Electron scattering in a zero-gap semiconductor

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A theory is developed for scattering, by a spherically symmetric potential, of electrons in a zero-gap semiconductor having a spectrum described by a Luttinger Hamiltonian. An exact solution of the scattering problem is obtained in the approximation $\beta = m_e/m_h \ll 1$ (m_e and m_h are the electron and hole masses) in the case of potentials $V(r) = U$ at $r < a$ and $V(r) = 0$ at $r > a$. It is shown that the results of the usual scattering theory do not hold in a wide range of incident-electron energies. The positions and widths of the quasilocal hole levels against the background of the conduction band are obtained for the potential well.

1. INTRODUCTION

The theory of kinetic effects in a zero-gap semiconductor is based as a rule on the Born approximation.[1] It will be shown here, however, that in this case the condition for the validity of the Born approximation is quite restricted. The reason is that, as a rule, the masses of the electrons and holes in a zero-gap semiconductor differ greatly. In HgTe, for example, the ratio of the electron and hole masses is $\beta = m_e/m_h \approx 0.06$ (Ref. 2). The energy dependence of the cross section for scattering of slow electrons is therefore by far not the same as in ordinary scattering theory, and this dependence cannot be described in the Born approximation (see Sec. 3).

We propose in this paper an exact solution of the problem of a spherically symmetric square potential well (or hump) within the framework of the Luttinger spherical Hamiltonian. To our knowledge this is the first case in which the Luttinger Hamiltonian could be diagonalized analytically and the wave functions of the quasilocal states could be obtained. The solution permits an analysis of the scattering phase shifts at all values of the energy and of the various parameters of the potential well. Moreover, it provides an idea of the character of scattering by a large class of potentials that can be roughly approximated by square wells or barriers. We consider this to be the main task of this paper.

To find the scattering amplitude we need a partial-wave method, which has not been developed for a zero-gap semiconductor, although it was found[3] for the valence band of a Ge-type band.[1)]

The specific feature of a zero-gap semiconductor is resonant scattering of electrons by quasilocal levels. The cross section for this scattering is determined by the level width. The width of the lowest level was obtained for the case of a Coulomb center by computer calculations in Ref. 4. In the present paper the widths and positions of the resonances were analyzed as functions of the well parameters (Sec. 4).

2. METHOD OF PARTIAL WAVES

The spectrum of a zero-gap semiconductor is described by the Luttinger Hamiltonian. The Schrödinger equation in an external potential is

$$\frac{1}{2m_0}\left[\left(\gamma_1+\frac{5}{2}\gamma\right)\hat{\mathbf{p}}^2-2\gamma(\hat{\mathbf{p}}\hat{\mathbf{J}})^2\right]\Psi+V(\mathbf{r})\Psi=E\Psi, \tag{2.1}$$

where $\hat{\mathbf{p}} = -i\hbar\nabla$; $\hat{\mathbf{J}}$ is the angular-momentum operator with value 3/2 (its projections are 4×4 matrices); Ψ is a four-component wave function; γ_1 and γ are the Luttinger parameters.

The Luttinger Hamiltonian commutes with the total-angular-momentum operator $\hat{\mathbf{F}} = \hat{\mathbf{L}} + \hat{\mathbf{J}}$, were $\hat{\mathbf{L}}$ is the orbital-momentum operator. In a centrosymmetric potential the wave functions are classified in accordance with the total angular momentum F and its projection M. The operator $\hat{\mathbf{L}}$ does not commute with the Hamiltonian, so that a wave function with fixed values of F and M is a superposition of four states with different l from $F-3/2$ to $F+3/2$. In addition, the parity operator $\hat{\mathbf{I}}$ commutes with the Hamiltonian. At a given parity I, this superposition contains only a pair of values of l of like parity. The general solution of (2.1) is

$$\Psi(r,\theta,\varphi)=\sum_{F,M,I}B_{FMI}R_{Fl_I}(r)\Psi_{FMl_I}, \tag{2.2}$$

where B_{FMI} are the expansion coefficients. The values of l_I are $F-3/2$ and $F+1/2$ for one parity and $F-1/2$ and $F+3/2$ for the other. The angle function is

$$\Psi_{FMl_I}=(2F+1)^{1/2}\sum_{m,\mu'}(-1)^{l_I+M-1/2}\times\begin{pmatrix} l_I & 3/2 & F\\ m & \mu' & -M\end{pmatrix}Y_{l_Im}(\theta,\varphi)\chi_z(\mu'). \tag{2.3}$$

Here $\chi_z(\mu)$ is an eigenvector of the matrix J_z: $\hat{J}_z\chi_z(\mu)=\mu\chi_z(\mu)$; The index μ takes on values $\pm 3/2$ and $\pm 1/2$, and the Wigner $3j$ symbols and the spherical functions are defined in the same manner as in Ref. 5. The radial functions R_{Fl_I} are defined for each parity value by a system of two equations[4]:

$$\begin{aligned}&(\gamma_1-2\gamma\cos\alpha_F)P_F^{+}P_FR_{F,F+1/2}+2\gamma\sin\alpha_FP_F^{+}P_{-F}R_{F,F-1/2}\\&\quad+(2m_0/\hbar^2)(E-V)R_{F,F+1/2}=0,\\&(\gamma_1+2\gamma\cos\alpha_F)P_{-F}^{+}P_{-F}R_{F,F-1/2}+2\gamma\sin\alpha_FP_{-F}^{+}P_FR_{F,F+1/2}\\&\quad+(2m_0/\hbar^2)(E-V)R_{F,F-1/2}=0;\end{aligned} \tag{2.4}$$

