Resonant scattering in gapless semiconductors

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The resonant scattering of an electron by a neutral acceptor in a gapless semiconductor is analyzed. The resonant scattering can be regarded as the capture of an electron by a neutral acceptor, followed by a decay of the charged acceptor into a neutral acceptor and an electron. The calculation of the effective scattering cross section must allow for inelastic scattering, which causes the quantum states of the neutral acceptor and of the electron to differ from those before the scattering. The Breit-Wigner expression is valid for the total scattering cross section.

1. The theory of acceptor states in gapless semiconductors is distinguished by the circumstance that there is unavoidably an acceptor level in the conduction band (Fig. 1). In the conventional approach,[1] the wave equation is solved in the effective-mass approximation with the Luttinger Hamiltonian and with the potential of a negative nucleus. The solutions are classified on the basis of the total angular momentum F, its projection M, and the parity I. We denote this set of three numbers by ν. At energies ε corresponding to the conduction band, the wave functions far from the nucleus oscillate as $\sin(kr+\delta_\nu)/r$, where $\hbar k=(2m_e\varepsilon)^{1/2}$, m_e is the effective mass of the electron, and δ_ν is the scattering phase shift. The acceptor levels $E_{\nu n}$ are characterized by the principal quantum number n in addition to the numbers ν. The levels are manifested in an energy dependence of the phase shift δ_ν which is characteristic of resonant scattering:

$$\delta_{\nu n}=\operatorname{arctg}\frac{\Gamma}{2(\varepsilon+E_{\nu n})}, \tag{1}$$

where Γ is the level width, and the energies $E_{\nu n}$ are assumed negative. This is the basis for the decay model of the acceptor state.[1]

We showed in Ref. 2 that the conventional model actually incorporates states with several charges at the acceptor and is disrupted by the electron-electron interaction. When this interaction is taken into account, it turns out that the state of the neutral acceptor is stable. The positive charge around the negative nucleus is at a distance on the order of the Bohr radius a_h, with the effective mass m_h of the valence band; it cannot go off to infinity. A charged acceptor, in contrast, is in a decaying state: A negative nucleus in a gapless semiconductor causes the spontaneous creation of an electron-hole pair; the electron goes off to infinity, while the hole localizes near the acceptor, converting the latter into a neutral acceptor. If an acceptor can bind two holes, spontaneous creation of two pairs will occur, and a positive charged acceptor will appear. If there is such a state, then it will, strictly speaking, be the ground state of the system.

In many regards this problem is analogous to that of superheavy nuclei in vacuum.[3] If an electron state lies in the position band, two electron-positron pairs will be created spontaneously, and electrons will localize near the nucleus, although the one-electron wave functions are again oscillatory far from the nucleus in this problem. Because of the large nucleus charge, the spatial distribution of the electron charge for a nucleus with localized electrons can be found by ignoring the electron-electron interaction. In the positron-scattering problem, however, we should solve the problem of the electron-positron field with an interaction.[4] In the acceptor problem, the electron-electron interaction is important even in finding the ground state. Another important distinction between these problems is that the masses of the electron and the hole are distinctly different in the acceptor problem: $m_e/m_h \ll 1$. It is essentially this condition which makes it possible to solve the problem.

The decay of charged acceptor is closely related to the resonant scattering of an electron by a neutral acceptor. We analyzed this question in Ref. 2, but made an error: We assumed that the scattering cross section could be calculated from the phase shift of the one-electron function. This approach loses the inelastic pathways. Resonant scattering may be thought of as the capture of an electron by a neutral acceptor, followed by the decay of the resulting charged acceptor into a neutral acceptor and an electron in quantum states different from those before the scattering. As we will show below, these processes influence the width of the resonant-scattering line. In §2 we analyze in detail the factors which cause all of these processes to be lost if we restrict the analysis to the solution of the Luttinger equation.

2. Electron and hole creation and annihilation operators a_ν^+, a_ν and $b_{\nu n}^+$, $b_{\nu n}$ were introduced in Ref. 2. The Hamiltonian is

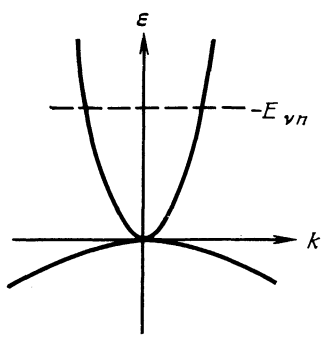

FIG. 1. Band diagram of a gapless semiconductor. The dashed line is an acceptor level.

