Electron passage through quantum-size structures in high-frequency fields

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Simple methods are developed for obtaining the solutions of the time-dependent Schrödinger equation that describe the passage of electrons through quantum-size structures in weak high-frequency fields both with and without a dynamic space charge. Problems with simple analytic solutions are examined as an example of application of the theory. The exact steady-state solutions of the time-dependent Schrödinger equation in free space with a strong uniform high-frequency field are found in the absence of a constant electric field and in the presence of such a field. Finally, a method is developed for solving problems of electron passage through systems of rectangular and triangular wells and barriers for an arbitrary amplitude of the uniform high-frequency field. © *1996 American Institute of Physics.* [S1063-7761(96)02005-7]

1. INTRODUCTION

The development of modern nanoelectronic technology has led to the emergence of new physical objects that make it possible to study macroscopic manifestations of quantum effects in experiments. In particular, in recent years devices such as semiconductor diodes and transistors with resonant electron tunneling have appeared in which the quantum mechanical interaction between the electron flux and a high-frequency (hf) electric field during passage of the electrons through semiconductor structures consisting of several potential wells and barriers (quantum-size structures) has a strong effect of the characteristics of the devices. In this connection a new broad class of problems of considerable physical and practical import has emerged, problems that require finding the steady-state solutions of the time-dependent Schrödinger equation. At low amplitudes of the hf field all these problems, at least in principle, can be solved by employing the techniques of standard time-dependent perturbation theory (described, for instance, in Refs. 1 and 2). To all appearances, however, the technical difficulties that emerge in analyzing such problems have ruled out the direct use of standard time-dependent perturbation theory, with the result that other methods are employed. The various approaches used, say, in analyzing the dynamics of resonant electron tunneling and based on the lifetime approximation,[3] the numerical calculation of the passage of Gaussian packets,[4] the Wigner kinetic equation,[5] the nonequilibrium Green's functions,[6] and the analytic properties of the transmission coefficient[9] either completely ignore the special features of the interaction of electrons and the hf field or are so complicated that they produce results contradictory in many respects even for double-barrier structures with a single quantum well (see, e.g., Refs. 5 and 6) and in most cases do not make it possible to obtain solutions in analytic form.

The irony of the situation is that before the author's papers[8,9] appeared, the basic problem of the passage of electrons through a rectangular potential barrier in the presence of a variable hf field had not been solved completely, notwithstanding its extreme simplicity and serious studies in this area of research.[10,11] In Ref. 8 only a sketchy description was given of a simple variant of the time-dependent perturbation theory, which thanks to the special features of the problems mentioned earlier makes it possible to find their solution in an extremely simple and graphic way. Moreover, some cases where the electrons pass through quantum-size structures give rise to problems that require solving the time-dependent Schrödinger and Poisson equations in a self-consistent manner. However, while various methods are available for the self-consistent solution of the time-independent Schrödinger equation with allowance for a space charge (for the case of double-barrier resonant-tunneling structures see, e.g., Refs. 12 and 13), practically no studies have been conducted of the effect of a static space charge (not to mention a dynamic space charge) on the interaction of the electrons with the hf field in such structures (a closely related problem has been studied only numerically[14]).

The aim of the present work is to give a description more general than that in Ref. 8 of a variant of the time-dependent perturbation theory applicable to problems in which the electrons interact with an hf field in quantum-size structures, and to demonstrate the application of this approach by simple and novel examples. A simple method is developed on the basis of this variant that allows us to obtain solutions of the self-consistent time-dependent Schrödinger and Poisson equations describing the passage of electrons through quantum-size structures in weak hf fields with a dynamic space charge. Also, a problem is given in which this solution can be obtained analytically. Finally, a simple method is presented that makes it possible in some cases to obtain solutions of the Schrödinger equation describing the passage of electrons through quantum-size structures in a uniform hf electric field of arbitrary amplitude.

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2. THE PERTURBATION-THEORY VARIANT

Let $\hat{H}_0$ be the time-independent Hamiltonian of an unperturbed system and let the time-dependent Schrödinger equation be

$$i\hbar\frac{\partial\psi}{\partial t}=\hat{H}_0\psi+\hat{V}\psi, \tag{1}$$

where $\hat{V}=V_-(x)e^{i\omega t}+V_+(x)e^{-i\omega t}$ is a small time-dependent periodic perturbation. We wish to find the steady-state solution of Eq. (1) that is independent of the initial conditions and corresponds to fixed boundary conditions (say, at $x=-\infty$ the flux of particles moving from left to right is fixed). The solution of the unperturbed problem is assumed to be known. What makes this problem special is that one must find not all solutions but only the steady-state ones. It is more natural, therefore, not to use the general formulas of standard perturbation theory (Ref. 1, Chap. VI) but rather to obtain the solution of the problem directly from the Schrödinger equation (just as is done when the potential energy is considered a perturbation; see Ref. 1, Chap. VI). Since the $V_\pm(x)$ are small, the solution of Eq. (1) can be sought in the form $\psi=\psi_0(x,t)+\psi_1(x,t)$, where $\psi_0(x,t)=\psi_0(x)e^{-i\omega t}$ is the solution of the unperturbed problem, and $|\psi_1|\ll|\psi_0|$, with $\omega_0=\varepsilon_0/\hbar$, and ε_0 the electron energy in the stationary state. The function ψ_1 satisfies the equation

$$i\hbar\frac{\partial\psi_1}{\partial t}=\hat{H}_0\psi_1+[V_-(x)e^{i\omega t}+V_+(x)e^{-i\omega t}]\psi_0. \tag{2}$$

We look for ψ_1 in the form[8]

$$\psi_1(x,t)=\psi_+(x)e^{-i(\omega_0+\omega)t}+\psi_-(x)e^{-i(\omega_0-\omega)t}.$$

The functions $\psi_\pm$ satisfy the equation

$$\hbar(\omega_0\pm\omega)\psi_\pm(x)=\hat{H}_0\psi_\pm+V_\pm(x)\psi_0(x). \tag{3}$$

Since the solution of the unperturbed problem is known, so are the general solutions of Eq. (3). A particular solution of Eq. (3) can be found by the variational method ,[15] and in many cases of practical interest (say, the passage of electrons through systems of rectangular or triangular barriers in a hf field whose coordinate dependence is described by a finite-degree polynomial), such solutions can be found analytically (see Sec. 2.3), while in other cases they can be expressed in terms of special functions (see Sec. 4) or in the form of power series.[16]

The continuity of the wave function and its derivative at each moment in time implies that the functions ψ_+ and ψ_- are independent of each other, a fact that enables finding these functions for given boundary conditions, and hence finding the wave function of the entire system.

The solutions of Eq. (3) can also be obtained by employing the Green's function, which in many cases may prove more convenient (say, in computer calculations).

Let us assess the applicability of the given method. Suppose that $|V_\pm^{\max}|$ is the maximum value of $|V_\pm|$. We examine Eq. (3) over a narrow range in which $V_\pm(x)\approx V_\pm^{\max}$. In this range it is natural to look for the particular solution of Eq. (3) among the class of functions close to ψ_0, which immediately leads to $\psi_\pm\sim\pm(V_\pm^{\max}/\hbar\omega)\psi_0$, and the necessary condition for the applicability of the perturbation theory is $|V_\pm^{\max}/\hbar\omega|\ll 1$.

Let us now take the important practical case in which the potential energy $U(x)$ in the unperturbed Hamiltonian and the perturbation $V_{\pm(x)}$ change significantly over the range $0<x<a$, while for $x<0$ we have $U(x)=V_\pm(x)=0$ (this situation is typical of most electronic devices mentioned above). The wave function of a stationary state normalized to one electron (for the sake of definiteness we assume that the electrons move from left to right) has the form

$$\psi_0(x)=\begin{cases}\exp(ikx)+D_0\exp(-ikx), & x<0,\\ A_0f(x,\omega_0)+B_0g(x,\omega_0), & 0<x<a,\\ C_0\exp[i\tilde{k}(x-a)], & x>a.\end{cases} \tag{4}$$

Here $f(x,\omega)$ and $g(x,\omega)$ are the linearly independent solutions of the equation $\hat{H}_0\psi=\varepsilon\psi$, $k=\sqrt{2m^*\varepsilon_0/\hbar^2}$, and $\tilde{k}=\sqrt{2m^*[\varepsilon_0-U(a)]/\hbar^2}$, with m^* the effective electron mass. Then the functions $\psi_\pm$ have the form

$$\psi_\pm(x)=\begin{cases}D_\pm\exp(-ik_\pm x), & x<0,\\ A_\pm f(x,\omega_0\pm\omega)+B_\pm g(x,\omega_0\pm\omega)+\chi_\pm(x), & 0<x<a,\\ C_\pm\exp[i\tilde{k}_\pm(x-a)]\pm\dfrac{V_\pm(a)}{\hbar\omega}C_0\exp[i\tilde{k}(x-a)], & x>a,\end{cases} \tag{5}$$

where

$$k_\pm=\sqrt{\frac{2m^*(\omega_0\pm\omega)}{\hbar}},\quad \tilde{k}_\pm=\sqrt{\frac{2m^*[\varepsilon_0-U(a)\pm\hbar\omega]}{\hbar^2}},$$

$\chi_\pm(x)$ are the particular solutions of Eq. (3) for $0<x<a$, $\pm[V_\pm(a)/\hbar\omega]C_0\exp[i\tilde{k}(x-a)]$ are the particular solutions of Eq. (3) for $x>a$, and the coefficients $A_\pm$, $B_\pm$, $C_\pm$, and $D_\pm$ are found by matching the wave function and its derivatives at the boundaries at each moment in time. In matrix form the system of equations for these coefficients is

$$\begin{pmatrix} 1 & -f(0,\omega_0\pm\omega) & -g(0,\omega_0\pm\omega) & 0 \\ ik_\pm & f'(0,\omega_0\pm\omega) & g'(0,\omega_0\pm\omega) & 0 \\ 0 & f(a,\omega_0\pm\omega) & g(a,\omega_0\pm\omega) & -1 \\ 0 & f'(a,\omega_0\pm\omega) & g'(a,\omega_0\pm\omega) & -i\tilde{k}_\pm \end{pmatrix} \begin{pmatrix} D_\pm \\ A_\pm \\ B_\pm \\ C_\pm \end{pmatrix} = \begin{pmatrix} \chi_\pm(0) \\ -\chi'_\pm(0) \\ -\chi_\pm(a)\pm\dfrac{V_\pm(a)}{\hbar\omega}C_0 \\ -\chi'_\pm(a)\pm i\tilde{k}\dfrac{V_\pm(a)}{\hbar\omega}C_0 \end{pmatrix}. \tag{6}$$

Expressions for higher-order perturbation-theory approximations can be obtained in a similar way. Moreover, the theory can be generalized in a natural manner to multifrequency fields and to the case where the potential energy in the unperturbed Hamiltonian has a complicated form and the general solution of Eq. (3) can be found analytically only if the interval from zero to a is partitioned into several characteristic regions.

