Theory of impurity states in a zero-gap semiconductor

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It is shown that the electron-electron interaction plays an important role in the description of the state of a neutral acceptor in a zero-gap semiconductor. This interaction causes strong localization of the wave function of the lowest state of the acceptor and makes its energy discrete. All this is true if we ignore the existence of a positively charged acceptor. However, if the energy representing the binding of an acceptor to two holes is negative, then the ground state of the system is a positive acceptor with an electron bound to it. The problem of the scattering of an electron by a neutral acceptor in the resonance and nonresonance regions is considered. It is shown that the line width describing the resonance scattering can be calculated in the one-electron approximation.

1. INTRODUCTION

In zero-gap semiconductors such as HgTe or α — Sn the states of impurities are within the continuous spectrum: acceptor states are in the conduction band and the donor states are in the valence band. Gel'mont and D'yakonov[1] considered acceptor states in the one-electron approximation describing them by the eigenfunctions of the Luttinger Hamiltonian, which includes the potential of the interaction of a particle with a Coulomb center. In the case of a zero-gap semiconductor all these functions correspond to the continuous spectrum. However, since the mass of a hole m_h is usually much greater than the mass of an electron m_e, we can say that these functions describe quasidiscrete levels lying against the background of the conduction band and the width of these levels is smaller than the binding energy by the factor $(m_e/m_h)^{3/2}$. The same logic leads to the conclusion that donor states are wide and, consequently, donors should be always ionized in a zero-gap semiconductor. This one-particle approximation, which ignores the exchange interaction, has made it possible to determine the positions of acceptor levels and their widths.

We shall show that in describing the ground state of an acceptor and the process of nonresonant scattering of an electron by a neutral acceptor we have to allow for the electron-electron interaction. In the one-electron treatment the virtual transitions creating electron-hole pairs give rise to a finite level width, whereas an allowance for the electron-electron interaction makes the lowest state of a neutral acceptor discrete, i.e., this level has no width at all at absolute zero, because it is the ground state of the whole system. This is justified if we ignore the possibility of formation of a positively charged acceptor to which two holes are bound. The possibility of formation of such a complex has the effect that the ground state of the system is a positive acceptor to which an electron is bound. All this cannot be deduced from the one-electron Hamiltonian, because in the Luttinger case the electron states can be as low as we please. An excited state of a neutral acceptor has a finite width, but this is not due to a transition to the continuous spectrum, but due to a transition to the ground state accompanied by the emission of an electron-hole pair. Therefore, for example, the line width in the case of optical excitation of a neutral acceptor should be different from the line width obtained in Ref. 1. We shall also assume that the presence of a continuous spectrum does not hinder the existence of a neutral donor.

We shall show later that the state of a charged acceptor splits into a neutral acceptor and an electron, and the width of a charged-acceptor level corresponding to such decay corresponds to the width obtained in Ref. 1 using the one-electron approximation.

The wave function describing the scattering of an electron by a neutral acceptor, obtained below, is identical at large distances with the wave function found using the one-electron approximation provided the electron energy is close to the acceptor energy, so that the scattering is of resonant nature. We shall find the cross section for such scattering and its angular dependence. However, far from a resonance the one-electron approximation fails to describe the scattering of an electron by a neutral acceptor because of the simultaneous interaction of an electron with a negatively charged center and with a hole, so that an acceptor behaves as a neutral particle. We shall estimate the order of magnitude of the cross section for nonresonant scattering of an electron by a neutral acceptor.

