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Treatment of Ionized Impurity Scattering in Degenerate Semiconductors. Combination of the Variational and Perturbational Technique in the Partial-Wave Method

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Using the variational technique for the calculation of the zeroth-order phase shift and the perturbational technique for obtaining the higher order phase shifts, an analytic expression is derived for the total scattering cross section of ionized impurity scattering in degenerate semiconductors. The formula obtained may be looked upon as resulting from a refinement of the first Born approximation and its significance lies in the fact that it is valid in a doping region where neither the uncorrected Born approximation nor the simplest form of the partial-wave method (based on using only a variationally determined zeroth-order phase shift) can be applied for the calculation of the resistivity of ionized impurity scattering.

I. INTRODUCTION

IN a previous paper,[1] hereafter referred to as I, ionized impurity scattering in degenerate semiconductors was discussed by making use of a variational approach in the partial-wave method. The analytic formula derived in I for the resistivity resulting from the scattering of electrons by ionized donors involved only the zeroth-order partial-wave shift, since it was assumed that the higher order phase shifts are very much smaller than the zeroth-order one. In the present paper a more exact resistivity expression is obtained that contains the contribution from all the higher order phase shifts too. The formula is arrived at by a combination of the variational and perturbational treatments of the partial-wave method and it may also be looked upon as resulting from a refinement of the first Born approximation.

II. THEORY

The scattering amplitude for the scattering of a particle by a spherically symmetric potential is given[2] by

$$f(\vartheta)=\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(e^{2i\eta_l}-1)P_l(\cos\vartheta)\,, \qquad (1)$$

where η_l is the lth partial wave shift, k is the wave number of the scattered particle, i is the imaginary unit, and $P_l(\cos\vartheta)$ is the lth Legendre polynominal.

Assuming that all phase shifts, except the zeroth-order one, are small compared to unity, as will be shown to be the case for degenerate semiconductors, one can approximate $e^{2i\eta_l}$ by $1+2i\eta_l$ and rewrite Eq. (1) as

$$f(\vartheta)=\frac{1}{2ik}\bigg\{(e^{2i\eta_0}-1)P_0(\cos\vartheta)+\sum_{l=1}^{\infty}(2l+1)(2i\eta_l)P_l(\cos\vartheta)\bigg\}\,, \qquad (2)$$

where for the present purposes the phase shifts are considered as unknown numerical quantities. For the zeroth-order phase shift, one may choose an approximate value η_{0v} such as obtained in I by the variational method, and for the higher order phase shifts one may take the approximate values η_{lB} given[3] by

$$\tan\eta_{lB}=-\frac{2m^*}{\hbar^2}k\int_0^{\infty}j_l^2(kr)V(r)r^2dr\,, \qquad (3)$$

where m^* is the mass of the scattered particle, $j_l(kr)$ is the spherical Bessel function of order l, and $V(r)$ is the interaction energy between the scattering center and the particle. The criterion for the validity of Eq. (3), which is the Born approximation expression for the partial-wave shifts, will be discussed later.

Approximating $\tan\eta_{lB}$ by η_{lB} and substituting Eq. (3) into Eq. (2), one obtains

$$f(\vartheta)=\frac{1}{2ik}\bigg\{(e^{2i\eta_{0v}}-1)P_0(\cos\vartheta)-2ik(2m^*/\hbar^2)\times\int_0^{\infty}r^2V(r)\bigg[\sum_{l=1}^{\infty}(2l+1)j_l^2(kr)P_l(\cos\vartheta)\bigg]dr\bigg\}. \qquad (4)$$