Another important feature of the problem must also be mentioned: the matrix of the system of equations (6) has the same form as the corresponding matrix describing the static passage of electrons in the given problem. Therefore, it can be expected that under certain conditions there will be a relationship between the special features of the static passage of electrons through the system and the dynamical properties of the same system.

Ignoring second-order terms and allowing for the form of the steady-state wave function and the hermiticity of the permutation operator, we arrive at the following expression for the current density ($j=j_0+j_\omega=j_0+j_{+\omega}+j_{-\omega}$) outside the interaction region:

$$j=\frac{q\hbar}{2m*}\{2\tilde{k}|C_0|^2+[(\tilde{k}+\tilde{k}_+)C_0C_+^* \times\exp[(\tilde{k}-\tilde{k}_+)(x-a)]+(\tilde{k}+\tilde{k}_-)C_0^*C \times\exp[i(\tilde{k}_--\tilde{k})(x-a)]]\exp(i\omega t)+\text{c.c}\}, \tag{7}$$

where q is the electron charge. The energy acquired by electrons from the hf field (or acquired by the field from the electrons) during an oscillation period $T=\omega/2\pi$ is

$$W=\frac{\hbar^2\omega T}{m^*}(\tilde{k}_+|C_+|^2+k_+|D_+|^2-\tilde{k}_-|C_-|^2-k_-|D_-|^2). \tag{8}$$

In some cases, however, say in designing electronic devices, it is convenient to describe energy transfer between electrons and the field in terms of what is known as the induced current[17]

$$j_i(t)=\frac{1}{a}\int_0^a j(x,t)dx.$$

Here in the quasistatic approximation we have

$$W=\left\langle\int_0^a j(x,t)E(x,t)dx\right\rangle T =\langle j_i(t)E(t)\rangle aT=T|j_i|Ea\cos\Delta\varphi_i,$$

where

$$E(t)=\frac{1}{a}\int_0^a E(x,t)dx$$

is the average electric field, $\Delta\varphi_i$ is the phase shift between the induced current and the field at frequency ω, and $\langle\cdots\rangle$ stands for averaging over an oscillation period. For further discussion it is convenient to introduce the complex-valued conductivity σ of the structure, equal to the ratio of the complex-valued amplitude of the output current and electric field. We denote the corresponding quantity for the induced current by σ_i. Then the expression for the transferred energy (the interaction energy) is

$$W=2TaE^2|\sigma_i|\cos\Delta\varphi_i=2TaE^2\text{Re}\sigma_i, \tag{10}$$

from which, with allowance for (8) and the form of the wave function, we obtain

$$\text{Re}\sigma_i=\frac{\hbar^2\omega}{2aE^2m^*}(\tilde{k}_+|C_+|^2+k_+|D_+|^2-\tilde{k}_-|C_-|^2 -k_-|D_-|^2). \tag{11}$$

This approach makes it possible to obtain only the real part of the conductivity, but it enables one to monitor separately the energy fluxes related to the interaction of the electrons and the hf field in the transmitted wave, $W(a)$, and the reflected wave, $W(0)$. To simplify the description, we formally introduce conductivities in the transmitted and reflected waves:

$$\text{Re}\sigma_i(a)=\frac{W(a)}{2TaE^2}=\frac{\hbar^2\omega}{2aE^2m^*}(\tilde{k}_+|C_+|^2-\tilde{k}_-|C_-|^2), \tag{12}$$

$$\text{Re}\sigma_i(0)=\frac{W(0)}{2TaE^2}=\frac{\hbar^2\omega}{2aE^2m^*}(k_+|D_+|^2-k_-|D_-|^2). \tag{13}$$

These formulas are valid only if $\hbar\omega<\varepsilon_0$ and $\hbar\omega<\varepsilon_0-U(a)$, in which case the general solutions of Eq. (3) for the ψ_- with $x<0$ and $x>0$ are plane waves. If $\hbar\omega>\varepsilon_0$ and $\hbar\omega>\varepsilon_0-U(a)$, the functions ψ_- assume the form

$$\psi_-(x)=\begin{cases} C_-\exp[-\tilde{\kappa}(x-a)]-\dfrac{V_\pm(a)}{\hbar\omega}C_0\exp[i\tilde{k}(x-a)], & x>a, \\ D_-\exp(\kappa x), & x<0, \end{cases}$$

$$\tilde{\kappa}=\sqrt{\frac{2m^*[\hbar\omega-\varepsilon_0+U(a)]}{\hbar^2}}, \quad \kappa=\sqrt{\frac{2m^*(\hbar\omega-\varepsilon_0)}{\hbar^2}},$$

thus leading to the appearance of a current

$$j_{-\omega}=\frac{q\hbar}{2m^*}(\tilde{k}+i\tilde{\kappa})C_0^*C_-\exp[-(i\tilde{k}+\tilde{\kappa}) \times(x-a)+i\omega t]+\text{ c.c.}, \tag{14}$$

which decays exponentially with distance. Here the solution ψ_- can be interpreted as a special state that appears in the region with the hf field (we call it a dynamically bound state), and in which electrons are localized. This becomes especially evident at $V_\pm(a)=0$, when the wave functions ψ_- for $x<0$ and $x>0$ have the same form as the wave functions of electrons in a well with a level $\mathcal{E}=\varepsilon_0-\hbar\omega$ (see also Sec. 2.2). Note that although in the steady-state regime for $\omega>\omega_0$ there can only be transitions with photon absorption, the localization of electrons in the hf field region and their motion in this region leads to generation of a variable field, which for a sufficiently high concentration of electrons in the wave incident upon the structure can become comparable to the field of the modulating signal, and this can significantly change the nature of the interaction of the entire electron flux with the hf field. (Generally, these aspects require additional investigation and lie outside the scope of the present work.)

As examples of application of the theory we examine the passage of electrons through a periodically varying jump in the potential, thin (delta function) and rectangular barriers, and double-barrier structures ($V_\pm(x)=-qEx$, where $2E$ is the field strength and q is the electron charge). For the sake of simplicity we assume that the edges of the region where the hf field is localized coincide the boundaries of the structure.

2.1. Periodically varying jump in the potential

Let us assume that the electrons interact with the high-frequency field within an interval of infinitesimal length a. Then the perturbation assumes the form $V_\pm(x)=-qEa\theta(x)$, where $\theta(x)$ is the Heaviside step function. In this case the perturbed part of the wave function has the form

$$\psi_\pm(x)=\begin{cases} D_\pm e^{-ik_\pm x}, & x<0, \\ C_\pm e^{ik_\pm x}\mp\dfrac{qEa}{\hbar\omega}e^{ikx}, & x>0. \end{cases} \tag{15}$$

The matching conditions for the wave function and its derivatives yield

$$C_\pm=\pm\frac{qEa}{\hbar\omega}\frac{k+k_\pm}{2k_\pm}, \quad D_\pm=\pm\frac{qEa}{\hbar\omega}\frac{k-k_\pm}{2k_\pm},$$

$$W=\frac{(qEa)^2}{2m^*\omega k_+k_-}(k_--k_+)(k^2-k_+k_-)T, \tag{16}$$

$$\text{Re }\sigma_i=\frac{q^2a}{4m^*\omega\, k_+k_-}(k_--k_+)(k^2-k_+k_-), \tag{17}$$

$$j_\omega=\frac{q^2Ea}{4m^*\omega k_+k_-}(k_--k_+)(k^2-k_+k_-)e^{i\omega t}+\text{ c.c.} \tag{18}$$

We see that in the interaction with a periodically varying jump in the potential the electrons give their energy to the field, and the shift of the current with respect to the field amounts to π. Note that since the interaction is point-like, the conductivities in the electronic and induced currents (see Eqs. (17) and (18)) are equal, and the energies given by the electrons to the field in the transmitted and reflected waves are also equal ($W(x<0)=W(x>0)$).

2.2. Tall thin barrier applied hf field

It has proved convenient in analytic studies to replace a tall thin barrier with a delta-function barrier of the same effective "strength" $\alpha=\int_0^a U(x)dx$. (The delta-function barrier approximation is applicable to thin and tall barriers when $2m^*\alpha a/\hbar^2\ll 1$, $\varepsilon\ll U$ or $k\hbar^2/a\gg U$; see Ref. 18.) Then Eq. (2) becomes

$$i\hbar\frac{\partial\psi_1}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi_1}{\partial x^2}+\alpha\delta(x)\psi_1-(e^{i\omega t}+e^{-i\omega t}) \times[\beta\delta(x)+\gamma\theta(x)]\psi_0, \tag{19}$$

where $\beta=qEa^2$, and $\gamma=qEa$. The perturbed part of the wave function has the same shape as in the previous case; the continuity conditions at the delta-function barrier (see Ref. 18) and the solution of the corresponding system of equations lead to the following result:[9]

$$C_\pm=C_0\frac{m^*\beta\pm\dfrac{m^*\gamma}{\hbar\omega}\left[\alpha-\dfrac{l\hbar^2}{2m^*}(k_\pm+k)\right]}{\alpha m^*-i\hbar^2k_\pm}. \tag{20}$$

Substituting (20) into (7) and allowing for the form of C_0, we find that

$$J_\omega=\frac{q^2Ea}{2m^*}\frac{k^2\hbar^5}{(m^*\alpha)^2+k^2\hbar^4} \times\left\{\frac{k_+-k_-}{\hbar\omega}+\frac{m^*}{2}\left[\frac{(k+k_+)a-2i}{\alpha m^*+i\hbar^2k_+} +\frac{(k+k_-)a+2i}{\alpha m^*-i\hbar^2k_-}\right]\right\}e^{i\omega t}+\text{ c.c.} \tag{21}$$

Analysis of (21) shows that this case differs dramatically from the previous one: as ω tends to zero, the phase shift $\Delta\varphi$ between field and current also tends to zero (note that here and in what follows we assume in all cases that $|qEa| \ll \hbar\omega$). The value of $\Delta\varphi$ increases with frequency, while for $\alpha \gg \hbar^2 k/m^*$ the phase shift is small, and the taller and thinner the barrier, the smaller the phase shift. This result agrees qualitatively with the expression for the time of flight of electrons through a barrier obtained in Ref. 11. At the same time, at low frequencies and for small barrier thicknesses ($m^*\alpha \ll \hbar^2 k_\pm$), (21) can be reduced to

$$j_\omega \approx \frac{q^2 Eka}{2m^*\omega_0}\left\{\frac{im^*\omega}{2k\hbar^2\omega_0}(2\alpha + a\hbar\omega_0) + \frac{\alpha m^* a}{\hbar^2} - \frac{1}{4}\left(\frac{\omega}{\omega_0}\right)^2\right\} e^{i\omega t} + \text{c.c.}, \tag{22}$$

which implies that for $\omega/\omega_0 > (4\alpha m^* a/\hbar^2)^{1/2}$, a thin potential barrier has negative dynamic conductivity (just as a periodically varying jump in the potential does).

