

Laser-Induced Localization of an Electron in a Double-Well Quantum Structure

Raanan Bavli and Horia Metiu

Department of Chemistry^(a) and Physics, University of California at Santa Barbara, Santa Barbara, California 93106
(Received 14 May 1992)

We integrate numerically the time-dependent Schrödinger equation and show that a semi-infinite laser pulse can be used to localize an electron in one of the wells of a double-well quantum structure.

PACS numbers: 71.50.+t

Grossmann, Dittrich, Jung, and Hänggi [1] have pointed out an interesting effect of a cw laser acting on an electron in a quartic double well. If the electron is initially localized in one of the wells, and if the laser power and frequency are chosen appropriately, the radiation field can prevent the electron from tunneling back and forth between the wells.

In this Letter we investigate a more complex question: Can a semi-infinite laser pulse act on a ground-state electron, localize it in one of the wells, and then keep it there? Previous work [1] was concerned with maintaining the localization but not with creating it and ignored the need to turn on the laser at given time.

We study an electron with an effective mass $m^* = 0.067m$ (m is the electron mass) trapped in the potential shown in Fig. 1. The parameters of the potential are typical of a double quantum well [2]. As in the previous study [1] we use a potential that does not allow the electron to escape from the two-well system.

The laser-electron interaction is

$$V(t) = \begin{cases} ezE_0 \exp[-(t-t_0)^2/(2\tau^2)] \cos[\omega t + \delta], & t \leq t_0, \\ ezE_0 \cos[\omega t + \delta], & t \geq t_0. \end{cases} \quad (1)$$

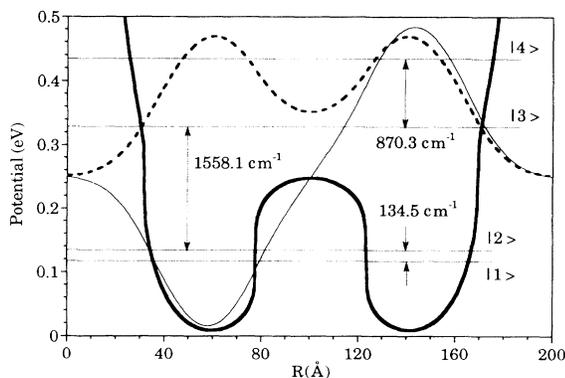


FIG. 1. The potential energy and the lowest two energy eigenstates. The energies of the first four states are shown by the horizontal lines. The barrier height is 240 meV and its width is 45 Å. The wells have about the same width as the barrier. The potential energy is $V(R) = 1000\{[(D+|D|)/2]^{1/4} - [(|D|-D)/2]^{1/4} + 1\} + \exp[30(R/L - \frac{1}{2})]$, where L is the total length of the structure ($=96\pi$ Å) and $D \equiv \cos(6.6R/L - 1.3\pi)$. The broken and solid lines show the lower two states of the system and the horizontal lines show the lowest four eigenenergies of the electron in the absence of the laser.

Here e and z are the electron charge and its coordinate along an axis perpendicular to the walls of the well. The laser parameters are the frequency ω , the rise time τ , and the phase δ . The parameter E_0 is specified by giving the photon energy flux $I_0 = 2ecE_0^2$ for $t > t_0$. If E_0 is given in statvolts/cm, $c = 3 \times 10^{10}$ cm/sec, and $\epsilon = 1/(4\pi)$, then I_0 is obtained in $\text{erg sec}^{-1} \text{cm}^{-2}$. We have not attempted to solve Maxwell equations to find the field inside the well, which should appear in the Schrödinger equation for the electron. For the strong fields used here Maxwell's equations are nonlinear and solving them is difficult. It is thus customary to use Eq. (1) and hope that the errors are not significant as long as the laser does not excite the electromagnetic resonances of the structure.