If in the right-hand side of Eq. (4) one adds and subtracts the quantity $(2i\eta_{0B})P_0(\cos\vartheta)$, then one finds that

$$f(\vartheta)=\frac{1}{2ik}(e^{2i\eta_{0v}}-2i\eta_{0B}-1)P_0(\cos\vartheta)-\frac{2m^*}{\hbar^2}\frac{1}{K}\int_0^{\infty}r\sin Kr\,V(r)dr\,, \qquad (5)$$

where $K=2k\sin(\frac{1}{2}\vartheta)$, since $\sum_{l=0}^{\infty}(2l+1)j_l^2(kr)P_l(\cos\vartheta)$ can be shown[3] to be equal to $\sin Kr/Kr$. The second term in Eq. (5) is just the well-known Born approximation expression for the scattering amplitude, and therefore, one may write Eq. (5) as

$$f(\vartheta)=f_{\mathrm{B}}(\vartheta)+\frac{1}{2ik}(e^{2i\eta_{0v}}-2i\eta_{0B}-1)\,, \qquad (6)$$

where it has been considered that $P_0(\cos\vartheta)=1$.

Using Eq. (6) the differential scattering cross section

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[1] P. Csavinszky, Phys. Rev. **126**, 1436 (1962).

[2] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., p. 105.

[3] See Ref. 2, p. 167.

is calculated[2] as

$$\sigma(\vartheta)=|f(\vartheta)|^2=[f_B(\vartheta)+(2ik)^{-1}(e^{2i\eta_{0v}}-2i\eta_{0B}-1)]\\ \times[f_B(\vartheta)-(2ik)^{-1}(e^{-2i\eta_{0v}}+2i\eta_{0B}-1)], \quad (7)$$

which upon some manipulation is brought to the form

$$\sigma(\vartheta)=k^{-2}(\eta_{0B}^2-\eta_{0B}\sin\eta_{0v}+\sin^2\eta_{0v})\\ +k^{-1}(\sin\eta_{0v}-2\eta_{0B})f_B(\vartheta)+f_B(\vartheta)^2. \quad (8)$$

If, for instance, the scattering of electrons by donor ions in degenerate semiconductors is considered and a screened Coulomb potential[4] is chosen for the donor ion then

$$V(r)=-(e_0^2/\kappa r)e^{-r/R}, \quad (9a)$$

with

$$R=\left(\frac{\pi}{3}\right)^{1/6}\frac{h\kappa^{1/2}}{4\pi e_0 m_0^{1/2}}\gamma^{-1/2}n^{-1/6}, \quad (9b)$$

where R is a screening length,[5] κ is the static dielectric constant of the semiconductor, n is the electron concentration, and $\gamma=m^*/m_0$ is the ratio of the effective electronic mass to the free electronic mass.

Using Eqs. (9a) and (9b) one finds that the scattering amplitude in the Born approximation is given by

$$f_B(\vartheta)=-\frac{2m^*}{\hbar^2}\frac{1}{K}\int_0^\infty r\sin KrV(r)dr\\ =\frac{2m^*e_0^2}{\hbar^2\kappa}\times\frac{1}{R^{-2}+K^2}. \quad (10)$$

The total scattering cross section, weighted for large angle scattering, is evaluated[1] from

$$Q=2\pi\int_0^\pi(1-\cos\vartheta)\sigma(\vartheta)\sin\vartheta d\vartheta, \quad (11)$$

which upon using Eqs. (8) and (10) is found to be

$$Q=2\pi\{k^{-2}(\eta_{0B}^2-\eta_{0B}\sin\eta_{0v}+\sin^2\eta_{0v})A\\ +k^{-1}(\sin\eta_{0v}-2\eta_{0B})(2m^*e_0^2/\kappa\hbar^2)B\\ +(4m^{*2}e_0^4/\kappa^2\hbar^4)C\}, \quad (12)$$