At first glance it would seem that the negative dynamic conductivity of a thin barrier is related exclusively to the harmonic variation of the potential behind the barrier, as is the case with a periodically varying jump in the potential. To check this assumption we eliminate any variation in the potential [we put $\gamma = 0$ in Eq. (19)]. Then, substituting (20) into (8), we find that here too, if $k_+ k_- > (\alpha m^*)^2/\hbar^4$, the electrons give their energy to the hf field, which means that periodic variation of the height (strength) of a thin barrier in itself is sufficient for negative dynamic conductivity to emerge. Moreover, in the absence of a barrier, i.e., $\alpha = 0$ (a delta-like source of oscillations), this effect is observed for all values of k and ω, as it is in the case of a periodically varying jump in the potential.

Harmonic delta-like variation of the potential can serve as a convenient object for studying dynamically bound states. Let us consider a delta-like potential well of strength α. Suppose that the frequency of the source exceeds the natural electron frequency, $\omega > \omega_0$. Then the perturbed part of the wave function ψ_- has the same form as the eigenfunction of electrons in the well:

$$\psi_-(x) = \begin{cases} D_- e^{\kappa x}, & x < 0, \\ C_- e^{-\kappa x}, & x > 0, \end{cases} \tag{23}$$

where C_- can be formally obtained from (2) by substituting $i\kappa$ for k_- and $-\alpha$ for α, i.e., $C_- = C_0 m^* \beta/(\hbar^2\kappa - \alpha m^*)$. However, the difference between an ordinary level in a well ($\kappa_0 = \alpha m^*/\hbar^2$) and a dynamically bound state is evident. As $\kappa \to \kappa_0$, $|C_-|$ tends to ∞, i.e., for an ordinary level there is resonant interaction between the electrons and the perturbation (the use of first-order perturbation theory in this case is clearly unjustified). For a dynamically bound state there is no resonance.

2.3. Resonant passage of electrons through a rectangular potential barrier in hf fields

In this case, just as with a periodically varying jump in the potential and with a barrier-free transit section,[19] one must directly use system (6). In the region where the Hamiltonian $\hat{H}_0$ is independent of the coordinates and its eigenfunctions are such that $\psi_0'' = \pm k^2\psi_0$ and $V_\pm(x) = Vx^n$, it is natural to look for the solution of Eq. (3) in the form

$$\psi_\pm = a_n^\pm x^n \psi_0 + b_{n-1}^\pm x^{n-1}\psi_0' + a_{n-1}^\pm x^{n-1}\psi_0 + \cdots + a_0^\pm \psi_0,$$

from which at $V_\pm(x) = -qEx$ we can find the particular solution of Eq. (3) in the form

$$\chi_\pm = \mp\frac{qEx}{\hbar\omega}\psi_0 + \frac{qE}{m^*\omega^2}\psi_0'. \tag{24}$$

This immediately yields expressions for $C_\pm$ and $D_\pm$. The problem has been examined in detail in Ref. 9, so that here we restrict our discussion to the example (not examined in Ref. 9) of the resonant passage of electrons above an AlGaAs rectangular barrier. As noted earlier, in this case the transmission coefficient G is small, and the phase shift between current and field for $\omega < \omega_0$ is small, too. Near the resonant passage of electrons above the barrier (Fig. 1) the nature of the dependences considered here changes considerably: below the resonance (at low frequencies) negative dynamic conductivity appears (Fig. 2). At high frequencies this effect can be observed even for electron energies at which the transmission coefficient increases with ε, i.e., there is no low-frequency negative dynamic conductivity; moreover, under certain conditions, the function $\mathrm{Re}\sigma_i(\omega)$ can take on negative values in several regions. Note that negative dynamic conductivity disappears at frequencies for which $G(\varepsilon - \hbar\omega) \approx G(\varepsilon + \hbar\omega)$, and, in addition, $\mathrm{Re}\sigma_i$ has its extrema approximately at those points where the function $f(\omega) = G(\varepsilon + \hbar\omega) - G(\varepsilon - \hbar\omega)$ has a maximum or minimum. The fluxes of electrons that have released or acquired the energy $\hbar\omega$ behave accordingly (here we are dealing with the total fluxes in the transmitted and reflected waves; Fig. 3): they have minima or maxima near the respective extrema of $G(\varepsilon \pm \hbar\omega)$. A similar picture is observed for double-barrier structures.[16,20]

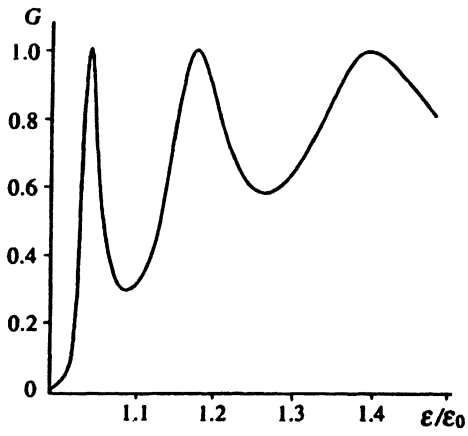

FIG. 1. The transmission coefficient for the passage of electrons through a rectangular potential barrier of thickness $a = 250$ Å and height $U = 200$ meV as a function of the normalized electron energy $\varepsilon/\varepsilon_0$ ($\varepsilon_0 = 200$ meV).

It appears that for the given problems the static transmission coefficient acts as a density of states: the probability of

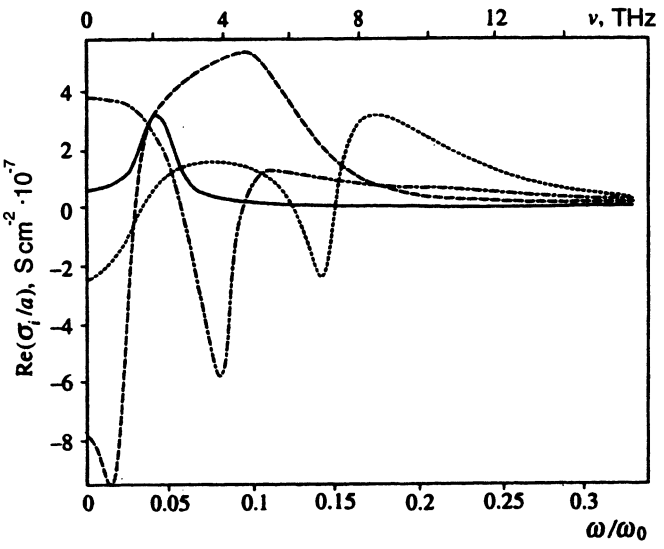

FIG. 2. Dependence on the normalized frequency ω/ω_0 ($\omega_0=\varepsilon_0/\hbar$) of the real part of induced-current conductivity, reduced to the barrier thickness, for electron passage through a rectangular potential barrier of thickness $a=250$ Å and height $U=200$ meV. Electron energies: $\varepsilon_0=200$ meV (solid curve), $\varepsilon=1.063\varepsilon_0$ (dashed curve), $\varepsilon=1.126\varepsilon_0$ (dot-dash curve), and $\varepsilon=1.189\varepsilon_0$ (dotted curve). Electron concentration: $n=10^{17}\text{cm}^{-3}$.

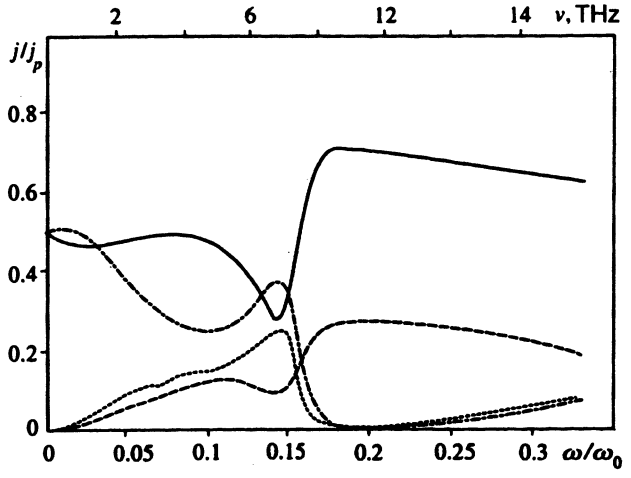

FIG. 3. Dependence on the normalized frequency ω/ω_0 ($\omega_0=\varepsilon_0/\hbar$, $\varepsilon_0=200$ meV) of the ratio of the fluxes of electrons that have interacted with the hf field in the transmitted wave, $j(\psi_+(a))$ (solid curve) and $j(\psi_-(a))$ (dot-dash curve), and the reflected wave, $j(\psi_+(0))$ (dashed curve) and $j(\psi_-(0))$ (dotted curve), to the total flux $|j_p|=|j(\psi_+(a))|+|j(\psi_-(a))|+|j(\psi_+(0))|+|j(\psi_-(0))|$ for electron passage through a rectangular potential barrier of thickness $a=250$ Å and height $U=200$ meV. Electron energy: $\varepsilon=237.8$ meV$=1.189\varepsilon_0$.

electrons moving into a region where the transmission coefficient is large is much higher than that of moving to a region where this coefficient is small. These features of time-dependent transport are mostly likely related to the fact that the matrices describing static and dynamic passage of electrons through a barrier are identical in form. In the case at hand, when the electrons pass through a rectangular potential barrier, the absolute value of the determinant of the matrix of (6), $|\Delta|$, has a minimum at exactly those electron energies $\varepsilon=\mathscr{E}_0$ at which $G(\mathscr{E}_0)$ is at its maximum. Since the absolute values of the determinants of the matrices obtained from the matrix of (6) by replacing the corresponding column with the column on the right-hand side of Eq. (6), $|\Delta_{C\pm}|$ and $|\Delta_{D\pm}|$, have no significant features at $\mathscr{E}_0$, $|C_+|=|\Delta_{C+}|/|\Delta|$ and $|D_+|=|\Delta_{D+}|/|\Delta|$ if $\varepsilon+\hbar\omega\approx\mathscr{E}_0$ or $|C_-|=|\Delta_{C-}|/|\Delta|$ and $|D_-|=|\Delta_{D-}|/|\Delta|$ if $\varepsilon-\hbar\omega\approx\mathscr{E}_0$ assume their corresponding maximum values.