The results reported in what follows are obtained by solving numerically [3] the time-dependent Schrödinger equation for the Hamiltonian defined above. A brief description of the strategy pursued is instructive. We start with the initial state $|L\rangle = (|1\rangle - |2\rangle)/2^{1/2}$ which is localized in the left well. $|1\rangle$ and $|2\rangle$ are the two lowest-energy eigenstates of the system in the absence of the laser. We drive the system with semi-infinite square laser pulse [i.e., $\tau = 0$ in Eq. (1)]. By numerical experimentation we find the laser power, frequency, and phase which will keep the electron in the left well. We find that, as in the case of a quartic double well [1], an electron initially located in the left well is maintained there by the action of the laser. At a laser intensity $I_0 = 347.22 \text{ MW/cm}^2$ and a phase $\delta = 1.5\pi$, localization is maintained for as many as 23 photon energies ranging from 26.28 to 1560.8 cm^{-1} (3.258–193.511 meV). In most of these cases the probability of finding the electron in the left well is never less than 70% and its average over time exceeds 80%. Prior work [1] used $\delta = \pi/2$ [i.e., it used $\sin(\omega t)$ for the time dependence of the field] and did not comment on the fact that the results are dependent on the laser phase. We find that the quality of localization is good (and the same) for $\delta = 1.5\pi$ and $\delta = 0.5\pi$ and is poor (but still over 50%) for $\delta = 0$ and $\delta = \pi$.

Once we find the conditions (laser power, frequency, and phase) which maintain the initially localized electron in its well, we start a new calculation in which the electron is initially in an eigenstate of the bare (i.e., no laser) double well and is exposed to a semi-infinite laser pulse with a finite rise time (i.e., $\tau > 0$). We use a pulse intensity and frequency for which the cw laser is capable of maintaining the electron localization (in a calculation in

which the electron is initially localized). The phase $\delta = -\omega t_0 \pm 2n\pi$ is chosen to give a maximum electric field $t = t_0$. Then, we pick a pulse rise time τ and we calculate, by solving the time-dependent Schrödinger equation, the wave function of the electron and monitor the time evolution of the probability that the electron is in the left well. We vary τ until we find a value for which the laser localizes the electron in a well and then keeps it there.

In Fig. 2 we show the probability $P_L(t)$ that the electron is in the left well, as a function of time. The electron started in the left well. The pulse properties are indicated in the figure. Let us examine the upper curve of Fig. 2(a). The electron is initially (i.e., at $t=0$) in the ground state and the wells are occupied with equal probability. The laser amplitude is a Gaussian which has a width τ , reaches a maximum at $t = t_0 = 3.5\tau$, and then levels off to a constant value. The value of τ for the upper curve in Fig. 2(a) is 585 fs. In the early times, when the laser intensity rises, $P_L(t)$ undergoes wild oscillations and the electron moves from one well to another. When the pulse

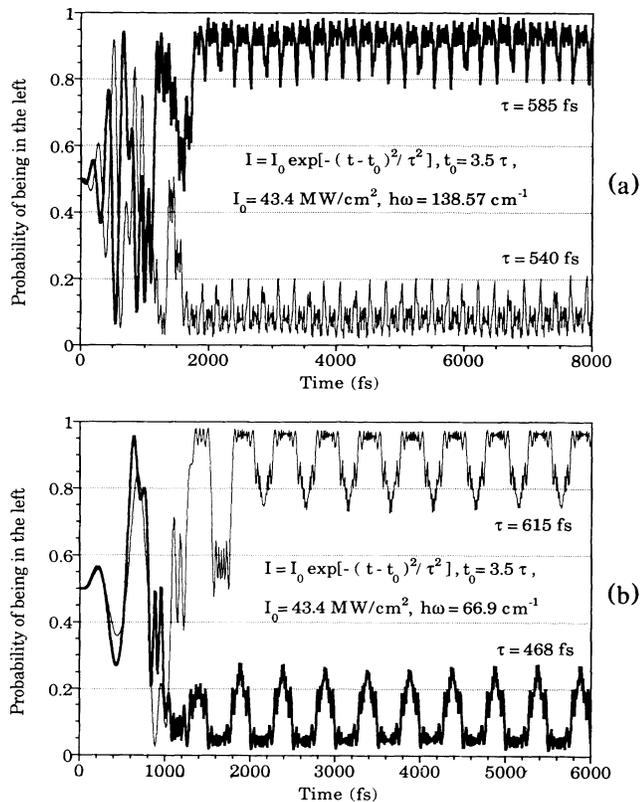


FIG. 2. The time dependence of the probability $P_L(t)$ that the electron is in the left well. The initial state is the bare ground state $|1\rangle$. The optical field is given by Eq. (1). The laser power when the pulse amplitude becomes constant is $I_0 = 347.22$ MW/cm². The photon energy is (a) 17.18 meV (138.57 cm⁻¹) and (b) 8.295 meV (66.9 cm⁻¹). Depending on the rise time of the pulse the electron is localized in the left well (upper curves) or in the right one (lower curves).

