Remarks on the Theory of the Electron Plasma in Semiconductors

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The scattering of current carriers by charged impurities is considered on the basis of the many-electron theory of semiconductors. In addition, the ionization energy of impurity centers of the third and fifth groups in germanium type semiconductors is calculated. It is shown that plasma screening produces an essential change in the character of the scattering at low temperatures. The ionization energy of impurity centers is found to be dependent on concentration, and to decrease when the latter increases.

1. INTRODUCTION

As HAS BEEN SHOWN previously[1, 2], the qualitative statements of the zone theory of homopolar semiconductors can be justified by using the picture of elementary excitations of a many-electron system. The "conduction electrons" and "holes", whose behavior is investigated in experiments, are actually excitations of the Fermi type; unlike the other electrons, they actually behave like independent particles, and it is legitimate to apply to them all the statements concerning the energy spectrum which are usually made in the zone theory. In particular, it is precisely their spectrum which is investigated in experiments on cyclotron resonance, etc. However, we must emphasize that the distinction between these excitations and "real" electrons is not merely a verbal distinction, but makes itself felt in various special features, of which the following two are of importance for us here:

a) the interaction of the fermions with an external field and with one another is screened; its Fourier expansion contains only wave numbers $k > k_0$, where k_0 is a certain limiting value;

b) in addition to the fermions, there is also a Bose branch of the spectrum[3], consisting of oscillations of the plasma type with wave numbers $k < k_0$. (We note that the effective charge of a plasma phonon is zero.)

The second item listed is essential in the theory of recombination of current carriers[2]; the first must be taken into account in the theory of local levels and, in particular, in studying the scattering of current carriers by charged impurities. (It is easy to see that the screening which is automatically obtained in the many-electron theory of semiconductors gives precisely that cutoff of the Rutherford scattering at small angles which, in the one-electron approximation, has to be introduced in more or less artificial *ad hoc* fashion[4]). In the present paper we shall consider the last two problems, and also the question of the estimate of the limiting wave number k_0.

2. EVALUATION OF k_0*

As shown in Ref. 2, the Hamiltonian of the many-electron system in a crystal can be brought to the form

$$H = H_1 + H_2 + H' + H'' + H''' + E_0, \quad (2.1)$$

where H_1 and H_2 are the energy operators of the non-interacting fermions and bosons, H', H'', H''' contain their various interactions with one another (and are treated as small perturbations), and E_0 is a constant.

We shall consider a semiconductor with current carriers of a single type, and for brevity we shall refer to them simply as electrons. This means, in particular, that we neglect the intrinsic conductivity. Thus in our case the plasma is made up of electrons (or holes) supplied by the impurity, and the positively (or negatively) charged impurity ions. The concentration, n, of electrons is then constant and equal to the concentration of impurities. We emphasize that this quantity in general does not coincide with the concentration of free current carriers, since some of the fermions may be localized near impurities.

In this case[2]

* The author is very grateful to L. E. Gurevich, D. N. Zubarev, V. V. Tolmachev and S. V. Tiablikov for discussion of this question.

$$H_1 = \sum_{r,\sigma} E_r A^*_{r,\sigma} A_{r,\sigma}, \quad (2.2)$$

$$H_2 = \sum_{\mathbf{k},k<k_0} W(k) B^*(\mathbf{k}) B(\mathbf{k}), \quad (2.3)$$

Here A^*, A and B^*, B are the Fermi and Bose operators of second quantization, σ is the spin quantum number, r denotes the remaining quantum numbers characterizing the electrons (which, for states in the band is simply the quasi-momentum $\hbar\mathbf{f}$),

$$W(k) = \sqrt{W_0^2 + (\hbar^2 k^2/2m)^2}, \quad (2.4)$$

$$W_0 = \hbar\sqrt{4\pi ne^2/\varepsilon m'}, \quad (2.5)$$

and m' is the effective mass of the electron.*

The eigenvalues E_r are determined from the "one-particle" Schroedinger equation for the fermion, with the Hamiltonian

$$H_{\text{ind}} = -\frac{\hbar^2}{2m}\nabla^2 + \sum_{\mathbf{k},k>k_0} \frac{b(\mathbf{k})}{V} e^{-i\mathbf{kr}}, \quad (2.6)$$

where $b(\mathbf{k})$ is the Fourier coefficient of the external field, V is the normalization volume (the usual periodicity conditions are imposed on the vector $\mathbf{k}$). In describing the fermions we shall use the method of effective masses (and regard the mass as isotropic).