$$\begin{aligned}&(\gamma_1-2\gamma\cos\tilde{\alpha}_F)P_{F+1}^{+}P_{F+1}R_{F,F+1/2}+2\gamma\sin\tilde{\alpha}_FP_{F+1}^{+}P_{-(F+1)}R_{F,F-1/2}\\&\quad+(2m_0/\hbar^2)(E-V)R_{F,F+1/2}=0,\\&(\gamma_1+2\gamma\cos\tilde{\alpha}_F)P_{-(F+1)}^{+}P_{-(F+1)}R_{F,F-1/2}\\&\quad+2\gamma\sin\tilde{\alpha}_FP_{-(F+1)}^{+}P_{F+1}R_{F,F+1/2}\\&\quad+(2m_0/\hbar^2)(E-V)R_{F,F-1/2}=0,\end{aligned} \tag{2.5}$$

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where

$$P_F=\frac{d}{dr}+\frac{F+{}^3/_2}{r},\qquad P_F^+=\frac{d}{dr}-\frac{F-{}^1/_2}{r};$$

$$\cos\alpha_F=\frac{2F-3}{4F},\quad \cos\tilde{\alpha}_F=-\frac{2F+5}{4(F+1)};\quad \sin\alpha_F,\ \sin\tilde{\alpha}_F>0.$$

The asymptotic forms of the functions R as $r\to\infty$ and at $E>0$ are

$$R_{F,F-1/2}=\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{k_e r}\sin\left[k_e r-\frac{\pi}{2}\left(F-\frac{3}{2}\right)+\delta_{FI}\right],$$

$$R_{F,F+1/2}=\operatorname{tg}\frac{\alpha_F}{2}R_{F,F-1/2}, \tag{2.6}$$

$$R_{F,F-1/2}=\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{k_e r}\sin\left[k_e r-\frac{\pi}{2}\left(F-\frac{1}{2}\right)+\delta_{FI}\right],$$

$$R_{F,F+1/2}=\operatorname{tg}\frac{\tilde{\alpha}_F}{2}R_{F,F-1/2}, \tag{2.7}$$

where $k_e=(2m_eE/\hbar^{1/2})$, and $m_e=m_0/(\gamma_1+2\gamma)$ is the electron mass. To introduce the scattering amplitude we must subtract from the function $\Psi(r,\theta,\varphi)$ [Eq. (2.2)] the wave function of the incident electron

$$\exp(ik_e z)\chi_z(\mu)=\sum_{F,M,I,l_I}(-1)^{l_I+M-1/2}\pi[(2F+1)(2l_I+1)]^{1/2}\times\begin{pmatrix} l_I & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}\left(\frac{2}{k_e r}\right)^{1/2}J_{l_I+1/2}(k_e r)\Psi_{FMl_I}. \tag{2.8}$$

Here $\mu=\pm 1/2$, corresponding to the conduction band. This equation is transformed into the usual expansion of a plane wave in spherical functions if allowance is made for the summation formula[5]:

$$\sum_{F,M}(2F+1)\begin{pmatrix} l & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}\begin{pmatrix} l & {}^3/_2 & F\\ m & \mu' & -M\end{pmatrix}=\delta_{\mu\mu'}\delta_{m0}. \tag{2.9}$$

The coefficient B_{FMI} must be chosen such that as $r\to\infty$ the general solution (2.2) be a sum of the plane wave (2.8) and a scattered and diverging waves, i.e.,

$$\Psi-\exp(ik_e z)\chi_z(\mu)=\sum_{F,M,I}\sum_{l_I}\left[B_{FMI}R_{Fl_I}-(-1)^{l_I+M-1/2}\pi[(2F+1)(2l_I+1)]^{1/2}\times\begin{pmatrix} l_I & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}\left(\frac{2}{k_e r}\right)^{1/2}J_{l_I+1/2}(k_e r)\right]\Psi_{FMl_I}=f_\mu(\theta,\varphi)\frac{\exp(ik_e r)}{r}, \tag{2.10}$$

where $f_\mu(\theta,\varphi)$ is a four-component column. In the case of a simple band all the radial functions are independent, so that the converging wave can be eliminated by suitably chosen numerical coefficient in each radial function. The specific feature of the case considered is that two radial functions with specified values of F and I have one and the same numerical coefficient B_{FMI} whose choice must eliminate the convergent wave in the difference (2.10) simultaneously for two different values of l_I. Let us verify that this can be done, using as an example the parity I to which correspond $l_I=F-3/2$ and $F+1/2$. Using (2.6), we write down the coefficients of the converging wave in the difference with $l_I=F-3/2$ and in the difference with $l_I=F+1/2$ respectively as $r\to\infty$:

$$\left(\frac{2}{\pi}\right)^{1/2}\exp\left[i\frac{\pi}{2}(F-{}^3/_2)-i\delta_{FI}\right]\times B_{FMI}-(-1)^{F+M-3}\pi[(2F+1)(2F-2)]^{1/2}\times\exp\left[i\frac{\pi}{2}(F-{}^3/_2)\right]\frac{2}{\sqrt{\pi}}\begin{pmatrix} F-{}^3/_2 & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix},$$

$$\left(\frac{2}{\pi}\right)^{1/2}\exp\left[i\frac{\pi}{2}(F-{}^3/_2)-i\delta_{FI}\right]B_{FMI}\operatorname{tg}\frac{\alpha_F}{2}-(-1)^{F+M-1}\pi[(2F+1)(2F+2)]^{1/2}\times\exp\left[i\frac{\pi}{2}(F+{}^1/_2)\right]\frac{2}{\sqrt{\pi}}\begin{pmatrix} F+{}^1/_2 & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}. \tag{2.11}$$