2. STATE OF A NEUTRAL ACCEPTOR

An acceptor impurity in a semiconductor captures an electron which joins an inner orbit and the acceptor becomes negatively charged. A hole which then appears in the valence band may be localized by the acceptor potential or it may be in a delocalized state. In the former state an acceptor is neutral, whereas as in the latter it is charged. The Hamiltonian of the system can be written down in the second quantization representation, in which it is convenient to allow for the Fermi occupancy:

$$H=\int \psi^{+}(\mathbf{r})\,[H_L(\hat{\mathbf{p}})+V(\mathbf{r})]\,\psi(\mathbf{r})\,d^3r+H_{ee}. \tag{1}$$

Here, $\psi^{+}(\mathbf{r})$ and $\psi(\mathbf{r})$ are the creation and annihilation operators for electrons, each of which represents a four-component vector, and H_L is the Luttinger Hamiltonian

$$H_L=\frac{\hbar^2}{2m_0}\left[\left(\gamma_1+\frac{5}{2}\gamma\right)\hat{p}^2-2\gamma(\hat{\mathbf{p}}\mathbf{J})^2\right], \tag{2}$$

where $\hat{\mathbf{p}}=i\hbar\nabla$; γ_1 and γ are the Luttinger parameters; m_0 is the mass of a free electron; the components of the vector J_x,

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J_y, and J_z represent a 4×4 matrix which describes an angular momentum 3/2. The Hamiltonian is written down in the spherical approximation. The quantity $V=e^2/\varkappa r$ is the potential of a negatively charged acceptor which is at the origin of the coordinate system, $\varkappa$ is the permittivity, and H_{ee} is the usual four-fermion Hamiltonian of the electron-electron interaction.

The four-component spinors $\chi_\alpha(\mu, \mathbf{p})$ which are the eigenfunctions of the Hamiltonian (2) are characterized by a wave vector p and a helicity μ. The helicity $\mu = \pm 1/2$ corresponds to an electron energy $\varepsilon_e(p)=p^2/2m_e$, where $m_e=m_0(\gamma_1+2\gamma)^{-1}$, whereas the helicity $\mu=\pm 3/2$ corresponds to holes:

$$\varepsilon_h(p)=p^2/2m_h, \qquad m_h=m_0(2\gamma-\gamma_1)^{-1}.$$

We shall now introduce the operators of the projection on electron and hole states:

$$\Lambda_{\alpha\beta}^{(e)}(\mathbf{p})=\sum_{\mu=\pm 1/2}\chi_\alpha(\mu,\mathbf{p})\chi_\beta^*(\mu,\mathbf{p})=\delta_{\alpha\beta}-\Lambda_{\alpha\beta}^{(h)}, \tag{3}$$

$$\Lambda_{\alpha\beta}^{(h)}(\mathbf{p})=\sum_{\mu=\pm 3/2}\chi_\alpha(\mu,\mathbf{p})\chi_\beta^*(\mu,\mathbf{p})=\frac{1}{2}\left[\frac{(\mathbf{pJ})^2}{p^2}-\frac{1}{4}\right]_{\alpha\beta}. \tag{4}$$

We can use them to introduce the creation and annihilation operators for electrons $\psi^{(e)+}$, $\psi^{(e)}$ and holes $\psi^{(h)+}$, $\psi^{(h)}$:

$$\psi=\psi^{(e)}+\psi^{(h)+}, \tag{5}$$

$$\psi^{(e)}=\Lambda^{(e)}\psi, \qquad \psi^{h+}=\Lambda^{(h)}\psi. \tag{6}$$

The new operators satisfy the following commutation relationships:

$$\begin{aligned}\{\psi_\alpha^{(e)}(\mathbf{r}),\psi_\beta^{(e)+}(\mathbf{r}')\}&=\Lambda_{\alpha\beta}^{(e)}(\mathbf{r}-\mathbf{r}'),\\ \{\psi_\alpha^{(h)+}(\mathbf{r}),\psi_\beta^{(h)}(\mathbf{r}')\}&=\Lambda_{\alpha\beta}^{(h)}(\mathbf{r}-\mathbf{r}'),\\ \{\psi_\alpha^{(e)+}(\mathbf{r}),\psi_\beta^{(h)}(\mathbf{r}')\}&=0,\end{aligned} \tag{7}$$

where $\{a, b\}=ab+ba$.

