Validity of the Born approximation for electron scattering by a Coulomb center in a gapless semiconductor

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A phase-shift analysis is presented of electron scattering by a Coulomb center in a gapless semiconductor whose band structure is described by the spherical Luttinger Hamiltonian in the limit where the electron mass is much smaller then the hole mass $m_e/m_h \ll 1$. It is shown that the Born approximation is valid for all energies greater than the electron Bohr energy, i.e., that its validity is determined by the mass of the lighter particle. This assertion is found to be valid everywhere except for a narrow energy region near the hole energy level in the case of scattering by a negatively charged center. Here the scattering is resonant, as was shown in the well-known paper by Gel'mont and D'yakonov.

1. In semiconductors, scattering by Coulomb centers is customarily described within the Born approximation. For the case of a degenerate band structure, however, the cross section differs from the Rutherford formula by a factor which depends on scattering angle;[1,2] this factor is related to the matrix character of the Hamiltonian. An interesting, and to our knowledge uninvestigated, problem is to determine the region of applicability of the Born approximation for this case.

In ordinary quantum mechanics (or the equivalent formalism for a nondegenerate parabolic band in a semiconductor) this problem does not arise, due to the "accidental" equality of the exact cross section and the cross section calculated according to the first Born approximation.[3] This is because the perturbation (Born) series for the scattering amplitude is simply the expansion of a pure phase which multiplies the Rutherford formula; the expansion parameters is $(E_B/E)^{1/2} \ll 1$, where E_B is the Bohr energy while E is the particle energy. Formally, however, the Born approximation is valid only for $E \gg E_B$.

In the case of a degenerate spectrum, it will be clear from what follows that for scattering by a Coulomb center the perturbation series for the scattering amplitude is not simply an expansion of a phase factor; consequently the Born approximation begins to be valid only at rather large energies $E \gg E_B$. However, since the carrier masses associated with the bands of a degenerate spectrum are very different as a rule, the problem of how to relate the convergence of the Born approximation to the masses of the scattered carriers is in fact one of some importance.

In this paper, electron scattering by a Coulomb center

$$V(r) = -Ze^2/\varkappa r \tag{1}$$

in a gapless semiconductor is investigated, where the semiconductor is described by the spherical Luttinger Hamiltonian[4] (sketched in Fig. 1) in the limit of very different carrier masses $m_e/m_h \ll 1$; m_e, m_h are the electron and hole masses, respectively, $\varkappa$ is the permittivity, and $Z = \pm 1$ is the charge of the center. The spectrum of the gapless semiconductor is degenerate only at the point $k = 0$.

What follows is a phase shift analysis of the wave function of an electron which is scattered by the potential (1). It is shown that the Born approximation is valid for all electron energies E greater than the electron Bohr energy $E_{Be} = m_e e^4/2\hbar^2\varkappa^2$, i.e., that the light particle mass determines the validity of the approximation. An exception is a narrow energy region in the case of scattering by a negatively charged center near the hole energy level. Within this region the Born approximation is not valid: the cross section has a resonant character, as shown by Gel'mont and D'yakonov. The energy level is determined in order of magnitude by the Bohr energy of a hole $E_{Bh} \gg E_{Be}$, while the resonance width is small compared to the parameter $(m_e/m_h)^{1/2}$.

2. The wave functions for the free-particle Hamiltonian are a plane "circularly-polarized" wave

$$|\mu, \mathbf{k}\rangle = |\mu(\mathbf{k})\rangle \exp(i\mathbf{kr}),$$

in which the helicity μ along the momentum $\hbar\mathbf{k}$ ($k = (2m_e E)^{1/2}/\hbar$) takes on the values $\pm 1/2$ for the electron band. The amplitude for scattering from an initial state $|\mu_0, \mathbf{k}_0\rangle$ into a final state $|\nu/\mathbf{k}\rangle$ at an angle $\hat{n} = \hat{\mathbf{k}_0\mathbf{k}}$ is determined by the scattering phase shifts[5]