Both expressions vanish at the same value of B_{FMI}, as can be verified using the identity

$$\left(\frac{F+1}{F-1}\right)^{1/2}\begin{pmatrix} F+{}^1/_2 & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}\Big/\begin{pmatrix} F-{}^3/_2 & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}=\begin{cases}-\operatorname{tg}(\alpha_F/2), & \mu=\pm{}^1/_2\\ \operatorname{ctg}(\alpha_F/2), & \mu=\pm{}^3/_2.\end{cases} \tag{2.12}$$

The parity corresponding to $l_I=F-1/2, F+3/2$ can be similarly treated. As a result we get

$$\mathbf{f}_\mu(\theta,\varphi)=\frac{\sqrt{\pi}}{ik_e}\sum_{F,M,I}(2F+1)^{1/2}[\exp(2i\delta_{FI})-1]\times\sum_{l_I}(-1)^{l_I+M-1/2}(2l_I+1)^{1/2}\times(-i)^{l_I}\begin{pmatrix} l_I & {}^3/_2 & F\\ 0 & \mu & -M\end{pmatrix}\Psi_{FMl_I}. \tag{2.13}$$

It can be seen from (2.13) that, in contrast to a simple band, the scattering amplitude $\mathbf{f}_\mu$ depends on the azimuthal angle φ. It is easy to verify, however, that $|\mathbf{f}_\mu|^2$ depends only on the polar angle θ.

The right-hand side of (2.13) can be made more compact by replacing the spinors $\chi_z(\mu')$ with the spinors $\chi_{\mathbf{n}}(\mu')$ that are eigenfunctions of the helicity operator $(\mathbf{n}\hat{\mathbf{J}})$, where $\mathbf{n}$ is a unit vector in the direction of the momentum $\mathbf{k}$ of the scattered wave. We have

$$\chi_z(\mu)=\sum_\lambda D^{1/2}_{\lambda\mu}(\mathbf{n})\chi_{\mathbf{n}}(\lambda), \tag{2.14}$$

where $D^{3/2}_{\lambda\mu}$ is the finite-rotation matrix[5] corresponding to the angular momentum 3/2. Substituting (2.14) in (2.13) we get

$$\mathbf{f}_\mu(\theta,\varphi)=\sum_{\mu'}f_{\mu\mu'}\chi_{\mathbf{n}}(\mu'), \tag{2.15}$$

where $f_{\mu\mu'}(\theta,\varphi)$ is the scattering amplitude of an electron with helicities μ and μ' in the initial and final states, respectively. It can be seen from Fig. 1 that in elastic scattering of an electron with positive energy ($|\mu|=1/2$) a transition is possible only into states with helicities $\mu'=\pm 1/2$. This is demonstrated in Appendix 1 by analyzing the explicit expression for $f_{\mu\mu'}$. It is also shown there that

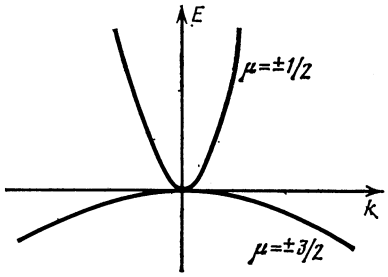

FIG. 1. Energy spectrum of zero-gap semiconductor. Positive energies correspond to electronic states with helicities $\mu = \pm 1/2$. Corresponding to holes (negative energies) are states with helicities $\mu = \pm 3/2$.

$$f_{\mu\mu'} = \frac{1}{4ik_e}\sum_{F,I}(2F+1)\,[\exp(2i\delta_{FI})-1]D^{F}_{\mu'\mu}(\mathbf{n})\,\delta_{|\mu|+|\mu'|,1}\xi, \tag{2.16}$$

where

$$\xi = \begin{cases} 1 & \text{for } l_I = F+1/2 \\ (-1)^{\mu-\mu'} & \text{for } l_I = F-1/2 \end{cases}. \tag{2.16a}$$

This is in fact the main result of the partial-wave method for the band structure of a zero-gap semiconductor. The general expression for the integral scattering cross section is[6]

$$\sigma(E) = \sum_{\mu'}\int d\Omega\,|f_{\mu\mu'}(\theta,\varphi)|^2 = \frac{2\pi}{k_e^2}\sum_{F,I}(2F+1)\sin^2\delta_{FI}. \tag{2.17}$$

We present explicit expressions for the scattering amplitude in the case of greatest importance for what follows, when it can be assumed that only one phase shift δ and $F = 3/2$ and $I = 1$ differs from zero:

$$f_{1/2,1/2} = \frac{1}{ik_e}(e^{2i\delta}-1)\,e^{-i\varphi/2}\cos\frac{\theta}{2}\left(3\cos^2\frac{\theta}{2}-2\right), \tag{2.18}$$

$$f_{-1/2,1/2} = \frac{1}{ik_e}(e^{2i\delta}-1)\,e^{i\varphi/2}\sin\frac{\theta}{2}\left(3\sin^2\frac{\theta}{2}-2\right). \tag{2.19}$$