In the new basis the Luttinger Hamiltonian becomes

$$H_L=\int d^3r\left[\psi^{(e)+}(\mathbf{r})\frac{p^2}{2m_e}\psi^{(e)}(\mathbf{r})+\psi^{(h)+}(\mathbf{r})\frac{p^2}{2m_h}\psi^{h}(\mathbf{r})\right]. \tag{8}$$

We shall define the vacuum state $|0\rangle$ so that

$$\psi^{(e)}|0\rangle=0, \qquad \psi^{(h)}|0\rangle=0. \tag{9}$$

In the occupation number representation the wave function of a neutral state of an acceptor is $\psi^{(h)+}|0\rangle$. Substituting Eqs. (5) and (6) into Eq. (1), we find that, without allowance for the electron-electron interaction, the Schrödinger equation for this function contains the Hamiltonian

$$H_A=\int d^3r\psi^{(h)+}(\mathbf{r})[\varepsilon_h(\hat{p})-V(r)]\psi^{(h)}(\mathbf{r}). \tag{10}$$

The state of a hole at an acceptor is described by the total momentum F, the projection of this momentum M, the parity I, and an analog of the principal quantum number n. We shall denote the set of numbers FMI by ν and represent the hole creation operator in the form

$$\psi^{(h)+}(\mathbf{r})=\sum_{\nu n}b_{\nu n}{}^{+}\varphi_{\nu n}^*(\mathbf{r}), \tag{11}$$

where $b_{\nu n}^{+}$ is the operator for the creation of a hole in a state νn related to the annihilation operator $b_{\nu n}$ by the usual expression

$$\{b_{\nu n}{}^{+}, b_{\nu' n'}\}=\delta_{\nu\nu'}\delta_{nn'},$$

where $\varphi_{\nu n}(\mathbf{r})$ satisfies the equation

$$\int d^3r'\Lambda^{(h)}(\mathbf{r}-\mathbf{r}')[\varepsilon_h(\hat{p}')-V(r')]\varphi_{\nu n}(\mathbf{r}')=E_{\nu n}\varphi_{\nu n}(\mathbf{r}). \tag{12}$$

Here, $\mathbf{p}'=i\hbar\partial/\partial\mathbf{r}'$ and $E_{\nu n}$ is the required energy of an acceptor center. This energy is negative in the case of bound states. Substituting Eq. (11) into Eq. (10), we obtain

$$H_A=\sum_{\nu n}E_{\nu n}b_{\nu n}{}^{+}b_{\nu n}. \tag{13}$$

It should be noted that these states have no width associated with a transition to the continuous spectrum.

We shall now turn to the electron-electron interaction. The states of energy lower than $E_B^{(e)}=m_e e^4/2\hbar^2\varkappa^2$ are strongly renormalized in a zero-gap semiconductor because of creation of electron-hole pairs. We shall be interested only in large energies of the order of the binding energy of an acceptor $m_h e^4/2\hbar^2\varkappa^2$. At such energies the creation of pairs is not favored by the energy considerations. Renormalization of the static permittivity (electron screening) is strong only at distances large compared with $a_e=\hbar^2\varkappa/m_e e^2$. The effective radius of an acceptor is of the order of $a_h=\hbar^2\varkappa/m_h e^2$ and if $m_e \ll m_h$, it is considerably less than a_e. Therefore, in studies of the ground state of a neutral acceptor there is no need to allow for the permittivity renormalization. Excited states of a neutral acceptor have a finite width because of a transition to the ground state accompanied by the creation of a pair. However, this width is small compared with the ground-state energy expressed in terms of the parameter m_e/m_h. We shall not calculate this width. The operator H_{ee} is important in the acceptor problem only because it renormalizes strongly the spectrum of holes.[2,3] Moreover, the electron-electron interaction should be allowed for in a study of nonresonant scattering of electrons by a neutral acceptor.

