Controlling the evolution of electronic states in nanostructures

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We investigate the evolution of electronic states of a system made up of quantum wells and tunneling-transparent barriers subjected to a time-dependent electric field. We establish that the dynamic evolution problem for a two-level system corresponds exactly to a static scattering problem, and demonstrate that it is possible for dynamic analogues of reflectionless potentials to exist. By solving the non-stationary Schröedinger equation numerically, we find conditions for the dissipationless relocation of the electron density in nanostructures under the action of a time-dependent electric field. We show that the character of the system evolution depends strongly on the phase structure of the wave function in the initial state. In order to describe how the wave function evolves in a nanostructure subjected to a periodically time-varying strong external field, we have developed a dynamic analogue of the Kronig-Penney model, which we use here to compute the dependence of the quasi-energy ε and the Floquet functions on the amplitude and period of the external field. We investigate how initial conditions influence the way the electron density is localized in the crossing regime (i.e., where branches of the quasi-energy intersect). We also study the evolution of electron states subjected to a slowly varying periodic signal (the switching-on regime) as the amplitude of the signal is varied. © *1995 American Institute of Physics.*

I. INTRODUCTION

Recently, there have been intensive efforts to develop bandgap engineering methods with the goal of creating nanostructures that exhibit a variety of quantum effects that resemble those of natural atomic systems but are considerably easier to observe.[1] One reason for the interest in such nanostructures is the possibility of changing their fundamental microscopic parameters, i.e., the distance between energy levels, the symmetry of wave functions, and the systems as a whole, in a controllable way.[2] There is special interest in the problem of describing the evolution of electronic states in time-dependent external potentials. In its practical implementation, this problem is closely related to investigations of new methods for processing and transforming information based on tuning the electron density of a quantum structure in a controllable way.[3]

In this paper, the specific objects of study are systems made up of quantum wells and barriers. Section 2 describes the evolution of electron states in an external field that varies monotonically with time. It is well known that a discontinuous change of applied voltage across a structure gives rise to spatial and temporal oscillations of the electron density.[4] The origin of these oscillations, which have the character of beating, is the fact that the initial state of the wave function, i.e., immediately after the field is switched on, differs from its steady-state value in the latter.[5] In particular, this type of time dependence can result in a transition to a stationary state in which the maxima of the wave-function amplitude are "relocated" as a result of energy relaxation, i.e., due to dissipation. In the opposite limit, when the change in the field is adiabatically slow, the wave function evolves in space and time while preserving the attributes of the given quantum state. In this case, the spatial restructuring of the electron density is dissipationless, but it takes place slowly, over a time $\Delta\tau$ much longer than the time during which the system energy levels satisfy the resonance (anticrossing) condition.[6] As noted by Landau,[7] the description of the time evolution of a quantum system in the adiabatic regime is formally analogous to the solution to a scattering problem in the quasiclassical approximation. In Sec. 2 we show that for a two-level system we can amplify this assertion and formulate the problem of dynamic evolution for an external potential that varies with time in an arbitrary manner as a scattering problem for the Schroedinger equation with a potential of special form, or as a problem in which an electromagnetic field propagates in a medium with a complex coordinate-dependent index of refraction. In this case we show that a regime of dynamic evolution is possible that is analogous to resonant tunneling in the scattering problem, for which dissipationless relocation is completed in a time Δt of the same order as the time $\Delta t \sim \hbar/\Delta E$ for quantum oscillations, i.e., considerably faster than the time for adiabatic changes, and without any quantum beating (the temporal analogue of a reflectionless potential).

Section 3 treats the evolution of electron states of a quantum system in a external field varying periodically in time. In a weak field, a resonance regime is identified in which the wave function executes slow temporal oscillations (Rabi oscillations[8]) between levels coupled by the resonance field. In the resonance approximation, a formally exact solution to the problem can be obtained by transforming to a rotating system of coordinates.[9] The more complicated and interesting case is when the external field is strong enough that the change in the position of the energy levels under the action of the field is comparable to the distance between levels in the absence of the field. In atoms such a field may cause ionization. The problem of an atom in a strong elec-

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tromagnetic field was solved by Keldysh,[10] who calculated the ionization probability of an atom and showed that, depending on the ratio of the time for tunneling through the decreased field of the potential barrier to the oscillation period of the field, the ionization could be viewed as the result either of a below-barrier tunneling transition or as an above-barrier multiphoton transition with absorption of photons. As we show in Sec. 3, the evolution of electronic states of a system of quantum wells in a periodically time-varying external field can be described in analogous terms. The difference lies in the fact that, whereas in the problem of ionization of an atom the final state is located at infinity, in the systems we will discuss the scale of spatial evolution of the wave function is bounded by the dimensions of the nanostructure. A unique feature of nanostructures is the possibility of strongly modifying the electron spectrum in fields that are weak compared to atomic values. (The characteristic distances between energy levels of a nanostructure decrease like $\Delta E \propto 1/D^2$ with increasing dimensions and increase like $\Delta E \propto e\mathscr{E}D$ with increasing external field $\mathscr{E}$.) For this reason, nanostructures are very attractive systems in which to create strong fields and study their effects.

The universal approach to describing a system in a strong periodically time-varying field is to introduce the concept of quasienergy and the Floquet basis.[11,12] In the quasienergy representation, the wave function ψ takes the form

$$\psi(r,t)=\exp(-i\varepsilon t/\hbar)\Phi(r,t) \tag{1}$$

where ε is the quasienergy and Φ is a function that is periodic in time (the Floquet function). A number of schemes have been proposed in the literature to compute the quasienergy spectrum and the Floquet functions.[13,14] In particular, it has been shown that as the force parameters vary (amplitudes or frequencies of the external signal) the system exhibits both anticrossing regimes, which are usual in the static problem (level repulsion at resonance) and crossing regimes (strict intersection of different branches of the quasienergy spectrum). These regimes are interesting because certain linear combinations of Floquet states that belong to different branches of the quasienergy spectrum can be spatially localized for all times. In other words, a periodic external field is capable of disrupting tunneling. Usually, determination of the quasi-energy spectrum is a task for numerical computations. In Sec. 3 we present and investigate a model that admits an analytical solution leading to a qualitative analysis of the basic properties of the quasienergy spectrum. The model is the temporal analogue of the Kronig-Penney model for the periodic potential of a crystal lattice. We investigate how the initial conditions for the wave function affect the character of localization of the electron density in the crossing regime, and determine the parameters of the external force that lead to a crossing regime for asymmetric nanostructures.

In Sec. 3.4 we investigate the evolution of electron states of a nanostructure subjected to a periodic force whose amplitude is smoothly switched on. Previous numerical experiments[15] have established that when such a system is subjected to a periodic field that corresponds to the crossing regime, the character and degree of localization of its electron states depend in a fundamental fashion both on the way the amplitude increases and on the phase of the field. We will show below that the mechanism for generating localized states is connected with dissipationless relocation and how the character of the evolution of the electron state depends on the phase structure of the wave function, both of which will be described in the next section.

2. DISSIPATIONLESS RELOCATION IN A MONOTONICALLY-VARYING EXTERNAL FIELD

2.1. Temporal evolution of a two-level system as the analogue of a stationary scattering problem

The time evolution of electronic states in a quantum structure (nanostructure) is described by the Schröedinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi, \tag{2}$$

where H is chosen to be the Hamiltonian used in the method of envelopes.[16] In a one-dimensional potential, the motions along the axis of the nanostructure (x) and in the plane of the layer (yz) are separable, $[\Psi(x,y,z,t)=\Psi_{\perp}(x,t)\Psi_{\parallel}(y,z,t)]$, and the stationary energy is the sum of the energy of free motion in the plane of the nanostructure $E(k_{\parallel})=h^2k_{\parallel}^2/2m^*$ and the size-quantized energy of longitudinal motion E_n. Under steady-state conditions the size-quantized energy is determined by solving a one-dimensional problem for the eigenstates:

$$\begin{aligned} &H(x)\psi(x)=-\frac{\hbar}{2m^*}\frac{d^2\psi}{dx^2}+\left(V(x)-ex\frac{U}{D}\right)\\ &\psi(x)=E_n\psi(x). \end{aligned} \tag{3}$$

Here m^* is the effective mass, and $V(x)$ is the potential of the quantum structure, which we assume to be one-dimensional (i.e., the structure consists of a sequence of quantum wells and barriers). $V(x)$ coincides with the position of the bottom of the conduction band (when we describe electrons) and the top of the valence band (when we describe holes); $U(t)$ is the voltage applied to the structure, D is the size of the structure, and $\mathscr{E}=U/D$ is the electric field intensity.

As the applied voltage varies, the potential energy profile changes. The subject of our investigation will be the resulting temporal evolution of the wave function. It is worth noting that control of this restructuring of the wave function in a quantum structure could lead to high-efficiency methods of processing and transforming information.[3]

It is comparatively easy to arrive at a qualitative picture of the dynamics of electron states in nanostructures by using an effective Hamiltonian. Let us expand the wave function of the system $\Psi(x,t)$ in a basis $\{\phi_i\}$ of wave functions for the isolated quantum wells of the problem without a field ($U=0$):

$$\psi(x,t)=\sum_i c_i(t)\phi_i(x). \tag{4}$$

Here $\phi_i(x)=\phi(x-x_i)$, where x_i is the coordinate of the center of the ith well. For weakly overlapping basis wave

functions we can neglect the interwell matrix elements of the external field compared to the intrawell matrix elements δ_i:

$$\delta_i = -\frac{eU(t)}{D}\int \phi_i(x)x\phi_i(x)dx \approx -\frac{eU(t)}{D}x_i. \qquad (5)$$

The most important features of the system behavior can be identified even within the two-well approximation, for which the non-stationary Schröedinger equation (2) has the following form in the basis chosen:

$$i\hbar\partial_t\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix} = \begin{pmatrix} \varepsilon-\delta(t) & W \\ W & -\varepsilon+\delta(t)\end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t)\end{pmatrix}. \qquad (6)$$

Here $\pm\varepsilon$ are the energy levels of isolated quantum wells measured from the average spacing between levels, W is the hopping integral between wells, and δ is the matrix element of the external potential $U(t)$. The stationary energy levels (δ=const) of the Hamiltonian (6) are

$$E_{1,2} = \mp E = \mp\sqrt{(\varepsilon-\delta)^2+W^2}. \qquad (7)$$

At resonance ($\varepsilon=\delta$) the distance between levels (7) is a minimum ($E_2-E_1=2W$); however, the levels do not intersect, i.e., level anticrossing takes place. The probability of observing an electron in the ith well is determined by the square of the absolute value $|c_i|^2$. Under steady-state conditions we have

$$|c_{1,2}|^2 = \frac{1}{2}\left(1\mp\frac{\varepsilon-\delta}{E}\right). \qquad (8)$$

By changing the value of the parameter δ we can bring about level inversion.

The time evolution of an electron state is quite simple to describe when the potential changes discontinuously (at $t=t_0$). The wave function immediately before the potential is switched on, i.e., $\psi(t=t_0)$, plays the role of an initial condition for the Schröedinger equation (2), which describes its subsequent evolution. We can evaluate the behavior of the electron state for $t>t_0$ by expanding the wave function in the basis of eigenfunctions of the Hamiltonian $H(t>t_0)$. In this case, the probability of finding an electron in a given quantum well exhibits beating at frequencies $\hbar\omega = E_n - E_{n'}$, where E_n, $E_{n'}$ are eigenvalues of the Hamiltonian $H(t>t_0)$.[5] If the stationary-state wave function of the system for $t<t_0$ differs greatly from the same function when $t>t_0$, the amplitude of this beating will be large, so that the electron density oscillates between the wells of the structure and can only be localized by dissipative recombination at the lower energy level.

