0$ or $\varphi = \pi$. Since $|\pm\rangle$ are eigenstates of the Hamiltonian (1), if Ω is suddenly switched off, the tunneling will start from the well-defined localized state previously prepared. Next, if Ω is suddenly switched on, again the tunneling will stop in the state $|\psi\rangle = a_+|+\rangle + a_-|-\rangle$ in which it is at the switching time. In particular, the tunneling can be stopped in one well if we choose a switching time when $a_+ = 1$ (or $a_- = 1$).

We implement this strategy in a tunneling system driven by two off-resonant pulse-shaped fields, of frequencies ω and its second harmonic 2ω (Fig. 1), of amplitudes $\mathcal{E}_1(t)$ and $\mathcal{E}_2(t)$, respectively, and of relative phase ϕ, leading to the total field $\mathcal{E}(t) = \mathcal{E}_1(t)\cos\omega t + \mathcal{E}_2(t)\cos(2\omega t + \phi)$. The effective Hamiltonian can be written in the three-photon resonant approximation as

$$H_{\rm eff}(t) = \hbar\begin{pmatrix} 0 & |\gamma|\mathcal{E}_2(t)\mathcal{E}_1(t)^2e^{i\varphi} \\ |\gamma|\mathcal{E}_2(t)\mathcal{E}_1(t)^2e^{-i\varphi} & \delta + S(t) \end{pmatrix} \qquad (6)$$

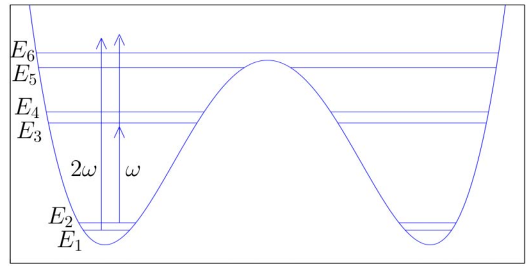

FIG. 1 (color online). Schematic diagram of the energy levels: E_1, E_2 are the energies of the two bare states $|1\rangle$, $|2\rangle$. The arrows represent the fields of frequencies ω and 2ω.

with

$$\varphi = \phi + \arg(\gamma), \qquad \arg(\gamma) = 0 \quad \text{or} \quad \pi, \qquad (7)$$

where the energy difference between the states $|2\rangle$ and $|1\rangle$ is denoted by δ and the relative Stark shift $S(t)$ (which is of second order in the field amplitudes) [14]. The off diagonal term $|\gamma|\mathcal{E}_2(t)\mathcal{E}_1(t)^2e^{i\varphi}$, of third order in field amplitude, is a three-photon coupling between the states $|1\rangle$ and $|2\rangle$. The construction of $H_{\rm eff}(t)$ requires in practice additional states in the model, which are taken into account by standard techniques of partitioning (or adiabatic elimination) [14,15]. This allows one to determine the coefficient γ and the relative Stark shift $S(t)$, which can both be chosen as real without loss of generality (see below for a concrete model). The Stark shifts will depend on the position of these additional states and on their couplings with $|1\rangle$ and $|2\rangle$. For instance, a single additional state $|3\rangle$ of energy E_3 coupled with the state $|2\rangle$ with the coupling element μ_{23}, by the field of frequency ω, with a positive detuning: $\hbar\Delta_{23} := E_3 - E_2 - \hbar\omega > 0$, will repel down the state $|2\rangle$ (of $-|\mu_{23}\mathcal{E}_1|^2/4\Delta_{23}$). Identifying (1) and (6) leads to $\Delta(t) \equiv \delta + S(t)$ and $\Omega(t)e^{i\varphi} \equiv |\gamma|\mathcal{E}_2(t)\mathcal{E}_1(t)^2e^{i\varphi}$. The condition (5) is well satisfied for the particular field amplitudes such that

$$\Delta \equiv \delta + S = 0 \qquad (8)$$

or for strong fields such that $|\gamma|\mathcal{E}_2\mathcal{E}_1^2 \gg |\delta + S|$. This latter condition is not considered in this work since in practice it requires generally very strong fields that would produce destructive processes, such as ionization. The condition (8) is expected to occur for specific values of field amplitudes if the frequency ω is appropriately chosen such that the Stark shift satisfies $S(t) < 0$.