Hence, basing our reasoning on the fact that the matrices describing static and dynamic passage of electrons through quantum-size structures have the same form, we expect that high-frequency negative dynamic conductivity can be observed not only in electron passage through rectangular potential barriers and double-barrier resonant-tunneling structures, but also through other quantum-size systems with a rapidly and nonmonotonically varying transmission coefficient.

2.4. Resonant interaction of electrons with an hf field in double-barrier structures

The above assumptions are confirmed in the case of the resonant interaction of electrons and a hf field in double-barrier resonant-tunneling structures. Here the system (6) contains not four but eight equations in eight unknowns. The problem can be simplified considerably, however, if the real barriers are replaced by delta-like barriers, as we did in Sec. 2.2.

For a symmetric double-barrier structure with thin barriers of height φ_b, thickness b, and strength $\alpha=\varphi_b b$ and with the distance between the barriers being a, the time-dependent Schrödinger equation has the form[16,20]

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2}+\alpha\delta(x)\psi+\alpha\delta(x-a)\psi+\hat{V}(x,t)\psi. \tag{25}$$

With a perturbation $\hat{V}(x,t)=V_-(x)e^{i\omega t}+V_+(x)e^{-i\omega t}$, for the given system the corrections to the ground-state wave function assume the form

$$\psi_\pm(x)=\begin{cases} D_\pm\exp(-ik_\pm x) & \text{if } x<0,\\ A_\pm\sin(k_\pm x)+B_\pm\cos(k_\pm x)+\chi_\pm(x) & \text{if } 0<x<a,\\ C_\pm\exp[ik_\pm(x-a)]+P_\pm\exp[ik(x-a)] & \text{if } x>a,\end{cases} \tag{26}$$

where $P_\pm = \pm(V_\pm(a)/\hbar\omega)\psi_0(a)$, and $\chi_\pm(x)$ are the corresponding particular solutions of Eq. (3). In matrix form the system of equations for the coefficients $A_\pm$, $B_\pm$, $C_\pm$, and $D_\pm$ is

$$\begin{pmatrix} 1 & 0 & -1 & 0 \\ ik_\pm - y & k_\pm & 0 & 0 \\ 0 & \sin(k_\pm a) & \cos(k_\pm a) & -1 \\ 0 & -k_\pm\cos(k_\pm a) & k_\pm\sin(k_\pm a) & ik_\pm - y \end{pmatrix} \times \begin{pmatrix} D_\pm \\ A_\pm \\ B_\pm \\ C_\pm \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}, \tag{27}$$

where

$$f_1 = \chi_\pm(0), \quad f_2 = -\chi'_\pm(0), \quad f_3 = P_\pm - \chi_\pm(a),$$
$$f_4 = (y - ik)P_\pm + \chi'_\pm(a),$$

with $y = 2m^*a/\hbar^2$. The solutions of Eq. (27) have a straightforward and yet somewhat cumbersome form, which makes them an inconvenient object for analytic studies. In some cases, however, they can be simplified considerably.

As is known, in double-barrier resonant-tunneling structures the transmission coefficient has a distinct resonant character, and the magnitude of the wave vector determining the resonant levels at which the transmission coefficient is unity can be found by solving the following transcendental equation:[18]

$$\tan(ka) = -\frac{k\hbar^2}{\alpha m^*} = -\frac{2k}{y}. \tag{28}$$

Here the unperturbed electron wave function normalized to the electron concentration n is

$$\psi_0(x) = \sqrt{n}\begin{cases} \exp(ikx), & x<0, \\ A_0\sin(kx) + B_0\cos(kx), & 0<x<a, \\ C_0\exp[ik(x-a)], & x>a, \end{cases} \tag{29}$$

where

$$A_0 = \frac{y}{k} + i, \quad B_0 = 1, \quad C_0 = \left(\frac{y}{k} + i\right)\sin(ka) + \cos(ka).$$

The determinant of the system (27) is

$$\Delta = (2k_\pm^2 - y^2)\sin(k_\pm a) - 2k_\pm y\cos(k_\pm a) + 2ik_\pm[k_\pm\cos(k_\pm a) + y\sin(k_\pm a)]. \tag{30}$$

Suppose that a monoenergetic electron beam passes through the resonant level with number K and that the frequency of the electric field corresponds to transitions to the resonant level with number M. For transitions to a nonresonant level $\Delta \sim k_\pm y$, while for sufficiently strong barriers ($y \gg k_\pm$) and a value of the wave vector corresponding to a resonant level, the determinant is small: $\Delta \approx 2ik_\pm^2(-1)^{M+1}$. Hence for narrow resonant levels ($y \gg k$) only the transition probability between two levels is important. In the case of wide levels ($y \sim k$), however, the probabilities of transitions with absorption or emission of quantum $\hbar\omega$ can become comparable. Moreover, the smallness of Δ in transitions to a resonant level implies that in nonresonant electron passage through a double-barrier resonant-tunneling structure, the probability of transitions to the energy range where the transmission coefficient is large is higher than to the range where the coefficient is small.

For $y \gg k_\pm$, the determinants needed for finding $C_\pm$ and $D_\pm$ ($D_\pm = \Delta_{D\pm}/\Delta$ and $C_\pm = \Delta_{C\pm}/\Delta$), with allowance for the form of the functions f in (27) and the fact that $V_\pm(x) = -qEx$ (see Eq. (24)), are approximately the same:

$$\Delta_{D\pm} \approx \frac{qE}{m^*\omega^2}(ik + y)(ik_\pm - y)k_\pm\sqrt{n} \times [\cos(k_\pm a) - \cos(ka)], \tag{31}$$

$$\Delta_{C\pm} \approx \frac{qE}{m^*\omega^2}(ik + y)(ik_\pm - y)k_\pm\sqrt{n} \times [\cos(k_\pm a)\cos(ka) - 1]. \tag{33}$$

From (28) it follows that $\cos(ka) < 0$ and $\sin(ka) > 0$ for odd resonant levels and $\cos(ka) > 0$ and $\sin(ka) < 0$ for even resonant levels, so that for a double-barrier resonant-tunneling structure with sufficiently strong barriers ($y \gg k_\pm$) we have

$$|\cos(k_\pm a) - \cos(ka)| \approx |\cos(k_\pm a)\cos(ka) - 1| \approx 2,$$

for transitions in which the level number changes from odd to even or from even to odd, and

$$|\cos(k_\pm a) - \cos(ka)| \approx |\cos(k_\pm a)\cos(ka) - 1| \approx 0,$$

for transitions in which the level number changes from odd to odd or from even to even. Hence, with $y \gg k_\pm$ only the first type of transition is important. This can be explained by the symmetry properties of the wave functions and the perturbation.

Using (11), we find the following expression for the active conductivity (without allowing for the space charge) of a double-barrier resonant-tunneling structure involved in electron transitions between resonant levels ($ak_\pm \approx \pi M$):

$$\mathrm{Re}\,\sigma_i^\pm \approx \pm\frac{8q^2m^*\alpha^4 n}{\pi M\hbar^6\omega^3}[1 - (-1)^{K-M}]. \tag{33}$$

A more rigorous calculation that allows in the expressions for $\Delta_{C\pm}$ and $\Delta_{D\pm}$ for terms not containing y yields

$$\mathrm{Re}\,\sigma_i^\pm \approx \pm\frac{q^2 n}{\pi M}\left\{\frac{8\alpha^2}{\hbar^3\omega^3}\left[\frac{m^*\alpha^2}{\hbar^3} + 2\omega_0 \pm \omega\right]\right\} \times [1 - (-1)^{K-M}]. \tag{34}$$

It would be interesting to see how accurate the above formulas are in describing conductivity in real structures. Figure 4 depicts the dependence of the relative error in active conductivity, as given by (33) and (34), on barrier thickness for electron passage through the eighth resonant level of a structure of width $a = 275$ Å. The dependence of $2k/y$ on barrier thickness is also depicted. We see that for thin barriers ($b < 20$ Å and $2k/y > 0.5$) in $8 \to 7$ transitions the conductivity is better described by (33). The reason is that in a structure with thin barriers not only are transitions to the

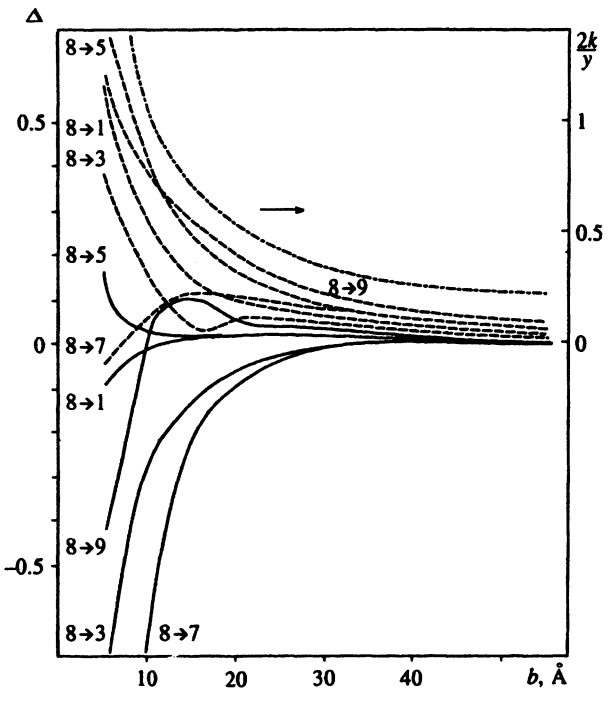

FIG. 4. Dependence on barrier thickness of the relative error $\Delta=(\sigma-\tilde{\sigma})/\sigma$ in calculations of the resonant active conductivity $\tilde{\sigma}_1$ with Eq. (34) (solid curves) and $\tilde{\sigma}_2$ with Eq. (33) (dashed curves) and of the parameter $2k/y$ (dot-dash curve) for electron passage through the eighth level of a double-barrier structure of width $a=275$ Å (the height of the barriers is $\varphi_b=1.04$ eV).