In the other limiting case, where the potential is slowly and adiabatically switched on, the quantum numbers of the quantum state where the electron is located remains invariant. The change in the probability distribution for finding an electron in various regions of the structure can be found by assuming the quantity δ in the Hamiltonian (6) depends parametrically on time. Consider the case of weak coupling: $\varepsilon \gg W$. When there is no external voltage (δ=0), an electron in the ground state is primarily localized in well 2. In the presence of a voltage δ such that $\delta-\varepsilon \gg W$, the maximum of the wavefunction amplitude in the ground state is now located in well 1. If we switch on the potential $\delta(t)$ adiabatically, the electron will execute dissipationless relocation from well 2 to well 1. The probability of dissipationless relocation P_0, i.e., the probability that the electron remains in the ground state, is

$$P_0 = 1-P_1,$$

where P_1 is the probability of exiting the ground state. We can estimate this probability in the standard way by using an analogy between the regime in which the Hamiltonian parameters vary adiabatically and the problem of scattering in the quasiclassical approximation.[7] For P_1 we have

$$P_1 \approx \exp\left\{\frac{2}{\hbar}\,\mathrm{Im}\int_C E(\tau)d\tau\right\},$$

where the integral is carried out in the complex time plane over a contour C that encloses the point τ_0 at which $E(\tau_0)=0$ [hence $E_1(\tau_0)=E(\tau_0)=E_2(\tau_0)=-E(\tau_0)$]. Specific calculations can be performed if we know how the potential depends on time. Let us consider a potential of the form:

$$\delta(t) = \varepsilon(1+\tanh(t/\theta)).$$

For the point τ_0 we have

$$\tau_0 = (i/\theta)\,\arctan(W/\varepsilon).$$

As a result, for P_1 we find

$$P_1 \approx \exp\left[-\frac{\pi\theta}{\hbar}\left(\sqrt{\varepsilon^2+W^2}-\varepsilon\right)\right]. \qquad (9)$$

From the condition $P_1 \ll 1$ we can estimate the characteristic time $t=\theta$ for adiabatic relocation of the electron density. When the parameters of the structure are $\varepsilon \sim W \sim 0.01$ eV, we find $\theta > 10^{-12}$ s.

The two-level model allows us to give a systematic description of the dynamic evolution of the system. By expressing the coefficients $c_{1,2}$ given in (6) in terms of one other, we arrive at the following differential equation:

$$-\hbar^2\partial_t^2 c_{1,2}(t) = (E^2 \mp i\hbar\partial_t\delta(t))c_{1,2}(t). \qquad (10)$$

Making the substitution $t \to x$ reveals that the equations for the probability amplitudes have the form of wave equations for an electromagnetic field propagating in a medium with a position-dependent complex index of refraction:

$$-\nabla^2\mathscr{E}_{1,2} = \frac{\omega^2}{c^2}(n^2(x)-\kappa^2(x)\pm 2in(x)\kappa(x))\mathscr{E}_{1,2}. \qquad (11)$$

Here the effective index of refraction n and the absorption κ can be expressed in the following way in terms of the parameters of the Hamiltonian (6):

$$\begin{aligned} &\frac{\omega^2}{c^2}(n^2(x)-\kappa^2(x)) \leftrightarrow (\varepsilon-\delta(t))^2+W^2 \\ &\frac{\omega^2}{c^2}2n(x)\kappa(x) \leftrightarrow \hbar\partial_t\delta(t). \end{aligned} \qquad (12)$$

These same equations can also be interpreted as time-independent Schröedinger equations with a nonhermitian

Hamiltonian whose imaginary part describes the mutual conversion of particles with conservation of the total probability:

$$|c_1|^2+|c_2|^2=1.$$

The direct analogy with the classical scattering problem leads us immediately to a qualitative description of how the probability amplitudes evolve with time in the dynamic problem. The general solution for the time-dependent wave function can be written as a linear combination of partial solutions, which in the scattering problem correspond to waves incident on the system from right to left and from left to right:

$$\begin{aligned} t\to-\infty:&\quad c_1=(\alpha R+\beta T')e^{-iE_-t}+\alpha e^{iE_-t},\\ t\to+\infty:&\quad c_1=\beta e^{-iE_+t}+(\alpha T+\beta R')e^{iE_+t}. \end{aligned} \tag{13}$$

Here $E_{+,-}=E(t\to\pm\infty)$, R, R' and T, T' are the reflection and transmission coefficients for waves incident from left to right and from right to left respectively, and α, β are numerical coefficients determined from the initial condition. Dissipationless relocation corresponds to values of the coefficients $\beta=0$ and $R=0$ in (13), i.e., to a reflectionless scattering potential in terms of the scattering problem.

More detailed information about the character of the dynamic evolution of the electronic states can be obtained from numerical solution of the time-dependent Schröedinger equation (2).

2.2. Results of numerical calculations

Let us discuss a structure consisting of a set of quantum wells separated by tunneling-transparent barriers (see the inset of Fig. 1). For $U=U_0=$const, the piecewise-constant nature of the potential $V(x)$ allows us to solve Eq. (2) conveniently by the method of separation of variables. In this case, the expression for $\psi(x,t)$ can be written in the form of a series

$$\psi(x,t)=\sum_{n=1}^{\infty} a_n \exp\left[-\frac{iE_nt}{\hbar}\right] X_n(x), \tag{14}$$

where $X_n(x)$ is the eigenfunction of the stationary Eq. (3) for $U=U_0$ corresponding to the eigenvalue E_n. The Fourier coefficients a_n result from expanding the eigenfunction $\psi(x,0)=\phi(x)$ of the original state in terms of the eigenfunctions $X_n(x)$.

If the wells have the same depth and the barriers have the same height, these calculations are most conveniently performed by introducing the dimensionless coordinate $\tilde{x}=x/\lambda$, where $\lambda=(2\pi^2\hbar^2/m^*\Delta E_c)^{1/2}$ and ΔE_c is the height of the barrier for electrons. For the system $GaAs/Al_xGa_{1-x}As$ we have $\lambda\approx 90$ Å for $x=0.3$ and $\lambda\approx 150$ Å for $x=0.1$.

The series (14) converges rather rapidly (often we only need those eigenvalues with $E_n<\Delta E_c$), and the summation is easily performed numerically. In this case, the basic procedure is to calculate E_n and $X_n(x)$ for the stationary Eq. (3).

The method given here can be used with a time-dependent external force $U(t)$ as well. In this case it is sufficient to approximate the function $U(t)$ by a piecewise-constant function $\tilde{U}(t)$, and to apply the procedure described above on each of the K segments where $\tilde{U}$ is constant, using as an initial value the solution $\psi(x,t)$ obtained for the previous interval.

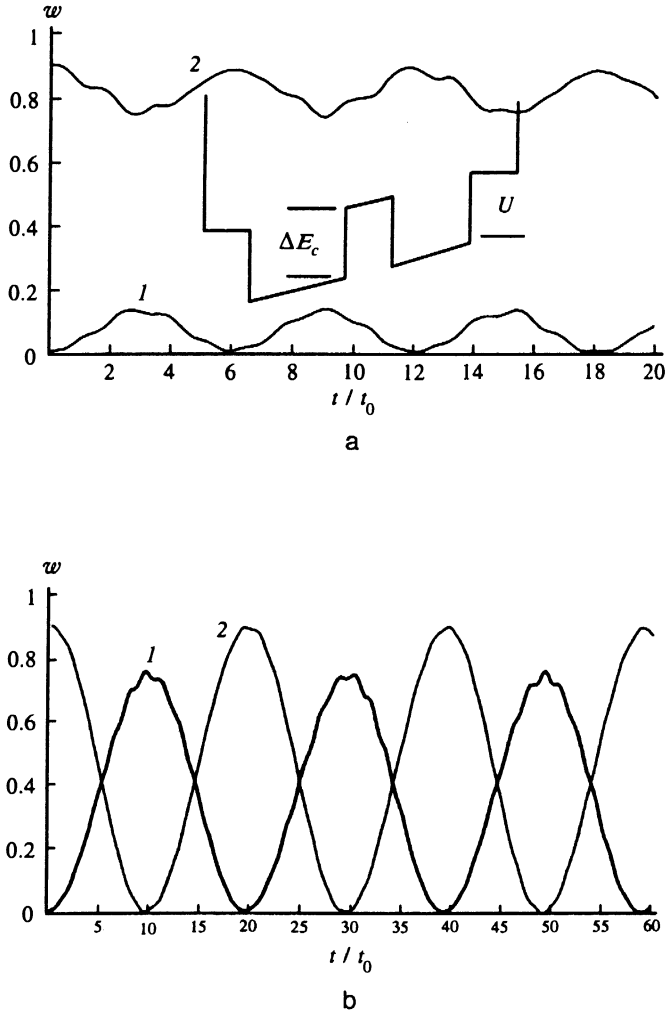


FIG. 1. Dependence of the probability w_i for observing an electron in the ith well on time t for a two-well structure with parameters $a_1=0.4\lambda$, $a_2=0.7\lambda$, $b=0.5\lambda$, when the voltage is switched on abruptly: $eU/\Delta E_c=0.5$ (a) and 0.15 (b). The inset to Fig. 1a shows a sketch of the structure under study.

We first investigate the evolution of the wave function in a system containing two quantum wells of different widths. Let us consider the situation where the potential across the structure changes discontinuously from zero to a certain U_0 that satisfies the condition $eU_0>E_2-E_1$. We will assume that the system is initially in the ground state for $U=0$. In this case the maximum of the wave function is localized in the second (deeper) well, while $\psi(x,0)$ is found to be close to the wave function of the stationary first excited state when the structure is in an external field $U=U_0$. Figure 1a shows the dependence of the probability of finding electrons in each of the wells $w_i(t)=\int|\psi(x,t)|^2dx$ the limits of integration are the limits of the ith well) obtained by solving Eq. (2) according to the method described above for a structure with $a_1=0.4\lambda$, $a_2=0.7\lambda$, $b=0.5\lambda$. It is clear from the figure

that the maximum of the electron density remains in the second well, undergoing oscillations as a result of electron tunneling through the barrier dividing the wells. The period of these oscillations is determined by the energy difference E_2-E_1 of the stationary states for $U=U_0$. In this case, in order to describe the relocation it is necessary to include dissipative processes in the discussion. The relaxation mechanism that mediates the relocation involves the emission of phonons. In this case, the characteristic time for interwell relaxation increases rapidly with increasing barrier width, due to the decrease in the overlap of the wave functions of the ground and excited states.[17] This time greatly exceeds the time for intrawell relaxation, which for transitions between spatially quantized levels in a well of width ~100 Å is 1 ps.[18] For a structure based on $Ga_{1-x}Al_xAs/GaAs$, the quantity $t_0=2\pi\hbar/\Delta E_c$ equals 0.016 ps for $x=0.3$ and 0.041 ps for $x=0.1$. In this case, the periods of oscillations in Fig. 1a are 0.1 and 0.25 ps respectively.

In Fig. 1b we show the time dependence of $w_{1,2}$ when the applied voltage corresponds to the resonance value U_r. By U_r we mean that value for which the spacing between the energy levels of the first excited stationary state and the ground stationary state is a minimum. In this case the probabilities for absorbing an electron in the first and second wells turn out to be similar for these states, due to resonant tunneling of electrons between the wells. As in the previous case, oscillatory behavior of $w_{1,2}(t)$ is observed. The oscillation period T_r is determined by the distance between energy levels at resonance and corresponds to 0.32 ps for $x=0.3$ and 0.82 ps for $x=0.1$. It is important to note that the minimum probability in the second well is practically reduced to zero, i.e., within one period of oscillation total relocation of the electron density takes place, so that the wells appear to have changed places.