$$f_{\mu\mu_0}(\hat{\mathbf{n}}) = \frac{1}{4ik} \sum_{F,I} (2F+1)\,[\exp(i\delta_{FI}) - 1]\, D^{F}_{\mu_0\mu}(\hat{\mathbf{n}})\, \xi\, \delta_{|\mu|+|\mu_0|,1}, \tag{2}$$

where F, I are eigenvalues of the operators of total angular momentum and parity ($F = 1/2, 3/2, \ldots$; $I = I_{1,2}$), $D^{F}_{\mu_0,\mu}(\hat{\mathbf{n}})$ are finite-rotation matrices,

$$\xi = \begin{cases} 1 & \text{for } I = I_1 \\ (-1)^{\mu-\mu_0} & \text{for } I = I_2 \end{cases}, \tag{2a}$$

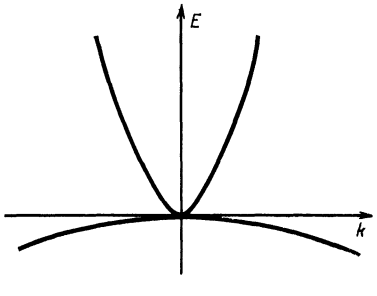

FIG. 1.

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while δ_{FI} are the scattering phase shifts of electron wave functions $Y_{FI}(r)$, which by virtue of the degenerate character of the bands are related to the hole functions $X_{FI}(r)$ in pairs for the two values of parity $I_{1,2}$ by the Gel'mont-D'yakonov equations,[4] by introducing the new functions

$$Y_{FI}(r)=\frac{(E-V(r))^{1/2}}{r}y_{FI}(r), \quad X_{FI}(r)=\frac{(E-V(r))^{1/2}}{r}x_{FI}(r), \tag{3}$$

we can write in the form ($F\neq 1/2$)

$$y_{FI}''+\left[\frac{2m_e(E-V)}{\hbar^2}-\frac{l_I(l_I+1)}{r^2}\right]y_{FI} = \frac{V'}{2r(E-V)}\left[\left(1-A_I+\frac{3}{2}\frac{rV'}{E-V}+\frac{rV''}{V'}\right)y_{FI}+B_Ix_{FI}\right], \tag{4a}$$

$$x_{FI}''-\left[\frac{2m_h(E-V)}{\hbar^2}+\frac{l_I(l_I+1)}{r^2}\right]x_{FI} - \frac{V'}{2r(E-V)}\left[\left(1+A_I+\frac{3}{2}\frac{rV'}{E-V}+\frac{rV''}{V'}\right)x_{FI}+B_Iy_{FI}\right]=0, \tag{4b}$$

where

$$l_{I_{1,2}}=F\mp 1/2, \quad I_{1,2}=(-1)^{l_{I_{1,2}}}, \quad A_{I_1}=2F\cos\alpha_{I_1},$$

$$A_{I_2}=2(F+1)\cos\alpha_{I_2},$$

$$B_{I_1}=2F\sin\alpha_{I_1}, \quad B_{I_2}=2(F+1)\sin\alpha_{I_2}, \quad \cos\alpha_{I_1}=\frac{2F-3}{4F},$$

$$\cos\alpha_{I_2}=-\frac{2F+5}{4(F+1)}, \quad \sin\alpha_I\geqslant 0.$$

For $F=1/2$, the equations decouple: the right side of (4a) reduces to zero, and $l_{I\,1,2}=1,2$.

In the case of scattering by a potential (1), as we will show below, the asymptotic behavior of the function $Y_{FI}(r)$ in the limit $r\to\infty$ exhibits a logarithmic term

$$y_{FI}(r)\underset{r\to\infty}{\longrightarrow}\sin\left(kr-\frac{\pi l_I}{2}+Z\left(\frac{E_{Be}}{E}\right)^{1/2}\ln 2kr+\delta_{FI}\right), \tag{5}$$

however, as in ordinary quantum mechanics, Eq. (2) remains valid.