where the integrals

$$A=\int_0^\pi(1-\cos\vartheta)\sin\vartheta d\vartheta;$$

$$B=\int_0^\pi(R^{-2}+K^2)^{-1}(1-\cos\vartheta)\sin\vartheta d\vartheta;$$

$$C=\int_0^\pi(R^{-2}+K^2)^{-2}(1-\cos\vartheta)\sin\vartheta d\vartheta$$

are evaluated as

$$A=2;$$

$$B=k^{-2}[1-(4k^2R^2)^{-1}\ln(1+4k^2R^2)];$$

$$C=\frac{R^2}{k^2(1+4k^2R^2)}+\frac{1}{4k^4}\ln(1+4k^2R^2). \quad (13)$$

The quantity η_{0B} is calculated from Eq. (3) and found to be

$$\tan\eta_{0B}=\frac{8\pi^2m^*e_0^2}{h^2\kappa}\frac{1}{k}G_1, \quad (14a)$$

where the integral

$$G_1=\int_0^\infty\frac{e^{-r/R}}{r}\sin^2krdr \quad (14b)$$

is evaluated[1] as

$$G_1=\tfrac{1}{4}\ln(1+4k^2R^2).$$

One also finds from Eq. (3) that the first few higher order phase shifts are given by

$$\tan\eta_{1B}=\frac{8\pi^2m^*e_0^2}{h^2\kappa}\frac{1}{k}\left[\left(1+\frac{1}{2k^2R^2}\right)G_1-\frac{1}{2}\right]$$

$$\tan\eta_{2B}=\frac{8\pi^2m^*e_0^2}{h^2\kappa}\frac{1}{k}\left[\left(1+\frac{3}{2k^2R^2}+\frac{3}{8k^4R^4}\right)G_1\\ -\left(\frac{3}{4}+\frac{3}{8k^2R^2}\right)\right]. \quad (15)$$

III. DISCUSSION

The derivation of Eq. (12), in terms of which the resistivity of ionized impurity scattering can be expressed,[1] was based on the assumption that η_{lB} is small compared to unity when $l\geqslant1$. For Ge with electron concentrations of 10^{18} and $5\times10^{18}\text{cm}^{-3}$, for instance, one finds from Eq. (15) (using an effective mass of $m^*=0.25m_0$ as in I) that the phase shifts (in rad) are

$$\eta_{1B}=0.16, \quad \eta_{2B}=0.057,$$

and

$$\eta_{1B}=0.15, \quad \eta_{2B}=0.055,$$

which, indeed, satisfy the above requirement. One may also show that the Born approximation expression for the higher order phase shifts, as given in Eq. (3), is a good approximation. For this to be the case the following condition[6] must be satisfied:

$$V(r)\ll\frac{l(l+1)}{r^2}\frac{\hbar^2}{2m^*}, \quad (16)$$

for r given by

$$kr=[l(l+1)]^{1/2}.$$

For Ge with $n=10^{18}\text{cm}^{-3}$ and $n=5\times10^{18}\text{cm}^{-3}$, respectively, one finds from Eqs. (9a) and (9b) that

$$V(r)_{l=1}=6.69\times10^{-15}, \quad V(r)_{l=2}=1.24\times10^{-15},$$

and

$$1.66\times10^{-14}, \quad 0.407\times10^{-14},$$

which shows that the left-hand side of Eq. (16) is, indeed, smaller than the right-hand side, whose value

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[4] R. B. Dingle, Phil. Mag. **46**, 831 (1955).

[5] R in Eq. (10) of I is misprinted. Where m_0 appears $m_0^{1/2}$ should be read; and where γ^{-1} appears $\gamma^{-1/2}$ should be read.

[6] N. S. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Clarendon Press, Oxford, England, 1949), 2nd ed., p. 127.

for the given electron concentrations is 23.2×10^{-15} and 6.79×10^{-14}, respectively.

Since in degenerate semiconductors the resistivity resulting from ionized impurity scattering is directly proportional[1] to the total scattering cross section, the ratio of the total scattering cross section containing only the zeroth-order phase shift as given in I to that of the expression given in Eq. (12) of the present paper will show the importance of the inclusion of the higher order phase shifts.