Comparing Figs. 1a and 1b, we may conclude that in order for dissipationless relocation of the electron density to occur in such a structure it is necessary first to apply a voltage to this system corresponding to the resonance, and then to discontinuously increase the voltage to a finite value $U=U_0$ when the minimum probability in the second well is reached (i.e., at $t=T_r/2$). In Fig. 2a we show the curves $w_{1,2}(t)$ for such a regime. It is clear from the figure that, in this case, although the relocation is essentially complete, a rather large oscillatory amplitude remains. We can decrease this by decreasing U_0. Note that dissipationless relocation occurs in an antiadiabatic regime (if the external voltage changes discontinuously in time).

As we showed above, characteristic times for the problem turn out to be the order of picoseconds, so that the stepwise change in the voltage for the structure is very complicated to implement. For this reason, it is worthwhile to follow the behavior of the system when the voltage is switched on smoothly. Furthermore, it is important to address the problem of picking the form of the switching pulse so as to decrease the oscillations in the final state. For this we solved Eq. (2) for a function $U(t)$ of the form

$$U(t)=U_0[\theta(\tau-t)(t/\tau)^\gamma+\theta(t-\tau)]$$

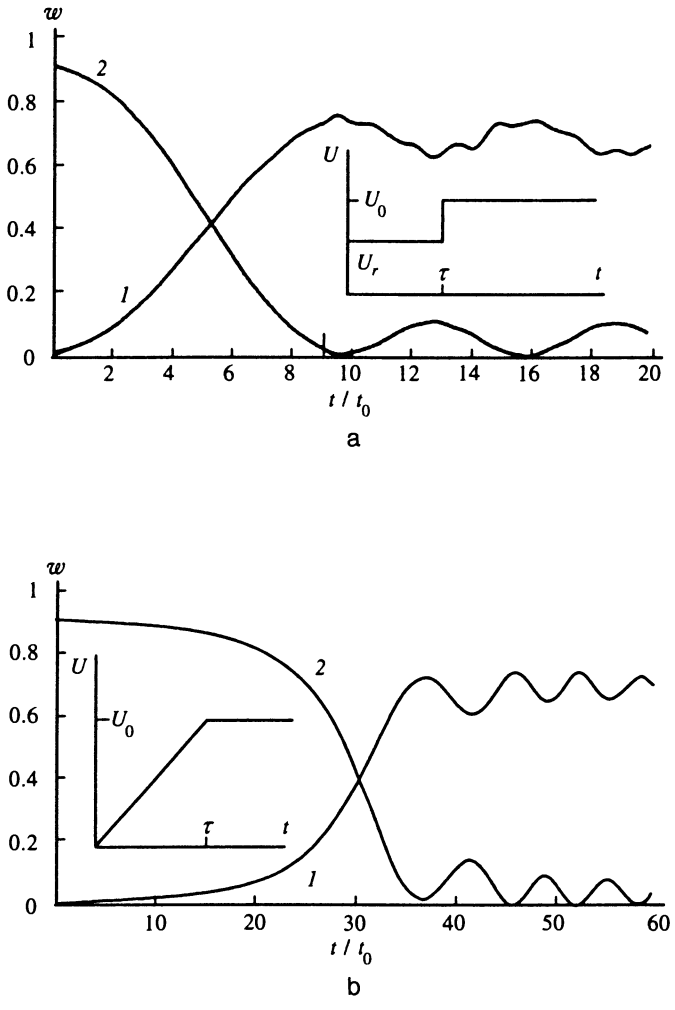


FIG. 2. Change in the probabilities $w_{1,2}$ (*1,2*) with time for a two-well structure for (a) stepwise switching on of the external voltage with $\tau=9t_0$, $U_1=U_r$, $U_0=0.5\Delta E_c$; (b) a linearly increasing potential with $\tau=50t_0$, $U_0=0.5\Delta E_c$. The inset shows the temporal shape of the switching pulse.

for $\gamma=0.5$, 1, and 2, i.e., signals with square-root, linear, and quadratic time dependence during the switch-on stage. For each γ we calculated $w_i(t)$, varying the rise time τ of the front and the magnitude U_0 of the steady-state signal. Figure 2b shows typical dependences $w_{1,2}(t)$ for the linear form of $U(t)$. The curves $w_{1,2}(t)$ have similar shapes for $\gamma=0.5$ and 2 as well. In order to achieve collisionless relocation we must have $\tau>T_r$ and $U_0>V_r$, while to obtain identical amplitudes for the residual oscillations $\tau_{0.5}<\tau_1<\tau_2$ is necessary. As τ increases, the amplitude of the oscillations decreases. The time τ required to achieve more or less complete relocation turns out to be two to three times larger than when the voltage is switched on in a stepwise manner. Despite this, it is clear from Fig. 2b that for $x=0.3$ it is 0.5 ps and 1.2 ps for $x=0.1$, i.e., it can be even smaller than the intrawell relaxation time.

Thus, by choosing a suitable regime for switching on the external voltage, we can bring about collisionless relocation of the electron density in asymmetric quantum-size struc-

tures. In this case, the switching time turns out to be a picosecond or less in order of magnitude.

In order to discuss the evolution of the states when the external electric field changes continuously, consider a system consisting of two identical wells separated by a barrier transparent to tunneling. In this case there are two evolution problems that are physically meaningful: first, when the system is in the ground state $\psi(x,0)=|1\rangle$ at $t=0$, and secondly, when the wave function in its initial state consists of a linear combination of functions corresponding to the ground and first excited states, i.e., $\psi(x,0)=(|1\rangle\pm|2\rangle)/\sqrt{2}$. First consider the case where the field amplitude is linearly increasing, so that when the potential U_0 reaches its constant value $U=U_0$, the value of U_0 ensures that the ground-state wave function is localized in the left-hand well. When $\psi(x,0)=|1\rangle$ holds, the probabilities for finding the electron in the two wells are equal in the initial state, i.e., $w_1(0)=w_2(0)$. When the switching-on of the voltage is sufficiently abrupt (small τ), the quantities $w_1(t)$ and $w_2(t)$ execute out-of-phase oscillations, such that $w_1>w_2$ always holds. The period of these oscillations is determined by the distance between levels for $U=U_0$. As the duration τ of the switching front increases, the amplitude of these oscillations decreases, and the final state of the system becomes more and more localized in the left-hand well. For example, if we consider a structure with parameters $a_1=a_2=0.50\lambda$, $b=0.3\lambda$, we find that when $U_0=0.5\Delta E_c$ and $\tau=20t_0$ the amplitude of the residual oscillations of w_1 is less than 10%, i.e., for this τ the switching regime is close to adiabatic. The system is initially in the ground state (with $w_1=w_2$); at the end of the adiabatic process it is once again in the ground state for the nonzero field U_0, which corresponds to $w_1\gg w_2$.

When the initial state is a combination of the ground and excited states, situations are possible for which either $w_1\gg w_2$ [when $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$] or $w_1\ll w_2$ [when $\psi(x,0)=(|1\rangle-|2\rangle)/\sqrt{2}$]. It is interesting that when the field is switched on sufficiently slowly, the evolution of the system at large times for these two cases is very similar: the probabilities $w_{1,2}$ in the steady-state regime oscillate out of phase around a value $\bar{w}=0.4$, i.e., on the average the electron is delocalized. Figure 3 shows the functions $w_i(t)$ for the case $\psi(x,0)=(|1\rangle-|2\rangle)/\sqrt{2}$, where the wave function is initially localized in the right-hand well. For $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$ the initial stage of the evolution of $w_i(t)$ is analogous to the previous case with the interchange $w_1\to w_2$, and in the steady-state regime (for $t>\tau$) the behavior of the system in both cases is practically identical. At first glance this result is unexpected. The fact is, these two cases can be realized by changing the polarity of the voltage applied to the system while leaving the initial condition unchanged (a wave function localized in the left-hand well). For the adiabatic regime, the results are as follows. When there is no field on the system, the initial state is made up of the ground and excited states with equal weights. That is, for a symmetric structure both the ground and the first excited state are delocalized when $U=0$. As the voltage is slowly switched on, the system evolves to a state that is also made up of the ground and excited states with equal weights, but now these are states of the system in the external field U_0. For $U=U_0$ the ground state is localized in one well and the excited state in another, but their combination turns out to be delocalized.

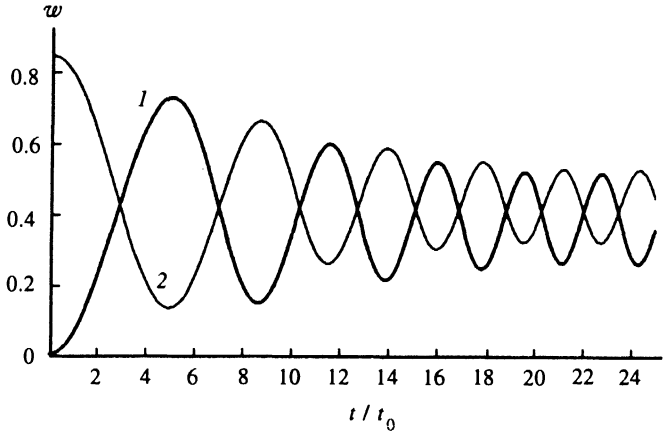


FIG. 3. Dependence of the probabilities $w_{1,2}$ (*1*,*2*) on time t for a two-well structure with parameters $a_1=a_2=0.5\lambda$, $b=0.3\lambda$ when the voltage is switched on linearly with $\tau=20t_0$ and the initial condition $\psi(x,0)=(|1\rangle-|2\rangle)/\sqrt{2}$.

In principle, we can prepare an initial state based on the more general combination $\psi(x,0)=(|1\rangle+\exp(i\phi)|2\rangle)/\sqrt{2}$. The cases discussed above correspond to $\phi=0$ and $\phi=\pi$. Calculations show that, for intermediate values of ϕ, the evolution for $t>\tau$ depends only weakly on ϕ when τ is sufficiently long. In particular, for $\phi=\pi/2$ [$\psi(x,0)=(|1\rangle+i|2\rangle)/\sqrt{2}$], although $w_1=w_2$ in the initial state (i.e., a situation analogous to the original ground state), in the steady-state regime the probabilities for finding an electron in each of the wells are close [rather than $w_1\gg w_2$, the case when $\psi(x,0)=|1\rangle$]. Thus, knowledge of the initial probability distribution in each well does not provide enough information to describe the time evolution. The fact is that the character of the evolution is determined by the distribution of the system over states.

3. PERIODIC FORCE AND QUASI-ENERGY SPECTRUM

3.1. Time-dependent analogue of the Kronig–Penney model

To investigate the evolution of quantum-size structures subjected to periodic time-dependent external forces, we will use the time-dependent analogue of the Kronig–Penney model, i.e., we will assume that a periodic sequence of rectangular pulses acts on the system:

$$U(t)=\begin{cases} U_1 & \text{for } nT<t<nT+\tau_1, \\ U_2 & \text{for } nT+\tau_1<t<(n+1)T, \end{cases} \tag{15}$$

where n is an integer and $T=\tau_1+\tau_2$ is the period of the force. As we show below, a time dependence of this form with $\tau_1=\tau_2$ and $U_1=-U_2$ can be used to describe all the features of processes that occur when $U(t)$ is harmonic. However, the computational methods for dealing with the model (15) turn out to be considerably simpler, and the results much easier to interpret. For structures in which the primary contribution to the evolution comes from the two first energy levels, a large number of important results can be

obtained analytically. In contrast, it can be seen from Refs. 13 and 14 that when the time dependence of the external signal is of the form $U(t)=U_0 \sin(\omega t)$, the problem of finding the quasi-energy spectrum is quite complicated even for the simplest two-level system and requires numerical calculations. Furthermore, by using this "temporal Kronig–Penney model," we can treat asymmetric forces as well ($\tau_1 \neq \tau_2$, $U_1 \neq -U_2$). Finally, this type of signal (or one close to it) can be realized in practice.