We illustrate the proposed mechanism to manipulate coherently the tunneling in the standard symmetric double-well model potential $\hat{H}_0 = p^2/2 - x^2/2 + x^4/(64D)$ (with $D = 2$ to approximately model the NH_3 tunneling), expressed here in dimensionless units. Choosing the polarization of the lasers in the x direction, we obtain for the driven Hamiltonian $\hat{H}(t) = \hat{H}_0 - x\mathcal{E}(t)$. The 2 + 1 field shows a bias for $\phi \neq \pi/2$ that allows the breaking of symmetry. Without loss of generality, we can choose a basis such that $|+\rangle$ and $|-\rangle$ represent the localization in the left and right wells, respectively: $|+\rangle \equiv |L\rangle$, $|-\rangle \equiv |R\rangle$. We choose the appropriate frequency $\omega = 1.71 \times 10^{14}$ Hz which is a one-photon near resonance between states $|2\rangle$ and $|3\rangle$, and a two-photon near resonance between states $|1\rangle$ and $|6\rangle$ (see Fig. 1). The coefficient γ and the Stark shift $S(t)$ can be estimated by partitioning, using the one-photon near resonances for simplification, under the condition $\Omega_{\max} \ll \Delta_{\rm nr}$, where $\Delta_{\rm nr}$ characterizes the minimum detuning associated to the one-photon near resonances and $\Omega_{\max}$ is the peak Rabi frequency. We obtain here that γ is proportional to $\mu_{16}\mu_{23}\mu_{36}$ and $\gamma < 0$; i.e., $\arg(\gamma) = \pi$. The dynamics can be considered as adiabatic inside the subspace spanned by $\{|1\rangle, |2\rangle\}$ if $\Delta_{\rm nr}T \gg 1$, where T stands for a characteristic duration of the pulse [e.g., the full width half maximum (FWHM) for a Gaussian pulse]. The adiabatic dynamics can be characterized by the quasienergy representation (associated to the Floquet Hamiltonian with the double-well driven potential) (see, e.g., [15] for a review of adiabatic dynamics for Floquet Hamiltonians) as a function of the two field amplitudes for a given frequency ω (see Fig. 2). One can see a (dark) region of avoided crossing for moderate field amplitudes, which corresponds approximately to the amplitudes for which the condition (8) is satisfied. This avoided crossing can be intuitively understood as follows: The Stark shifts, which are the elements of lowest order in the field amplitudes, push the two Floquet eigenenergies, connected to the bare states $|1\rangle$ and $|2\rangle$, closer to each other. They subsequently repel since they are coupled (by the three-photon resonance) approximately when the effective Δ becomes zero. A choice of the envelope and peak fields correspond to a specific path in Fig. 2. An additional condition on the speed of the dynamics, which is determined by numerical simulation, has also to be fulfilled to reach adiabatically this avoided crossing.

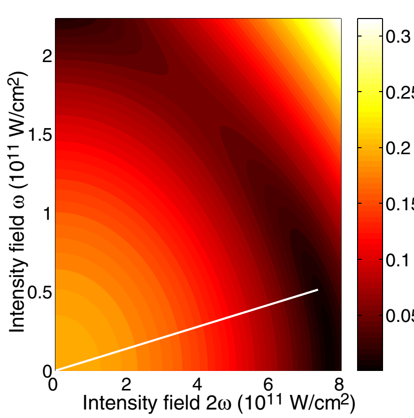

FIG. 2 (color online). Contour plot of the difference of the quasienergies connected to the bare states $|2\rangle$ and $|1\rangle$. The darker region is the considered line of avoided crossings. The white straight line corresponds to the dynamics used to achieve localization.

To achieve localization, we use nanosecond super-Gaussian ramps of shape $\Lambda(t) = \exp[-(t/\tau)^8]$ (here of FWHM 55.8 ns), which include a quasiplateau [see Fig. 4(b), left frame; note that the width of the rising of this super-Gaussian pulse is approximately 15 ns, which gives here for the adiabatic factor $\delta T \approx 565$), and of peak intensities 51 and 740 GW/cm^2 for I_1 and I_2, respectively. They allow (i) the use of the effective Hamiltonian (6) and (ii) adiabatic passage until the avoided crossing. The choice of the relative phase ϕ allows one to choose the well of localization.

As shown in Fig. 3, we obtain the localization of the wave packet from the initial state $|2\rangle$ in the right (left) well for $\phi = 0$ ($\phi = \pi$). The localization is quite robust with respect to the relative phase ϕ: We have observed numerically that the localization probability decreases from 1 to 0.97 when the relative phase is taken as 2.83 instead of π. Figure 4(a) (left frame) shows the localization for a population initially prepared in state $|1\rangle$. The population is localized in the left (right) well for $\phi = 0$ ($\phi = \pi$). Depending on the initial state, we create the target localized state by choosing the relative phase of the two pulses.

To control the subsequent starting and suppression of the tunneling oscillations, we use suddenly switched pulses since the localized states are eigenstates of the Floquet Hamiltonian (see Fig. 4). In practice this is ob-