3. ELECTRON SCATTERING BY A POTENTIAL WELL

Consider a potential well in which $V(r) = U$ at $r < a$ and $V(r) = 0$ at $r > a$. The most interesting results are obtained in scattering of slow electrons, for which $k_e a \ll 1$. In this case, at any fixed value of F, the system (2.4), which contains the function $R_{F,F-3/2}$ with minimal orbital angular momentum $l = F - 3/2$ yields a phase $(k_e a)^{-2}$ times larger than the system (2.5). We turn therefore to the system (2.4). Its solution is

$$R_{F,F+1/2} = \frac{1}{\sqrt{r}}\begin{cases} AJ_{F+1}(\varkappa_h r)+CI_{F+1}(\varkappa_e r), & r<a, \\ BK_{F+1}(k_h r)+DJ_{F+1}(k_e r)+GN_{F+1}(k_e r), & r>a, \end{cases}$$

$$R_{F,F-1/2} = \frac{\operatorname{ctg}(\alpha_F/2)}{\sqrt{r}} \tag{3.1}$$

$$\times\begin{cases} \operatorname{tg}^2(\alpha_F/2)\,AJ_{F-1}(\varkappa_h r)+CI_{F-1}(\varkappa_e r), & r<a, \\ -\operatorname{tg}^2(\alpha_F/2)\,BK_{F-1}(k_h r)-DJ_{F-1}(k_e r)-GN_{F-1}(k_e r), & r>a, \end{cases}$$

where

$$\varkappa_e = [2m_e(U-E)/\hbar^2]^{1/2}, \quad \varkappa_h = [2m_h(U-E)/\hbar^2]^{1/2},$$
$$k_h = (2m_h E/\hbar^2)^{1/2},$$
$$m_h = m_0/(2\gamma-\gamma_1)$$

is the hole mass. It is convenient to determine the coefficients A, B, C, D, and G from the conditions that the functions (3.1), as well as the function X_F and Y_F (Ref. 4), viz.,

$$X_F = \cos(\alpha_F/2)\,P_F R_{F+1/2} - \sin(\alpha_F/2)\,P_{-F}R_{F-1/2},$$
$$Y_F = -\beta^{-1}[\sin(\alpha_F/2)\,P_F R_{F+1/2} + \cos(\alpha_F/2)\,P_{-F}R_{F-1/2}] \tag{3.2}$$

be continuous at the point $r = a$. These conditions are

$$AJ_{F+1}(\varkappa_h a) - BK_{F+1}(k_h a) - GN_{F+1}(k_e a)$$
$$= -CI_{F+1}(\varkappa_e a) + DJ_{F+1}(k_e a),$$
$$\operatorname{tg}^2(\alpha_F/2)\,AJ_{F-1}(\varkappa_h a) + CI_{F-1}(\varkappa_e a) + \operatorname{tg}^2(\alpha_F/2)\,BK_{F-1}(k_h a)$$
$$+ DJ_{F-1}(k_e a) = -GN_{F-1}(k_e a), \tag{3.3}$$
$$C\varkappa_e I_F(\varkappa_e a) - Dk_e J_F(k_e a) - Gk_e N_F(k_e a) = 0,$$
$$A\varkappa_h J_F(\varkappa_h a) + Bk_h K_F(k_h a) = 0.$$

It can be seen from (2.6), (2.7), and (3.1) that

$$\operatorname{tg}\delta_F = G/D. \tag{3.4}$$

It can be shown that at $U \ll \hbar^2/m_e a^2$ (i.e., at $\varkappa_e a \ll 1$ and $k_e a \ll 1$) the terms in the right-hand sides of the first two equations in (3.3) can be neglected, and in the left hand sides it is necessary to expand in powers of $k_e a$ and $\varkappa_e a$. Solving the system in this approximation, we get

$$\operatorname{tg}\delta_F = \frac{(-1)^{1/2+F}\Gamma(1-F)}{2^{2F}\Gamma(1+F)}(k_e a)^{2F}Q_F(1+\nu)$$
$$\times\left[Q_F\left(\operatorname{tg}^2\frac{\alpha_F}{2}-\nu\right)-\frac{2F}{(k_h a)^2}\operatorname{tg}^2\frac{\alpha_F}{2}(1+\nu)\right]^{-1}, \tag{3.5}$$

$$Q_F = \frac{J_{F+1}(\varkappa_h a)}{(\varkappa_h a)J_F(\varkappa_h a)} + \frac{K_{F+1}(k_h a)}{(k_h a)K_F(k_h a)}, \qquad \nu = \frac{k_e^2}{\varkappa_e^2} = \frac{E}{U-E}. \tag{3.5a}$$

Equation (3.5) was obtained under the assumption that $\varkappa_e a \ll 1$ and $k_e a \ll 1$. It was assumed in addition that $U > E$. At $U < E$ expression (3.5) retains the same form, but we must substitute $J_\mu(\varkappa_h a) \to I_\mu(|\varkappa_h|a)$ in (3.5a). The ratio of $\varkappa_e a$ and $k_e a$ can be arbitrary. If $\varkappa_e a \gg k_e a$, we must put $\nu = 0$ in (3.5). It can be shown that Eq. (3.5) with $\nu = 0$ remains valid also at $\varkappa_e a \gg 1$ (but $k_e a \ll 1$).

At $U > 0$ the denominator of (3.5) vanishes at certain values of the energy. This leads to resonant peaks in the energy dependence of the scattering cross section. The positions and widths of the resonances are analyzed in the next section, and now we consider energy regions far from the resonances.

