Scattering of slow electrons by centers with Coulomb and short-range potentials

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A calculation is reported of the amplitude and cross section for the scattering of electrons with wave vector k ($ka_0 \ll 1$) by two centers separated by a distance $R \gg a_0$, where a_0 is the Bohr radius. One of these centers has a Coulomb potential (attractive or repulsive) and the other has a short-range δ-function potential[1]. It is shown that, when $k^2Ra_0/2 \ll 1$, so that the wave function of the electron in the Coulomb field differs appreciably from a plane wave (see Refs. 6 and 7), the scattering amplitude due to the δ-function potential in the attractive Coulomb field, $f^c(R)$, is substantially greater in absolute magnitude than the corresponding free-electron amplitude f_δ (Ref. 1). As k is reduced, the ratio $|f^c(R)|/|f_\delta|$ is found to increase in proportion to k^{-1}. The dependence of $f^c_\delta(R)$ on the angle between the vectors **k** and **R** and on the scattering angle is investigated. The relation between $f^c_\delta(R)$ and the Born scattering amplitude is found. It is shown that the change in the scattering amplitude due to the δ-function center at distances $R \gg a_0$ from the Coulomb center may be detectable experimentally in weakly-doped semiconductors at low temperatures at which it gives rise to an increase in the electron scattering and trapping cross section of small neutral impurities located near attracting centers.

1. This paper is devoted to the determination of the scattering amplitude and cross section for electrons interacting with a system of two centers (a pair) separated by a distance R. It is assumed that one of the centers has a purely Coulomb (attractive or repulsive) potential $V_1 r)$, whereas the potential $V_2(r)$ of the second center has a decay length a that is much smaller than the de Broglie wavelength of the electron, i.e., $V_2(r)$ is a short-range potential. The interaction of an electron with the second center will be treated within the framework of the zero-range model potential (δ-function potential),[1] and we shall refer to the second center as the δ-center. We shall concentrate our attention on slow electrons with wave vectors $k = \hbar^{-1}(2mE)^{1/2}$ satisfying the condition

$$ka_0 \ll 1, \tag{1}$$

where a_0 is the Bohr radius ($a_0 > a$) and E is the energy of the electron. The scattering amplitude will be calculated for the pair in the case where the separation R between the Coulomb and δ-centers is large:

$$R/a_0 \gg 1, \tag{2}$$

but has the upper bound

$$R \ll R_k \equiv 2/k^2a_0 = 2a_0(E_0/E), \tag{3}$$

where E_0 is the ionization energy of the Coulomb center in its ground state.

2. An example of a system for which the present results may be relevant is a semiconductor with donor density $N_D \ll a_0^{-3}$ and low degree of compensation.[1)] In equilibrium, at temperatures T such that $T_1 \leqslant T \leqslant E_0$, where $T_1 = 2E_0 N_D^{1/3} a_0$, the density N_+ of positively charged donors is approximately equal to the density N_- of negatively charged acceptors, and both are much smaller than the density N_0 of neutral donors. Charged donors D^+ and acceptors A^- are then located at distances $\sim R_+ \equiv N_+^{-1/3}$ and $\sim R_- \equiv N_-^{-1/3}$ from one another. The centers D^+ and A^- are also separated by distances $\sim R_+$ when, for $T \ll T_1$, external illumination of sufficient intensity is present.[3] In such cases, a sphere of radius $\sim R_+$ around each charged center contains $\sim N_0/N_+ \gg 1$ neutral donors characterized, by analogy with the hydrogen atom, by a short-range potential.[3] The interior of this sphere is then dominated by the Coulomb potential of "its own" charged center which forms pairs of size R with neutrals, where $R_0 \lesssim R \lesssim R_+$ and $R_0 = N_0^{-1/3}$. We shall suppose that electrons are mostly scattered by neutral impurities and partly by charged impurities. It is commonly assumed that these scattering mechanisms are independent, and the mobility is found by calculating the individual scattering cross sections of the Coulomb and neutral centers.[4,5] Our results show that, for electrons of low enough energy, the scattering amplitude and cross section, obtained for a center of small radius at a large but bounded [see (2) and (3)] distance from the Coulomb center, are substantially different from the corresponding amplitude and cross section in the absence of the Coulomb center.[1,4,5] This difference is due to the influence of the Coulomb potential on the electron wave function near the center with the short-range potential. The consequence of this is that the magnitude and energy dependence of the scattering cross section of neutral impurities turn out to depend on the presence of charged impurities. The question of applications of our results will be examined in greater detail at the end of this paper.