Let us write the phase in the form of a sum $\delta_{FI}=\sigma_{FI}+\eta_{FI}$. The first term corresponds to Eq. (4a) when the right side is zero. In this case, Eq. (4a) coincides with the usual Schroedinger equation in a Coulomb potential, and consequently[3] $\sigma_{FI}=\sigma_{lI}^c$, where

$$\sigma_l^c=\arg\Gamma(l+1-iZ(E_{Be}/E)^{1/2}) \tag{6}$$

is the Coulomb phase shift. The second term corresponds to the right side of Eq. (4a). We emphasize that for $F=1/2$ the additional phase is $\eta_{FI}=0$.

Let us rewrite the amplitude (2) for the cases of scattering with and without change in helicity (corresponding to $\mu=\pm\mu_0$) by substituting expression (2a) into Eq. (2). We obtain

$$f_{\mu\mu}(\hat{\mathbf{n}})=f_{\mu\mu}^{(1)}(\hat{\mathbf{n}})+\frac{1}{4ik}\sum_{F=1/2,I}^{\infty}(2F+1) \times\exp\{2i\sigma_{FI}\}(\exp\{2i\eta_{FI}\}-1)D_{\mu\mu}^{F}(\hat{\mathbf{n}}), \tag{7a}$$

$$f_{\mu-\mu}(\hat{\mathbf{n}})=f_{\mu-\mu}^{(1)}(\hat{\mathbf{n}})+\frac{1}{4ik}\sum_{F=1/2}^{\infty}(2F+1)\{[\exp\{2i(\sigma_{FI_1}+\eta_{FI_1})\} - \exp\{2i(\sigma_{FI_2}+\eta_{FI_2})\}]-[\exp\{2i\sigma_{FI_1}\}-\exp\{2i\sigma_{FI_2}\}]\}D_{-\mu\mu}^{F}(\hat{\mathbf{n}}), \tag{7b}$$

where $f_{\mu\mu_0}^{(1)}(\hat{\mathbf{n}})$ is a quantity determined only by the Coulomb phase shifts:

$$f_{\mu\mu}^{(1)}(\hat{\mathbf{n}})=\frac{1}{4ik}\sum_{F=1/2,I}^{\infty}(2F+1)[\exp(2i\sigma_{FI})-1]D_{\mu\mu}^{F}(\hat{\mathbf{n}}),$$
$$f_{\mu-\mu}^{(1)}(\hat{\mathbf{n}})=\frac{1}{4ik}\left[\sum_{F=1/2}^{\infty}+\sum_{F=3/2}^{\infty}\right][(2F+1)(\exp\{2i\sigma_{FI}\} - \exp\{2i\sigma_{FI_2}\})]D_{-\mu\mu}^{F}(\hat{\mathbf{n}}). \tag{8}$$

We will make an important assertion here: for energies $E\gg E_{Be}$ the scattering amplitude is determined by the term $f_{\mu\mu_0}^{(1)}(\hat{\mathbf{n}})$ in (8), which leads (as is shown in the Appendix) to the equation

$$f_{\mu\mu_0}(\hat{\mathbf{n}})\approx f_{\mu\mu_0}^{(1)}(\hat{\mathbf{n}})\approx\frac{Z(E_{Be}/E)^{1/2}}{2k\sin^2\theta/2}D_{\mu_0\mu}^{1/2}(\hat{\mathbf{n}}), \tag{9}$$

which corresponds to the Born approximation[1,2,5] where θ is the scattering angle. It remains for us to show that in comparison to (8) the terms dependent on the additional phase shift η_{FI} in Eq. (7a), (7b) give a small contribution to the scattering amplitude when the conditions $E\gg E_{Be}$ and $m_e/m_h\ll 1$ are fulfilled. In what follows, it will be clear that for all of these phases the inequality $\eta_{FI}\ll 1$ will be valid, thanks to which we can calculate them using plane waves; in addition, we can assume that the phases from the sum of terms of the right-hand part of Eq. (4a) are additive.