For the determination of k_0 we should, strictly speaking, minimize the free energy of the whole system (including the perturbation terms describing the interactions of the various types of excitations). However, we shall limit ourselves to evaluating the limiting admissible values of k_0. In the first place, the screened interaction between fermions must be small; this gives the obvious condition $k_0 \gg n^{1/3}$. Secondly, the coupling between fermions and bosons must be small. This coupling is contained in one of the perturbation terms, and also in the supplementary condition which is imposed when the "superfluous" variables are introduced. (*Cf.* Ref. 3.) This coupling shows itself in particular in the fact that a certain electrical current is associated with the plasma quanta. But it is clear that the effective charge of a plasma quantum must be equal to zero. In an exact treatment of the problem, the current carried by the bosons becomes zero automatically. We take the supplementary condition into account approximately by requiring that this current be negligibly small.* This gives a second inequality: $k_0^4 \ll 16\pi nme^2/\hbar^2$. Thus the approximate condition for the applicability of our computation is

$$n^{1/3} \ll k_0 < 2(\pi nme^2/\hbar^2)^{1/4}. \quad (2.7)$$

This proves to be adequate for the evaluation of the magnitude of the effects we are interested in. Actually we shall use the lower bound, thus obtaining somewhat reduced values for the "plasma" effects.

* Strictly speaking, because of exchange effects, the interaction potential between the "excess" electrons is not purely a Coulomb interaction, so that we should write in (2.4) $\nu(k) = 4\pi e^2/k^2 + f(k)$, $f(0) \neq \infty$. However, this will not change the result.

* L. E. Gurevich pointed out to the author that in general this approximate treatment is inadequate. However, it can apparently be used for the problem treated in the present paper.

3. SCATTERING BY CHARGED IMPURITIES INCLUDING THE EFFECT OF PLASMA SCREENING

In accordance with (2.6), the motion of a current carrier in the field of a defect with charge Ze ($b(k) = 4\pi Ze/\epsilon k^2$; the values of Z may be either positive or negative) is described by a "one-particle" Schroedinger equation with the Hamiltonian

$$H_{\text{ind}} = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{Ze^2}{\varepsilon r}\left(\frac{2}{\pi}\int_{k_0 r}^{\infty} \frac{\sin u}{u}\,du\right). \quad (3.1)$$

The actual mass of the electron is here replaced by the effective mass of the fermion, taking into account the effect of the periodic field of the lattice. (In general, the effective mass does not coincide with m'.)

Obviously, the presence of the screening factor (the factor in brackets) in the potential energy results in: a) the elimination of the logarithmic divergence in the reciprocal relaxation time which is characteristic for pure coulomb scattering; b) a drastic change in the character of the scattering when the average thermal momentum p of the electron becomes of the order of or less than $\hbar k_0$.

This last situation occurs if

$$T \sim \hbar^2 k_0^2/m^*\varkappa.$$

Thus at helium temperatures we should expect significant deviations from the usual Conwell-Weisskopf formula because of plasma screening. (This remark retains its validity even when we take into account modifications introduced when we include the interference of waves scattered by different defects[5]. We also emphasize that, unlike the Debye screening, the plasma screening is purely mechanical.) To illustrate the type of dependence obtained, we shall treat the scattering from the screened potential in (3.1) by means of the Born approximation.*