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$$H=\sum_{\nu}\int_{0}^{\infty}d\varepsilon\varepsilon a_{\nu}^{+}(\varepsilon)a_{\nu}(\varepsilon)+\sum_{\nu n}E_{\nu n}b_{\nu n}^{+}b_{\nu n}$$

$$+\sum_{\nu n}\int_{0}^{\infty}d\varepsilon[V_{\nu n}a_{\nu}^{+}(\varepsilon)b_{\nu^{*}n}+V_{\nu n}^{*}b_{\nu^{*}n}^{+}a_{\nu}(\varepsilon)]+H_{ee}. \quad (2)$$

Here the $E_{\nu n}$ are the energies of the holes localized at an acceptor. All are negative. The continuous spectrum of holes can be ignored. The matrix elements $V_{\nu n}$ were written in Ref. 2; ν^{*} differs from ν in the replacement of M by $-M$. The operators a and b satisfy the standard commutation relations for fermions. The operator (Z) representing the charge of the electron-hole system minus the charge of the completely filled valence band is

$$Z=e\left[\sum_{\nu n}b_{\nu n}^{+}b_{\nu n}-\sum_{\nu}\int_{0}^{\infty}d\varepsilon a_{\nu}^{+}(\varepsilon)a_{\nu}(\varepsilon)\right], \quad (3)$$

where e is the magnitude of the electron charge. As was shown in Ref. 5 (see also Ref. 2), a calculation of $E_{\nu n}$ must incorporate the circumstance that the electron-electron interaction renormalizes the hole spectrum. The other terms of the interaction operator are incorporated in H_{ee}. For the analysis below it is sufficient to consider the terms of "Hubbard" form,

$$H_{ee}=\sum_{\nu n\neq\nu' n'}U_{\nu n,\nu' n'}b_{\nu n}^{+}b_{\nu n}b_{\nu' n'}^{+}b_{\nu' n'}, \quad (4)$$

where all the elements of the matrix U are positive.

In semiconductors in which an acceptor level is in the energy gap, the states of the neutral acceptor are described by the function $b_{\nu n}^{+}|0\rangle$, where the state $|0\rangle$ is determined by the condition

$$a_{\nu}|0\rangle=b_{\nu n}|0\rangle=0. \quad (5)$$

It can be seen from (3) that the electron charge Z of the state $b_{\nu n}^{+}|0\rangle$ is $+1$. The coordinate wave functions were found in Ref. 2; they are localized near the acceptor, so that the negative charge of the acceptor is neutralized by the charge of a hole at a distance on the order of the Bohr radius of the hole.

In a gapless semiconductor, in contrast, these states are solutions of a Schrödinger equation if we ignore the electron-electron interaction. By virtue of the third term in Hamiltonian (2), the state $b_{\nu n}^{+}|0\rangle$ is at resonance with states of the type

$$\sum_{\nu'}a_{\nu'}^{+}(E_{\nu' n'})b_{\nu^{*}n^{*}}^{+}b_{\nu n}^{+}|0\rangle \quad (6)$$

and with other states which are found through the creation of electron-hole pairs. Since the Hamiltonian of the effective-mass method ignores the interaction of holes at the acceptor, states of the type in (6) have the same energy as $b_{\nu n}^{+}|0\rangle$. For this reason, the states $b_{\nu n}^{+}|0\rangle$ are not solutions of the equation of the effective-mass method in a gapless semiconductor.

As we showed in Ref. 2, incorporating the electron-electron interaction has the consequence that the states $b_{\nu n}^{+}|0\rangle$ describe a neutral acceptor in a gapless semiconductor. The repulsion of holes at an acceptor causes states of the type (6) to deviate from the resonance, so that a state $b_{\nu n}^{+}|0\rangle$ satisfies the Schrödinger equation to within small terms of order m_e/m_h.

We now consider the form of the solutions of the Luttinger equation with a Coulomb center for a gapless semiconductor in the second-quantization representation. For this purpose we should diagonalize Hamiltonian (2), ignoring the term H_{ee}. The eigenfunction of the Hamiltonian can be written

$$\Phi_{\nu n}=\left[\int_{0}^{\infty}A_{\nu n}(\varepsilon)a_{\nu}^{+}(\varepsilon)d\varepsilon+B_{\nu n}b_{\nu n}\right]\Phi_{0}, \quad (7)$$

where the function

$$\Phi_{0}=\prod_{\nu n}b_{\nu n}^{+}|0\rangle \quad (8)$$

corresponds to a state in which all the levels of the acceptor are filled with holes. We should print out immediately that such a state is meaningless when we take the repulsion of the holes into account.