As can be seen from (3.5), at $k_e a \ll 1$ we can confine ourselves to one phase with angular momentum $F = 3/2$. In the case of a simple band the condition $k_e a \ll 1$ also means that we can confine ourselves to one phase corresponding to scattering with zero orbital momentum. In this case the scattering cross section is known to be

$$\sigma = 4\pi a^2, \quad U \gg \hbar^2/m_e a^2, \tag{3.6}$$

$$\sigma = {}^{16}/_{9}\pi a^2 (m_e U a^2/\hbar^2)^2, \quad U \ll \hbar^2/m_e a^2. \tag{3.7}$$

Equation (3.6) corresponds to scattering by a hard sphere. Equation (3.7) is obtained in the Born approximation, which is applicable at $k_e a \ll 1$ if $U \ll \hbar^2/m_e a^2$.

Analysis of (3.5) shows that Eqs. (3.6) and (3.7) are not valid for electron scattering in a zero-gap semiconductor. It

turns out that the Born approximation can be used only under the much more stringent condition $U \ll \hbar^2/m_h a^2$ at $E \ll \hbar^2/m_h a^2$ or $U \ll E$ at $\hbar^2/m_h a^2 \ll E \ll \hbar^2/m_e a^2$. In this case we obtain from (3.5) and (2.17)

$$\sigma = {}^8/_9 \pi a^2 (m_e U a^2/\hbar^2)^2, \tag{3.8}$$

which is half the value for the case of a simple band. The same result is obtained in Appendix 2, where a Born approximation is constructed for electron scattering in a zero-gap semiconductor by a potential of arbitrary form.

If the conditions for the applicability of the Born approximation are not satisfied, i.e., if $U \gg \hbar^2/m_h a^2$ at $E \ll \hbar^2/m_h a^2$ or $U \gg E$ at $\hbar^2/m_h a^2 \ll E \ll \hbar^2/m_e a^2$, we obtain from (3.5) and (2.17) the following expressions for the scattering cross section and phase:

$$\operatorname{tg} \delta_{1/2} \approx \delta_{1/2} \approx {}^1/_3 (k_e a)^3 [1 + 3/k_h a + 3/(k_h a)^2], \tag{3.9}$$

$$\sigma = 8\pi a^2 (m_e/m_h)^2 [1 + k_h a + (k_h a)^2/3]^2. \tag{3.10}$$

These expressions, just as Eq. (3.6) in the case of a simple band, correspond to scattering by a hard sphere. They can be obtained from (3.1) under the assumption that the functions $R_{3/2,0}$ and $R_{3/2,2}$ vanish at $r = a$. We note that in contrast to the usual scattering theory the cross section (3.10) is much less than the square of the geometric dimension of the well. At $E \ll \hbar^2/m_h a^2$

$$\sigma \approx 8\pi a^2 (m_e/m_h)^2,$$

and at $\hbar^2/m_h a^2 \ll E \ll \hbar^2/m_e a^2$

$$\sigma \approx {}^{32}/_9 \pi a^2 (m_e E a^2/\hbar^2)^2,$$

i.e., the cross section increases as the square of the energy, again contrary to the usual scattering theory.

We have considered so far the case $k_e a \ll 1$. At $k_e a \gg 1$ the main contribution to the scattering cross section is made by phases with large values of the angular momentum. In this case the cross section is described by the usual scattering theory and is given by

$$\sigma = 2\pi a^2, \quad U \gg (\hbar^2 E/m_e a^2)^{1/2}, \tag{3.11}$$

$$\sigma = (\pi\hbar^2/m_e E)(m_e U a^2/\hbar^2)^2, \quad U \ll (\hbar^2 E/m_e a^2)^{1/2}. \tag{3.12}$$

A scheme that indicates the values of the scattering cross sections at all energies and well parameters is shown in Fig. 2.

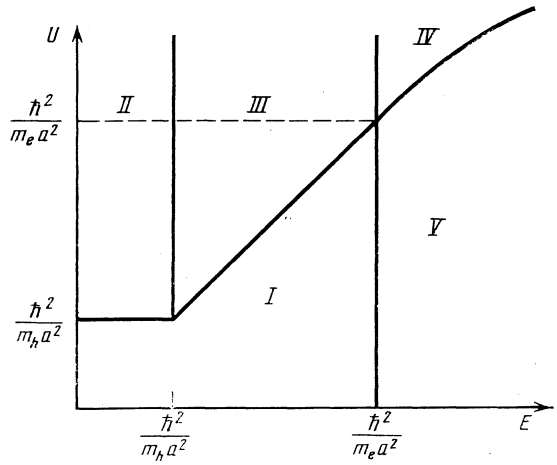

FIG. 2. Illustration of the dependence of the cross section for scattering of an electron on its energy and on the potential: region I—Eq. (3.8); region II—$\sigma = 8\pi a^2 (m_e/m_h)^2$; region III—Eq. (3.10). The usual scattering theory is valid in regions IV [Eq. (3.11) and V [Eq. (3.12)].

4. RESONANCES AND THEIR WIDTHS

As noted by Gel'mont and D'yakonov,[4] in a zero-gap semiconductor there can exist quasilocal levels with positive energy. They have a finite width Γ, since they are against the background of a continuous electron spectrum, but this width is small to the extent that the electron mass is small. In our calculation scheme these levels occur as poles of the function (3.5) as well as of another function, not written out here, that corresponds at fixed F to the solution with the other parity. It differs from (3.5) in that F is replaced by $F + 1$ and α_F by $\tilde{\alpha}_F$.