Then the probability of scattering per unit time with momentum change $\mathbf{p} - \mathbf{p}'$ is equal to

$$P(\mathbf{p}, \mathbf{p}') = \frac{2\pi^3\hbar^3 e^4 N Z^2}{\varepsilon^2 p^4 \sin^4(\theta/2)} \delta(E_p - E_{p'}) f\left(\frac{2p}{\hbar}\sin\frac{\theta}{2} - k_0\right), \quad (3.2)$$

where θ is the angle between the vectors $\mathbf{p}$ and $\mathbf{p}'$, N is the concentration of scattering centers,

$$f(z) = \begin{cases} 1 & \text{for } Z > 0 \\ 0 & \text{for } Z < 0. \end{cases}$$

Thus the scattering is actually "cut off" at $\theta/2 = \arcsin(\hbar k_0/2p)$. For the reciprocal relaxation time, $1/\tau$, we get (*cf.* Ref. 7).

$$\frac{1}{\tau} \frac{p^2(dp/dE)}{(2\pi)^2\hbar^3} \int_0^\pi \sin\theta(1-\cos\theta) P(\theta)\, d\theta = \frac{2\pi N e^4 Z^2}{\sqrt{2m^*}\,\varepsilon^2} E_p^{-3/2} \ln\left(\frac{2p}{\hbar k_0}\right) f\left(1 - \frac{\hbar k_0}{2p}\right). \quad (3.3)$$

Thus there is no scattering when $p < \hbar k_0/2$. Of course this result should not be taken too literally: it is changed if we take into account both the correction to the Born approximation and the small term H' which was dropped in (2.6) and (3.1). However there is no doubt about the fact (which is obvious beforehand) that there is a marked decrease in scattering for $p \sim \hbar k_0$. Under these circumstances we must take account of other possible scattering mechanisms, the most important of which (at low temperatures) is scattering by uncharged impurities. The corresponding relaxation time was calculated in Ref. 8 (without including screening). Since in the present case the forces are short range, the plasma screening is unimportant, so that we can use the formula of Ref. 8 for our estimate:

$$1/\tau_0 = 20\varepsilon\hbar^3 N_0 / m^{*2} e^2 \quad (3.4)$$

(The subscript 0 refers to quantities characterizing neutral impurity centers.)

Remembering the illustrative nature of our computation, we may assume that only one scattering mechanism acts for each value of p (on charged impurities for $p < \hbar k_0/2$, and on uncharged impurities for $p > \hbar k_0/2$). Then we get for the microscopic mobility μ, the Hall coefficient R, and the Hall mobility μ_H.

$$\mu = \frac{8e\tau_0}{3m^*\sqrt{\pi}}\chi(u_0) + \frac{4\varepsilon^2\varkappa^{3/2}\psi(u_0)T^{3/2}e^{-u_0^2/2}}{\sqrt{m^*}\,\pi^{3/2}e^2 N \ln(2\sqrt{7m^*\varkappa T}/\hbar k_0)},$$

$$R = R'\frac{64}{945\sqrt{\pi}} \frac{\varphi(u_0)e^{-u_0^2/2} + \tau_0^2\alpha^{-2}(\varkappa T)^{-3}\chi(u_0)}{[\psi(u_0)e^{-u_0^2/2} + {}^1/_3\tau_0\alpha^{-1}(\varkappa T)^{-3/2}\chi(u_0)]^2}, \quad (3.5)$$

$$\mu_H = \mu_H' \frac{64}{945\sqrt{\pi}} \frac{\varphi(u_0)e^{-u_0^2/2} + \tau_0^2\alpha^{-2}(\varkappa T)^{-3}\chi(u_0)}{\psi(u_0)e^{-u_0^2/2} + {}^1/_3\tau_0^2\alpha^{-1}(\varkappa T)^{-3/2}\chi(u_0)},$$

where R' and μ_H' are the values obtained from the Cornell-Weisskopf formula, neglecting the scattering by uncharged impurities ($R' = 1.93/n_c ec$, n_c is the concentration of current carriers),

$$\alpha = \sqrt{2m^*}\,\varepsilon^2 / 2\pi N e^4 Z^2 \ln\frac{2\sqrt{7m^*\varkappa T}}{\hbar k_0},$$

$$\varphi(u_0) = \frac{945\sqrt{\pi}}{64}\left[1 - \operatorname{erf}\left(\frac{u_0}{\sqrt{2}}\right)\right]e^{u_0^2/2} + \frac{u_0}{32\sqrt{2}}(u_0^8 + 9u_0^6 + 63u_0^4 + 315u_0^2 + 945), \quad (3.6)$$