We note that, in the literature, the scattering of particles with wave vector $k \ll a^{-1}$ by a Coulomb and a short-range potential has been considered only on the assumption that $R = 0$, i.e., when the potentials originate at the same point,[6–8] so that the scattering system has spherical symmetry. The analysis given under these conditions in Refs. 6 and 7 was concerned with the scattering of protons by protons, whereas Ref. 8 was concerned with scattering of electrons in semiconductors by deep (nonhydrogenlike) impurities. In the discussion given below, we shall briefly investigate the general expressions for the scattering amplitude (17), (18) in

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the special case when $R=0$. The scattering of electrons by systems which, as in our case, are not spherically symmetric (several δ-centers or two oppositely charged Coulomb centers, i.e., a dipole) has been investigated in several papers. They are reviewed in Ref. 9.

The distance R_k and the inequality given by (3) have a simple physical interpretation: At $r=R_k$, the potential energy of the electron in the Coulomb field $V_1(r)$ is equal in absolute magnitude to its total energy, so that R_k is the classical turning point.[1,7] In other words, the δ-center lies in the interval of distances in which the motion of electrons in the Coulomb field is essentially different from free motion. We note that inequalities (1) and (2) are actually the conditions for the validity of the quasiclassical approximation to the motion of particles in a Coulomb field at distances R from the Coulomb center.[7]

3. The basic results of the present paper relate to the total amplitude f^c for the scattering of electrons by a δ-center at a large but bounded distances from the Coulomb center [see (2) and (3)]. We shall show that, generally speaking, f_δ^c depends on R, the angle of scattering ϑ, and the angle β between the wave vector $\mathbf{k}$ of the incident electron and the vector $\mathbf{R}$ (the origin lies at the Coulomb center and the δ-center lies at the point $r=R$; see Fig. 1). In an attractive field, the modulus $|f_\delta^c|$ is then much greater than the modulus $|f_\delta|$ of the amplitude for the scattering of a free electron by a δ-center.[1] For example, for small angles β and $\vartheta\simeq\pi$ (backward scattering), we have $|f_\delta^c|/|f_\delta|\sim(2\pi/ka_0)\gg1$. When $\beta\ll1$ and $\vartheta\ll1$ (forward scattering), the ratio is

$$|f_\delta^c|/|f_\delta|\sim(2\pi/ka_0)^{1/2}(2/k^2Ra_0)^{1/4}\gg1.$$

Finally, for large angles β, we have

$$|f_\delta^c|/|f_\delta|\sim(2/k^2Ra_0)^{1/2}\gg1.$$

This means that the presence of an attractive Coulomb center produces a change in the energy dependence and an increase in the amplitude of scattering by the δ-center located far from the attractive center. There is also a corresponding change in the energy dependence of the differential and total cross sections of the δ-center. Moreover, the amplitude and cross section become functions of R. In a repulsive field, the ratios of the moduli of the amplitude contain the further factor $\exp(-\pi/ka_0)$ and are small. In other words, scattering by the δ-center is, in this case, completely masked by Coulomb repulsion. This is in qualitative agreement with the results obtained in Refs. 6 and 7 (Section 138 of the latter) in the case of scattering by equally charged particles for $R=0$.

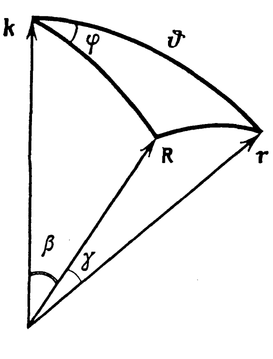

FIG. 1

The change in the scattering amplitude of the δ-center in a Coulomb field is actually due to the fact that the free-electron Coulomb wave function $\psi_k^+(r)$ corresponding to wave vector k satisfying (1) is very different from a plane wave both for $r=0$ and for the distances defined by (2) and (3). Thus, in the case of the attractive fields, the ratio of the moduli of these functions for $r=0$ is[7]

$$|\psi_k^+(0)|/|\psi_k(0)|=u_1\approx(2\pi/ka_0)^{1/2}. \tag{4}$$

For distances $R>0$, and bounded in accordance with (3), the ratio of the moduli is

$$\frac{|\psi_k^+(\mathbf{R})|}{|\psi_k(\mathbf{R})|}=u_2\approx\left(\frac{2\pi}{ka_0}\right)^{1/2}J_0\left[\left(\frac{8R}{a_0}\right)^{1/2}\sin\frac{\beta}{2}\right] \tag{5}$$

(J_0 is the zero-order Bessel function). In the case of the repulsive field, the ratios given by (4) and (5) acquire the additional factor $\exp(-\pi/ka_0)$, which ensures that the scattering amplitude is reduced.

4. Henceforth, we shall use Coulomb units. Let the electron wave function be denoted by $\varphi_k(r)$. It satisfies the Schrödinger equation

$$\left(-\frac{1}{2}\nabla^2+\frac{\alpha}{r}-E\right)\varphi_k(\mathbf{r})=-2\pi L\delta(\mathbf{r}-\mathbf{R})\frac{\partial}{\partial\rho}(\rho\varphi) \tag{6}$$

with boundary condition[1,10,11]

$$\frac{1}{\rho\varphi}\frac{\partial}{\partial\varphi}(\rho\varphi)_{\rho\to0}=-\frac{1}{L}\equiv-\varkappa,\quad \rho=|\mathbf{r}-\mathbf{R}|. \tag{7}$$

In Eqs. (6) and (7), L is the scattering length for an electron incident on a small-radius center. It is considered to be positive when the electron forms a bound state with the well (negative ion), and negative in other cases.[10] The parameter α is equal to unity for the repulsive potential and to -1 for an attractive potential.