The equation $H\Phi_{\nu n}=E\Phi_{\nu n}$ has a solution for all energies. The energy E is conveniently measured from the eigenvalue corresponding to the function Φ_0. The coefficients $A_{\nu n}$ and $B_{\nu n}$ are easily determined under the condition that the energy E is close to that of one of the levels $-E_{\nu n}$. The coefficient $B_{\nu n}$, thought of as a function of E, represents a Lorentz contour centered at $E=-E_{\nu n}$. The width of this contour,

$$\Gamma_{\nu n}=2\pi|V_{\nu n}|^{2} \quad (9)$$

contains the small parameter of the problem, $(n_e/m_h)^{3/2}$, and is much smaller than the distance between levels. Consequently, only a single level is incorporated in expression (7).

States (7) were actually also found in Ref. 1 through a solution of the Luttinger equation in coordinate space. It is important to note that these states are characterized by quantum numbers F, M, I, n. When the operator H acts on $\Phi_{\nu n}$, particles with $\nu'\neq\nu$, $n'\neq n$ are not created since all the hole states with $\nu'\neq\nu$, $n'\neq n$ are filled. Far from the center, the coordinate wave functions oscillate; their phase shift $\delta_{\nu n}$ is related to the width Γ by the ordinary relation for resonant scattering [relation (1)]. We used these phase shifts in Ref. 2 to calculate the cross section for the resonant scattering of an electron by a neutral acceptor. As we have already mentioned here, that approach is incorrect. Actually, an electron can undergo changes in quantum numbers ν during resonant scattering, and this possibility must be taken into account in a calculation of the scattering cross section. This phenomenon cannot be taken into account in the equations of the effective-mass method.

3. We now consider the resonant scattering of an electron by a neutral acceptor. We seek the wave function in the form

$$\Phi=A|0\rangle+\sum_{\nu n}\int_{0}^{\infty}d\varepsilon C_{\nu n}(\varepsilon)a_{\nu}^{+}(\varepsilon)b_{\nu^{*}n}^{+}|0\rangle, \quad (10)$$

where A and $C_{\nu n}$ are coefficients determined by the Schrödinger equation $H\Phi=E\Phi$. Using (2), we find

$$(\varepsilon+E_{\nu n}-E)C_{\nu n}(\varepsilon)+V_{\nu n}A=0, \tag{11}$$

$$\sum_{\nu n}\int_0^\infty d\varepsilon V_{\nu n}(\varepsilon)C_{\nu n}(\varepsilon)-EA=0. \tag{12}$$

From (11) we find

$$C_{\nu n}(\varepsilon)=\{(E-\varepsilon-E_{\nu n})^{-1}+z_{\nu n}\delta(E-\varepsilon-E_{\nu n})\}V_{\nu n}(\varepsilon)A, \tag{13}$$

and from (12) we find an equation for $z_{\nu n}$:

$$\sum_{\nu n}\left\{\int d\varepsilon\frac{|V_{\nu n}(\varepsilon)|^2}{E-\varepsilon-E_{\nu n}}+|V_{\nu n}(E-E_{\nu n})|^2 z_{\nu n}\right\}=E. \tag{14}$$

We restrict the analysis below to states with a total angular momentum $F=3/2$. This is the angular momentum of the ground state of the acceptor. Furthermore, the matrix elements $V_{\nu n}$ reach a maximum at $F=3/2$. For other values of the angular momentum, these matrix elements contain additional powers of m_e/m_h. Equations (10)–(14) can be used to find the electron scattering amplitude. We assume that the neutral acceptor is in the state $\nu_0 n_0$ before the scattering. The coordinate wave function of the electron in the scattering pathway in which the acceptor is in state ν, n after the scattering is

$$\int_0^\infty d\varepsilon C_{\nu n}(\varepsilon)\varphi_\nu^{(e)}(\varepsilon,\mathbf{r}), \tag{15}$$

where $C_{\nu n}$ is determined by (13), and $\varphi_\nu^{(e)}(\varepsilon,\mathbf{r})$ is the wave function of the free electron, given by expression (22) of Ref. 2. According to Ref. 2, at large values of r we have

$$\varphi_\nu^{(e)}(\varepsilon,\mathbf{r})\propto \sin kr/r\sqrt{k},\qquad \hbar k=(2m_e\varepsilon)^{1/2}.$$

It can be seem from (22) and (35) of Ref. 2 that $V_{\nu n}(\varepsilon)\propto k$. It follows that (15) has an integral of the type

$$\int_0^\infty d\varepsilon \sin kr[(E-\varepsilon-E_{\nu n})^{-1}+z_{\nu n}\delta(E-\varepsilon-E_{\nu n})]$$
$$=z_{\nu n}\sin p_{\nu n}r-\pi\cos p_{\nu n}r, \tag{16}$$

where the wave vector is

$$p_{\nu n}=\hbar^{-1}(2m_e(E-E_{\nu n}))^{1/2}\approx\hbar^{-1}(-2mE_{\nu n})^{1/2},$$

since for resonant scattering we have $|E|\ll|E_{\nu n}|$.