seventh level important, but so are transitions to the ninth resonant level, and a maximum in conductivity is realized at an energy somewhat below the resonant value (Fig. 5). Here, however, Eq. (34) provides a better description of the maximum possible conductivity in $8\rightarrow 7$ transitions. In transitions

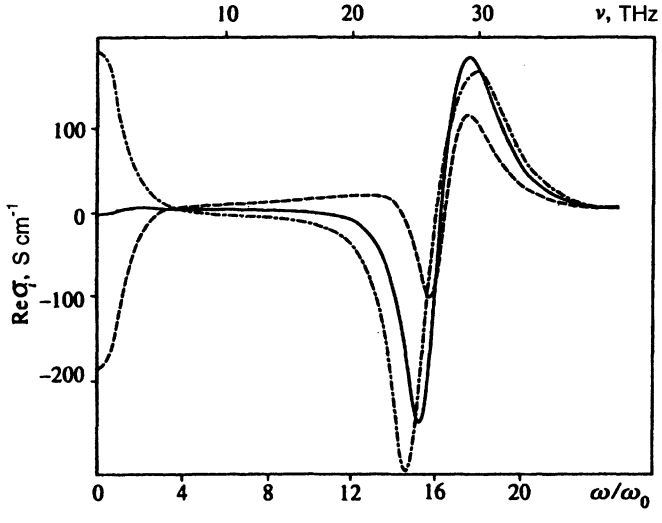

FIG. 5. Dependence of the active conductivity of a double-barrier resonant-tunneling structure on the normalized frequency ω/ω_0 ($\omega_0=\varepsilon_0/\hbar$) for electron passage through the eighth level of the structure ($a=275$ Å, $\varphi_b=1.04$ eV, and $b=11$ Å). Electron energies: $\varepsilon=\mathcal{E}_8=64.8\varepsilon_0$ (solid curve), $\varepsilon=64.2\varepsilon_0$ (dashed curve), and $\varepsilon=65.4\varepsilon_0$ (dot-dash curve), with $\varepsilon_0=6.91$ meV.

to other (narrower) resonant levels, Eq. (34) is essentially always more accurate. For thicker barriers (20 Å$<b<$40 Å and $0.25<2k/y<0.5$), Eq. (34) describes the conductivity much more accurately than (33). When the thickness of the structure is increased still further, calculations with (33) and (34) are essentially identical, as expected, and the formulas provide an extremely accurate value of conductivity.

3. SELF-CONSISTENT SOLUTION OF THE SCHRÖDINGER EQUATION

Here we must find a steady-state solution of Eq. (1) that is independent of the initial conditions and agrees with the given boundary conditions with allowance for a dynamic space charge. We assume that the solution of the unperturbed problem is known.

With the first-order perturbation theory for calculating the corrections to the ground-state wave function,

$$\psi_1(x,t)=\psi_+(x)e^{-i(\omega_0+\omega)t}+\psi_-(x)e^{-i(\omega_0-\omega)t},$$

the variation in the electron concentration has the form

$$\Delta n(x,t)=[\psi_0\psi_+^*+\psi_0^*\psi_-]e^{i\omega t}+[\psi_0^*\psi_++\psi_0\psi_-^*]e^{-i\omega t}$$
$$=2\Delta n(x)\cos[\omega t+\beta(x)]. \qquad (35)$$

Let us consider the case in which the potential energy $U(x)$ in the unperturbed Hamiltonian and the perturbation $V_\pm(x)$ vary considerably in the region $0<x<a$, with $U(x)=V_\pm(x)=0$.

Let $\xi_1(x),\ldots,\xi_L(x)$ be a complete set of functions over the interval $[0,a]$ for which the potential energies are known:

$$\varphi_m(x)=-\frac{q^2N}{\kappa}\int_0^x\int_0^{x'}\xi_m(x'')dx'dx''+G_m^1x+G_m^2,$$

where κ is the dielectric constant of the semiconductor, N is the normalization constant with dimensions of concentration, and the constants G_m^1 and G_m^2 are found for each specific case from the boundary conditions. The number L of basis functions employed is determined by the desired accuracy. Suppose that we know the particular solutions $\chi_\pm^m(x)$ of Eq. (3) at $V_\pm\frac{1}{2}\varphi_m(x)$, which means we know the corresponding corrections $\psi_\pm^m(x)$ to the wave functions and the solution of the problem for a uniform hf field, $\hat{V}=-qE_0x(e^{i\omega t}+e^{-i\omega t})$. In this case, each solution $\psi_\pm^m(x)$ corresponds to a definite variation of concentration, $\Delta n_m(x,t)=\Delta n_m(x)\cos[\omega t+\beta_m(x)]$, shifted in relation to the main signal by $\beta_m(x)$, a variation that can be represented as

$$\Delta n_m(x,t)=\sum_{k=1}^{L}n_m^k\xi_k(x)\cos(\omega t+\beta_m^k).$$

We have the following correspondence:

$$-qE_0x\cos\omega t\rightarrow\Delta n_0(x,t)=\sum_{k=1}^{L} n_0^k\xi_k(x)\cos(\omega t+l^k),$$

$$\varphi_1(x)\cos\omega t\rightarrow\Delta n_1(x,t)=\sum_{k=1}^{L} n_1^k\xi_k(x)\cos(\omega t+\beta_1^k),$$

$$\vdots$$

$$\varphi_L(x)\cos\omega t\rightarrow\Delta n_L(x,t)=\sum_{k=1}^{L} n_L^k\xi_k(x)\cos(\omega t+\beta_L^k). \tag{36}$$

Let a uniform electric field $E(t)=E_0\cos\omega t$ act on the interval $0<x<a$. This field changes the concentration by

$$\Delta n(x,t)=\sum_{k=1}^{L} n_0^k\xi_k(x)\cos(\omega t+l^k)+\sum_{k=1}^{L}\alpha_k\xi_k(x)\cos(\omega t+\gamma^k) \tag{37}$$

and brings about a corresponding change in the potential energy:

$$V(x,t)=-qE_0x\cos(\omega t)+\sum_{k=1}^{L}\alpha_k\varphi_k(x)\cos(\omega t+\gamma^k)+\sum_{k=1}^{L} n_0^k\varphi_k(x)\cos(\omega t+l^k). \tag{38}$$

On the other hand, this variation in potential energy corresponds to the following variation in concentration:

$$\Delta\tilde{n}(x,t)=\sum_{k=1}^{L} n_0^k\xi_k(x)\cos(\omega t+l^k)+\frac{1}{N}\sum_{k=1}^{L}\alpha_k\sum_{j=1}^{L} n_k^j\xi_j(x)\cos(\omega t+\gamma^k+\beta_k^j)+\frac{1}{N}\sum_{k=1}^{L} n_0^k\sum_{j=1}^{L} n_k^j\xi_j(x)\cos(\omega t+l^k+\beta_k^j). \tag{39}$$

To obtain a self-consistent equation we equate the right-hand sides of Eqs. (37) and (39). The result is

$$\sum_{k=1}^{L}\alpha_k\xi_k(x)\cos(\omega t+\gamma^k)=\frac{1}{N}\sum_{k=1}^{L}\alpha_k\sum_{j=1}^{L} n_k^j\xi_j(x)\cos(\omega t+\gamma^k+\beta_k^j)+\frac{1}{N}\sum_{k=1}^{L} n_0^k\sum_{j=1}^{L} n_k^j\xi_j(x)\cos(\omega t+l^k+\beta_k^j). \tag{40}$$

Equation (40) must hold for each coordinate at every point, so that it splits into a system of L equations:

$$\alpha_1\cos(\omega t+\gamma^1)=\sum_{k=1}^{L}\frac{\alpha_k n_k^1}{N}\cos(\omega t+\gamma^k+\beta_k^1)+\sum_{k=1}^{L}\frac{n_0^k n_k^1}{N}\cos(\omega t+l^k+\beta_k^1),$$

$$\alpha_2\cos(\omega t+\gamma^2)=\sum_{k=1}^{L}\frac{\alpha_k n_k^2}{N}\cos(\omega t+\gamma^k+\beta_k^2)+\sum_{k=1}^{L}\frac{n_0^k n_k^2}{N}\cos(\omega t+l^k+\beta_k^2), \tag{41}$$

$$\vdots$$

$$\alpha_L\cos(\omega t+\gamma^L)=\sum_{k=1}^{L}\frac{\alpha_k n_k^L}{N}\cos(\omega t+\gamma^k+\beta_k^L)+\sum_{k=1}^{L}\frac{n_0^k n_k^L}{N}\cos(\omega t+l^k+\beta_k^L).$$

Each equation in (41) must hold at any moment in time, so it splits into two equations each of which contains terms only with $\cos(\omega t)$ or only with $\sin(\omega t)$. After determining the values of α_i and γ^i from the $2L$ equations we can use (38) to find the potential at $x=a$, and then find the corresponding perturbed wave functions.

Let us examine the simplest case, in which only one basis function ξ_1 ($L=1$) is needed to describe the space charge. (Note that usually this approximation is sure to be invalid for conductivities $|\sigma|\gg\omega\kappa$, when the space charge has a strong effect on electron dynamics.) Then the system (41) becomes

$$\alpha_1\cos(\omega t+\gamma^1)=\frac{\alpha_1 n_1^1}{N}\cos(\omega t+\gamma^1+\beta_1^1)+\frac{n_0^1 n_1^1}{N}\times\cos(\omega t+l^k+\beta_1^1). \tag{42}$$

By equating the coefficients of $\cos(\omega t)$ and of $\sin(\omega t)$, we arrive at the following expressions for the coefficients α_1 and γ_1:

$$\cot\gamma^1=\frac{N\cot(l^1+\beta_1^1)-n_1^1[\cot(l^1+\beta_1^1)\cos\beta_1^1+\sin\beta_1^1]}{N+n_1^1[\cot(l^1+\beta_1^1)\sin\beta_1^1-\cos\beta_1^1]},$$

$$\alpha_1=\frac{n_0^1 n_1^1\cos(l^1+\beta_1^1)}{N\cos\gamma^1-n_1^1\cos(\beta_1^1+\gamma^1)}. \tag{43}$$

We can now use (37) to find $\Delta n(x,t)$, and then determine the perturbed part of the system's wave function $\psi_\pm=\psi_\pm(E_0)+\psi_\pm[\varphi_1(\Delta n(x,t))]$.