3. A characteristic length which appears in analyzing the equations (4) is the quantity $r_0=e^2/\varkappa E$—the length for which the potential energy (1) is comparable to the electron energy E. The additional phase shift is conveniently expressed as a sum of two terms: a contribution $\eta_{FI}^{(1)}$ connected with the right side of Eq. (4a) at large ($r>r_0$) distances, plus a contribution $\eta_{FI}^{(2)}$ from the right side for $r\lesssim r_0$.

Let us obtain an estimate of $\eta_{FI}^{(1)}=\eta_{FI}^{(h)}+\eta_{FI}^{(e)}$. The first term is related to the hole function $X_{FI}(r)$ in the right side of (4a); when the conditions $E\gg E_{Be}$, $m_e/m_h\ll 1$ and $r>r_0$ are fulfilled, it is easy to show from equation (4b) that

$$x_{FI}\approx-\frac{\hbar^2}{2m_hE}\frac{Zr_0}{2r^3}B_Iy_{FI}. \tag{10}$$

Let us substitute (10) into Eq. (4a), and calculate the phase $\eta_{FI}^{(h)}$ of a plane wave in the first Born approximation:

$$\eta_{FI}^{(h)}\approx\frac{\pi}{2}\frac{\hbar^2}{2m_hE}\frac{B_I^2r_0^2}{4}\int_0^{\infty}[J_{l_I+1/2}(kr)]^2\frac{dr}{r^5}\sim\frac{m_e}{m_h}\frac{E_{Be}}{E} \tag{11}$$

(we recall that $l_I\geqslant 1$). In the integral (11), the characteristic length over which the integrand varies is $r\sim 1/k\gg r_0$, so that it does not depend on r_0; hence the integration can be extended down to zero. Because the phase (11) is smaller than the Coulomb phase (6) $\sigma_{FI}\sim(E_{Be}/E)^{1/2}$ for $E\gg E_{Be}$, it follows that the correction to the scattering amplitude from the term on the right side of Eq. (4), which is proportional to X_{FI} for $r>r_0$, is small compared to (8).

Let us obtain an estimate for the quantity $\eta_{FI}^{(e)}$, the scattering phase from the potential

$$U(r)=\frac{\hbar^2}{2m_e}\frac{Zr_0}{2r^3}\begin{cases}F-1/2, & I=I_1\\ -(F+3/2), & I=I_2\end{cases} \tag{12}$$

which is the contribution from terms in the right side of Eq. (4a) for $r > r_0$, which are independent of the hole functions. Within the Born approximation it is easy to obtain

$$\eta_{FI_1}^{(e)} \approx -\eta_{FI_2}^{(e)} \approx -Z(E_{Be}/E)^{1/2}/(2F+1), \tag{13}$$

i.e., it is found that the phase $\eta_{FI}^{(e)}$ is a quantity of the same order of magnitude as the Coulomb phase. However, as is clear from Eq. (7a), (7b), the correction to the amplitude from the phase $\eta_{FI}^{(e)}$ to a first approximation equals zero, and in subsequent approximations is small, of order the parameter $(E_{Be}/E)^{1/2}$.

4. The correction $\eta_{FI}^{(2)}$ from the right-hand part of Eq. (4a) for small distances $r \lesssim r_0$ can be estimated based on the inequality $(kr_0) \sim (E_{Be}/E)^{1/2} \ll 1$. In ordinary quantum mechanics for scattering by a potential of radius a, when the condition $ka \ll 1$ holds we can introduce a single parameter—the scattering length—and express the scattering phases in terms of it.[3] Beyond the resonance region the scattering length is of order a, and all the phases are small in the parameter ka. They can be found in the hard-sphere approximation by using the condition that the wave function reduce to zero at the potential boundary. As bound levels appear in a given potential, the scattering length becomes much larger than the radius of the potential, and the cross section increases sharply, which signals the onset of the resonance.