In I, for $n=10^{18}$ and $5\times10^{18}\text{cm}^{-3}$ the approximate expression

$$Q_0{}^F=(4\pi/k_F{}^2)\sin^2\eta_{0v},$$

(F refers to electrons on top of the Fermi surface) is found to be 8.90×10^{-13} and 2.41×10^{-13} cm^2, respectively, while Eq. (12) leads to the values of 16.8×10^{-13} and 3.28×10^{-13} cm^2, which gives for the ratio $Q^F/Q_0{}^F$ the values of 1.88 and 1.36. It is thus seen that though the higher order phase shifts are small compared to the zeroth-order one, their consideration still leads to an increase in the total scattering cross section and, consequently, in the resistivity by a factor of between 1 and 2.

At this point, attention is drawn to some of the shortcomings of the theory of ionized impurity scattering in degenerate semiconductors. First, an effective scalar electronic mass was used throughout which is a simplification of the actual band structure of the semiconductor. Second, the dielectric constant κ and the effective mass (whether scalar or tensor) might depend on the electron concentration, n, which is not considered. Third, at the electron concentration of 10^{18}cm^{-3}, for instance, the screening length is 29.4 Å, which is not so large compared to several nearest-neighbor distances in the semiconductor in which region the space dependence[7] of the dielectric constant, $\kappa=\kappa(r)$, might also have some importance on the magnitude of the total scattering cross section. Fourth, the calculation[4] of $V(r)$ is based on a series expansion of the Fermi-Dirac integral which becomes invalid at a certain value of $r=r_0$. The condition for the validity of the expansion can be expressed[8] as

$$\frac{1}{k_BT}\frac{e_0{}^2}{\kappa r}e^{-r/R}\ll1, \tag{17}$$

where k_B is Boltzmann's constant and T is the absolute temperature. At $n=10^{18}\text{cm}^{-3}$ and $T=100$°K, for instance, one finds from Eq. (17) that $r_0\sim R$. For this reason the use of the screened Coulomb potential in the region $r<R$ is not strictly justified and amounts to using an asymptotically correct expression in all regions of space.

Fifth, one may ask to what degree is the picture of individual scattering correct. Some considerations of this problem have been given elsewhere.[9] Here it is only added that the wavelength of an electron on top of the Fermi surface in Ge doped to an electron concentration of 10^{18}cm^{-3}, for instance, is $\lambda_F\sim200$ Å, while the "average distance" of impurities (calculated from $\frac{3}{4}\rho^3\pi n=1$) is $2\rho\sim120$ Å, which would suggest that the picture of individual scattering acts is marginal.

Finally, one may also note that ionized impurity scattering should also be augmented by dipole scattering when a screened Coulomb potential is used for the donor ion. The reason for this is twofold. First, when the electron approaches the screened donor ion, the electron cloud surrounding the ion undergoes polarization and, consequently, a dipole is created whose magnitude is a function of the electron's position. Since the total energy of the system of a screened donor ion and an electron must be conserved, this process is only possible if the energy for the creation of the time-varying dipole is supplied from the kinetic energy of the electron which means that the scattering process is no longer elastic though the kinetic energy of the electron before and after the scattering act is the same.

Second, as pointed out by Koenig,[10] the thermal motion of the impurity also creates a dipole since the screening around the ion does not rigidly follow the motion of the impurity. While the previous mechanism for dipole scattering should be temperature-independent, this latter one should show a temperature dependence since the rms displacement of the ion is a function of the temperature.

IV. CONCLUSIONS

In summary, one may conclude that consideration of the higher order phase shifts in the resistivity calculation is important and that this may be achieved by a combination of the variational and perturbational treatments of the partial-wave method. As far as the theory of strong ionized impurity scattering as a whole is concerned, a number of as yet not investigated features appear whose consideration may or may not have a significant bearing on the numerical result.

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[7] K. Weiser, Bull. Am. Phys. Soc. **6**, 156 (1961).

[8] T. Morimoto and K. Tani, J. Phys. Soc. Japan **17**, 1121 (1962).

[9] P. Csavinszky, J. Phys. Soc. Japan **16**, 1865 (1961).

[10] S. H. Koenig, in *Proceedings of the International Conference on the Physics of Semiconductors, Exeter* edited by A. C. Strickland. (The Institute of Physics and the Physical Society, London, 1962), p. 10.