All the levels $(2F + 1)$ are multiply degenerate in the angular-momentum projection. The ground state corresponds to $F = 3/2$ and $I = 1$, for only in this state does a radial wave function with zero angular momentum enter. The system of levels with $F = 3/2$ and $I = 1$ is obtained from the solution of the transcendental equation

$$\left(1 - \frac{k_h^2}{\varkappa_h^2}\right)\left(\frac{1}{1 - \varkappa_h a \operatorname{ctg} \varkappa_h a} - \frac{1}{1 + k_h a}\right) + \frac{3}{\varkappa_h^2 a^2}\left(1 + \frac{k_h^2}{\varkappa_h^2}\right) = 0 \tag{4.1}$$

relative to the energy $E_{3/2} = \hbar^2 k_h^2/2m_h$, where $k_h^2 + \varkappa_h^2 = 2m_h U/\hbar^2$. As in an ordinary three-dimensional well, the levels appear only starting with a certain well size $W = 2m_h U a^2/\hbar^2$. The first level $E^{(0)}_{3/2}$ appears at $W = W_0 = 4.86$, almost double the value for a simple well with mass m_h. Its goes deeper with increasing U in accordance with the law

$$E_{1/2} = 0.83 \frac{\hbar^2}{m_h a^2}\left(\frac{W - W_0}{W_0}\right)^2. \tag{4.2}$$

In a simple well the numerical coefficient in the equation analogous to (4.2) is $\pi^4/128$. The dependence of the ground-state energy on the well size is shown in Fig. 3 (curve 1).

From (3.5) we can also find the quasilocal-level widths $\Gamma^{(n)}_F$, where n is the number of the level. To this end we must expand the denominator in (3.5) near the value $E = E^{(n)}_F$, representing (3.5) in the form

$$\operatorname{tg} \delta_F = \Gamma^{(n)}_F / (E - E^{(n)}_F). \tag{4.3}$$

For levels described by the system (2.4), it is convenient to express the width $\Gamma^{(n)}_F$ in the form

$$\Gamma^{(n)}_F = \beta^F E^{(n)}_F G^{(n)}_F (W), \tag{4.4}$$

where $G^{(n)}_F(W)$ is a function that depends only on the size of the well. For levels described by the system (2.5) we have $\Gamma^{(n)}_F \propto \beta^{F+1}$. It can be seen from (4.4) that at $\beta = m_e/m_h \ll 1$ the level width is small compared with the energy. It is interesting to note that this property is preserved also at low energies, when the level just appears in the well, and its position is described by Eq. (4.2). It can be shown that $G^{(0)}_{3/2}(W)$ tends to a value 2 as $W \to W_0$, in accordance with

$$G^{(0)}_{1/2}(W) = 2 + 2.56[(W - W_0)/W_0], \tag{4.5}$$

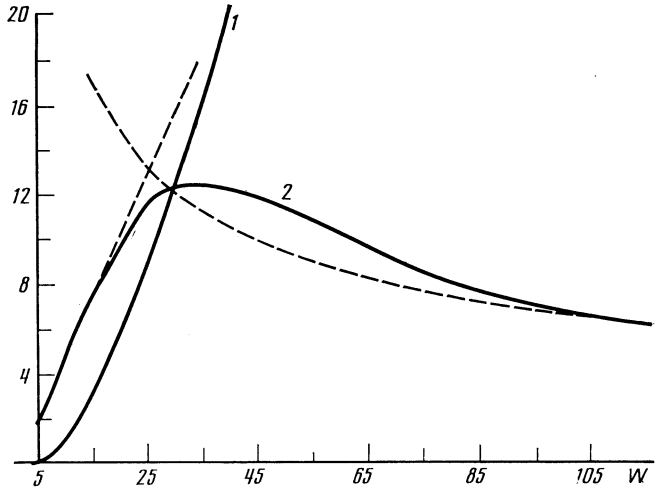

FIG. 3. Curve 1—dependence of ground-state energy in units of $2m_h E^{(0)}_{3/2} a^2/\hbar^2$ on the well size. Curve 2—dependence of the quantity $G^{(0)}_{3/2}$, which characterizes the width of the quasilocal level in the potential well [see Eq. (4.4)] on the size W of the well. The dashed curves are the asymptotic values of (4.5) and (4.6) for $G^{(0)}_{3/2}$ as $W \to W_0$ and $W \to \infty$, respectively.

so that the ratio $\Gamma^{(0)}_{3/2}/E^{(0)}_{3/2}$ tends to the value $2\beta^{3/2} \ll 1$. As $W \to \infty$. The width of the ground level in the well tends to zero:

$$\Gamma^{(0)}_{1/2}/E^{(0)}_{1/2} \approx 66.4\beta^{3/2} W^{-1/2}. \tag{4.6}$$

Curve 2 of Fig. 3 shows $G^{(0)}_{3/2}$ as a function of W as well as (dashed) the asymptotic forms of (4.5) and (4.6).