If we are dealing with an inelastic pathway, $\nu\neq\nu_0$ or $n\neq n_0$, the wave function at large r must be of the form

$$f_{\nu_0 n_0}^{\nu n}\frac{\exp(ip_{\nu n}r)}{r}\delta_{\mu M_0}, \tag{17}$$

where f is the amplitude for inelastic scattering. It follows from (16) and (17) that

$$z_{\nu n}=-\pi i, \tag{18}$$

where $\nu\neq\nu_0$ or $n\neq n_0$. This is the condition that there be no incoming waves in the inelastic pathways. The phase shift $z_0\equiv z_{\nu_0 n_0}$ can be found from Eq. (14). The first term of this equation describes the renormalization of the energy of the acceptor levels and can be ignored. Furthermore, in examining resonant scattering we may assume $|E|\ll -E_{\nu n}$; we then have

$$z_0=\frac{2\pi E}{\Gamma}+2\pi^2 i\sum_{\nu n}{}'\frac{|V_{\nu n}|^2}{\Gamma}, \tag{19}$$

where Γ is determined by (6) with $\nu=\nu_0$ and $n=n_0$. The prime on the summation sign means that the term $|V_{\nu_0 n_0}|^2$ is excluded. The argument of $V_{\nu n}$ is $E_{\nu n}$.

In an elastic pathway the wave function at large r must be of the form

$$e^{ipz}\chi_z(\mu)+\delta_{\mu M_0}f_{\nu_0 n_0}^{\nu n}\frac{\exp(ipr)}{r}, \tag{20}$$

where $\chi_z(\mu)$ is the eigenfunction of the operator I_z with the eigenvalue $\mu=\pm 1/2$. If $M_0=\pm 3/2$, an electron with momentum along z does not undergo resonant scattering.

Using (15) with $\nu=\nu_0$ and $n=n_0$; with the explicit expression for $\varphi_\nu^{(e)}(\varepsilon,\mathbf{r})$; and with Eqs. (16), (19), and (20), we can find the coefficient A and the scattering amplitude. The result is

$$f_{\nu_0 n_0}^{\nu n}=-\frac{V_{\nu n}}{V_{\nu_0 n_0}}\frac{2\pi^{3/2}}{(z_0+\pi i)(pp_{\nu n})^{1/2}}[\Psi_{\nu l_1}+\Psi_{\nu l_2}], \tag{21}$$

The $\hbar p$ is the momentum of the incident electron. The ground state of the acceptor corresponds to $I=1$, $l_1=0$, $l_2=2$. The normalized angular wave functions are

$$\Psi_{\nu l}=2\sum_{m\mu}(-1)^{l+M-3/2}\begin{pmatrix} l & 3/2 & 3/2\\ m & \mu & -M\end{pmatrix}Y_{lm}(\theta,\varphi)\chi_z(\mu), \tag{22}$$

where $\mu=\pm 3/2$, $\pm 1/2$, and θ and φ are the scattering angles. The total cross section for elastic scattering is

$$\sigma^e=\int d\Omega|f_{\nu_0 n_0}^{\nu_0 n_0}|^2=\frac{2\pi\Gamma^2}{p^2(E^2+\Gamma_t^2/4)},$$

$$\Gamma_t=2\pi\sum_{\nu n}|V_{\nu n}|^2,\qquad \Gamma=2\pi|V_{\nu_0 n_0}|^2, \tag{23}$$

where Γ_t is the total width, and Γ the elastic width.

The integrated cross section for scattering accompanied by a transition to the state νn is

$$\sigma_{\nu n}=\frac{(2\pi)^2|V_{\nu n}|^2\Gamma}{p^2(E^2+\Gamma_t^2/4)}, \tag{24}$$

and the total cross section is

$$\sigma^t=\frac{2\pi\Gamma\Gamma_t}{p^2(E^2+\Gamma_t^2/4)}. \tag{25}$$

Expressions (23)–(25) are the standard Breit-Wigner expressions for the case with inelastic scattering pathways (§142 in Ref. 6).

The coefficient A in (10) can be found by normalizing the function $\Phi(E)$ by means of the condition

$$\Phi^+(E)\Phi(E')=\delta(E-E'). \tag{26}$$

We find

$$A(E)=\frac{\Gamma}{2\pi(E^2+\Gamma_t^2/4)}. \tag{27}$$

From this study we conclude that the Luttinger equation can be used only to find the energy of an impurity state in a gapless semiconductor in the lowest approximation in m_e/m_h. The electron-electron interaction must be taken

into account in order to calculate the wave functions and the decay time of a charged acceptor into a neutral acceptor and an electron.

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