In principle, we could immediately solve the periodic-force problem for any set of parameters using the solution algorithm described below for the time-dependent Schrödinger equation. Analysis of the possible situations is greatly simplified if we use the concept of quasi-energy. Knowledge of the quasi-energy spectrum allows us to draw conclusions about the character of the time evolution without solving the full time-dependent problem.

In order to find the quasi-energy spectrum and Floquet functions, let us consider the solution to the time-dependent Schröedinger Eq. (2) with $U(t)$ in the form (15) on a time interval consisting of a single period $[0,T]$. In each of the regions $[0,\tau_1]$ and $[\tau_1,T]$ where the potential is constant, we can represent the wave function in the form of an expansion over the steady-state eigenfunctions in the fields $U=U_i$. These expansions have the form (14) when we make the replacements $a_n \to a_n^{(i)}$, $E_n \to E_n^{(i)}$, $X_n \to X_n^{(i)}$, where $i=1, 2$ corresponds to U_1, U_2 in Eq. (15). Using the condition of continuity at $t=\tau_1$, we can express the coefficients $a_n^{(2)}$ in terms of $a_n^{(1)}$, and then make use of the Floquet theorem in the form

$$\psi(x,T)=\exp(-i\varepsilon T/\hbar)\psi(x,0). \tag{16}$$

Substituting the expansion for ψ in terms of $X_n^{(i)}(x)$ into (16), multiplying the right and left sides of the equation by $X_m^{(1)}(x)$, and integrating over x, we are led to the following eigenvalue problem

$$\sum_{k,n=1}^{\infty} a_n \exp\left[-\frac{i}{\hbar}(E_n^{(1)}\tau_1+E_k^{(2)}\tau_2)\right]\mu_{kn}\mu_{km}=\lambda a_m, \tag{17}$$

where

$$\lambda=\exp(-i\varepsilon T/\hbar), \quad \mu_{kn}=\int_{-\infty}^{\infty} X_n^{(1)}(x)X_k^{(2)}(x)dx.$$

It is easy to show that the following relation holds for the μ_{kn}:

$$\sum_{n=1}^{\infty} \mu_{kn}\mu_{mn}=\delta_{km}.$$

The eigenvalues (17) determine the quasi-energy spectrum ε_j, while the eigenvectors determine the Floquet functions $\Phi_j(x,t)$.

For a system of two quantum wells separated by a tunneling transparent barrier, we can choose the parameters of the structure such that the primary contribution to the expansion of the wave function (14) comes from the first two size-quantized levels both for $U=U_1$ and $U=U_2$. In this case we can limit ourselves to the first two terms of the sum in (17). In this case, the equation for the eigenvalues takes the simple form

$$\tilde{\lambda}^2-\tilde{\lambda}\{\mu_{11}[1+y_1y_2-y_1-y_2]+y_1+y_2\}+y_1y_2=0, \tag{18}$$

where

$$\tilde{\lambda}=\lambda \exp[i(E_1^{(1)}\tau_1+E_1^{(2)}\tau_2)/\hbar)],$$

$$y_{1,2}=\exp[-i\Delta_{1,2}\tau_{1,2}/\hbar],$$

$$\Delta_1=E_2^{(1)}-E_1^{(1)}, \quad \Delta_2=E_2^{(2)}-E_1^{(2)}.$$

Let us discuss the limit $U_1=-U_2 \to 0$. In this case we have $\mu_{11} \to 1$, and (18) reduces to

$$\tilde{\lambda}^2-\tilde{\lambda}(1+y^2)+y^2=0, \tag{19}$$

whose solutions are $\tilde{\lambda}_1=1$, $\tilde{\lambda}_2=y^2$, or to within terms of order $n\hbar\omega$,

$$\varepsilon_1=E_1, \quad \varepsilon_2=E_2.$$

That is, for $U \to 0$ the quasi-energy coincides with the energy as we should expect. For arbitrary U_1 and U_2, the solution to (18) offers no difficulty, i.e., the problem of finding the quasi-energies for the two-level system can be solved analytically when the force is a periodic sequence of rectangular pulses.

The quasi-energy concept allows us to describe the evolution of this system for an arbitrary initial condition. To do so, we simply need to find the expansion of the initial function $\psi_0(x)$ in terms of the Floquet functions $\Phi_j(x,0)$ at time $t=0$. The wave function at an arbitrary time then will have the form

$$\psi(x,t)=\sum_{m=1}^{\infty} g_m \exp(-i\varepsilon_m t/\hbar)\Phi_m(x,t), \tag{20}$$

where g_m are the coefficients of the expansion of the function $\psi_0(x)$ in the basis $\Phi_m(x,0)$. This approach has a considerable advantage over direct methods of solving the time-dependent Schroedinger equation when it is necessary to obtain the function $\psi(x,t)$ over long intervals of time, or to obtain a solution over a wide set of initial conditions. Here we need only find the quasi-energy spectrum and the corresponding Floquet functions once by solving the time-dependent Schröedinger equation over a single period, and then use Eq. (20).

The most interesting situation is when two (or more) quasi-energy levels coincide. It is clear from (20) that the time dependence of the wave function is not periodic in general, because the values of the quasi-energy are usually not commensurate. When the primary contribution to (20) comes from the first two levels and $\varepsilon_1=\varepsilon_2$, the behavior of $\psi(x,t)$ becomes close to periodic, with a period T equal to the period of the external force. As is easy to see from (18), the quasi-energies of the "two-level" system coincide when the following relation holds:

$$y_1=y_2=1. \tag{21}$$

Elementary analysis shows that this is the only possible situation in which the quasi-energies can coincide. Using the definition of y, we can rewrite condition (21) in the form

$$\Delta_1\tau_1=2\pi\hbar l, \quad \Delta_2\tau_2=2\pi\hbar m. \tag{22}$$

The value of the quasi-energy in this case equals

$$\varepsilon=(E_1^{(1)}\tau_1+E_1^{(2)}\tau_2)/T. \tag{23}$$

As we noted above, the period of free oscillations T_i^0 for the wave function when a constant electric field U_i is applied to the structure is determined by the separation between system energy levels Δ_i through the relation:

$$T_i^0=2\pi\hbar/\Delta_i. \tag{24}$$

Comparing (22) and (24), it is easy to see that the quasi-energies intersect if, within each time τ_i during which the action of the voltage is constant, each component of the periodic signal of the system executes an integer number of oscillations. In this case, the system has returned to its original state when the next pulse arrives. These considerations hold for each pulse. As a result, the system is in the ground state after each period, and the absolute value of the wave function is a periodic function with period T. In principle we may conclude this without analyzing the quasi-energy spectrum; however, qualitative discussions do not tell us if this the only kind of periodic behavior possible. In contrast, the analysis given above shows that the solution (22) is unique. For a symmetric system subjected to a symmetric periodic force ($\Delta_1=\Delta_2=\Delta$, $\tau_1=\tau_2=\tau$), we may write condition (22) in the form

$$\Delta=2m\hbar\omega, \tag{25}$$

where $\omega=2\pi/T$ is the frequency of the force and m is an integer. It is clear from (25) that the intersection of quasi-energies can be compared to a multiquantum process of order to $2m$.

Suppose that, in the absence of the external force, the distance between system levels Δ_0 satisfies the condition

$$[\Delta_0/\hbar\omega]=k \tag{26}$$

(the notation [ ] denotes the integer part of a number), i.e., as $U\to 0$ the energy levels can be intermixed as a result of the k-quantum process. The first intersection of the quasi-energies at a finite amplitude of the periodic force takes place when condition (25) is fulfilled. Since $\Delta>\Delta_0$ holds for the symmetric structure, the first intersection corresponds to

$$\begin{aligned} &2m=k+1 \text{ when } k \text{ is odd,}\\ &2m=k+2 \text{ when } k \text{ is even.}\end{aligned} \tag{27}$$

It follows from (27) that for $k=0$ and $k=1$ the first intersection corresponds to a two-quantum process, for $k=2$ and $k=3$ to a four-quantum process, etc.

It is also easy to obtain the condition for when more than two quasi-energies coincide, using Eq. (17). For a symmetric system and a symmetric two-pulse force, N quasi-energies will intersect as some parameter is changed when the following condition holds:

$$(E_n-E_{n-1})T=4\pi\hbar k, \tag{28}$$

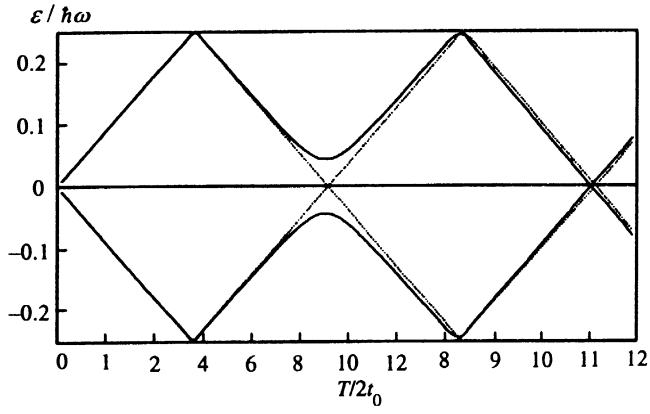


FIG. 4. Quasi-energy ε as a function of the period of the force T for a structure with $a_1=a_2=0.5\lambda$, $b=0.3\lambda$, when $U_0\to 0$ (dotted) and $eU_0=0.02\Delta E_c$.

where k is an integer, which can be different for different pairs of levels. The simplest example of such a system is a system with equidistant levels. By choosing the parameters of the multiwell structure, we can ensure that (28) holds. In what follows we will illustrate this for the example of a three-well structure.

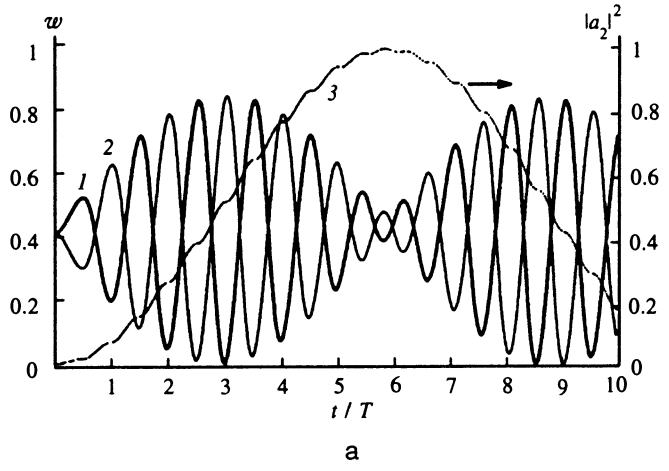
3.2. Symmetric structures

As an example, let us consider a symmetric system consisting of two identical quantum wells with dimensions $a_1=a_2=0.5\lambda$, $b=0.3\lambda$. For these dimensions, in the energy interval below the barrier height, there are only two energy levels whose wave functions are localized in the ground states of the wells. Therefore, we can initially limit ourselves to the first two terms of the summation (17) and find the eigenvalues from (18). We will assume the force to be symmetric, i.e., $U_1=-U_2=U_0$, $\tau_1=T/2$. Let us trace how the values of the quasi-energy change for this system as external parameters such as the amplitude U_0 and period T of the force change. As $U_0\to 0$, the dependence of the quasi-energy on T (or $\hbar\omega$) can be written in the form

$$\varepsilon_i/\hbar\omega=E_i/\hbar\omega-[E_i/\hbar\omega]\equiv T/\tau_0-[T/\tau_0],$$

where τ_0 is the period of free oscillations of the system without a field. For $U_0\neq 0$ the function $\varepsilon_i(T)$ is easily obtained by solving (18).