We shall define a normal operator product

$$N[\psi(\mathbf{r}_1)\ldots\psi^+(\mathbf{r}_N)]$$

as a sequence in which all the operators $\psi^{(e)+}$, $\psi^{(h)+}$ are on the left of $\psi^{(e)}$, $\psi^{(h)}$. Applying Eqs. (5)–(7), we can easily show that

$$\psi_\alpha^+(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2)=N[\psi_\alpha^+(\mathbf{r}_1)\psi_\beta(\mathbf{r}_2)]+\Lambda_{\alpha\beta}^{(h)}(\mathbf{r}_2-\mathbf{r}_1). \tag{14}$$

Application of the Wick theorem[4] transforms H_{ee} to

$$\begin{aligned}H_{ee}=\frac{e^2}{2\varkappa}\int\frac{d^3r_1\,d^3r_2}{|\mathbf{r}_1-\mathbf{r}_2|}\{&N[\psi^+(\mathbf{r}_1)\psi^+(\mathbf{r}_2)\psi(\mathbf{r}_2)\psi(\mathbf{r}_1)]\\ &-2\Lambda^{(h)}(\mathbf{r}_2-\mathbf{r}_1)N[\psi^+(\mathbf{r}_2)\psi(\mathbf{r}_1)]\}.\end{aligned} \tag{15}$$

Equation (15) is derived assuming that the terms containing $\Lambda^{(h)}(0)$ should be dropped from the neutrality conditions. The second term of Eq. (15) results in renormalization of both the hole and electron spectra. We must bear in mind that it contains integrals which diverge in the effective mass method. They should be normalized by altering the point from which energy is measured, i.e., by adding to the Hamiltonian the following counter-term which commutes with the Hamiltonian:

$$\frac{e^2}{4\pi^2\varkappa}\int\frac{d^3q}{q^2}\int d^3rN[\psi^+(\mathbf{r})\psi(\mathbf{r})], \tag{16}$$

where the integration with respect to q is limited to the first Brillouin zone. After this normalization the energies of electron and hole excitations are measured from the point $p=0$. When Eq. (16) is added to the second term of Eq. (15), both the electron and hole spectra become renormalized. In particular, $\varepsilon_h(p)$ in the Hamiltonian of Eq. (10) should be replaced with

$$\varepsilon_h(p)=p^2/2m_h+3\pi^2e^2p/32\varkappa\hbar. \tag{17}$$

Such renormalization of the hole spectrum was first obtained in Refs. 2 and 3. The process of renormalization of the electron spectrum is very similar, but in the range of energies of interest to us it is a small effect.

We can expand formally in respect of the parameter m_e/m_h provided we assume that $|\psi^{(e)}|\ll|\psi^{(h)}|$. In fact, averaging over a quantity containing $\psi^{(e)}$ gives rise to an electron density of states containing $m_e^{3/2}$. Therefore, the main term in the normal product of Eq. (15) contains only the operators $\psi^{(h)}$ and $\psi^{(h)+}$. However, such a term gives zero result when it is applied to the neutral acceptor function. The other terms contain $\psi^{(e)}$ and $\psi^{(e)+}$ and we shall ignore them.

The ground state of an acceptor corresponds to the momentum 3/2. The wave function of this state $\varphi^0(\mathbf{r})$ can be represented in the form[5]

$$\varphi^0(\mathbf{r})=\frac{1}{(2\pi)^{3/2}}\int d^3qe^{i\mathbf{qr}}f(q)\Lambda^{(h)}(\mathbf{q})\chi_M. \tag{18}$$

The function $f(q)$ depends only on the modulus of q, and χ_M is the eigenfunction of the momentum projection operator $J_z\chi_M=M\chi_M$. The ground state is quadruply degenerate in respect of M. The function $f(q)$ and the energy E_0 are given by the equation

$$\left(\frac{p^2}{2m_h}+\frac{3\pi e^2}{32\varkappa\hbar}p-E_0\right)f(p)$$

$$-\frac{e^2}{8\pi^2\varkappa\hbar}\int\frac{d^3q}{(\mathbf{p}-\mathbf{q})^2}f(q)\left[1+\frac{3(\mathbf{pq})^2}{p^2q^2}\right]=0, \tag{19}$$

which is obtained on substitution of Eqs. (17) and (18) in Eq. (12). This equation was first obtained and solved by Gel'mont.[5] A variational calculation gives $E_0=-0.085m_he^4/\varkappa^2\hbar^2$.