For scattering by a short-range potential[5] of radius a the situation in a gapless semiconductor is almost the same. As in ordinary quantum mechanics, outside a resonance region the hard-sphere approximation is valid so long as $ka \ll 1$. The difference lies in the fact that the resonance corresponds to the appearance of a hole level in the potential which is of short range for electrons. However, the width of the resonance, which is proportional to the probability of a transition from a local state to the continuum, is small, scaling with the density of final states in the electron band.[6]

The analogous situation also obtains in our case for $r \lesssim r_0$. In the hard-sphere approximation, we must subject the electron wave function $y_{FI}(r)$ to the boundary condition $y_{FI}(r_0) = 0$. The function y_{FI} is a superposition of Coulomb functions which, as we have noted already, we can replace by spherical Bessel functions with the same boundary condition. From this it is easy to verify that even the largest of the phases $\eta_{3/2}^{(2)}{}_{,I_1} \sim (E_{Be}/E)^{3/2}$ is small compared to the phases (6), i.e., even at small distances there is no contribution to the cross section for $E \gg E_{Be}$. However, this holds only in the region outside the resonance region.

We have already said that the hard-sphere approximation is valid outside the resonance region. For energies close to resonance, as for the case of scattering by a short-range potential,[5] it is necessary to "mix in" the hole wave function to the superposition of electron wave functions depending on the electron parameters (there will be a non-Coulomb function involved in the exact solution even for $r \sim r_0$); because of this, the cross section at the resonance point will be much larger than its Born approximation value, and will be approximately equal to the squared wave length of an electron.[4–6] Therefore, in the resonance region the long-range character of the Coulomb potential cannot enter in any way. The scattering amplitude can be cast in the form of a sum of the Born term (8) and a resonance term in the case where the resonant phase is small compared to unity, i.e., outside the width of the resonance. For energies within the width of the resonance, this representation is not valid, because it is not correct to treat the scattering phases from a sum of potentials as additive when these phases are not small. However, the correction due to the principal resonance term coincides in order to magnitude with the Born term, because the resonance is described by only one phase.[4–6]

5. Thus, we have shown that for electron scattering by a Coulomb center in a gapless semiconductor, the Born approximation works for electron energies $E \gg E_{Be}$. In the case of a negatively charged center there is an exceptional region of energies near the hole level. Thus, the principle contribution which limits the validity of the Born approximation arises from those terms in Eq. (4a) which do not depend on the hole function X_{FI}, in contrast with the energy region near resonance.

An alternative to the approach we give here is to analyze the perturbation series for the scattering amplitude. Such a discussion is outside the framework of our paper. We remark only that this approach is found to be constructive in the case of the Kane Hamiltonian, i.e., when taking into account nonparabolicity of the conduction band. In place of the ratio $(E_{Be}/E)^{1/2}$ for the Born parameter we use the quantity $(e^2/\varkappa P)[(E-E_g)/E_g]^{1/2}$, where P is the Kane matrix element and E_g is the spacing between the symmetry points Γ_6 and Γ_8 (in ordinary semiconductors, i.e., with nonzero gaps, the quantity E_g is positive and plays the role of a forbidden gap). For $E_g > 0$ and a large inband electron energy $\varepsilon = E - E_g$ ($\varepsilon \gg |E_g|$), corrections to the Born approximation are determined by the "fine structure constant" $e^2/\varkappa P$ of the Kane Hamiltonian, which was already noted in Ref. 7. In ordinary quantum mechanics, this case corresponds to scattering of a relativistic electron by a Coulomb potential.

In conclusion, I am deeply grateful to A. L. Efros for posing this problem, and for a multitude of useful discussions along with his support and friendship. I am also appreciative of very useful discussions with B. G. Gel'mont, M. A. Zhusupov, M. Yu. Kuchiev and M. E. Raikh.