We shall seek the solution of (6) in the form of the sum

$$\varphi_k(\mathbf{r})=\psi_k^+(\mathbf{r})+A_k(\mathbf{R})G_k(\mathbf{r},\mathbf{R}), \tag{8}$$

where $\psi_k^+(r)$ is the Coulomb wave function of the continuous spectrum, corresponding to a plane wave and a diverging spherical wave at infinity, $G_k(r,R)$ is the Coulomb Green's function corresponding to the diverging wave $\exp(ikr)/r$ at infinity, and the factor $A_k(R)$ is determined by the boundary condition (7). Substituting (8) in (7), and recalling that $G_k(r,R)\to1/2\pi|r-R|$ as $\mathbf{r}\to\mathbf{R}$, we obtain

$$A_k(\mathbf{R})=-\frac{2\pi\psi_k^+(\mathbf{R})}{\varkappa+\Lambda_k(R)}, \tag{9}$$

where

$$\Lambda_k(R)=2\pi\frac{\partial}{\partial\rho}[\rho G_k(\mathbf{r},\mathbf{R})]_{\rho\to0}. \tag{10}$$

In deriving (9), we took into account the fact that $\psi_k^+(r)$ is a continuous function of r as $r\to R$, so that $\rho\partial\psi_k^+/\partial\rho\to0$ for $\rho\to0$.

5. The quantity $A_k(R)$ will now be shown to determine the scattering amplitude. For the moment, we shall not use assumptions (1)–(3). In its contracted form, the Coulomb Green's function is given by (see, for example, Ref. 12)

$$G_k(\mathbf{r},\mathbf{R})=\frac{\Gamma(1-\eta)}{2\pi|\mathbf{r}-\mathbf{R}|}\left(\frac{\partial}{\partial ikx}-\frac{\partial}{\partial iky}\right)W_{\eta,1/2}(-ikx)M_{\eta,1/2}(-iky). \tag{11}$$

where

$$\eta=\alpha/ik,\quad x=r+R+|\mathbf{r}-\mathbf{R}|,$$
$$y=r+R-|\mathbf{r}-\mathbf{R}|,$$

and $W_{\eta,\frac{1}{2}}$, $M_{\eta,\frac{1}{2}}$ are the Whittaker functions.[13] (The subscripts $\eta,\frac{1}{2}$ on the functions W, M and their derivatives W', M' will not, as a rule, be indicated explicitly.) To obtain the scattering amplitude, we expand the expressions for x and y into a series in powers of R/r, and retain only the zero- and first-order terms. We thus obtain

$$G_k(\mathbf{r},\mathbf{R})\approx\frac{1}{2\pi r}\Gamma(1-\eta)\left[W\left(\frac{2r}{\eta}\right)M'\left(\frac{R(1+\cos\gamma)}{\eta}\right)-W'\left(\frac{2r}{\eta}\right)M\left(\frac{R(1+\cos\gamma)}{\eta}\right)\right],\qquad(12)$$

where γ is the angle between the vectors $\mathbf{r}$ and $\mathbf{R}$ (see Fig. 1). The asymptotic forms of W and W' are[13]

$$W\left(\frac{2r}{\eta}\right)\approx e^{-r/\eta}\left(\frac{2r}{\eta}\right)^{\eta}\left(1+\frac{\eta(1-\eta)}{2r/\eta}\right),\qquad(13)$$

$$W'\left(\frac{2r}{\eta}\right)\approx\frac{1}{2}e^{-r/\eta}\left(\frac{2r}{\eta}\right)^{\eta}\left(-1+\frac{\eta(1+\eta)}{2r/\eta}\right).\qquad(14)$$

It is usual in scattering theory (see Ref. 7) to neglect terms $\eta^3/r\sim(k^3r)^{-1}$ and $\eta^2/r\sim(k^2r)^{-1}$. Adopting this approximation, we obtain

$$G_k(\mathbf{r},\mathbf{R})\approx\frac{1}{2\pi r}\Gamma(1-\eta)e^{-r/\eta}\left(\frac{2r}{\eta}\right)^{\eta}B(R,\gamma),\qquad(15)$$

where

$$B(R,\gamma)=M'(R(1+\cos\gamma)/\eta)+{}^1/_2M(R(1+\cos\gamma)/\eta).\qquad(16)$$