The conclusion that a neutral acceptor represents the ground state of a system is valid only if we ignore the existence of a positively charged acceptor, i.e., an acceptor which binds two holes. If a state of this kind does exist, then a neutral acceptor may decay into a positive acceptor and an electron. The ground state of the system is then represented by a positive acceptor and the associated electron. If the electron mass is very small, a positive acceptor can be regarded as a point nucleus. If the acceptor concentration is finite, then an increase in this concentration causes the electron states to overlap so that a Fermi occupancy of the conduction band is established. The number of electrons is equal to the number of acceptors. However, as soon as the Fermi energy exceeds the binding energy of a positive acceptor, the formation of such acceptors and, consequently, an increase in the acceptor concentration becomes undesirable and the state of a neutral stabilizes. Unfortunately, the binding energy of a positive acceptor in a complex energy band is not yet known. If we assume, by analogy with a negative hydrogen ion, that it is $0.1|E_0|$, then the effects discussed here can hardly be important under modern experimental conditions. For this reason we shall ignore the existence of a positive acceptor and assume that the ground state is represented by a neutral acceptor.

It should be noted that without an allowance for the electron-electron interaction the lowest state of a neutral acceptor has a finite width even if we ignore the possibility of a positively charged acceptor. This finite width appears because of creation of a pair: a second hole with an energy E_0 and a different value of M, bound to the acceptor, and an electron of energy $|E_0|$. This is exactly the origin of the width of one-electron solutions of the Luttinger Hamiltonian. In fact, this width exists only because of the possibility of the positive acceptor and it is of different order of magnitude.

3. RESONANT SCATTERING OF ELECTRONS BY NEUTRAL ACCEPTORS

If the positive energy of a free electron is close to the binding energy of an acceptor $|E_0|$, the system formed by an electron and a neutral acceptor has an energy close to the energy of the vacuum state, which we shall call the state of a charged acceptor. The terms of the Hamiltonian (1) describing creation of electron-hole pairs provide the coupling between these states. It therefore follows that we can expect processes resulting in decay of a charged acceptor into an electron and a neutral acceptor or in resonant scattering of an electron by a neutral acceptor.

The main term of the Hamiltonian (1) relating the states in resonance is

$$\int d^3rV(r)[\psi^{(e)+}(\mathbf{r})\psi^{(h)+}(\mathbf{r})+\psi^{(h)}(\mathbf{r})\psi^{(e)}(\mathbf{r})]. \tag{20}$$

We shall expand the operator $\psi^{(e)+}$ in terms of the wave functions of a free electron $\varphi_\nu^{(e)}(\mathbf{r},\varepsilon)$ in the form

$$\psi^{(e)+}(\mathbf{r})=\sum_\nu\int d\varepsilon a_\nu^+(\varepsilon)\varphi_\nu^{(e)*}(\mathbf{r},\varepsilon), \tag{21}$$

where $a_\nu^+(\varepsilon)$ is the electron creation operator in a state ν with an energy ε, and

$$\varphi_\nu^{(e)}(\mathbf{r},\varepsilon)=\left(\frac{2m_e}{r}\right)^{1/2}\sum_{l_I,m}(-1)^{l_I-1/2+M}\begin{pmatrix} l_I & 3/2 & F\\ 0 & 1/2 & -1/2\end{pmatrix}$$

$$\times\begin{pmatrix} l_I & 3/2 & F\\ m & \mu & -M\end{pmatrix}[(2F+1)(2l_I+1)]^{1/2}Y_{lm}(\mathbf{r})J_{l+1/2}(pr)\chi_\mu. \tag{22}$$