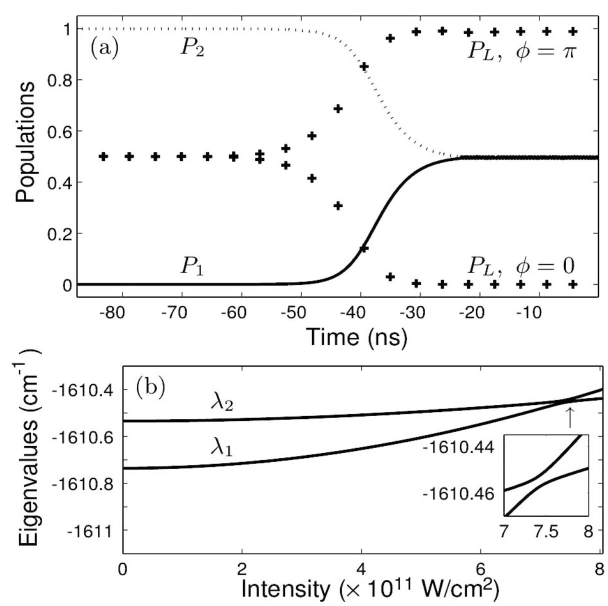

FIG. 3. (a) Numerical simulation of the localization of the populations as a function of time, respectively P_1 (P_2) of the states $|1\rangle$ ($|2\rangle$) in the full (dotted) line with $|2\rangle$ as initial condition. The + lines represent the population P_L localized on the left for the phases $\phi = 0$ and $\phi = \pi$. (b) Floquet eigenvalues λ_1, λ_2, respectively, connected to the bare energies E_1 and E_2, as functions of the intensity of the pulse 2 for a fixed value of the intensity of the pulse 1: $I_1 = 0.51 \times 10^{11}$ W/cm^2. The inset shows an enlargement of the avoided crossing of the Floquet eigenvalues.

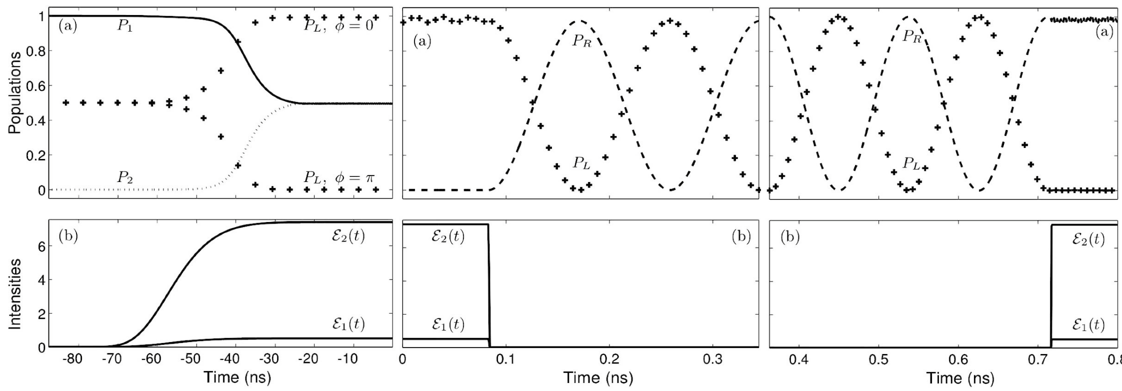

FIG. 4. (a) Left frame: same as Fig. 3(a), but with $|1\rangle$ as the initial condition. Middle and right frames: time continuation of the left frame. The plus (minus) line represents the population localized on the left (right) with the choice $\phi = 0$. (b) Intensities (in 10^{11} W/cm^2) of the pulses as a function of time. The middle (right) frame shows the tunneling starting (suppression) induced by fields suddenly switched off (on).

tained with Gaussian ramps of short FWHM T_s such that $\delta T_s \ll 1$ and $\Delta_{\rm nr} T_s \gg 1$ to avoid the appearance of other resonances. The population is initially prepared in the left well by adiabatic passage (see the left frame of Fig. 4). Tunneling (of period 176 ps) starts when the fields are suddenly switched off ($T_s = 2$ ps is used, which gives here $\delta T_s \approx 0.08$ and $\Delta_{\rm nr} T_s \approx 6$). After three and a half periods, the pulses suddenly switched on (with the same intensities used to localize) induce the suppression of the tunneling and the localization in the right well. This result is in agreement with the CDT by two fields of different frequencies predicted in the context of classical mechanics and with numerical quantum simulations of a localized initial Gaussian wave packet [12]. Since we have localized the wave packet, we have access to the subsequent times of localization, and we can thus start and suppress the tunneling at controlled times. Reversing time in Fig. 3 and in the left frame of Fig. 4 shows that the wave packet can be alternatively redelocalized by adiabatic passage in state $|1\rangle$ or $|2\rangle$ if the fields are switched off adiabatically when the wave packet is in state $|+\rangle$ or $|-\rangle$. The choice of the final state is made by the appropriate choice of the phase $\phi = 0$ or $\phi = \pi$, depending on the state before switching off.

This process of localization by adiabatic passage does not depend on the absolute phase of the total field, nor on the ramp area.

In conclusion, we have shown that it is possible to achieve the localization and suppression of tunneling by adiabatic passage. This controlled switching process can be adapted to the molecular alignment versus orientation. In this context, alignment is obtained by the Stark shifts induced by the two fields and oriented molecules correspond to localized states [16]. The tunneling, which is an oscillation between the two possible orientations, can be obtained by switching off one of the two fields, the other one maintaining the alignment. This scheme of controlled tunneling, reinterpreted as controlled manipulation of superposition of states, can have applications in the context of quantum computing.

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