Recalling the form of $\psi_k^+(r)$ at large distances,[7] the wave scattered by a Coulomb and a δ-center can be written in the form

$$\varphi_{\mathrm{pacc}}(\mathbf{r})=\frac{1}{r}[f_c(\vartheta)+f_\delta{}^c(\beta,\mathbf{R})]\exp\left(ikr+\frac{i}{k}\ln 2kr\right),\qquad(17)$$

where $f_c(\vartheta)$ is the Coulomb scattering amplitude[7] and the quantity

$$f_\delta{}^c(\beta,R)=-\psi_{\mathbf{k}}{}^+(\mathbf{R})\frac{\Gamma(1-i/k)}{\varkappa+\Lambda_k(R)}\exp\left(\frac{\pi}{2k}\right)B(R,\gamma)\qquad(18)$$

can be referred to as the scattering amplitude for a δ-center located at a distance R from the Coulomb center (cf. Ref. 7). It depends on the angle β between the vectors $\mathbf{k}$ and $\mathbf{R}$ [through the factor $\psi_{\mathbf{k}}^+(\mathbf{R})$] and on the angle γ between the vectors $\mathbf{r}$ and $\mathbf{R}$ [through the factor $B(R,\gamma)$], i.e., the dependence of f_δ^c on the angles β and γ can be factorized. We note that a similar factorization obtains in the Born approximation to the scattering by a δ-center if the "free motion" wave functions are taken to be the Coulomb function $\psi_k^+(\mathbf{r})$ and $\psi_{k'}^-(\mathbf{r})$, where $\psi_k^+(\mathbf{r})$ corresponds to the incident electron, $\psi_{k'}^-(\mathbf{r})$ to the scattered electron, and $|\mathbf{k}|=|\mathbf{k}'|$ (Ref. 7; see below for further details). The dependence on the scattering angle ϑ is implicit and appears through the dependence on γ. In the case of the repulsive field, the wave function is obtained from (17) and (18) by simultaneously reversing the signs of k and r. The function $\psi_{\mathbf{k}}^+(\mathbf{r})$ then describes a divergent wave in the repulsive field.[7] We note once again that (17) and (18) were obtained without using the assumptions (1)–(3). The essential assumption used in deriving them is the replacement of the actual short-range potential $V_2(r)$ with the zero-range potential.

6. Let us now examine some of the general properties of the amplitude f_δ^c. For the moment, we shall not assume the validity of (1)–(3). Let us first find the equation for the poles of the amplitude in the case of the attractive fields. It is clear from (18) that, in this case, the δ-center scattering amplitude, like the Coulomb scattering amplitude $f_c(\vartheta)$, has poles for $k=i/n$, where n is a positive integer, i.e., when the energy coincides with the discrete levels in the Coulomb field.[7] The other family of poles is determined in accordance with (18) and (9), using the equation

$$2\pi\frac{\partial}{\partial\rho}[\rho G_k(\mathbf{r},\mathbf{R})]_{\rho\to0}=-\varkappa.\qquad(19)$$

This equation can be used to determine the bound-state energies $[E(R)<0]$ for an electron in the combined Coulomb and δ-center potentials.[1] There is extensive literature (see for example, Refs. 11, 14, and 15) devoted to the determination of the energies that satisfy (19) and are different from the energies of excited Coulomb states. It investigates in detail the behavior of $E(R)$ for $R\gg a_0$.

Let us now consider f_δ^c in the attractive field in the special case $R=0$. This case was examined formally in Refs. 6–8 by a somewhat different method. Using the expression for $\psi_{\mathbf{k}}^+(0)$ (Ref. 7) and for $G_{\mathbf{k}}(\mathbf{r},0)$ (Ref. 12), and using the behavior of the function M for small values of the argument,[13] we find from (18) and (16) that

$$f_\delta{}^c(\vartheta)=-\frac{2\pi}{k}e^{2i\delta_0^c}\frac{1}{1-e^{-\pi/2k}}\times\left[\varkappa+\frac{\partial}{\partial r}\Gamma\left(1-\frac{i}{k}\right)W_{i/k,{}^1/_2}(-2ikr)\right]^{-1},\qquad(20)$$

where $\delta_0^c=\arg\Gamma(1-i/k)$ is the zero-order scattering phase in the Coulomb field.[2)] If we substitute $k\to-k$ and $r\to-r$, we find that (20) becomes identical with the scattering amplitude obtained in Refs. 6 and 7 for the repulsive field. We draw attention to the fact that, for slow particles with $ka_0\ll1$, the amplitude f_δ^c in the attractive field increases with decreasing k, in accordance with the expression $|f_\delta^c|\sim k^{-1}$, which differs from the behavior in the case of the repulsive field.[6,7] Moreover, if we investigate the equation for the pole of f_δ^c in (20) by the method used in Ref. 6, we can readily verify that the "Coulomb + δ" potential well contains bound states with energies different from those of the Coulomb levels. The equation for the energies of the bound states is identical with that obtained in Ref. 16 by a different method.