Figure 4 shows how $\varepsilon_{1,2}$ depend on T as $U_0\to 0$ (dotted curve) and for $U_0=0.02\ \Delta E_c$ (solid curve). Because ε_i and $\varepsilon_i+n\hbar\omega$ are equivalent, the representation of ε_i is not unique. In Fig. 4 we have chosen a representation for which the branches ε_1 and ε_2 corresponding to minimum distance between quasi-energies, since it is this quantity that determines the time evolution of the wave function, and the values of $\Delta\varepsilon$ and $\hbar\omega\pm\Delta\varepsilon$ are equivalent. As $U_0\to 0$ a crossing occurs at $T=n\tau_0$, which corresponds to an n-quantum process. As we noted above, the real points of intersection of the quasi-energy correspond to $2n$-quantum processes. It is this that explains the change of situation when $U_0\neq 0$: real intersection of quasi-energies leads to anticrossing. This causes



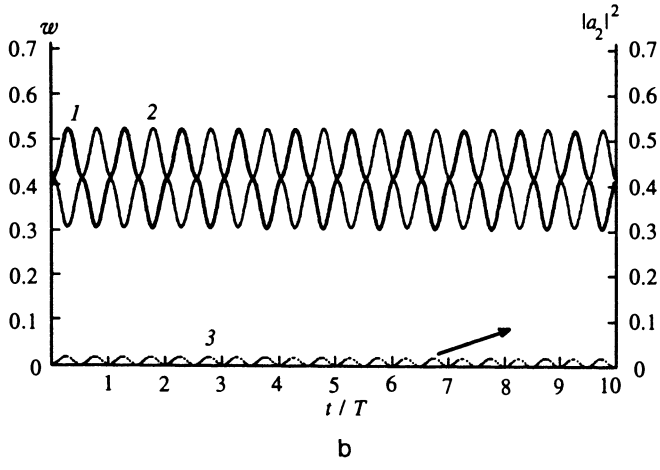


FIG. 5. Temporal evolution of the probabilities for finding an electron in the wells $w_{1,2}$ (curves *1*, *2*) and occupation probabilities for the excited energy level $|a_2|^2$ (*3*) for $eU_0=0.02\Delta E_c$ when the period of the force $T=T_{ac}=11.2t_0$ (a) and $T=T_{cr}=22.4t_0$ (b).

the time evolution of the wave functions for $T=T_{cr}=2k\tau_0$ (crossing) and $T=T_{ac}=(2k+1)\tau_0$ (anticrossing) to vary greatly. In Figs. 5a and 5b we show how the probabilities of observing an electron in the left and right wells depend on time for $U_0=0.02\Delta E_c$ (in Fig. 5a, $T=11.2t_0=\tau_0$, while $T=22.4t_0=2\tau_0$ in Fig. 5b) when the system is initially in the ground state for $U=0$. The dotted curve in Figs. 5a, 5b shows the square of the absolute value of the coefficient a_2 appearing in the expansion of the wave function $\psi(x,t)$ in eigenfunctions of the unperturbed state. At a point of anticrossing, despite the smallness of the force amplitude, there are times when the wave function is localized in one of the wells; in this case the function $w(t)$ has the typical beating form. Within a period of this beating the terms reverse: in the initial state $a_1=1$, $a_2=0$, while for $t\cong 5.8t_0$, $a_1\cong 0$, $a_2\cong 1$. At a crossing point, $w(t)$ is of course a periodic function with period T; its oscillation amplitude $w(t)$ is small, $|a_1(t)|^2$ remains close to unity, and $|a_2(t)|^2$ is close to zero. For $T=2k\tau_0$ (k is an integer) the system behavior is analo-

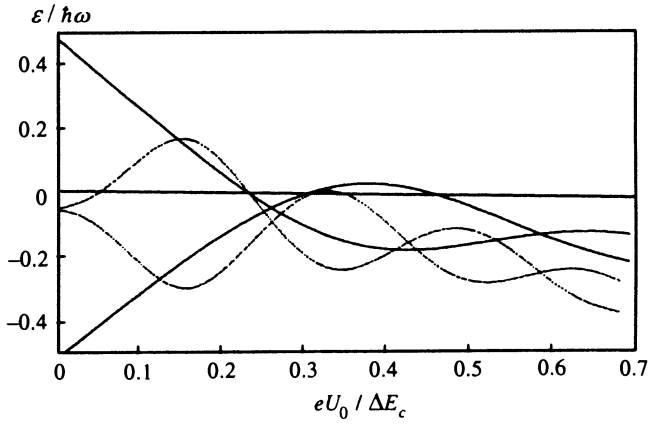


FIG. 6. Dependence of the quasi-energies $\varepsilon_{1,2}$ on the periodic signal amplitude U_0 for a symmetric structure ($a_1=a_2=0.5\lambda$, $b=0.5\lambda$) when $T=11.2t_0$ (solid curves) and $T=22.4t_0$ (dotted curves).

gous to Fig. 5a; for $T=(2k+1)\tau_0$ it is analogous to Fig. 5b.

For intermediate values of the force period, the functions $w_i(t)$ also have a characteristic beating form, but the amplitude of the oscillations decreases smoothly as we move away from the crossover point. The maximum value of $|a_2(t)|^2$ abruptly decreases as we move away from T_{ac}, dropping to zero as $T\to T_{cr}$. Thus if the amplitude of the force is small, the anticrossing points ($n\hbar\omega=\Delta_0$) are identified by the fact that, in this case, the average probability of observing an electron in the excited state is a maximum and equals 0.5.

If the electron is initially localized, e.g., $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$, then at an anticrossing point the functions $w_i(t)$ and $|a_i(t)|^2$ are close in form to the curves shown in Fig. 5a, but displaced by half a beat period. At the crossing points, the $w_i(t)$ oscillate between a maximum value equal to $w_1(0)\approx 0.9$ and a minimum of zero; $|a_1(t)|^2$ and $|a_2(t)|^2$ oscillate out of phase around an average value equal to 0.5.

Figure 6 shows how the quasi-energy depends on the amplitude of the force U_0 for two values of the period: $T\cong\tau_0$ (solid curves) and $T\cong 2\tau_0$ (dotted curves), obtained from (18). The points where the curves intersect are deter

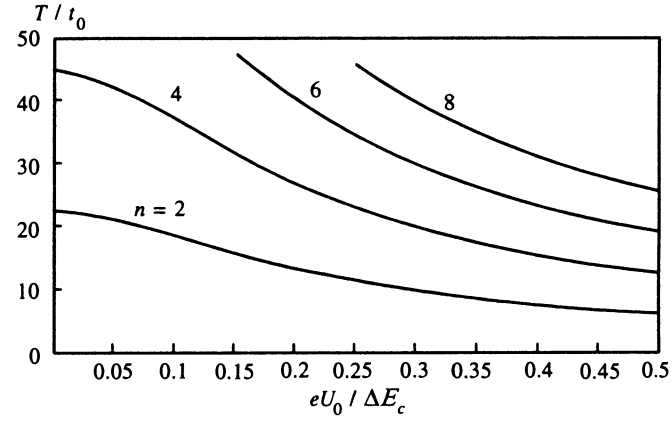


FIG. 7. Geometric position of crossing point on the plane (T,U_0) for a symmetric two-well structure.

mined by Eqs. (22), and the corresponding value of ε by Eq. (23). For small amplitudes, the anticrossing points correspond to quasi-energies as close as possible to the neighboring Brillouin zones; for the first zone this corresponds to points with maximum spacing between quasi-energies. Therefore it is natural to refer to points at which the distance between quasi-energies in the first Brillouin zone is a maximum as anticrossing points for finite amplitudes as well. Let us analyze Fig. 6 using Eqs. (26), (27). The curves for $T=\tau_0$ correspond to $k=1$; therefore, the first intersection of the quasi-energies takes place when the condition $\Delta_1=2\hbar\omega_1$ holds, i.e., this point corresponds to a two-quantum process. For $T=2\tau_0$, $k=2$ and the first point of intersection corresponds to a four-quantum process: $\Delta_2=4\hbar\omega_2$; however, $\omega_2=\omega_1/2$ holds i.e., at these points we have $\Delta_1\cong\Delta_2$, and they are observed for nearby values of the force amplitude. Analogous considerations show that for $T=\tau_0$ the second intersection should be observed at the same U_0 as the three intersections for $T=2\tau_0$.

The most characteristic points on the curves $\varepsilon(U_0)$ are the crossing points. Because the points of intersection of quasi-energies are so important to the system evolution, we have showed the geometric position of these points on the plane (U_0,T) in Fig. 7, determined according to Eq. (22) using the function $\Delta(U_0)$ obtained by solving the time-independent Schröedinger equation.

In the previous discussion we have limited ourselves everywhere to two quasi-energy levels, for which the calculations can be done analytically. Including more than two levels requires numerical solution of the eigenvalue equations. Such calculations show that including a larger number of levels changes the function $\varepsilon(U_0)$ only slightly, as is clear from Fig. 6 (except for bounded regions where crossing or anticrossing with higher levels occurs). We must emphasize that, in this case, the locations of the points where the first quasi-energy levels intersect are practically unchanged. An analogous situation obtains for other structures as well (two-well structures for which the number of energy levels exceeds two, three-well structures, etc.). This tells us that most of the information about the character of the system evolution may be obtained by analyzing the behavior of the first few quasi-energy levels. Confirmation of this assertion comes from numerical calculations of the wave-function evolution by direct solution of the time-dependent Schröedinger equation using methods of Sec. 2.2. Here the number of terms of the series (14) is chosen to ensure convergence and achieve the required computational accuracy. In order to guarantee high accuracy this number should be of order 10. The calculations show that for force parameters corresponding to the crossing points obtained by taking into account two quasi-energy levels, periodic behavior of $w(t)$ is observed when (2) is solved numerically for various initial conditions.