settles to a constant value, $P_L(t)$ oscillates with a small amplitude around a mean value larger than 0.9. The period of these small oscillations is the laser frequency. The second graph in Fig. 2(a) shows that if we change the rise time from $\tau = 585$ fs to $\tau = 540$ fs, but keep all other parameters unchanged, the electron will be localized in the right well. We have found, for $I_0 = 347.22$ MW/cm² and $\omega = 138.57$ cm⁻¹, about 20 values of the rise time τ for which the electron is localized in one of the wells. Fewer rise times leading to localization were found when the laser frequency is 66.9 cm⁻¹, and none for frequencies higher than 138.57 cm⁻¹.

The ability of the laser to localize the electron depends on the phase δ of the laser electric field. For laser parameters (i.e., rise time, frequency, and power) that localize the electron in the left well for $\delta = -\omega t_0 \pm 2n\pi$, the electron is localized in the right well if $\delta = -\omega t_0 \pm (2n + 1)\pi$; if $\delta \neq -\omega t_0 \pm n\pi$, the localization is very poor. Note that a change of phase by π is equivalent to a change in the sign of z [see Eq. (1)] hence a conversion of left into right; this explains why an electron localized in one well for a phase δ is localized in the other well if the phase is $\delta \pm \pi$. This phase dependence may appear surprising because a change of phase in the time-dependent Schrödinger equation is equivalent to a change of time origin. If the laser amplitude is constant the choice of time origin is irrelevant. However, such a constant amplitude is physically impossible: The laser must start acting on the system at some time and the outcome will depend on the laser phase which controls the initial direction of the force acting on the electron.

Unless one works at a very low temperature the excited state $|2\rangle$ is initially populated. For this reason we have also investigated the effect of a semi-infinite pulse in the case when the electron starts in $|2\rangle$. We find that a pulse having a set of parameters that localize an electron starting in $|1\rangle$ in the left well will localize an electron starting in $|2\rangle$ in the right well. If the same pulse acts on an electron in thermal equilibrium the population in the left well will exceed that in the right one by a Boltzmann (or a Fermi) factor.

The extent of the trapping is rather sensitive to the parameters of the pulse. As illustrated by Fig. 2, relatively small changes in τ [e.g., 40 fs for Fig. 2(a) and 147 fs in Fig. 2(b)] can change the localization from the left to the right well. Small deviations from the frequency required to localize the electron in the left well cause $P_L(t)$ to drift slowly from about 0.9 to about 0.1 and back. In calculations using a photon energy close to 17.18 meV the period of this drift is of order $1/\Delta\omega$, where $\Delta\omega$ is the difference between the photon frequency used in the calculation and the frequency (i.e., 17.18 meV) at which the localization is achieved. At lower photon energies this drift is faster: If the laser frequency is close to 104.27 meV the drifting period is about 3 times longer than $1/\Delta\omega$.

We have also calculated the dipole $\mu(t) = \langle \Psi, t | x | \Psi, t \rangle$