7. We shall now find the amplitude for scattering of slow electrons by a δ-center located at a distance R from the Coulomb center. We shall begin with $\Lambda_k(R)$, given by (10), which we shall transform with the aid of the equation for the Whittaker functions. This gives (cf. Refs. 10, 11, and 14)

$$\Lambda_k(R)=2\pi\frac{\partial}{\partial\rho}(\rho G)_{\rho\to 0}=2\frac{\Gamma(1-\eta)}{\eta}$$
$$\times\left\{\left(-\frac{1}{4}+\frac{\eta}{z}\right)W(z)M(z)+W'(z)M'(z)\right\},\quad z=\frac{2R}{\eta}. \tag{21}$$

The function $M(2R/\eta)$ can be written in the form of a series in terms of Bessel functions J_ν (see Ref. 13, p. 265):

$$M_{\eta,1/2}\left(\frac{2R}{\eta}\right)=\left(\frac{2R}{\eta^2}\right)^{1/2}\sum_{n=0}^{\infty}A_n\left(\frac{R}{2\eta^2}\right)^{n/2}J_{n+1}((8R)^{1/2}), \tag{22}$$

where $A_0=1$, $A_1=0$, $A_2=1$, and the remaining A_n $(n\geqslant 3)$ are given by

$$A_{n+1}=A_{n-1}-[2\eta/(n+1)]A_{n-2}.$$

When n is a multiple of three, A_n is a polynomial in η of degree $n/3$. For example, $A_3=-2\eta/3$, $A_4=1$, $A_5=-16\eta/15$, $A_6=1+2\eta^2/9$, and so on.

For simplicity, we shall confine our attention to the first term in (22). This is valid when the inequality

$$\left|\frac{2}{3}\eta\left(\frac{R^2}{2\eta^2}\right)^{3/2}\right|=\left(\frac{2}{9}R\right)^{1/2}\frac{k^2R}{2}\ll 1 \tag{23}$$

is satisfied simultaneously with (2) and (3).

We shall now use the expansion of $W(2R/\eta)$ into a series for large absolute values of η, i.e., for $ka_0\ll 1$. This gives[13]

$$W_{\eta,1/2}(2R/\eta)\approx\Gamma(1/2+\eta)(2R/\eta)^{1/2}(-1)$$
$$\times[\cos\pi\eta J_1((8R)^{1/2})+\sin\pi\eta N_1((8R)^{1/2})], \tag{24}$$

where N_1 is the Neumann function and the terms neglected in (24) are of order[13] $(ka_0)^{1/2}$.

For large values of R [see (2)], we obtain, using the asymptotic form of J_1 and N_1 and neglecting terms $\sim R^{-1/2}$:

$$\Lambda_k(R)\approx 2\pi\,\mathrm{ctg}\,\pi\eta(J_1^2+J_1'^2)\approx(2/R)^{1/2}\,\mathrm{ctg}\,\pi\eta. \tag{25}$$

This expression could also have been obtained from the Green's function for weakly bound states ($E<0$), found in Ref. 17. It is clear from the above calculation that, when $(8R/a_0)^{1/2}\gg 1$, the derivation of (25) involves not only the assumption that $(|E|/E_0)^{1/2}\ll 1$ (see Ref. 17), but also the two conditions given by (3) and (23).

Since $\eta=\alpha/ik$ for small $k\ll a_0^{-1}$ [see (1)], we finally obtain

$$\Lambda_k(R)\approx i\alpha(2/R)^{1/2}. \tag{26}$$

Consequently, the term Λ_k in the denominator of (18) is important only for $|L|\gtrsim(R/2)^{1/2}$.

We shall now write out the remaining factors in the scattering amplitudes (for brevity, only for the attractive fields). When conditions (1), (3), and (23) are satisfied, the function $\psi_k^+(R)$ is proportional to the Bessel function:

$$\psi_{\mathbf{k}}^+(\mathbf{R})\approx\exp(\pi/2k)\Gamma(1-i/k)e^{i\mathbf{kR}}J_0(\sin(\beta/2)(8R)^{1/2}), \tag{27}$$

i.e., its modulus oscillates as R and β vary. Under the same conditions,

$$B(R,\gamma)\approx{}^1/_2\{y_1^{-1/2}J_1(2y_1^{1/2})+J_0(2y_1^{1/2})-J_2(2y_1^{1/2})\}, \tag{28}$$

where $y_1=R(1+\cos\gamma)=2R\cos^2(\gamma/2)$. Finally, when (1)–(3) and (23) are satisfied in the attractive field, we obtain, after transforming to dimensionless units,

$$f_\delta^c(k,R,\beta)$$
$$=-\frac{2\pi}{ka_0}e^{2i\delta_0^c}e^{i\mathbf{kR}}B(R,\gamma)\frac{J_0(\sin(\beta/2)(8R/a_0)^{1/2})}{[\varkappa-ik(2/k^2Ra_0)^{1/2}]}. \tag{29}$$

In the repulsive field, f_δ^c differs from (29) by the factor $\exp(-\pi/ka_0)$ and the replacement $k\to -k$.