3.1. Space charge in transit sections and double-barrier structures

We demonstrate the application of the method by studying the simple examples of a short transit section with a localized hf field and a double-barrier of width a with thin (delta-like) barriers, assuming that $\Delta n(x,t)=\Delta\, n(x)\cos(\omega t+\zeta)$ ($L=1$) and that the dynamic space charge is independent of the coordinates ($\Delta n(x)=\Delta n=\text{const}$). In this case it is convenient to calculate the concentration variation using the current flowing

across the boundaries of the structure, $j(0,t)$ and $j(a,t)$, instead of Eq. (35). Indeed, $qa(\partial\Delta n/\partial t)=j(0,t)-j(a,t)$, so that

$$\Delta n\cos(\omega t+\zeta)=\frac{1}{qa\omega}\{|j(0)|\sin[\omega t+\zeta(0)] -|j(a)|\sin[\omega t+\zeta(a)]\}. \quad (44)$$

Note that the approximation $\Delta n(x)=\Delta n=\text{const}$ is inapplicable when $\Delta n(x)$ changes sign along the structure's length (this is possible when the structure is much longer than one-half of the electron's wavelength).

Calculations of the passage of electrons through a transit section and a double-barrier structure in hf fields has been described in detail in Ref. 16 and 19, so that here we discuss only the features related to the space charge. Allowing for the symmetry of the structure and perturbation, we get

$$\varphi_1(x)=-\frac{q^2\Delta n}{2\kappa}(ax-x^2). \quad (45)$$

When $0<x<a$ the particular solutions of Eq. (3) for such structures at $V_\pm=-qEx$ have the form (24), while at $V_\pm(x)=-q^2\Delta n x^2/2\kappa=Vx^2$ they have form

$$\chi_\pm=\pm\frac{Vx^2}{\hbar\omega}\psi_0-\frac{2Vx}{m^*\omega^2}\psi_0^1-\frac{V}{m^*\omega^2}\left(1\pm\frac{4\omega_0}{\omega}\right)\psi_0. \quad (46)$$

For different forms of the potential we have the following correspondence:

$$-qE_0x\cos\omega t\rightarrow n_0^1\cos(\omega t+l^1),$$

$$-\frac{q^2N}{2\kappa}(ax-x^2)\cos\omega t\rightarrow n_1^1\cos(\omega t+\beta_1^1), \quad (47)$$

from which, combining (43) and (37), we find the variation of the electron concentration and the correction to the system's wave function.

Figure 6 depicts the frequency dependence of the active conductivity Re σ_i of a gallium arsenide transit section of length $a=100$ Å calculated for different electron concentrations at an electron energy $\varepsilon=20$ meV. The results imply that allowing for a space charge at this electron energy changes the sign of Re σ_i at low frequencies, and the higher the electron concentration, the greater the frequency at which negative dynamic conductivity appears. Note that as assumed in Ref. 19, allowing for a space charge removes the divergence in Re σ_i when $\omega\rightarrow\omega_0$. Here the lower the electron concentration, the larger the value of $|\text{Re }\sigma_i|$.

Figure 7 depicts the results of calculating Re $\sigma_i(\omega)$ for a double-barrier GaAs/AlGaAs structure with barrier height $\varphi_b=1.04$ eV, barrier width $b=11$ Å, and distance between barriers $a=65$ Å (the first resonant level is at $\mathcal{E}_1\approx 101$ meV) for different electron energies. The electron concentration in the flux of monoenergetic electrons passing through the structure is $n=10^{17}$ cm^{-3}. We see that the field of the electron space charge can have a strong effect on the interaction of the electrons and the hf field, changing Re σ_i and lowering the upper frequency at which negative dynamic conductivity still exists. Figure 8 depicts the frequency dependence of Re σ_i for different electron concentrations. We

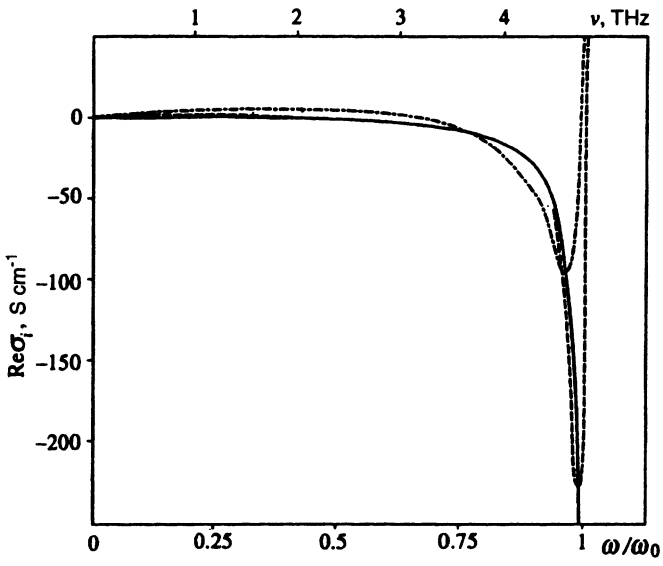

FIG. 6. Dependence on the normalized frequency ω/ω_0 of the active conductivity of a transit section of length $a=100$ Å with a localized hf field ($\omega_0=\varepsilon_0/\hbar$, with $\varepsilon_0=20$ meV). Calculations without a space charge (solid curve) were done for an electron concentration $n=5\times10^{17}$ cm^{-3}. Calculations with a space charge were done for $n=5\times10^{17}$ cm^{-3} (dashed curve) and $n=10^{18}$ cm^{-3} (dot-dash curve).

see that here an increase in electron concentration, and hence an increase in the space-charge effect, lead to a change in the frequency at which the active conductivity is at its maximum: for Re $\sigma_i>0$ this frequency rises, while for Re $\sigma_i<0$ it falls.

3.2. Effect of a dynamic space charge on resonant interaction with the hf field in double-barrier structures

As noted earlier, the approximation $\Delta n(x)=\text{const}$ works if a concentration perturbation does not change the sign

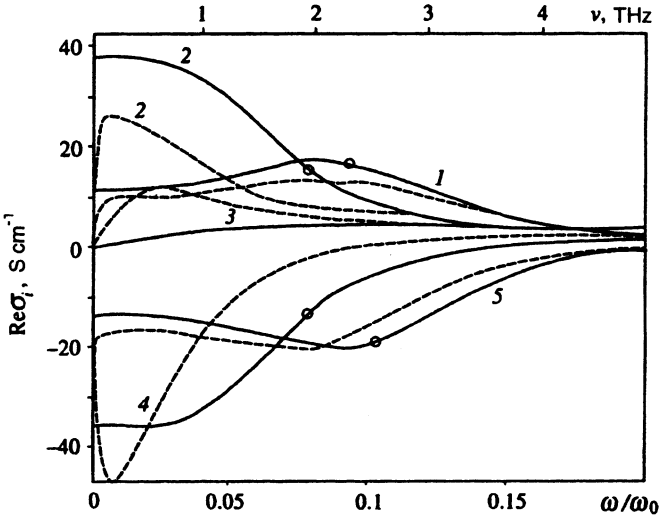

FIG. 7. Dependence of the active conductivity of a double-barrier structure on the normalized frequency $\omega/\omega_0(\omega_0=\varepsilon_0/\hbar)$. The solid curves represent calculations without a space charge, and the dashed curves calculations with a space charge. Electron energies: curve *1*—$\varepsilon=0.90\mathcal{E}_1$, curve *2*—$\varepsilon=0.95\mathcal{E}_1$, curve *3*—$\varepsilon=\mathcal{E}_1$, curve *4*—$\varepsilon=1.05\mathcal{E}_1$, and curve *5*—$\varepsilon=1.1\mathcal{E}_1$ (the first resonant level is at $\mathcal{E}_1=\varepsilon_0\approx 101$ meV).

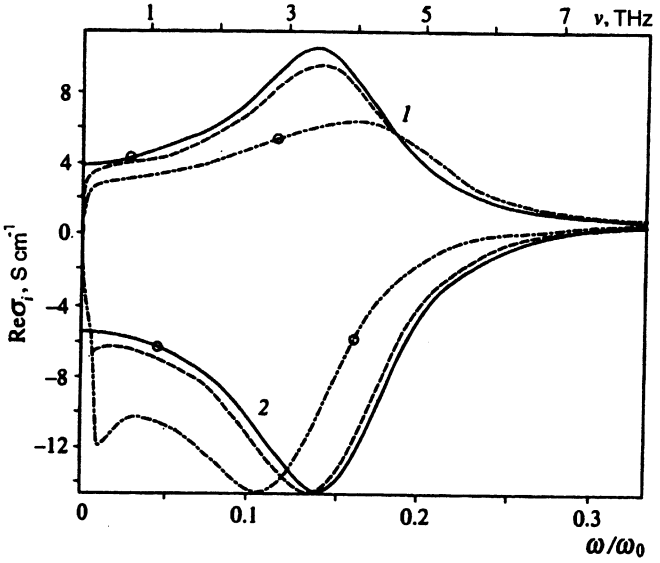

FIG. 8. Dependence of the active conductivity of a double-barrier structure on the normalized frequency $\omega/\omega_0(\omega_0=\varepsilon_0/\hbar)$. Calculations without a space charge for an electron concentration $n=10^{17}$ cm^{-3} are represented by the solid curves. Calculations with a space charge: $n=10^{17}$ cm^{-3} (dashed curves), and $n=5\times10^{17}$ cm^{-3} (dot-dash curves); for convenience Re $\bar{\sigma}=$Re $\sigma_i/5$ is also shown. Electron energies: curves *1*—$\varepsilon=0.85\mathscr{E}_1$, and curve *2*—$\varepsilon=1.15\mathscr{E}_1$ (the first resonant level is at $\mathscr{E}_1\approx101$ meV).

along the length of the structure. As applied to a double-barrier resonant-tunneling structure, this means that all the electrons, those that have interacted with the hf field and those that have not, pass near the first resonant level. For this reason the approximation is inapplicable in one of the most interesting cases, the resonant interaction of the electrons in the double-barrier structure and the hf field. But for a structure with thin and fairly tall barriers the problem of the effect of a space charge on the resonant interaction of electrons and the hf field allows for a rigorous analytic solution. Let us discuss this problem in greater detail.