APPENDIX

In what follows, we use the relation[3]

$$D_{\mu\mu'}^{F}(\hat{n}) = e^{i\mu\alpha} d_{\mu\mu'}^{F}(\hat{n}) e^{i\mu'\gamma}. \tag{A1}$$

Here, α, β, γ are the Euler angles (θ is the scattering angle), and

$$d_{\mu\mu'}^{F}(\theta) = \xi_{\mu\mu'} \begin{cases} \cos(\theta/2)\, P_{F-1/2}^{(0,1)}(\cos\theta), & \mu = \mu' \\ \sin(\theta/2)\, P_{F-1/2}^{(1,0)}(\cos\theta), & \mu = -\mu' \end{cases}, \tag{A2}$$

where $|\xi_{\mu\mu'}| = 1, P_n^{(i,j)}(x)$ are Jacobi polynomials.

Let us begin with the case $\mu = \mu_0$, and turn to the first of Eqs. (8). Taking into account the relation

$$\sum_{F=1/2,\, I}^{\infty} (2F+1)\, d_{\mu\mu}{}^{F}(\theta) = 4\delta(1-\cos\theta) \tag{A3}$$

(a proof of this is given below), and also the relation $\sigma_{FI} = \sigma_{II}^{c}$ ($F \neq \frac{1}{2}$), $\sigma_{1/2,I_{1,2}} = \sigma_{1,2}^{c}$, where σ_1^c are the Coulomb phases (6); the quantity $f_{\mu\mu}^{I}(\hat{\mathbf{n}})$ can be written in the form

$$f_{\mu\mu}^{(4)}(\hat{\mathbf{n}})=\frac{1}{4ik}\Big\{\sum_{F=1/2}^{\infty}(2F+1)\,(\exp\{2i\sigma_{F-1/2}^{c}\}$$

$$+\exp\{2i\sigma_{F+1/2}^{c}\})D_{\mu\mu}^{F}(\hat{\mathbf{n}})$$

$$+2(\exp\{2i\sigma_1{}^{c}\}+\exp\{2i\sigma_2{}^{c}\})D_{\mu\mu}{}^{1/2}(\mathbf{n})\}. \qquad \text{(A4)}$$

Substituting the expressions (A1) and (A2) into this latter equation, and using the relation[8] $N=F-\frac{1}{2}$:

$$(n+1)P_n^{(0,1)}(x)+nP_{n-1}^{(0,1)}(x)=(2n+1)P_n(x), \qquad \text{(A5)}$$

where $P_n(x)$ are the Legendre polynomials, and then the summation formula for $P_n(x)$ which leads to the Rutherford formula,[3] we obtain

$$f_{\mu\mu}^{(1)}(\hat{\mathbf{n}})=-\frac{2\cos(\theta/2)}{4ik}\exp(2i\sigma_0{}^{c})\Big[\frac{Z(E_{Be}/E)^{1/2}}{\sin^2(\theta/2)}$$

$$\cdot\exp\Big\{2iZ\Big(\frac{E_{Be}}{E}\Big)^{1/2}\ln\sin\frac{\theta}{2}+i\pi\Big\}$$

$$+\frac{1}{i}(1-\exp\{2i(\sigma_2{}^{c}-\sigma_0{}^{c})\})\Big]\xi_{\mu\mu'}$$

$$\times\exp\{i\mu\alpha+i\mu'\gamma\}. \qquad \text{(A6)}$$

Substituting for σ_0^c and σ_2^c from equation (6) into this formula, we obtain the final Eq. (9) with $\mu=\mu_0$ as $(E_{Be}/E)^{1/2}\to 0$.

In deriving equation (9) for $\mu=\mu_0$, we must use the relation[8]

$$(n+1)P_n^{(1,0)}(x)-nP_{n-1}^{(1,0)}(x)=(2n+1)P_n(x). \qquad \text{(A7)}$$

The remaining procedures of the derivation are analogous to those presented above.

Expression (A3) follows from (A5) together with the well-known summation formula for Legendre polynomials.[3]

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