The quantity l_I assumes the value $F-3/2$, $F+1/2$ for one parity I and the value $F-1/2$, $F+3/2$ for the other parities; $p=(2m_e\varepsilon)^{1/2}$; Y_{lm} are spherical functions; $j_{l+1/2}$ are Bessel functions; χ_μ are the eigenvectors of the operator J_z. The $3j$ Wigner symbols are used in the expansion. Equation (22) can be derived using Eqs. (2.2), (2.6), (2.7), and (2.12) from Ref. 6. The functions (22) are normalized by the condition

$$\int d^3r\varphi_\nu^{(e)*}(\mathbf{r},\varepsilon)\varphi_{\nu'}^{(e)}(\mathbf{r},\varepsilon')=\delta_{\nu\nu'}\delta(\varepsilon-\varepsilon'). \tag{23}$$

The Hamiltonian H_r describing the resonance scattering consists of the neutral acceptor Hamiltonian (13), the Hamiltonian of free electrons [representing the first term in Eq. (8)], and the binding Hamiltonian (20). Using Eqs. (11) and (21) we obtain

$$H_r = \sum_{\nu} \int d\varepsilon a_\nu^+(\varepsilon) a_\nu(\varepsilon) + \sum_{\nu,n} E_{\nu n} b_{\nu n}^+ b_{\nu n} + \sum_{\nu n} \int d\varepsilon [V_{\nu n}(\varepsilon) a_\nu^+(\varepsilon) b_{\nu n}^+ + V_{\nu n}^*(\varepsilon) b_{\nu n} a_\nu(\varepsilon)], \quad (24)$$

where

$$V_{\nu n}(\varepsilon) = \frac{e^2}{\varkappa} \int \frac{d^3r}{r} \varphi_\nu^{(e)*}(\mathbf{r}, \varepsilon) \varphi_{\nu n}(\mathbf{r}). \quad (25)$$

The eigenfunction Φ_ν of the Hamiltonian of Eq. (24) represents a superposition of resonant states, and the quantities F, M, and I are—as before—good quantum numbers:

$$\Phi_\nu = A_\nu |0\rangle + \sum_n d\varepsilon C_{\nu n}(\varepsilon) a_\nu^+(\varepsilon) b_{\nu n}^+ |0\rangle. \quad (26)$$

We find from the equation $H_r \Phi = E\Phi$ that

$$\begin{aligned} &(E_{\nu n} + \varepsilon - E) C_{\nu n}(\varepsilon) + V_{\nu n}(\varepsilon) A_\nu = 0, \\ &\sum_n \int d\varepsilon V_{\nu n}^*(\varepsilon) C_{\nu n}(\varepsilon) + E A_\nu = 0. \end{aligned} \quad (27)$$

We shall show later that the width of a resonance is less than the separation between the acceptor levels. Therefore, we can assume that an electron interacts only with one level and we shall assume that this is the ground state with the energy E_0. The corresponding matrix element $V_{\nu n}$ will be denoted by V_0. Its energy dependence can be ignored.

The system of equations (27) can be solved by a method suggested by Fano[7] for the problem of self-detachment of an electron when it is scattered by a negative ion. The results are of the form:

$$C_0(\varepsilon) = \frac{\sin \Delta}{\pi (E - E_0 - \varepsilon)} - \cos \Delta \delta (E - E_0 - \varepsilon), \quad (28)$$

$$A_0 = \sin \Delta / \pi V_0. \quad (29)$$

Here, Δ is the electron scattering phase found from the asymptotic behavior of the wave function at large distances from an acceptor. This phase is

$$\Delta = -\operatorname{arctg}(\Gamma/2E), \quad (30)$$

where

$$\Gamma = 2\pi |V_0|^2. \quad (31)$$

The formula (30) describes resonant scattering of an electron by a neutral acceptor. A resonance appears when the energy of the incident electron is equal to the binding energy of the acceptor $E = \varepsilon + E_0 = 0$ [we are ignoring here a slight shift of the acceptor level as a result of the system of equations (27)]. Substituting Eq. (30) into Eq. (29), we obtain

$$|A_0|^2 = \frac{\Gamma}{2\pi} \left(E^2 + \frac{\Gamma^2}{4} \right)^{-1}. \quad (32)$$

We can see from Eqs. (30) and (32) that the quantity Γ represents the width of the resonant scattering, whereas the quantity $\hbar/\Gamma$ is the lifetime of a charged acceptor which decays into an electron and a neutral acceptor.