The amplitudes of the resonant scattering at $F = 3/2$ can be obtained with the aid of Eqs. (2.18), (2.19), (4.3), and (4.4). The integral cross section has the usual form (see the review 7 and the literature therein):

$$\sigma = \frac{2\pi}{k_e^2} \frac{4(\Gamma^{(n)})^2}{(E-E^{(n)})^2 + (\Gamma^{(n)})^2} \tag{4.7}$$

(we omit the subscript 3/2 of $E^{(n)}$ and $\Gamma^{(n)}$). The phase and the cross section for resonant scattering, as can be seen from (4.3) and (4.7), tends to zero at $|E - E^{(n)}| \gg \Gamma^{(n)}$. It is clear, however, that at energies far from resonance, the phase and the cross section tend to their nonresonant values (3.9) and (3.10). By using (3.5) we can obtain for the cross section an equation valid both near and off resonance,

$$\sigma = \frac{8\pi}{k_e^2} \frac{[\Gamma^{(n)} + (E-E^{(n)})\delta]^2}{(E-E^{(n)})^2 + [\Gamma^{(n)} + (E-E^{(n)})\delta]^2}. \tag{4.8}$$

The phase δ of the nonresonant scattering is given by (3.9). It can be seen that Eq. (4.8) goes over into (4.7) at energies close to the resonance at $|E - E^{(n)}| \ll \Gamma^{(n)}/\delta$, and coincides with (3.10) at $|E - E^{(n)}| \gg \Gamma^{(n)}/\delta$. It is interesting to note that at $E - E^{(n)} = -\Gamma^{(n)}/\delta$ the cross section (4.8) vanishes (antiresonance), and then the phase shift δ of the scattering with angular momentum $F = 3/2$ and parity $I = 1$ assumes a value that is a multiple of π. The total cross section (2.17), however, does not vanish exactly, but is determined by a contribution from other scattering phase shifts, which is parametrically small, to the extent that $\beta \ll 1$. When there are many levels in the well ($\varkappa_h a \gg 1$), the distance between the positions of the resonance and the antiresonance is of the order of $\hbar^2/m_h a^2$. It is much larger than the resonance width Γ, but much smaller than the distance, of the order of $(\varkappa_h a)\hbar^2/m_h a^2$, to the next resonance.

APPENDIX 1

We expand the angle functions $\Psi_{FM_I}(\theta, \varphi)$ in the eigenfunctions of the helicity operator. Substituting this expansion in (2.13) we get (2.16). We use Eq. (2.14) and the connection between the spherical functions and the rotation matrices[5]:

$$Y_{lm}(\theta, \varphi) = Y_{lm}(\mathbf{n}) = i^l \left(\frac{2l+1}{4\pi}\right)^{1/2} D_{0m}{}^{l}(\mathbf{n}). \tag{A1.1}$$

The angle functions (2.3) take the form

$$\Psi_{FMl_I} = i^{l_I} \left[\frac{(2F+1)(2l_I+1)}{4\pi}\right]^{1/2} (-1)^{l_I+M-1/2} \times \sum_{\mu',\lambda,m} \begin{pmatrix} l_I & 1/2 & F \\ m & \mu' & -M \end{pmatrix} D_{0m}{}^{l_I}(\mathbf{n}) D^{1/2}_{\lambda\mu'}(\mathbf{n}) \chi_{\mathbf{n}}(\lambda). \tag{A1.2}$$

Substituting in (A1.2) the equation[8]

$$D_{0m}{}^{l_I}(\mathbf{n}) D^{1/2}_{\lambda\mu'}(\mathbf{n}) = \sum_{F',M',M''} (2F'+1) \begin{pmatrix} l_I & 1/2 & F' \\ 0 & \lambda & -M' \end{pmatrix} \times \begin{pmatrix} l_I & 1/2 & F' \\ m & \mu' & -M'' \end{pmatrix} D^{(F')^*}_{-M',-M''}(\mathbf{n}), \tag{A1.3}$$

changing the order of the summation, and using the equations[5]

$$\sum_{\mu',m} \begin{pmatrix} l_I & 1/2 & F \\ m & \mu' & -M \end{pmatrix} \begin{pmatrix} l_I & 1/2 & F' \\ m & \mu' & -M'' \end{pmatrix} = \frac{1}{2F+1} \delta_{FF'} \delta_{MM''} \times D^{(F')^*}_{-M',-M''}(\mathbf{n}) = (-1)^{M''-M'} D^{F'}_{M',M''}(\mathbf{n}), \tag{A1.4}$$

we obtain the expansion of the angle function (2.3) in the rotated basis $\chi_{\mathbf{n}}(\lambda)$

$$\Psi_{FMl_I}(\theta, \varphi) = i^{l_I} \left[\frac{(2F+1)(2l_I+1)}{4\pi}\right]^{1/2} \sum_{\lambda} (-1)^{l_I+2M-1/2-\lambda} \times \begin{pmatrix} l_I & 1/2 & F \\ 0 & \lambda & -\lambda \end{pmatrix} D_{\lambda M}{}^{F}(\mathbf{n}) \chi_{\mathbf{n}}(\lambda). \tag{A1.5}$$

Substituting (A1.5) in (2.13) and using the definition (2.15) we obtain the amplitude $f_{\mu\mu'}(\theta, \varphi)$ of scattering of an electron with helicity μ in the initial state into a state with helicity μ':

$$f_{\mu\mu'}(\theta, \varphi) = \frac{1}{2ik_e} \sum_{F,I} (2F+1)[\exp(2i\delta_{FI}) - 1] D^{F}_{\mu'\mu}(\mathbf{n}) Z_I^{\mu\mu'}, \tag{A1.6}$$

where

$$Z_I^{\mu\mu'} = (-1)^{\mu-\mu'} \sum_{l_I} (2l_I+1) \begin{pmatrix} l_I & 1/2 & F \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} l_I & 1/2 & F \\ 0 & \mu' & -\mu' \end{pmatrix}. \tag{A1.7}$$