In Fig. 8 we show the functions $w_i(t)$ for a symmetric two-well structure when $T=22.28t_0$ and $U_0=0.26\Delta E_c$, which corresponds to the first crossing point (see Fig. 6). Figure 8a corresponds to $\psi(x,0)=|1\rangle$, Fig. 8b to $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$. The periodicity of the $w_i(t)$ is clearly apparent. Furthermore, Fig. 8 illustrates a number of features of

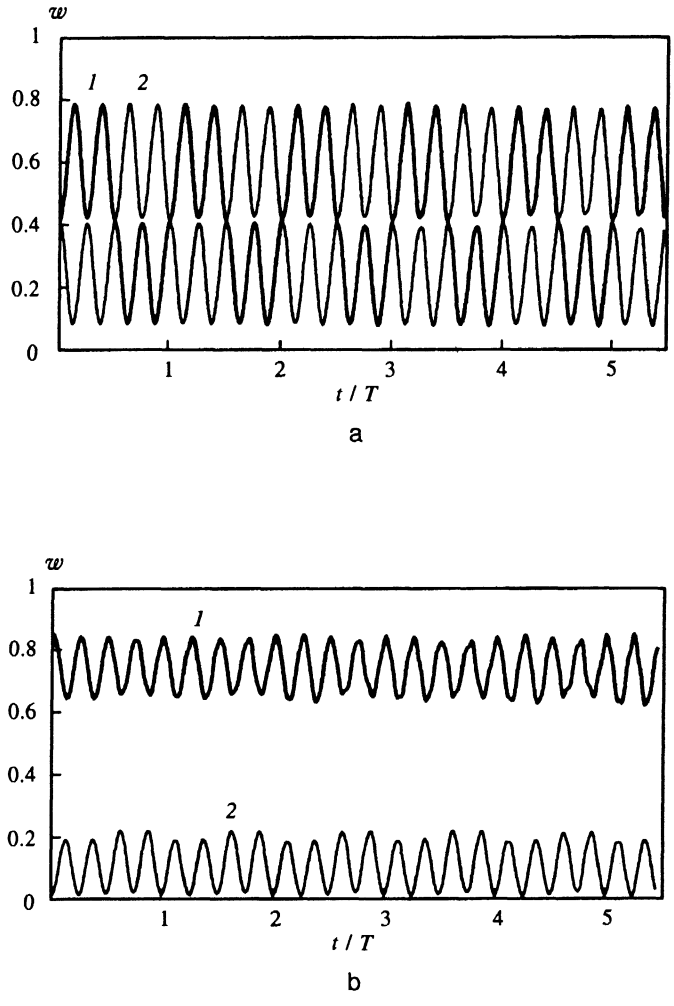


FIG. 8. Probabilities $w_{1,2}$ of finding an electron in wells *1* and *2* as a function of time t when $T=22.4t_0$, $eU_0=0.26\Delta E_c$ (crossing point), for $\psi(x,0)=|1\rangle$ (a) and $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$ (b).

the evolution of a system subjected to a periodic force with finite amplitude. It is clear from the figure that for the initial ground state (Fig. 8a) the amplitude of oscillations of the $w_i(t)$ turns out to be considerably larger than for the case of small U_0 (Fig. 5b). Conversely, for an initially localized state the amplitude decreases with increasing U_0. In the latter case, an electron can be localized in the well by the periodic force.[14] For this it is necessary to satisfy the crossing condition for a rather large force amplitude.

Figure 8 reveals a characteristic feature of $w_i(t)$: the obvious presence of the fourth harmonic. This is because the crossing point we have chosen corresponds to a four-photon process, i.e., a situation where the period of the force is four times larger than the period of the eigenmodes. Thus, frequency multiplication of the external force occurs at a crossing point. The multiplication coefficient depends on the amplitude of the force, i.e., such structures can be used for analog-digital conversion.

In Sec. 2 we discussed the evolution of $w_i(t)$ when the variation of the potential $U(t)$ is smooth and monotonic, for a wave function with the initial form $\psi(x,0)=(|1\rangle$

$+e^{i\phi}|2\rangle)/\sqrt{2}$, and showed that for $t>\tau$ the system behavior depends weakly on ϕ. A different situation obtains for periodic forces. In this case, the choice $\phi=0$ leads to localization of the electron in the left-hand well, whereas for $\phi=\pi$ the periodic force localizes the electron in the right-hand well. As calculations show, for intermediate ϕ the probability $\bar{w}_1$ of observing an electron in the left-hand well averaged over a period changes smoothly from a maximum value at $\phi=0$ to a minimum value close to zero at $\phi=\pi$; in this case, $\bar{w}_2$ increases from zero to a maximum value. The amplitude of the oscillations around the average value is a minimum for $\phi=0$ and $\phi=\pi$, and a maximum for $\phi=\pi/2$, where $\bar{w}_1=\bar{w}_2$ holds. Thus, in this case the evolution is a strong function of the phase ϕ. A state with a specified value of ϕ can be prepared from the state $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$ by delaying the switching on the signal, i.e., allowing the system to execute free oscillations for a time $t=\hbar\phi/(E_2-E_1)$.

When the excitation amplitude lies outside the crossing region, the evolution of $w(t)$ results from the superposition of oscillations corresponding to at least two Floquet modes with different frequencies (in general, incommensurate). The function $w(t)$ has the characteristic beating form, whose frequency is determined by the spacing between quasi-energies for the first few Floquet modes. In this case, the contribution of higher modes is also significant. The form of $w(t)$ turns out to be very complicated, the behavior of the system is close to chaotic, and the variation of $w(t)$ is large. The probability of observing an electron in the excited state $|a_2(t)|^2$ for a force with finite amplitude always turns out to be rather large, reaching a maximum at the anticrossing point.

Everywhere above we have treated a sequence of rectangular pulses, for which we are able to carry out a rather complete and comparatively simple analysis of the system behavior. In contrast, the signal dependence usually encountered in the literature is harmonic, of the form $U(t)=U_0\sin\omega t$. As we demonstrated in the previous sections, the time-dependent Kronig-Penney model allows us to describe all the features of the evolution that result from a harmonic signal.[13–15] Our method of solving the time-independent Schröedinger equation allows us to compute $\psi(x,t)$ for an arbitrary function $U(t)$ as well, simply by approximating this function by a piecewise-constant function. The basic results in this case turn out to be the same as for a sequence of rectangular pulses.

3.3. Asymmetric structures

In asymmetric structures, the regimes of crossing and anticrossing are no longer directly associated with even-order multiquantum transitions. We can illustrate the connection between nth order multiquantum transitions and crossing and anticrossing regimes at the qualitative level by considering an effective Hamiltonian written in the basis $\{\phi_m\}$ of eigenstates of the system without an external field. In this case the anticrossing regime corresponds to the resonance approximation; in the weak-field limit this is described by the following two-level effective Hamiltonian:

$$H=\begin{pmatrix} \varepsilon & \lambda^{(n)}e^{-in\omega t} \\ \lambda^{(n)}e^{in\omega t} & -\varepsilon \end{pmatrix}$$

$$=\varepsilon\sigma_z+\lambda(\sigma_x\cos n\omega t+\sigma_y\sin n\omega t). \qquad (29)$$

Here $\pm\varepsilon$ are the energy levels coupled by the resonance field, which in general may also include transverse dispersion ($k_\perp$). For $n=1$, the resonance interaction amplitude is $\lambda=e\mathscr{E}P_{12}/\omega$, where P_{12} is the interband matrix element of the pulse (for an interaction with a field of the form $A\nabla$, where A is the vector potential). Using the canonical transformation U

$$U=\exp(i\sigma_z\omega t/2),$$

corresponding to transforming to a rotating system of coordinates, we can reduce the time-dependent problem to a time-independent problem with the Hamiltonian

$$\bar{H}=(\varepsilon-\omega/2)\sigma_z+\lambda\sigma_x.$$

The spectrum of this Hamiltonian $\bar{H}$ has the form $E=\pm\sqrt{(\varepsilon-\omega/2)^2+\lambda^2}$, which under resonance conditions ($\varepsilon\approx\omega/2$) describes level anticrossing. If the wave function is initially in one of the stationary states of the Hamiltonian without a field, then it will oscillate between resonantly coupled states in the anticrossing regime with an amplitude $a(t)=(\lambda/E)\sin(Et/\hbar)$.[7]

For $n>1$ ($n\omega\approx2\varepsilon$) the anticrossing regime can also be described by using the resonant Hamiltonian (29) if we compute the nondiagonal components to the order of perturbation theory required by the condition $n\omega\approx2\varepsilon$. When a center of inversion is present in the system without a field, the diagonal matrix elements of the term that describes the interaction of the system with the field ($A\nabla$ or $e\mathscr{E}x$) vanish, and nondiagonal components appear only in odd orders:

$$\lambda_{\text{eff}}^{(3)}\sim P_{12}P_{21}P_{12}.$$

In the absence of a center of inversion ($P_{11}\neq0$), resonant components appear in the even orders as well:

$$\lambda_{\text{eff}}^{(2)}\sim P_{11}P_{12}.$$

Thus, once the center of inversion of the system is eliminated, we can observe transitions from the crossing regime to the anticrossing regime, with a corresponding change in the character of the time evolution of the electron states. In a symmetric nanostructure this can be achieved by applying a constant electrical bias along the nanostructure axis.

Let us discuss the dependence of the quasi-energy on the signal amplitude for an asymmetric system, both for a symmetric force and for a nonsymmetric one.

In Fig. 9 (curves *1*, *2*) we show the functions $\varepsilon(U_0)$ for an asymmetric structure with dimensions $a_1=0.49\lambda$, $a_2=0.50\lambda$, $b=0.3\lambda$ subjected to a symmetric force. If we compare these curves with the analogous functions for a symmetric structure (see Fig. 6), we see that in the presence of asymmetry, crossing can convert to anticrossing. Curves *3*, *4* in Fig. 9 illustrate the fact that by choosing the duration of the positive and negative half-waves of the periodic signal we can bring about intersection of the quasi-energies for an asymmetric structure. The parameters of the structure were

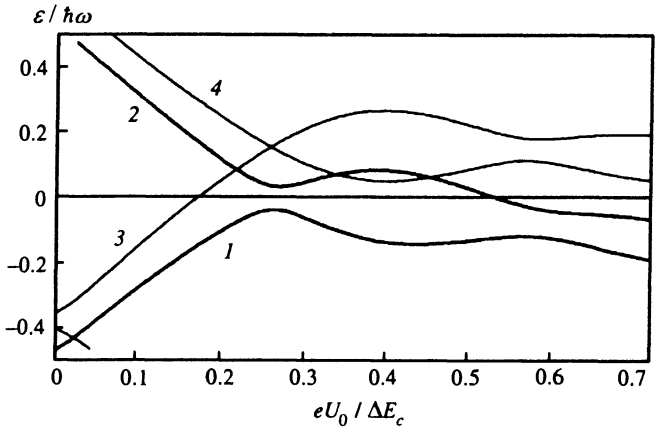


FIG. 9. Quasi-energies $\varepsilon_{1,2}$ as functions of the amplitude of the periodic force U_0 for an asymmetric structure ($a_1=0.49\lambda$, $a_2=0.5\lambda$, $b=0.3\lambda$). Here *1*, *2* are for a symmetric force with $\tau_1=\tau_2=5.57t_0$, *3*, *4* are for an asymmetric force with $\tau_1=5.49t_0$, $\tau_2=5.93t_0$.

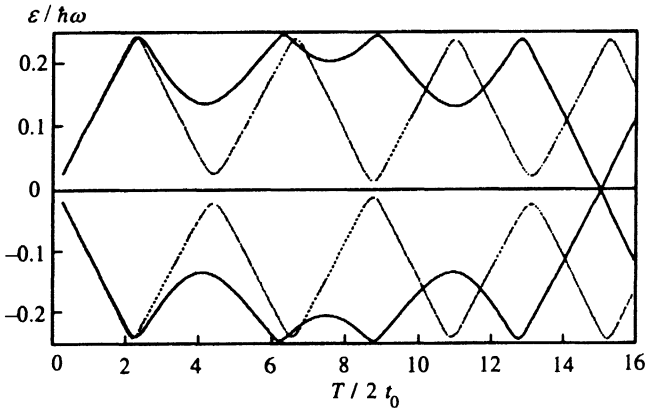


FIG. 10. Dependence of the quasi-energies $\varepsilon_{1,2}$ on the amplitude of a symmetric periodic force for an asymmetric structure ($a_1=0.4\lambda$, $a_2=0.5\lambda$, $b=0.4\lambda$) when $eU_0=0.02\Delta E_c$ (dots) and $eU_0=0.15\Delta E_c$ (solid curves).

$a_1=0.49\lambda$, $a_2=0.50\lambda$, $b=0.3\lambda$; the duration of the positive half-wave was $\tau_1=5.49t_0$; and the negative half-wave duration was $\tau_0=5.93t_0$. The magnitudes of τ_1 and τ_2 were chosen so that Eq. (24) holds for $U=0.25\Delta E_c$. It is for this value of the amplitude that the quasi-energies intersect in Fig. 9. In contrast to a symmetric two-well structure, where several crossing points are observed in this range of U_0, in this case there is only a single point where the quasi-energies intersect.