The active conductivity Re σ_i of a quantum-size structure (determined by the ratio of probabilities of absorption and emission of a quantum $\hbar\omega$ by an electron) and the density $j(a)$ of the current exiting the structure with the wave functions (4) and (5) are described by Eqs. (7) and (11). Comparison of these equations with allowance for Eqs. (31) and (32) shows that in a double-barrier structure with resonant transitions between the narrow levels the induced current, which determines the active conductivity, is much higher than the current flowing across the boundaries of the structure (Re $\sigma_i\propto y^4$ and $j\propto y^2$). The space charge outside the double-barrier structure therefore has no significant effect on the resonant interaction of electrons and the hf field.

In studying the effect of a spatial charge on the resonant interaction of the electrons and the hf field, we restrict our discussion, to simplify calculations, to transitions from the second to the first resonant level ($K=2$ and $M=1$). Then for the wave function (26) we have

$$B_-(E)\approx D_-(E)\approx C_-(E)\approx\frac{qEy^2}{im^*\omega^2k_-}\sqrt{n}, \tag{48}$$

$$A_-(E)\approx\frac{qEy^3}{im^*\omega^2k_-^2}\sqrt{n}. \tag{49}$$

Substituting these equations into (26) and leaving only terms in the highest power of y, from (35) we get

$$\Delta n(E)\approx\frac{2qEy^4n}{m^*\omega^2k_-^2k}\sin(\omega t)\sin(kx)\sin(k_-x). \tag{50}$$

According to this relation, the perturbation of the electron concentration does indeed change sign along the length of the structure and, since $q<0$, lags behind the variation of the field by $\frac{3}{2}\pi(l^1=-\frac{3}{2}\pi)$ and behind the variation of the potential by $\frac{1}{2}12\pi$.

For variations of concentration of the form $N\sin(kx)\sin(k_-x)$ and with allowance for the fact that the field of the space charge is weak at the boundaries of the structure (in contrast to the two cases considered earlier), the potential is

$$\varphi(x)=\frac{qN}{\kappa}\left\{\frac{\cos[(k-k_-)x]}{2(k-k_-)^2}-\frac{\cos[(k+k_-)x]}{2(k+k_-)^2}-\frac{2kk_-}{(k-k_-)^2(k+k_-)^2}\right\}. \tag{51}$$

The sine and cosine expansions of the functions $\psi_0[(k-k_-)x]$ and $\psi_0\cos[(k+k_-)x]$ contain terms with the wave vector k_- that is the characteristic number of Eq. (3) for the given structure.[21] Since $k\approx2k_-$ and $\omega\approx\frac{3}{4}\omega_0$ in structures with thin and tall barriers ($k\ll y$) involved in resonant transitions from the second level to the first, here the perturbation $V_-(x)=q\varphi(x)$ can be represented as

$$V_-(x)\approx V\left[\frac{\cos(k_-x)}{2}-\frac{\cos(3k_-x)}{18}-\frac{4}{9}\right]. \tag{52}$$

Substituting (59) into (3) and allowing for the fact that for the given stricture k_- is a characteristic number of Eq. (3), we find the particular solution of Eq. (3):

$$\chi_-=-\frac{4V}{9\hbar\omega}\psi_0-\frac{V}{\hbar\omega_0}\{\psi_0kx\sin(k_-x)+x\psi_0'\cos(k_-x)+\psi_0\cos(k_-x)\}-\frac{V}{36\hbar\omega_0}\left\{\psi_0kx\sin(3k_-x)+x\psi_0'\cos(3k_-x)+\frac{1}{3}\psi_0\cos(3k_-x)\right\}, \tag{53}$$

from which, calculating the function f in (27), we obtain

$$D_-(V)\approx C_-(V)\approx\frac{5Vay^2}{48ik_-\hbar\omega}\sqrt{n}, \tag{54}$$

$$A_-(V)\approx\frac{5Vay^3}{48ik_-^2\hbar\omega}\sqrt{n}. \tag{55}$$

For the variation of the electron concentration (35) with allowance for (26), (29), (54), and (55) we obtain

$$\Delta n(V)\approx\frac{5aVy^4n}{24\hbar\omega k_-^2k}\sin(\omega t)\sin(kx)\sin(k_-x). \tag{56}$$

We see that the variation of the electron concentration caused by the potential of the space charge lags behind the potential of the space charge ($\beta_1^1 = -\frac{1}{2}\pi$) by $\frac{1}{2}\pi$ and has the same form as the variation of the concentration associated with a uniform electric field. Hence, using only one basis function, $\xi_1(x) = \sin(kx)\sin(k_-x)$, for an accurate description of the variation of the concentration proves sufficient in such a structure with resonant interaction of the electrons and the hf field and with $k \ll y$. Here for the coefficients n_0^1 and n_1^1 in (42) we have

$$n_0^1 = -\frac{qEy^4 n}{m^*\omega^2 k_-^2 k}, \quad n_1^1 = \frac{5q^2 N a y^4 n}{48\kappa\hbar\omega k_-^4 k}. \tag{57}$$

Combining (42) and the relations $l^1 = -3/2\pi$ and $\beta_1^1 = -1/2\pi$, we obtain

$$\tan\gamma^1 = -\frac{n_1^1}{N}, \quad \alpha_1 = \frac{n_0^1 n_1^1}{N}\cos\gamma^1. \tag{58}$$

For further calculations it proves convenient to introduce the complex-valued charge and potential:

$$n(t) = (N_x + iN_y)e^{i\omega t} + \text{c.c.}, \tag{59}$$

$$\varphi(a,t) = [\varphi_x(a) + i\varphi_y(a)]e^{i\omega t} + \text{c.c.} \tag{60}$$

In this case

$$N_x = \alpha_1\cos\gamma^1, \tag{61}$$

$$N_y = n_0^1 + \alpha_1\sin\gamma^1, \tag{62}$$

$$\varphi(a) = \varphi(E) + \varphi(N_x) + i\varphi(N_y), \tag{63}$$

which when combined with the form (51) of $\varphi(N)$ and (52) yield

$$\varphi_x = -aE - \frac{8q}{9\kappa k_-^2}N_x, \tag{64}$$

$$\varphi_y = -\frac{8q}{9\kappa k_-^2}N_y. \tag{65}$$

As in (63), for the constant C_- in (26) we can write

$$C_- = C_-(E) + C_-(V(N_x)) + iC_-(V(N_y)). \tag{66}$$

Next, substituting (48) and (54) into (66), allowing for (61), (62), and (57), and introducing the notation (see (33))

$$\sigma_E = -\frac{16q^2 m^* \alpha^4 n}{\pi\hbar^6\omega^3}, \quad \zeta = \frac{|\sigma_E|}{\kappa\omega}, \quad \eta = \frac{45\pi^2}{256}, \tag{67}$$

we obtain

$$C_- = C_-(E)\left(\frac{1}{1+\eta^2\zeta^2} - i\frac{\eta\zeta}{1+\eta^2\zeta^2}\right), \tag{68}$$

$$\varphi = -aE\left(\frac{1+(\eta^2-\eta)\zeta^2}{1+\eta^2\zeta^2} - i\frac{\zeta}{1+\eta^2\zeta^2}\right). \tag{69}$$

Generally, in calculations involving a space charge one should use not the specific active conductivity Re σ_i as related to the amplitude of the variable field, Re $\sigma_i = 2W/aE^2$, but the specific active conductivity $G = 2W/U^2$ as related to the amplitude of the variable voltage U applied to the structure (here W is the power imparted to the electrons by the hf field or imparted by the electrons to the hf field), although here we can also formally introduce the average field $E = U/a$, and Re $\sigma_i = aG$. Hence, combining (68) and (69) and allowing for the fact that $|C_-| = |D_-|$, we find that

$$G = \frac{\sigma_E}{a}\frac{1+\eta^2\zeta^2}{1+(1+2\eta^2-2\eta)\zeta^2+\eta^2(1-\eta)^2\zeta^4}, \tag{70}$$

or

$$G = -\frac{\omega\kappa}{a}\frac{\zeta+\eta^2\zeta^3}{1+(1+2\eta^2-2\eta)\zeta^2+\eta^2(1-\eta)^2\zeta^4}$$

$$\approx -\frac{\omega\kappa}{a}\frac{\zeta+3.01\zeta^3}{1+3.55\zeta^2+1.62\zeta^4} = -\frac{\omega\kappa}{a}F(\zeta). \tag{71}$$

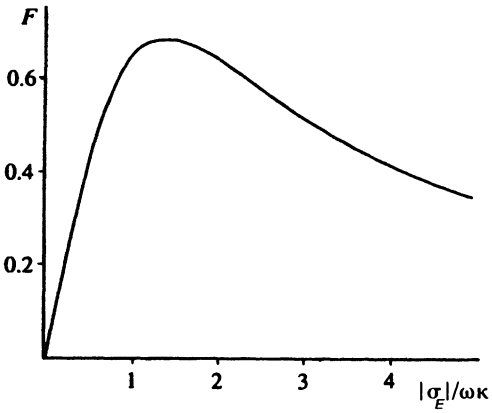

FIG. 9. F vs $|\sigma_E|/\omega\kappa$ for electron transitions from the second resonant level to the first.

Figure 9 depicts F as a function of $|\sigma_E|/\omega\kappa$. We see that the active conductivity of a double-barrier structure with resonant transitions from the second level to the first has a maximum $|G_{\max}| \approx 0.68\omega\kappa/a$ at $|\sigma_E| = 1.36\omega\kappa$. For $|\sigma_E|/\omega\kappa < 0.7$ the space charge has a small effect on the probability of such transitions. As parameter $|\sigma_E|/\omega\kappa$ grows, the space charge first limits the transition probability and then drives it down.