8. Let us investigate the dependence of f_δ^c in (29) on R, the electron energy, and the angles β and γ (see figure). This will enable us to exhibit some of the properties of scattering by a δ-center in a Coulomb field.

Let the angle β between the vectors $\mathbf{k}$ and $\mathbf{R}$ be so small that $\beta(2R/a_0)^{1/2}\ll 1$. The function J_0 in (29) is then close to its maximum value, which is of the order of unity, and there are no oscillations. The angle γ is then virtually equal to the scattering angle ϑ. Consider scattering through an angle ϑ close to π and suppose that

$$2R\cos^2(\gamma/2)\approx 2R\cos^2(\vartheta/2)\ll 1,\quad B(R,\gamma)\approx 1$$

[see (28)]. The "backward-scattering" amplitude can then be obtained from (29) in the form

$$|f_\delta^c|=\frac{2\pi}{ka_0}\frac{|L|}{(1+2L^2/Ra_0)^{1/2}}, \tag{30}$$

from which it is clear that, when $Ra_0\gtrsim 2L^2$, the "backward-scattering" amplitude of the δ-center has increased in absolute value by a factor of approximately $(2\pi/ka_0)\gg 1$ as compared with the analogous quantity for a free electron, i.e., $|f_\delta|=|L|/(1+k^2L^2)^{1/2}$. Let us now compare (30) with the modulus of the Coulomb backward-scattering amplitude $|f_c(\pi)|=a_0/2(ka_0)^2$. From (30), we have

$$\frac{|f_\delta^c|}{|f_c(\pi)|}=\frac{4\pi|L|}{a_0}\frac{ka_0}{(1+2L^2/Ra_0)^{1/2}}. \tag{31}$$

The ratio $|L|/a_0$ is usually of the order of a few times unity. For example, for the hydrogen atom, the scattering length in the singlet state is $|L_s|\simeq 6a_0$ (Ref. 1). It is readily seen that, when (1)–(3) are satisfied, the ratio given by (31) may substantially exceed unity in this case.

Let us now suppose that the angle β is small, as before, but the angles γ and ϑ are close to zero, so that $\cos^2(\gamma/2)\simeq 1$, and let us consider forward scattering at small angles. We then have

$$B(R,\gamma)\approx J_0((8R/a_0)^{1/2})$$
$$\approx(2/\pi)^{1/2}(a_0/8R)^{1/4}\cos((8R/a_0)^{1/2}-\pi/4)$$

[see (28)]. From (29), we have

$$|f_\delta^c|=\left(\frac{2\pi}{ka_0}\right)^{1/2}|L|\left(\frac{2}{k^2Ra_0}\right)^{1/4}\frac{|\cos((8R/a_0)^{1/2}-\pi/4)|}{(1+2L^2/Ra_0)^{1/2}}. \tag{32}$$

In this case, the scattering amplitude for a δ-center oscillates rapidly as a function of R/a_0 and vanishes for certain definite values of this ratio. For example, this occurs for $R=R_1=3.8a_0$ and $R=R_2=9.3a_0$. By virtue of (1)–(3), the maximum value of (32) with respect to R is much greater than the free-electron scattering amplitude of a δ-center. The reasons for the appearance of the large factors $u_1=(2\pi/$

$ka_0)^{1/2}$ and $u_2 = (2/k^2Ra_0)^{1/4}$ in the amplitudes were discussed at the beginning of this paper. Here, we note that $u_1/u_2 = (2\pi^2R/a_0)^{1/4} \gg 1$.

Let us now suppose that the angle β is close to π, i.e., the electron is incident from the side of the δ-center. For small values of γ, for which the scattering angle is close to π, we then find from (29) that

$$|f_\delta^c| \approx \left(\frac{2}{k^2Ra_0}\right)^{1/2} \frac{|L|}{(1+2L^2/Ra_0)^{1/2}} \cos^2\left[\left(\frac{8R}{a_0}\right)^{1/2} - \frac{\pi}{4}\right]. \quad (33)$$

In otherwords, the factor u_2 becomes important when the electron does not pass close to the Coulomb center, but is incident on the δ-center and reflected from it. The scattering amplitude then oscillates as a function of R/a_0. We draw attention to the fact that, in contrast to the free-electron scattering amplitude $f_\delta = -L/(1+ikL)$ (Ref. 1), the amplitude f_δ^c increases in absolute magnitude in proportion to $(ka_0)^{-1}$ as ka_0 is reduced.