Another example of a nonsymmetric force is

$$U(t)=(U_0+\Delta U)\theta(\tau-t)-(U_0-\Delta U)\theta(t-\tau).$$

For a symmetric structure, the crossing becomes anticrossing when ΔU is not equal to zero. When $e\Delta U=0.02\Delta E_c$, the functions $\varepsilon(U_0)$ are analogous to curves *1*, *2* of Fig. 9.

Intersection of quasi-energy levels can also be achieved when symmetric pulses ($\tau_1=\tau_2$) act on an asymmetric structure. It is easy to see that Eq. (22) will hold if the amplitude is chosen so that the ratio Δ_-/Δ_+ (where $\Delta_{+,-}$ are the separations between the energy levels of the first two stationary states when $U=\pm U_0$) equals the ratio of two integers l/m, and the period equals $T=4l\hbar/\Delta_+$. In contrast to a symmetric structure, the conditions for crossing in this case will no longer be satisfied on a curve in the plane (T,U_0), but only at discrete points.

In Fig. 10 we show the dependence of the quasi-energies on the force for an asymmetric structure with the parameters $a_1=0.4\lambda$, $a_2=0.5\lambda$, $b=0.4\lambda$, and amplitudes $U_0=0.02\Delta E_c$ (dotted curves) and $U_0=0.15\Delta E_c$ (solid curves). It is clear from the figure that by varying the voltage U_0 we can cause the anticrossing point to become a crossing point. At the crossing point shown in Fig. 10 we have $\Delta_-/\Delta_+=3$, $T=30t_0$. The parameters of the system are chosen so that the quasi-energies intersect at the resonance $U_0=U_r$.

Figure 11 shows the time evolution of the probability of finding an electron in the wells for this intersection point, under the condition that the system is initially in the ground state. In the first half-period, the system executes a single oscillation, while in the second it executes three. This is because $\Delta_+/\Delta_-=3$. During the positive half-wave the voltage equals its resonance value; hence, the amplitude of the oscillations $w_{1,2}$ is large. The number of points of intersection of quasi-energies as U_0 varies will increase as the resonant distance between the stationary energy levels decreases. This can easily be ensured by increasing the barrier width. Figure 12 (which is analogous to the diagram shown in Fig. 7 for the symmetric structure) shows the geometric location of crossing points in the plane (T,U_0) for a structure with parameters $a_1=0.4\lambda$, $a_2=0.5\lambda$, $b=0.7\lambda$.

There is a certain analogy between the problem we are discussing, in which the relocation of electrons from one quantum well to another is controlled externally, and the problem of ionization of atoms (departure of an electron to infinity). In this case, instead of discussing excitation from a localized ground state to a state of the continuous spectrum, we discuss the case where a transition occurs from one localized state to another.

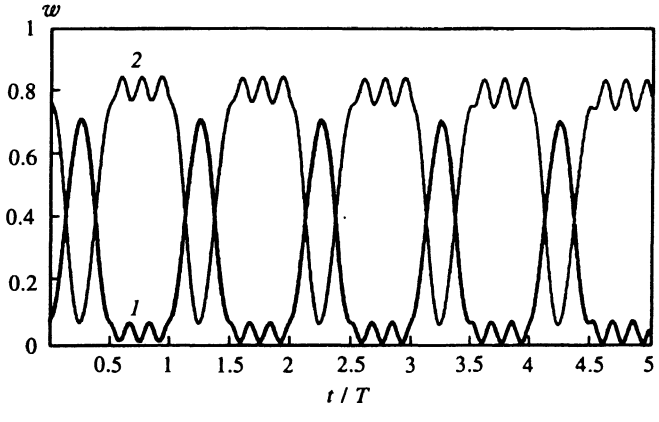


FIG. 11. Temporal evolution of the probabilities $w_{1,2}$ for an asymmetric structure when a symmetric force acts at the point of quasi-energy crossing: $T=30t_0$, $eU_0=0.15\Delta E_c$.

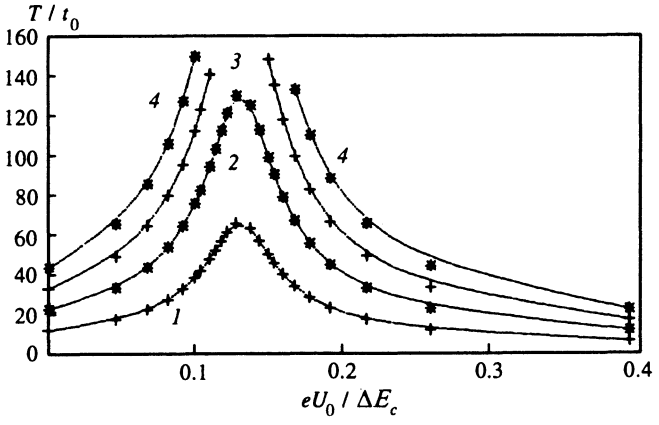


FIG. 12. Position of the crossing (*) and anticrossing (+) points on the plane (T,U_0) for an asymmetric structure ($a_1=0.4\lambda$, $a_2=0.5\lambda$, $b=0.4\lambda$) and a symmetric force.

Ionization of atoms proceeds by two alternative mechanisms: multiphoton ionization (including one-photon), and tunneling ionization. In the paper Ref. 10, L. V. Keldysh obtained a general expression for the ionization probability, which in the limit $\omega \ll \omega_{\text{tun}}$ (where $1/\omega_{\text{tun}}$ is proportional to the tunneling time) reduces to the expression $w = (B/\sqrt{\mathscr{E}})\exp(-C/\mathscr{E})$ for tunneling ionization, where B, C are certain constants and $\mathscr{E}$ is the electric field intensity in the wave. In the opposite limit $\omega \gg \omega_{\text{tun}}$, Keldysh obtained the expression for multiphoton ionization $w = \alpha\varepsilon^{2k_0}$, where α is the cross section for the multiphoton process and k_0 is the number of photons involved. In this case the argument turns on the smallness of the probabilities. In our case it makes sense to speak of a relocation or of a transition from the ground state to an excited state when the corresponding probabilities are of order unity. The technique we are using, i.e., Floquet functions and the quasi-energy representation, allows us to describe the electron dynamics in general, including multiphoton behavior and tunneling, over the entire physically interesting range of transition probabilities. Of the curves that show the dependence of the frequency on field intensity, those that correspond to the anticrossing condition exhibit probabilities for these transitions of order unity.

On these curves, in the weak-field limit it is the corresponding multiphoton processes that are responsible for the transition. The tunneling contribution (resonant tunneling) will dominate the multiphoton contribution for asymmetric structures when the distance between electronic levels in the system, which determines the value of $\mathscr{E}d_{12}$ under conditions of resonant tunneling, significantly exceeds the value of the tunneling-induced splitting of the level, which decreases exponentially as the width of the barrier increases. The most favorable conditions for relocation and excitation are realized along the curve $\omega(U_0)$ corresponding to anticrossing with a low frequency determined by the tunneling-induced splitting. In this case, the dependence on frequency within this range is actually rather weak (perhaps with the exception of crossing points).

Let us turn to the situation where the number of quantum wells in the system is more than two. In this case we are no longer able to obtain simple analytic expressions for the quasi-energies, but they are easily computed numerically. For multiwell structures, we are most interested in finding structure parameters for which the intersection of several (more than two) quasi-energy levels takes place. In this connection, let us compute the spectra of quasi-energies $\varepsilon(U_0)$ for three- and four-well structures.

For the three-well structure, we choose the parameters of the wells so that there are three energy levels below the barrier height in the unperturbed system. Our basic interest is in the behavior of the three lowest quasi-energy levels. Calculations show that for a symmetric system with three identical wells there are regions where all three levels approach very close to one another, although there are no exact simultaneous intersections. As we noted previously, the simultaneous intersection of several quasi-energy levels within the time-dependent Kronig–Penney model requires that the energy levels of the system be equidistant when the constant field is equal in magnitude to the amplitude of the periodic force. This is easily achieved for a three-well structure by varying the width of the center well. For example, for a system with well sizes $a_1=a_2=a_3=0.5\lambda$, $b_1=b_2=0.3\lambda$, the first approach of the quasi-energy levels is observed for $eU_0\approx 0.2\Delta E_c$. By solving the stationary Schrödinger equation, we easily find that for this constant external bias the energy levels become equidistant if we change the size of the center well to 0.4925λ. In this case we observe the simultaneous intersection of three quasi-energy levels when $eU_0=0.25\Delta E_c$, i.e., the first anticrossing is converted to a crossing. Since the distance between energy levels in steady state depends on the value of the external field, the levels are not equidistant for other U_0, and, in contrast to the two-well structure, only one crossing point occurs.

As in the case of the two-well structure, calculations show that the main features of the function $\varepsilon(U_0)$ for the first three levels are preserved even when we take into account a larger number of levels. We made analogous calculations for four-well structures. For a system of identical wells and identical barriers, there are no crossing points. Intersection is achieved by varying the width of the wells and barriers. Thus, our investigations are in agreement with the conclusion that a superlattice made up of identical elements in a periodic external field exhibits only an approximation of band collapse (due to inclusion of only nearest neighbors).[13,19]

3.4. A regime for switching on a periodic signal

The features of most interest to us are the points of intersection of the first quasi-energy levels. In this case, the behavior of the system is close to periodic over a wide set of initial conditions (if the primary contribution to the expansion of the initial state in Floquet modes includes modes that correspond to quasi-energies that intersect). The details of the behavior of the probability of finding an electron in a particular well depend on the specific form of the initial state. For this reason, it is interesting to trace the behavior of the system as we switch on a periodic signal. For the time-

dependent analogue of the Kronig–Penney model, a good way to describe the switching front of the signal is to use the following expression:

$$U(t)=U_n G(t),$$

where $G(t)$ is the periodic step function (15) with $U_1=-U_2=1$, and

$$U_0=\begin{cases} U_0 & \text{for } n>N, \\ U_0 n/(N+1) & \text{for } n\leq N, \end{cases}$$

i.e., the first N pulses have amplitudes that increase linearly with N. We will consider the evolution for two types of initial conditions: a) $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$, and b) $\psi(x,0)=|1\rangle$.

Figure 13 shows the time dependence of the probability of observing an electron in the first and second wells for case a) when N equals 7, 8, and 10 respectively. The period of the force is $T=22.23t_0$, and its amplitude in the steady-state regime is $eU_0=0.42\Delta E_c$. These conditions correspond to the second crossing point shown in Fig. 6, and are chosen because the amplitude of the force in steady state will be rather large for an electron to be localized and relocated in the wells (of course, this is possible only at a crossing point). Especially noteworthy is the change in the behavior of the system in the steady-state regime for small changes in the number of pulses at the switch-on stage. Both relocation into the second well (Fig. 13a) and localization in the first well (Fig. 13c) are possible. Furthermore, it is possible to have a situation where rather strong oscillations occur in the probabilities in each of the wells in steady state, although the average values of these numbers remain close (Fig. 13b). Similar behavior is obtained for case b) as well.

In order to illustrate the behavior of this system over a broader range of N, we plotted the dependence of the time-averaged values of the probabilities for observing an electron in the first well ($\bar{w}_1$) and second well ($\bar{w}_2$) for $n>N$ versus the number of periods N in the switch-on stage. Figure 14 shows the functions $\bar{w}(N)$ when the system is initially in the ground state ($\psi(x,0)=|1\rangle$). It is clear from the figure that there is a rather broad region where either localization in the first well or relocation into the second is possible, and a narrow region where the probabilities in the two wells are equal. This reflects the fact that for a periodic force the evolution of the wave function depends strongly on its initial distribution. The role of the transient stage, in this case, reduces to preparing the initial state for the periodic regime. In contrast to the regime where the external constant field is switched on adiabatically, in this case we do not find that $\bar{w}$ approaches a definite limit as N goes to infinity, and different initial conditions do not produce appreciably different behaviors of $w(t)$.