Let us prove that

$$Z_I^{\mu\mu'} = \frac{1}{2} \begin{cases} \xi, & |\mu| = |\mu'| = 1/2 \\ 0, & |\mu| \neq |\mu'| \end{cases}, \tag{A1.8}$$

where ξ is defined in (2.16a). Let the given parity I in (A1.7) correspond to orbital angular momentum values $l_I = F - 3/2, F + 1/2$. Then

$$Z_I^{\mu\mu'} = (-1)^{\mu-\mu'} 2(F-1) \times \begin{pmatrix} F-3/2 & 3/2 & F \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} F-3/2 & 3/2 & F \\ 0 & \mu' & -\mu' \end{pmatrix} A, \tag{A1.9}$$

$$A = \frac{F+1}{F-1} \begin{pmatrix} F+1/2 & 3/2 & F \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} F+1/2 & 3/2 & F \\ 0 & \mu' & -\mu' \end{pmatrix} \Big/ \begin{pmatrix} F-3/2 & 3/2 & F \\ 0 & \mu & -\mu \end{pmatrix} \begin{pmatrix} F-3/2 & 3/2 & F \\ 0 & \mu' & -\mu' \end{pmatrix} + 1.$$

It can be seen from (2.12) that A vanishes at $|\mu| \neq |\mu'|$ and is equal to $\tan^2(\alpha_F/2) + 1$ at $|\mu| = |\mu'| = 1/2$. Direct calculation of the factor preceding A leads to Eq. (A1.8). The calculation for the other parity is similar. From (A1.6) and (A1.8) follows the expression (2.16).

APPENDIX 2

The scattering cross section for a zero-gap semiconductor takes in the Born approximation the form

$$|f_{\mu\mu'}(\theta, \varphi)|^2 = \frac{4\pi m_e^2}{\hbar^4} \int_0^\infty \frac{dk}{(2\pi)^3} k |\langle \mathbf{k}, \mu | V(r) | \mathbf{k}', \mu' \rangle|^2 \delta(k^2 - k'^2), \tag{A2.1}$$

where

$$|\mathbf{k}, \mu\rangle = e^{i\mathbf{k}\mathbf{r}} \chi_{\mathbf{k}}(\mu) \tag{A2.2}$$

is the wave function of the free motion of an electron with helicity μ. We transform the matrix element contained in (A2.1) by using (2.14):

$$\langle \mathbf{k}, \mu | V(r) | \mathbf{k}'\mu' \rangle = D^*_{\mu'\mu}(\theta) \int d^3r V(r) e^{i\mathbf{q}\mathbf{r}}, \tag{A2.3}$$

where θ is the scattering angle (between $\mathbf{k}$ and $\mathbf{k}'$); $\mathbf{q} = \mathbf{k}' - \mathbf{k}$, and $q' = 2k \sin(\theta/2)$. From (A2.1) and (A2.3) we get

$$|f_{\mu\mu'}(\theta, \varphi)|^2 = \left[\frac{2m_e}{\hbar^2} \int_0^\infty V(r) \frac{\sin qr}{q} r\, dr \right]^2 |D^*_{\mu'\mu}(\theta)|^2. \tag{A2.4}$$

It can be seen that in scattering of slow electrons ($k_e a \ll 1$) by a potential well the angular dependence of the cross section is determined by the factor $|D^{3/2}_{\mu'\mu}(\theta)|^2$, as follows from the general formula [see (2.18) and (2.19)]. It is easy to obtain the total cross section for scattering by the potential well

$$\sigma = \sum_{\mu'} \int d\Omega |f_{\mu\mu'}(\theta, \varphi)|^2 = \begin{cases} {}^8/_9 \pi a^2 (m_e U a^2/\hbar^2)^2, & k_e a \ll 1, \\ (2\pi/k_e^2)(m_e U a^2/\hbar^2)^2, & k_e a \gg 1. \end{cases} \tag{A2.5}$$

We note that for fast particles the answer coincides with the known result for a simple band. Scattering in a complicated well was first considered in the Born approximation by Bir, Normantas, and Pikus.[9]

[1)]We thank A. M. Kogan for pointing out Ref. 3 to us.

[1]J. G. Broerman, Phys. Rev. **B1**, 4568 (1970). W. Zawadski, Mechanisms of Electron Scattering in Semiconductors, Warsaw, 1979. V. L. Gel'mont, V. I. Ivanov-Omskiĭ, B. T. Kolomiets, *et al.*, Fiz. Tekh. Poluprov. **5**, 266 (1971) [Sov. Phys. Semicond. **5**, 228 (1971)].

[2]I. M. Tsidil'kovskiĭ, Elektrony i dyrki v poluprovodnikakh (Electrons and Holes in Semiconductors), Nauka, 1972.

[3]H. I. Ralph, Philips Res. Repts. **32**, 160 (1977).

[4]B. L. Gel'mont and M. I. D'yakonov, Zh. Eksp. Teor. Fiz. **62**, 713 (1972) [Sov. Phys. JETP **35**, 377 (1972)].

[5]L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Nonrelativistic Theory, Pergamon, 1978.

[6]B. L. Gel'mont, Impurity States and Kinetic Effects in Semiconductors with Band-Spectrum Singularities, Doctoral dissertation, Leningrad, 1974.

[7]L. Liu, in: Physics of Narrow-Gap Semiconductors, Proc. 3d Intern. Conf., Warsaw, Polish Scient. Publ., 1978, p. 151.

[8]E. M. Lifshitz and L. P. Pitaevskii, Relativistic Quantum Theory, part 1, Pergamon, 1974.

[9]G. L. Bir, E. Normantas, and G. E. Pikus, Fiz. Tverd. Tela (Leningrad) **4**, 1180 (1962) [Sov. Phys. Solid State **4**, 867 (1962)].

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