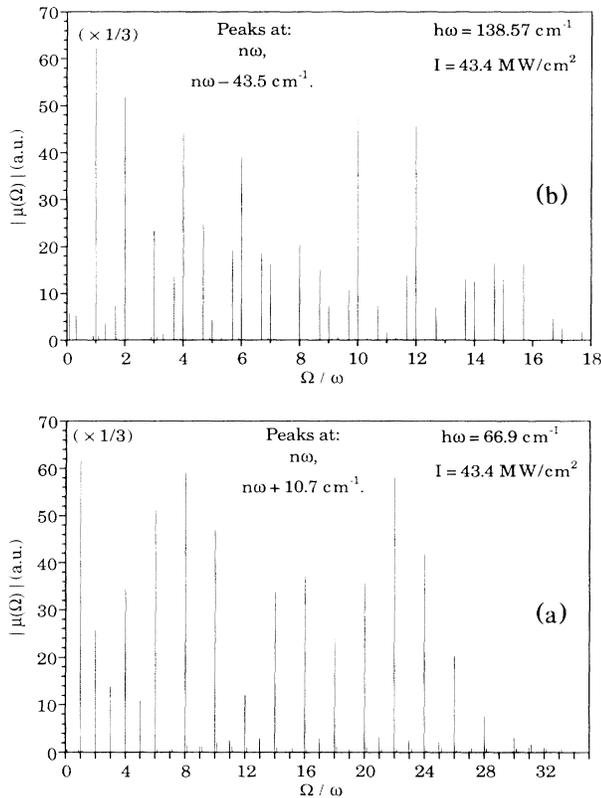


FIG. 3. The peak positions and heights in $\mu(\Omega)$ (see the definition given in the text). The calculations in (a) and (b) were performed for the parameters used in Figs. 2(b) and 2(a).

of the sample, where $|\Psi, t\rangle$ is the wave function of the electron at time t . In Fig. 3 we show

$$\mu(\Omega) = \left| \int_{-\infty}^{+\infty} dt e^{-i\Omega t} W(t-t') \mu(t) \right|.$$

The width and the center t' of the Gaussian window function W are chosen to cut off the values of $\mu(t)$ at times when the pulse intensity is still rising. $\mu(\Omega)$ has peaks of Gaussian shape (i.e., the transform of the window function) centered at the frequencies at which the Fourier components of $\mu(t)$ are nonzero. In Fig. 3 we show only the positions and heights of these peaks. The parameters for the laser pulse (indicated in the figure) are those that lead to localization if the initial state was the bare ground state. The transform in Fig. 3(a) has a large number of peaks forming two progressions: one at $n\omega$ (ω is the laser

frequency) and the other at $n\omega + 10.7 \text{ cm}^{-1}$, where n is an integer. There are several striking features. The amplitudes of the terms in the progression $n\omega$ are larger for n even. The intensity of the harmonics does not decay with n as one would expect if high-order perturbation theory had any validity. For example, the intensity of the 22nd harmonic is a third of that of the Rayleigh (i.e., having the same frequency as the incident laser) peak. Similar results are obtained for a laser frequency of 138.57 cm^{-1} , a power of 347.22 MW/cm^2 , and a rise time that leads to electron localization [Fig. 3(b)]. We see two progressions at $n\omega$ and $n\omega - 43.37 \text{ cm}^{-1}$ (or $n\omega + 95.2 \text{ cm}^{-1}$). There are substantial differences between these two cases but we still see high harmonics (the peak at 12ω is about one-fourth of the largest peak which appears at the frequency of the incident light).

This work was supported by the NSF CHE9112926 and in part by the Office of Naval Research. We became interested in this problem after listening to talks by Jim Allen and Martin Holthaus given at the QUEST Science and Technology Center and in Walter Kohn's group seminar. Discussions with Walter Kohn, Jim Allen, Mark Sherwin, and especially with Martin Holthaus are gratefully acknowledged.

(a) Address for correspondence.

- [1] F. Grossmann, T. Dittrich, P. Jung, and P. Hänggi, *Phys. Rev. Lett.* **67**, 516 (1991); F. Grossmann, T. Dittrich, and P. Hänggi, *Physica (Amsterdam)* **175B**, 293 (1991); F. Grossmann and P. Hänggi, *Z. Phys. B* **85**, 315 (1991); F. Grossmann, P. Jung, T. Dittrich, and P. Hänggi, *Europhys. Lett.* **18**, 571 (1992); related work was also performed by D. Neuhauser, "Coherent Destruction of Tunneling—Physical Origin" (to be published); M. Holthaus, "Pulse-Shape-Controlled Tunneling in a Laser Field" (to be published).
- [2] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Halsted, New York, 1988); C. W. J. Beenakker and R. Van Houten, in *Semiconductor Heterostructures and Nanostructures*, edited by G. Ehrenreich and D. Turnbull (Academic, New York, 1991).
- [3] J. A. Fleck, Jr., J. R. Morris, and M. D. Feit, *Appl. Phys.* **10**, 129 (1976); M. D. Feit, J. A. Fleck, Jr., and A. Steiger, *J. Comput. Phys.* **47**, 412 (1982); M. D. Feit and J. A. Fleck, Jr., *J. Chem. Phys.* **78**, 2578 (1984).