9. We note that the basic features of $|f_\delta^c|$ given by (30), (32), and (33) can also be obtained by a more graphic method. Thus, let us suppose that the short-range potential $V_2(r)$ is a perturbation producing transitions between states ψ_i and ψ_f in the continuous spectrum of an electron in the Coulomb field. According to Ref. 7 (Section 136), the amplitude for the transition from the state with momentum $\hbar\mathbf{k}$ to the state with momentum $\hbar\mathbf{k}'$ can be obtained by replacing $\psi_i(r)$ with the function $\psi_k^+(r)$ [cf. (27)] and replacing $\psi_f(r)$ with

$$\psi_{\mathbf{k}'}^-(\mathbf{r}) = (\psi_{-\mathbf{k}'}^+(\mathbf{r}))^* = \exp(\pi/2k'a_0)\Gamma(1+i/k'a_0) \times \exp(i\mathbf{k}'\cdot\mathbf{r})\, F(-i/k'a_0, 1, -i(\mathbf{k}'\mathbf{r}+k'r)).$$

This corresponds to the presence of plane and converging spherical waves at infinity. The modulus of the amplitude for a transition in a short-range potential [for example, $V_2(r) = (\hbar^2L/2ma^3)e^{-r/a}$] in the first Born approximation is then given by

$$|f_\delta^c| \approx |L\psi_k^+(\mathbf{R})(\psi_{k'}^-(\mathbf{R}))^*| \approx L(2\pi/ka_0) \times J_0((8R/a_0)^{1/2}\sin(\beta/2))J_0((8R/a_0)^{1/2}\cos(\gamma/2)). \quad (34)$$

The vector $\mathbf{k}'$ in this expression lies along the vector $\mathbf{r}$ (see figure), and we have taken account of the fact that $|\mathbf{k}| = |\mathbf{k}'|$. Formula (34) leads to (30), (32), and (33) for different β and γ, except that the factor $(1 + L^2/Ra_0)^{-1/2}$ is replaced with unity. The reason for this difference is quite clear: the term L^2/Ra_0 in the denominators of (30), (32), and (33) corresponds to the inclusion of the imaginary term in the denominator of the scattering amplitude. This term is not present in the first Born approximation.[18] The factorization of the dependence of $|f_\delta^c|$ on the angles β and γ, mentioned above, is clear from (34), where the dependence on β reflects the behavior of the initial wave function $\psi_{\mathbf{k}}^+(r)$, and the dependence on γ reflects the behavior of the final wave function. The initial and final wave functions are then large for $\beta \to 0$ and $\gamma \to \pi$, respectively. Both functions oscillate for large values of the ratio R/a_0 with a k-independent period.

10. We must now find the differential electron scattering cross section of the "Coulomb + δ" pair. Using the well-known expression for the amplitude $f^c(\vartheta)$ (Ref. 7), we obtain

$$\frac{d\sigma}{d\Omega} = |f_c(\vartheta)+f_\delta^c|^2 = |f_c(\vartheta)|^2 + |f_\delta^c(\beta,R,\vartheta)|^2 + |f_c|\,|f_\delta^c(\beta,R,\vartheta)|\cos[\mathbf{k}\cdot\mathbf{R} - (2/ka_0)\ln\sin(\vartheta/2)], \quad (35)$$

where the last term is the interference term, whose magnitude oscillates with the angles β, γ, φ (see figure).

We now assume that, in addition to (1)–(3) and (23), we also have

$$kR \gg 1. \quad (36)$$

In the situation described in Section 1, there were pairs with different R and different mutual orientation of the vectors $\mathbf{k}$ and $\mathbf{R}$. We shall therefore average the cross section $d\sigma/d\Omega$ over a small interval of the angle ϑ and over the small interval $\Delta R \sim k^{-1} \ll R$. The cross section averaged in this way (denoted by $d\bar{\sigma}/d\Omega$) does not contain the interference term if the angle ϑ is appreciably different from π, or if the angle β is appreciably different from $\pi/2$. The cross section $d\bar{\sigma}/d\Omega$ then splits into the sum of the differential cross sections $(d\bar{\sigma}/d\Omega)_c$ (isolated Coulomb center) and $(d\bar{\sigma}/d\Omega)_\delta^c$ (δ-center in the Coulomb field). This enables us to find the corresponding total cross sections σ_c and σ_δ^c and the transport cross sections $(\sigma_c)_{tr}$ and $(\sigma_\delta^c)_{tr}$ separately. However, the presence of the Coulomb center is clearly reflected in σ_δ^c and $(\sigma_\delta^c)_{tr}$.