Since we are considering the interaction with the ground state of an acceptor, Eq. (30) corresponds to the phase of a partial wave with the momentum $F = 3/2$ and the parity $I = 1$. All other phases vanish in this approximation. An expression for the scattering amplitude expressed in terms of phases is obtained in Ref. 6 for a zero-gap semiconductor. In the case under discussion we have

$$f_{\mu\mu'} = \frac{1}{2^{5/2} ip} (e^{2i\Delta} - 1) e^{i\mu\varphi/2} (1 + 4\mu\mu' \cos\theta)^{1/2} (1 - 12\mu\mu' \cos\theta), \quad (33)$$

where $f_{\mu\mu'}$ is the amplitude of the scattering of an electron from a state with a helicity μ to a state with a helicity μ', whereas φ and θ are the scattering angles. The integral scattering cross section is

$$\sigma(E) = \frac{2\pi\Gamma^2}{p^2} \left[E^2 + \frac{\Gamma^2}{4} \right]^{-1}. \quad (34)$$

The value of Γ for an acceptor in its ground state can be expressed in terms of the function $f(p)$ which satisfies Eq. (19). This can be done by substituting Eq. (18) into Eqs. (22) and (25) and by assuming that $F = 3/2$ and $I = 1$. Since the electron wavelength is considerably greater than the radius of an acceptor state, it follows that we can simplify the function $\varphi_\nu^{(e)}(\mathbf{r}, \varepsilon)$ by substituting $r = 0$. This gives

$$V_0 = \frac{e^2}{\varkappa (2\pi)^{1/2}} \int \frac{d^3q}{q^2} f(q) \varphi_\nu^{(e)*}(0, |E_0|) \chi_M, \quad (35)$$

where ν includes $F = 3/2$, $I = 1$, as well as the number M which is the same as for χ_M. Using Eq. (19), we obtain

$$\frac{\Gamma}{2} = \pi |V_0|^2 = \pi^2 (2m_e)^{3/2} |E_0|^{5/2} f^2(0). \quad (36)$$

The variational function f obtained in Ref. 5 yields

$$\Gamma/2|E_0| = 4(m_e/m_h)^{3/2}. \quad (37)$$

We shall show in the Appendix that quasidiscrete one-electron states representing a solution of the Luttinger Hamiltonian with a Coulomb center have a width Γ which is identical with Eq. (36).

4. NONRESONANT SCATTERING OF ELECTRONS BY A NEUTRAL ACCEPTORS

When nonresonant scattering is considered, it is necessary to include in the Hamiltonian the term $\psi^{(e)+} V \psi^{(e)}$ which describes the interaction of an electron with a charged acceptor, the term

$$-\frac{e^2}{\varkappa} \int \frac{d^3r_1 d^3r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_\alpha^{(e)+}(\mathbf{r}_1) \psi_\alpha^{(e)}(\mathbf{r}_1) \psi_\beta^{(h)+}(\mathbf{r}_2) \psi_\beta^{(h)}(\mathbf{r}_2),$$

describing the direct Coulomb interaction of an electron with a hole, and the term

$$\frac{e^2}{\varkappa} \int \frac{d^3r_1 d^3r_2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_\alpha^{(e)+}(\mathbf{r}_1) \psi_\beta^{(e)}(\mathbf{r}_2) \psi_\alpha^{(h)+}(\mathbf{r}_1) \psi_\beta^{(h)}(\mathbf{r}_2),$$

describing the exchange interaction. The operators $\psi^{(h)}$ should be substituted in the form of an expansion given by Eq. (11) and an allowance should be made for the fact that an acceptor is in the ground state. Then, if the electron energy is not affected by the scattering, Eq. (11) consists only of the sum over M.

As a rough approximation the effective potential acting on an electron is equivalent to a potential well of size of the acceptor radius a_h and of depth of the order of the binding energy $|E_0|$. We shall confine ourselves to an estimate of the cross section for the scattering of slow electrons, which is characterized by $pa_h\hbar^{-1}\ll 1$. This estimate can be obtained within the framework of the Born approximation or from the results of Ref. 6. We thus obtain

$$\sigma=ca_h^2(m_e/m_h)^2, \tag{38}$$

where c is a numerical factor which requires detailed calculation.