*Strictly speaking, the Born approximation is not applicable under the conditions of interest to us; it can nevertheless give us a description of the true state of affairs. In addition, it hardly makes sense to carry out exact calculations of the scattering and then to use a kinetic equation whose criterion of applicability[6] is rather poorly satisfied at those temperatures and impurity concentrations of interest to us.

$$\psi(u_0) = 1 + u_0^2/2 + u_0^4/8 + u_0^6/48,$$

$$\chi(u_0) = \frac{3\sqrt{\pi}}{8}\,\mathrm{erf}\left(\frac{u_0}{\sqrt{2}}\right) - \frac{u_0}{4\sqrt{2}}\,e^{-u_0^2/2}\,(u_0^2+3),$$

and $u_0^2 = \hbar^2 k_0^2/8\,m^* \varkappa T$.

From Eq. (3.5) it is clear that for $u_0^2/2 \ll 1$ the plasma screening plays no part ($R \to R'$, $\mu_H \to \mu_H'$); however if the temperature is sufficiently low (of the order of 1° K for $n \sim 10^{15}$ cm^{-3}), the scattering has nothing in common with the Conwell-Weisskopf scattering. Thus, for example, if we determine the concentration of current carriers, n_c, from measurements of the Hall constant in the usual way ($n_c \sim 1/Rec$), then what is actually determined is the effective concentration

$$n_{\text{eff}} = n_c \frac{945\sqrt{\pi}}{64} \frac{[\psi(u_0)\,e^{-u_0^2/2} + {}^1/_3\,\tau_0\alpha^{-1}(\varkappa T)^{-3/2}\chi(u_0)]^2}{\varphi(u_0)\,e^{-u_0^2/2} + \tau_0^2\,\alpha^{-2}(\varkappa T)^{-3}\chi(u_0)}. \tag{3.7}$$

When $u_c \gtrsim 1$ this quantity has nothing in common with n_c; under suitable conditions, the factor multiplying n_c can even increase exponentially with temperature (for $N/N_0 \sim 10^{-2}$). Possibly this is one of the causes of the (apparent) decrease in activation energy which is observed for high concentrations of impurities ($n \sim 10^{18}$ cm^{-3}). In this latter case the plasma screening becomes particularly important, and its inclusion is apparently necessary not only at helium, but also at hydrogen temperatures.*

4. LOCAL LEVELS WHEN PLASMA SCREENING IS INCLUDED

The deviation of the potential of the interaction between the fermion and the impurity center from the Coulomb form naturally shows itself not only in scattering but also in the structure of the local levels produced by the center. Within the realm of the so-called "hydrogen-like" model, the energy of the local level (measured from the bottom of the zone) is determined by a wave equation with the Hamiltonian (3.1) with $Z = -1$. For not too large values of k_0 it is natural to represent the potential energy in (3.1) in the form

$$-\frac{e^2}{\varepsilon r} + \frac{e^2}{\varepsilon r}\left\{1 - \frac{2}{\pi}\int_{k_0 r}^{\infty}\frac{\sin u}{u}\,du\right\}$$

and to treat the second term as a perturbation. We then find for the ground state energy E_0 in first approximation:

$$E_0 = -\frac{m^* e^4}{2\varepsilon^2\hbar^2}\left\{1 - 2\left[\frac{1}{\pi}\,\frac{k_0 a_0}{1+(k_0 a_0/2)^2} + 1 - \frac{2}{\pi}\tan^{-1}\frac{2}{k_0 a_0}\right]\right\}, \tag{4.1}$$