Let us now consider how the presence of charged impurities affects the momentum relaxation time τ_0 on neutral donors (i.e., the mobility) in the situation described in Section 1. Usually, τ_0 is calculated on the assumption that scattering by different neutral centers is independent, i.e., that (36) is satisfied for the average distances between them. Two expressions[4,5] are used for the scattering by an individual neutral center:

$$\sigma_0 = 20a_0^2/ka_0, \quad (37a)$$

$$\sigma_0 \approx \pi(L_s^2 + 3L_t^2). \quad (37b)$$

The first of these was obtained by numerical calculation of the cross section of the hydrogen atom for slow electrons (see Ref. 4). It is shown in Ref. 5 that, for electrons with $E \ll E_0$, a good approximation is to take σ_0 as the sum of the singlet and triplet cross sections: $\sigma_0 = \sigma_s/4 + 3\sigma_t/4$, where each cross section is obtained for the zero-range potential: $\sigma_s \simeq 4\pi L_s^2$, $\sigma_t \simeq 4\pi L_t^2$ (Ref. 1). This leads to (37b), where L_s, L_t are the singlet and triplet scattering lengths. The factors 1/4 and 3/4 represent the corresponding degeneracy factors.

We must now take into account the influence of the positively charged center on the scattering cross section of neutral donors at distances $R < R_+$ from it. The average of σ_δ^c over the angle β can be obtained only by numerical methods. To estimate the lower limit for the effect, let us take the modulus of f_δ^c from (30), (32), and (33). Replacing L with L_s and with L_t, and taking the average value for the fourth power of the cosine, we obtain

$$\sigma_\delta^c = \frac{3}{8}\pi a_0^2\left[\left(1+\frac{Ra_0}{2L_s^2}\right)^{-1} + 3\left(1+\frac{Ra_0}{2L_t^2}\right)^{-1}\right]\frac{E_0}{E}. \quad (38)$$

The cross section σ_δ^c decreases with increasing R. We note that, for $(kL_s)^2 \ll 1$, $(kL_t)^2 \ll 1$, and $R \simeq R_{\max}$, where $R_{\max}$ is given by $k^2 R_{\max} a_0/2 = 3/8$ [cf. (2)], the cross section (38) turns out to be equal to σ_0, as given by (37b). Hence, it follows that the cross section (38) of each of the neutral centers within the sphere of radius R, $R \lesssim R_+ < R_{\max}$ centered on the attractive center is greater than σ_0. This difference appears when the density of attractive centers satisfies the condition

$$(N_+ a_0^3) > (E/E_0)^3 \approx (T/E_0)^3. \quad (39)$$

The scattering cross section of neutral centers at a distance $R \lesssim R_-$ from the repulsive center is then exponentially smaller than the cross section $\sigma_\delta^c(R)$ given by (38).

Thus, at low temperatures $T \ll E_0$, the electrons are scattered mainly by neutral centers lying near the attractive center and are practically unaffected by those near the repulsive center. The effect associated with the change in the scattering cross section of neutral centers will be appreciable when the relaxation time on charged centers is greater than or of the order of τ_0. This imposes an upper limit on the ratio N_+/N. Estimates show that the increase in the scattering by neutral centers in the Coulomb field can be noticeable, for example, in p-Si if $T/E_0 \sim 5 \times 10^{-3}$ (i.e., $T \sim 2$ K), we have $Na_0^3 \lesssim 10^{-5}$ (i.e., $N_0 \sim 10^{15}$ cm^{-3}) and $N_-/N \sim N_+/N \sim 10^{-3}$. The quantity kR_0 then amounts to a few units, and interference between waves scattered by different neutral centers should be small.

The results of our analysis may also be useful in the study of the trapping of slow electrons by small neutral centers in weakly doped and weakly compensated semiconductors as a result of the emission of acoustic phonons.[19] The trapping cross section $\sigma_t(E)$ was found in Ref. 19 on the assumption that the potential due to the neutral center was in the form of a δ-function. The presence of charged centers was not taken into account, and the free-electron wave function $\varphi_k(r)$ was taken in the form of the sum of a plane wave and a wave scattered by the δ-center, i.e., $\varphi_{\mathbf{k}}(\mathbf{r}) = \exp(i\mathbf{k} \cdot \mathbf{r}) + (f_\delta/r)\exp(ikr)$. It was found that the main contribution to $\sigma_t(E)$ was provided by the second term and, as $E \to 0$, the cross section became $\sigma_t(E) \sim E^{-1/2}$ (Ref. 19). Let us now consider how the presence of charged centers will affect $\sigma_t(E)$. It is clear from the derivation of (18) that the increase in the modulus of the free-electron wave function near neutral centers within the sphere of radius $R < R_+$ around the nearest attractive center [i.e., the replacement $\exp(ik \cdot R) \mapsto \psi_k^+ + (R)$] should lead to an increase in the electron trapping cross section on these neutral centers and to a stronger, as compared with Ref. 19, energy dependence for $E \to 0$, i.e., $\sigma_t(E) \sim E^{-1}$. Conversely, the trapping cross section of centers at distances $R < R_-$ from the repulsive center should be exponentially small. The total rate of trapping by neutral centers should then be determined both by the density N_0 of neutral particles and the density N_+ of attractive centers.

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[1)]Another example is, obviously, the weakly ionized low-temperature dense plasma.[2]

[2)]The derivative in (20) must be taken at $r = a$ (Refs. 6–8).

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