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APPENDIX

We shall consider the problem of determination of the width of resonance levels of an acceptor in the one-electron approximation. The Schrödinger equation for two energy bands differing in respect of the sign of the mass is

$$\left[\frac{p^2}{2m_e}\Lambda^{(e)}(\mathbf{p})-\varepsilon_h(p)\Lambda^{(h)}(\mathbf{p})+\frac{e^2}{\varkappa r}-E\right]g=0. \tag{A.1}$$

When the mass ratio is $m_e/m_h\ll 1$, the width of a resonance level can be explained in terms of the wave function of a hole at an acceptor, obtained in the limit $m_e/m_h\to 0$. We shall do this by representing the wave function in the form

$$g=g^{(h)}+g^{(e)},\quad g^{(h)}=\Lambda^{(h)}g,\quad g^{(e)}=\Lambda^{(e)}g. \tag{A.2}$$

The equations for $g^{(h)}$ and $g^{(e)}$ are

$$(\varepsilon_h(p)+E)g^{(h)}-\Lambda^{(h)}(\mathbf{p})\frac{e^2}{\varkappa r}g=0, \tag{A.3}$$

$$\left(\frac{p^2}{2m_e}-E\right)g^{(e)}+\Lambda^{(e)}(\mathbf{p})\frac{e^2}{\varkappa r}g=0. \tag{A.4}$$

If $m_e/m_h\ll 1$, we have $g^{(e)}\ll g^{(h)}$. In the zeroth order with respect to m_e/m_h, the function $g^{(h)}$ is identical with the function $\varphi^{(0)}$ which was determined earlier and which can be found from Eq. (12) (in the same way as the resonance level position). The function $g^{(e)}$ can be found from Eq. (A.4). Substituting it in Eq. (A.3), we can deduce the width from the imaginary part of the equation:

$$\frac{\Gamma}{2}=\frac{\pi e^4}{\varkappa^2}\int d^3r\varphi^0(r)\cdot\frac{1}{r}\Lambda^{(e)}(\mathbf{p})\delta\left(\frac{p^2}{2m_e}-|E_0|\right)\frac{1}{r}\varphi^0(r). \tag{A.5}$$

According to Eq. (18), the function $\varphi^{(0)}$ can be expressed in terms of the function $f(g)$, which satisfies Eq. (19). In this way we obtain

$$\frac{\Gamma}{2}=\frac{2}{(2\pi)^3}\left(\frac{e^2}{\varkappa}\right)^2\int d^3p_1\,d^3p_2\,d^3p f(p_1)f(p_2)(\mathbf{p}-\mathbf{p}_1)^{-2}$$
$$\times(\mathbf{p}-\mathbf{p}_2)^{-2}\delta\left(\frac{p^2}{2m_e}-|E_0|\right)\chi_M^*\Lambda^{(h)}(\mathbf{p}_1)\Lambda^{(e)}(\mathbf{p})\Lambda^{(h)}(\mathbf{p}_2)\chi_M. \tag{A.6}$$

In the integral with Eq. (A.6), we have $p_1\sim p_2\sim\hbar/a_h\gg p\sim(m_e|E_0|)^{1/2}$. Ignoring p compared with p_1 or p_2, we obtain

$$\frac{\Gamma}{2}=\frac{e^4}{4(2\pi)^3\varkappa^2}\int d^3p\,\delta\left(\frac{p^2}{2m_e}-|E_0|\right)\left(\int\frac{d^3q}{q^2}f(q)\right)^2. \tag{A.7}$$

The integral in Eq. (A.7) is related to $f(0)$ by

$$\int\frac{d^3q}{q^2}f(q)=\frac{4\pi^2\varkappa}{e^2|E_0|}f(0). \tag{A.8}$$

Substitution in Eq. (A.7) gives Eq. (36).

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