4. SOLVING THE SCHRÖDINGER EQUATION FOR AN HF FIELD OF ARBITRARY AMPLITUDE

The linearly independent solutions of the time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2} - U\psi\cos\omega t, \tag{72}$$

with $U = \text{const}$ are given by the wave functions[11]

$$\psi(x,t,\omega_0) = \exp\left(\pm ikx - i\omega_0 t + \frac{iU}{\hbar\omega}\sin\omega t\right). \tag{73}$$

When electrons travel through the barrier-free section with a localized uniform hf field ($\psi_0(x,t) = \exp(ikx - i\omega_0 t)$), to within second-order terms the electron wave function (24) is

$$\psi(x,t)=\psi_0(x,t)\left[1+\frac{2iqEx}{\hbar\omega}\sin\omega t+\frac{2iqEk}{m^*\omega^2}\cos\omega t\right]. \tag{74}$$

We can assume that the exact solution of the equation

$$i\hbar\frac{\partial}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2}-qEx\psi\cos\omega t \tag{75}$$

can be represented as follows:

$$\psi(x,t)=\psi_0(x,t)\exp\left[\frac{iqEx}{\hbar\omega}\sin\omega t+\frac{iqEk}{m^*\omega^2}\cos\omega t+f(t)\right], \tag{76}$$

where for the time being $f(t)$ is an unknown function. Substituting (76) into (75) and equating the left- and right-hand sides, we get

$$\psi(x,t)=\exp\left[ikx-i\omega_0 t+\frac{iqEx}{\hbar\omega}\sin\omega t-\frac{iqEk}{m^*\omega^2}\cos\omega t-\frac{i(qE)^2}{4m^*\hbar\omega^3}\left(\omega t-\frac{\sin 2\omega t}{2}\right)\right]. \tag{77}$$

The second linearly independent solution of Eq. (75) can be obtained from (77) by substituting $-k$ for k.

When electrons travel through triangular potential barriers or other regions with a static uniform field such that the coordinate part of a periodic perturbation has the form $V_{\pm}(x)=Vx^n$, the particular solution of Eq. (3) can be found in the form of power series.[16] But in the case of a uniform hf field it is more convenient to obtain this solution from the exact solution of the Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2}-qE_0x\psi-qEx\psi\cos\omega t. \tag{78}$$

As in the previous case, if we take advantage of the properties of the Airy functions[22] $\mathrm{Ai}(x)$, we can look for a solution in the form

$$\psi(x,t)=\mathrm{Ai}[-\xi+\beta(t)]\exp\left[-i\omega_0 t+\frac{iqEx}{\hbar\omega}\sin\omega t+f(t)\right], \tag{79}$$

where $\xi=(2m^*qE_0/\hbar^2)^{1/3}(x+\varepsilon/qE_0)$ (see Ref. 1, Chap. III), and the functions $\beta(t)$ and $f(t)$ are yet to be found. Substituting (79) into (78) and equating the left- and right-hand sides, we get

$$\beta(t)=-\left(\frac{2m^*qE_0}{\hbar^2}\right)^{1/3}\frac{qE}{m^*\omega^2}\cos\omega t, \tag{80}$$

$$f(t)=-\frac{iq^2EE_0}{m^*\hbar\omega^3}\sin\omega t-\frac{i(qE)^2}{4m^*\hbar\omega^3}\left(\omega t-\frac{\sin 2\omega t}{2}\right). \tag{81}$$

The final result is

$$\psi(x,t)=\mathrm{Ai}\left[-\left(\frac{2m^*qE_0}{\hbar^2}\right)^{1/3}\left(x+\frac{\varepsilon}{qE_0}+\frac{qE}{m^*\omega^2}\cos\omega t\right)\right]\times\exp\left[-i\omega_0 t+\frac{iqEx}{\hbar\omega}\sin\omega t-\frac{iq^2EE_0}{m^*\hbar\omega^3}\sin\omega t-\frac{i(qE)^2}{4m^*\hbar\omega^3}\left(\omega t-\frac{\sin 2\omega t}{2}\right)\right]. \tag{82}$$

The second linearly independent solution of Eq. (78) can be found from (82) by substituting Bi for Ai (see Ref. 22). Expanding (82) in a power series in the small parameter, we arrive at the solution of Eq. (3) at $\psi_0=\mathrm{Ai}(\xi)$:

$$\psi_{\pm}=\mp\left(\frac{qEx}{\hbar\omega}-\frac{q^2EE_0}{m^*\hbar\omega^3}\right)\mathrm{Ai}\left[-\left(\frac{2m^*qE_0}{\hbar^2}\right)^{1/3}\left(x+\frac{\varepsilon}{qE_0}\right)\right]-\left(\frac{2m^*qE_0}{\hbar^2}\right)^{1/3}\left(\frac{qE}{m^*\omega^2}\right)\mathrm{Ai}'\left[-\left(\frac{2m^*qE_0}{\hbar^2}\right)^{1/3}\times\left(x+\frac{\varepsilon}{qE_0}\right)\right]. \tag{83}$$

The wave functions (73), (77), and (82) make it possible to solve rather simply the problem of electron passage through systems of rectangular and triangular wells and barriers in a strong uniform variable field. Suppose that a uniform hf field is localized in the region $0<x<a$. There can either be no constant field in this region (the transit section, rectangular barrier or well), or such a field may be present (the transit section with the field, a triangular barrier or well), and electrons with energy $\varepsilon=\hbar\omega_0$ move from left to right. Then the wave function at $x<0$ consists of a set of plane waves:

$$\psi_1(x,t,\varepsilon)=\exp(ikx-i\omega_0 t)+\sum_{j=-\infty}^{\infty}D_j\exp[ik_jx-i(\omega_0+j\omega)t]. \tag{84}$$

At $x>0$ the wave functions have the form

$$\psi_3(x,t,\varepsilon)=\sum_{j=-\infty}^{\infty}C_j\psi_U(x,t,\omega_0+j\omega), \tag{85}$$

where the ψ_U are the solutions of Eq. (72) at $U=qEa$. Finally, at $0<x<a$ we have

$$\psi_2(x,t,\varepsilon)=\sum_{j=-\infty}^{\infty}A_j\psi_{E1}(x,t,\tilde{\omega}_0+j\omega)+B_j\psi_{E2}(x,t,\tilde{\omega}_0+j\omega), \tag{86}$$

where ψ_{E1} and ψ_{E2} are the corresponding linearly independent solutions of Eq. (75) or (78), and $\tilde{\omega}_0=\omega_0-(qE)^2/4m^*\hbar\omega^2$.

In Eqs. (84)–(86) the index j formally runs through all values from $-\infty$ to $+\infty$, but it is obvious that starting with a certain number n depending on the amplitude of the hf field, multiphoton processes in which the number of participating photons is greater than n have a low probability of occurrence.

Here is a simple estimate:

$$\psi_U(x,t,\omega_0)=\psi_0(x,t)\exp\left(\frac{iqEa}{\hbar\omega}\sin\omega t\right), \tag{87}$$

$$\exp\left(\frac{iqEa}{\hbar\omega}\sin\omega t\right)=\sum_{-\infty}^{\infty}\left(\frac{iqEa}{\hbar\omega}\right)^n\frac{1}{n!}\left(\frac{e^{i\omega t}-e^{-i\omega t}}{2i}\right)^n. \tag{88}$$

Since in factorizing $[(e^{i\omega t}-e^{-i\omega t})/2i]^n$ the terms with the maximum frequency have the form $e^{in\omega t}/(2i)^n$ and $e^{-in\omega t}/(2i)^n$, it is obvious that for $(qEa/2\hbar\omega)^n/n!\ll 1$, terms with $|j|>n$ can be ignored in (85). Similar estimates can be made for (77) and (82). Hence, depending on the required accuracy of the solution, the number of terms in Eqs. (84)–(86) can always be kept finite.

The matching conditions imposed on the wave functions at the boundaries of the region lead to the following system of equations:

$$\begin{aligned}
&\psi_1(0,t,\varepsilon)=\psi_2(0,t,\varepsilon),\\
&\frac{\partial}{\partial x}\psi_1(0,t,\varepsilon)=\frac{\partial}{\partial x}\psi_2(0,t,\varepsilon),\\
&\psi_2(a,t,\varepsilon)=\psi_3(a,t,\varepsilon),\\
&\frac{\partial}{\partial x}\psi_2(a,t,\varepsilon)=\frac{\partial}{\partial x}\psi_3(a,t,\varepsilon),
\end{aligned} \tag{89}$$

which must hold at all times. The solution of this system yields the desired wave function describing the passage of electrons through a given structure.

There are at least three ways of solving the system of equations (89).

(1) Functions are equal if all the corresponding Fourier components are. Expanding the functions ψ_2 and ψ_3 in an appropriate way, we can reduce (89) to a system of linear equations for the coefficients A_j, B_j, C_j, and D_j and solve the new system with the required accuracy. However, while for functions like (73) the Fourier expansions exist in a convenient form,[11] for functions like (77) or (82) these expansions have apparently yet to be found.

(2) Functions are equal if at a certain moment all their time derivatives are. Differentiating the system (89) the required number of times at an arbitrary moment, we arrive at a system of linear equations for the coefficients A_j, B_j, C_j, and D_j.

(3) However, the simplest way to solve the system (89) is to employ the requirement that the equations in the system be valid at all times. Partitioning the period $T=2\pi/\omega$ into M intervals, with M determined by the required accuracy, and calculating the functions in (89) at each moment $t=Ts/M$ $(s=0,1,\ldots,M-1)$, we can reduce (89) to a system of linear equations for the coefficients A_j, B_j, C_j, and D_j.

The problem for structures consisting of an arbitrary number of rectangular and triangular wells and barriers can be solved in a similar way.

5. CONCLUSIONS

We have developed simple methods for obtaining the solutions of the time-dependent Schrödinger equation, which describes the passage of electrons through quantum-size structures in weak hf fields both with and without a dynamical space charge. For an example illustrating the use of the theory we obtained analytic expressions for the hf current and the energy transferred by electrons to the field during their passage through a jump in the potential that varies periodically with time, through thin barriers, and through the resonant levels of double-barrier structures. We demonstrated the negative dynamic conductivity of a potential jump and of the thin potential barriers, and the localization of electrons in the regions with a hf field.

We studied the resonant interaction of electrons and the hf field in the passage of electrons through rectangular potential barriers, and double-barrier structures. We showed that the probability of interaction increases sharply at frequencies corresponding to transitions to the range of energies at which the transmission coefficient is at its maximum.

We investigated the effect of dynamic space charge on the passage of electrons through the transit sections and double-barrier structures. We found analytic solution of the self-consistent time-dependent Schrödinger and Poisson equations describing the resonant interaction of the electrons and the hf field in double-barrier structures. We showed that in such structures, a dynamic space charge limits the probability of resonant interaction of the electrons and the hf field.

Finally, we found exact steady-state solutions of the time-dependent Schrödinger equation in free space in a strong uniform hf field, in the absence of a constant electric field and in the presence of such a field. We developed a method of solving for the passage of electrons through systems of rectangular and triangular wells and barriers in a uniform hf field of arbitrary amplitude.

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