A similar dependences on the width of the front over which the amplitude of the periodic excitation increases was observed in Ref. 15. There it was noted that localization in the regime of increasing fields takes place only for certain values of the phase of the external field. Our calculations imply that this stems from the way the wave function evolution depends on its intrinsic phase structure rather than any direct dependence on the phase of the external field. In this

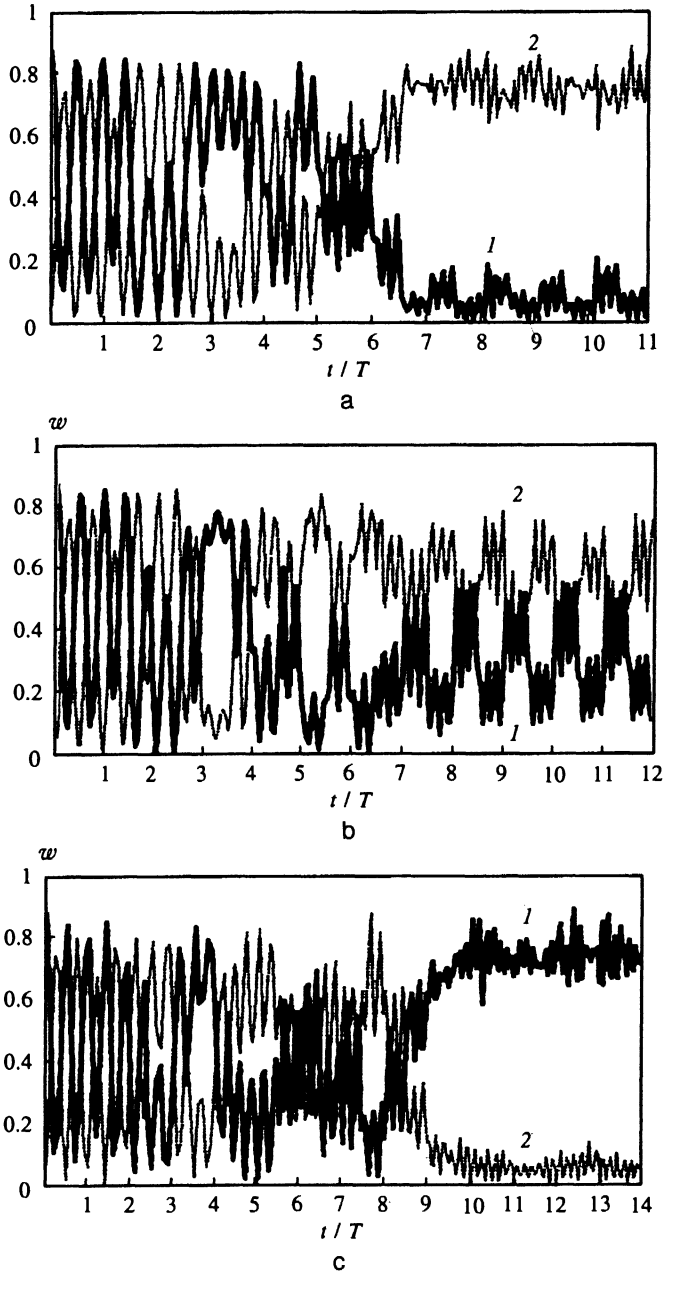


FIG. 13. Time dependence of the probabilities of finding an electron in the wells $w_{1,2}$ for a structure with $a_1=a_2=0.5\lambda$, $b=0.3\lambda$, when $T=22.23t_0$, $eU_0=0.42\Delta E_c$ for a pulsed regime with pulse amplitudes that increase linearly for the first N periods; the values of N are 7 (a), 8 (b), and 10 (c). The initial condition is $\psi(x,0)=(|1\rangle+|2\rangle)/\sqrt{2}$.

case, the following mechanism for generating localized states will be involved. Our study of the relocation process given in Sec. 2, and our calculation of the quasi-energy spectrum, indicate that an external potential causes relocation of the electron density only for a sufficiently large force amplitude, comparable to the distance between energy levels of the unperturbed states. Just as during dissipationless relocation, discontinuous (Fig. 2a) and smooth (Fig. 2b) forces lead to physically similar results: up to a certain critical value in the amplitude, when the excitation is periodic a smooth increase is qualitatively equivalent to a discontinuous increase. In

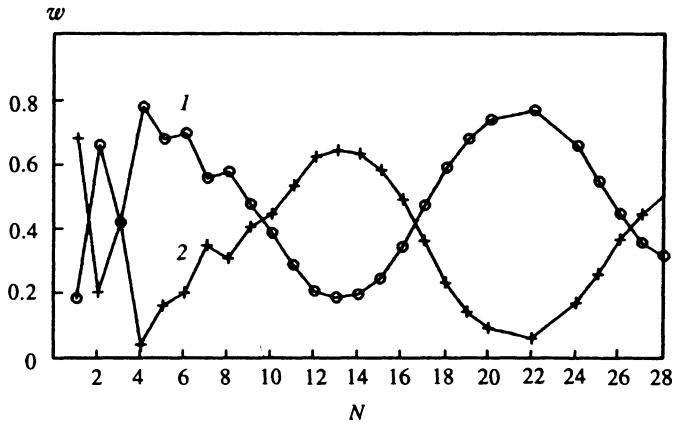


FIG. 14. Dependence of the average probabilities $\bar{w}_{1,2}$ of observing an electron in wells *1* and *2* on the number of periods N involved in the transient signal for $\psi(x,0)=|1\rangle$.

turn, it follows from Fig. 8 that when the periodic force is switched on discontinuously, the subsequent evolution of the electron state varies smoothly with the initial phase structure of the wave function. However, our calculations imply that the dependence of the evolution on the phase of the intrinsic field is completely insignificant. The phase structure of a wave function formed by a superposition of stationary eigenstates of the system is determined by how long it has been evolving:

$$\psi=\exp(-iE_1t)[|1\rangle+\exp(i(E_1-E_2)t|2\rangle].$$

It is possible to choose a relative phase that leads to mixing of various states at a specified time by choosing the initial phase structure of the wave function. From this we may conclude that the evolution of an electron state depends on the phase of the field when the latter is switched on smoothly, as we observed in numerical experiments,[15] because for different values of the phase of the field the wave function is able to acquire different relative phase shifts $\exp[i(E_1-E_2)t]$ up to a time t_0 when the amplitude of the field becomes large enough to cause relocation or localization.

4. CONCLUSIONS

The results we have obtained in this work show that superlattices are convenient objects for studying the behavior of quantum systems in a strong electromagnetic field. We have established that the evolution of electronic states in quantum structures placed in an external field is determined by a combination of two factors: quantum-mechanical tunneling, which dominates in strong slowly varying fields, and multiphoton transitions between energy levels of the system, which determine the dynamics in the limit of weak field amplitudes. In strong rapidly oscillating fields these two effects are interdependent, since the field modifies the energy spectrum significantly. The characteristic scale ΔE of the distances between energy levels for the quantum structures we have discussed is of order 0.01 to 0.1 eV. In this case a strong field is one with intensity 10^4–10^5 V/cm. At this time, such fields are easily attainable experimentally.[20]

The time-dependent behavior of a system in a strong field is conveniently described in terms of the quasi-energy spectrum and Floquet functions. By using the formalism developed in this paper based on the dynamic analogy with the Kronig-Penney model, we can analytically investigate the quasi-energy spectrum of quantum structures subjected to a periodic force. In this case the most interesting situation involves crossing, i.e., rigorous intersection of quasi-energy levels, for which the electron density can be dynamically localized in a specific part of the quantum structure. The quasi-energy structure of an energy spectrum that consists of a set of equidistant levels should manifest itself in tunneling experiments as well.[21] The tunneling admittance of a superlattice in a strong AC field was investigated in Ref. 22. The asymmetry in the current–voltage characteristics observed in this paper coincides qualitatively with our calculations (see Figs. 6, 9).

In this paper we have further developed the analogy between problems of dynamic evolution in quantum mechanics on the one hand and static scattering problems in optics and quantum mechanics on the other. Along with the dynamic analogue of the Kronig–Penney model, in this paper we have also constructed dynamic analogues of reflectionless potentials, which describe dissipationless relocation of the electron density for a rapid (antiadiabatic) change in the external voltage on the structure. The conjunction of dissipationless relocation and dynamic localization in the crossing regime allows us to explain the dependence of the localization character on the phase of the external force when the amplitude of the latter increases monotonically, which we saw previously in numerical experiments.

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[1] *Localization and Confinement of Electrons in Semiconductors*, F. Kachar, H. Heinrich, and G. Bauer eds., Springer-Verlag, Berlin, 1990.
[2] A. A. Gorbatsevich, V. V. Kapaev, and Yu. V. Kopaev, JETP Lett. **57**, 565 (1993) [JETP Lett. **57**, 580 (1993)].
[3] A. A. Gorbatsevich, V. V. Kapaev, and Yu. V. Kapaev, Silicon Microelectronics 23, 17 (1994) [in Russian].
[4] C. Juang, Phys. Rev. B **44**, 1076 (1991).
[5] E. O. Kane, in the book *Tunnelling Phenomena in Solids*, E. Burstein and S. Lundqvist eds. Russ. transl. Mir, Moscow, 1973.
[6] J. Von Neumann and E. Wigner, Phys. Z. **30**, 467 (1929).
[7] L. D. Landau and E. M. Lifshits, *Quantum Mechanics (Nonrelativistic Theory)*, Nauka, Moscow, 1974 [Pergamon Press, Oxford, 1977].
[8] I. I. Rabi, Phys. Rev. **51**, 652 (1964).
[9] I. I. Rabi, N. F. Ramsey, and J. Schwinger, Rev. Mod. Phys. **26**, 167 (1966).
[10] L. V. Keldysh, Zh. Éksp. Teor. Fiz. **47**, 1945 (1964) [Sov. Phys. JETP **20**, 1307 (1965)].
[11] J. H. Schirley, Phys. Rev. **138**, 979 (1965).
[12] Ya. B. Zel'dovich, Zh. Éksp. Teor. Fiz. **51**, 1492 (1966) [Sov. Phys. JETP **24**, 1006 (1967)]; V. Ritus, Zh. Éksp. Teor. Fiz. **51**, 1544 (1966) [Sov. Phys. JETP **24**, 1041 (1967)].
[13] M. Holthaus and D. Hone, Phys. Rev. B **47**, 6499 (1993).
[14] F. Grossmann, P. Jung, T. Dittrich, and P. Hanggi, Z. Phys. B: Condens. Matter **84**, 315 (1991).
[15] R. Bavli and H. Metiu, Phys. Rev. Lett. **69**, 1986 (1992).

[16] G. Bastard, J. A. Brum, and R. Ferreira, *Solid State Physics,* **44**, 229. Academic Press, 1991.
[17] B. Weil and B. J. Vinter, Appl. Phys. **60**, 3227 (1986).
[18] D. Y. Oberli, D. R. Wake, M. V. Klein, J. Klem, T. Henerson, and H. Morkoç, Phys. Rev. Lett. **59**, 696 (1987).
[19] D. H. Dunlap and V. M. Kenkre, Phys. Rev. B **34**, 3625 (1986).
[20] F. Keilmann, Solid State Commun. **92**, 223 (1994).
[21] V. A. Chitta *et al.*, J. Phys. Condens. Matter **6**, 3945 (1994).
[22] P. S. S. Guimarâes, B. J. Keay, J. P. Kaminski *et al.*, Phys. Rev. Lett. **70**, 3792 (1993).

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