where

$$a_0 = \varepsilon\hbar^2/m^* e^2.$$

For small values of $k_0 a_0$ (which are the only values for which the use of perturbation theory is meaningful), (4.1) becomes

$$E_0 = -(m^* e^4/2\varepsilon^2\hbar^2)\{1 - (4\varepsilon\hbar^2 k_0/\pi m^* e^2)\}, \tag{4.2}$$

or, using the lower limit in (2.7) for a rough estimate,

$$E_0 = -\frac{m^* e^4}{2\varepsilon^2\hbar^2} + \Delta E, \quad \Delta E = \frac{2e^2 k_0}{\pi\varepsilon} \geqslant \frac{2e^2}{\pi\varepsilon}\,n^{1/3}. \tag{4.3}$$

We get the well-known[9] relation ΔE = const. $n^{1/3}$, with a reasonable value for the constant ($\sim 10^8$ if ΔE is measured in electron volts and n in cm^{-3}). We emphasize that the "plasma" level shift treated here should occur not only at high impurity concentrations, but also at low concentrations if the concentration of carriers forming the plasma is raised by some other means. This should make it possible experimentally to distinguish the "plasma" mechanism for shift of the levels from the effect of formation of impurity bands.

Summarizing, we must recognize that "plasma" effects already become significant for current carrier concentrations $\sim 10^{15} - 10^{16}$ cm^{-3}; for still higher concentrations (and also at low temperatures), their inclusion is absolutely essential.

* However, one should remember that the use of the kinetic equation for these values of impurity concentration is already entirely inadmissible.

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227

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On the Dependence of the Motion of Bodies in a Gravitational Field on Their Mass

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The Lagrangian function for the motion of a body of small mass, in the fixed field of n other bodies of finite mass, is derived to the second approximation of gravitational theory. This function is compared with the Lagrangian function for the motion of a body of finite mass in the gravitational field of all $n + 1$ bodies. It is found that in the approximation under consideration, the Lagrangian function for the motion of a finite mass depends in an essential way on the value of that mass.

IN ACCORDANCE WITH the principle of the geodesic line, the motion of a body in a fixed gravitational field* is determined by the requirement that

$$\delta \int \mathscr{L}\, dt = 0, \tag{1}$$

where

$$\mathscr{L} = mc^2\left(1 - \frac{1}{c}\sqrt{g_{00} + 2g_{0i}\dot{x}_i + g_{ik}\dot{x}_i\dot{x}_k}\right) \tag{2}$$

is the Lagrangian function of the mechanical problem. Here m is the mass of the body under consideration, $x_i(t)$ the Cartesian coordinates of the center of mass of m at the instant t and g_{00}, g_{0i}, g_{ik} the components of the fundamental tensor as determined by the Einstein equations of gravitation; the Latin indices i, k take the values 1, 2, 3 and summation over a repeated index is understood. A superior dot indicates a time derivative.

In order to find an approximate expression for the Lagrangian function $\mathfrak{L}$ for the motion of a small mass in the fixed field of n other finite (not small) masses, we shall use an approximate solution of the Einstein equations of gravitation, obtained by Fock[1].

We consider spherically symmetric, nonrotating bodies, whose linear dimensions are much smaller than the distances between them; and we retain only quantities of order v^2/c^2, where v^2 is the square of the velocity of translational motion of one of the bodies. We then obtain the following expressions for the components of the fundamental tensor:

$$g_{00} = c^2 - 2U + (2U^2 - 2S^*)/c^2, \quad g_{0i} = 4U_i/c^2,$$

$$g_{ik} = -(1 + 2U/c^2)\,\delta_{ik}. \tag{3}$$

* The field of a system of bodies is regarded as fixed, with respect to a given body, if the motion of each of the bodies of the system that produces the field is supposed independent of the motion of the given body.