J. Phys. Chem. Solids Pergamon Press 1962. Vol. 23, pp. 875–880. Printed in Great Britain.

DENSITY MATRIX APPROACH TO A SIMPLE HOT ELECTRON PROBLEM

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(*Received* 4 *December* 1961)

Abstract—A transport theory of non-ohmic conductivity in semiconductors is developed in a form which is closely related to Kohn–Luttinger theory of ohmic conductivity. The theory is limited to a very simple case in which the energy surfaces are spherically symmetric and the conduction electron is scattered by acoustic vibrations. The interaction between the conduction electron and the lattice vibration is considered in the lowest order of the coupling constant. The density matrix of the system is expanded by a power series of the intensity of the external field F, and an equation is derived for each order of F. By solving these equations we find that the quantum transport equation is equivalent to the Boltzmann transport equation in any order of F.

1. INTRODUCTION

THE PROBLEM of electrical conductivity is usually treated on the basis of a transport equation. Recently, the foundation of the equation has been thoroughly investigated by many authors from a quantum theoretical point of view, and the nature of the approximations is well understood, as long as ohmic conductivity is concerned. On the other hand, a study of a non-ohmic current in semiconductors is one of the subject of active research in semiconductor physics, and many experimental and theoretical works have been published on this subject. In a pioneer work on hot electron phenomena in semiconductors, Shockley developed a theory of the hot electron on the basis of a naïve energy balance condition on the electron system, and this approach was afterwards developed by several investigators. Another approach based on the Boltzmann transport equation was also developed and the theoretical results seem to be in reasonable agreement with experiments. However, the transport equation used in non-ohmic problems was derived by a formal extension of the ohmic one, so that the foundation of the equation is still ambiguous. Therefore, our next problem is to examine a transport equation of the non-ohmic conductivity from the quantum theoretical point of view. The purpose of the present paper is to investigate the foundation of the Boltzmann transport equation of hot electron problems on the basis of the quantum theory. We shall, however, confine ourselves to treat a very simple case in order to illustrate a possibility that the usual transport equation is still applicable to some non-ohmic problems as it can be applied to many transport phenomena in the ohmic region.

2. MODELS AND ASSUMPTIONS

In the following we shall develop a transport theory of non-ohmic conductivity in semiconductors in a form which is closely related to the Kohn–Luttinger theory[1] of ohmic conductivity. We assume that the density of conduction electrons is so low that we can safely neglect the effect of the Coulomb interaction between the conduction electrons. Then every electron may be treated as completely independent of all other electrons. We assume also that the structure of a conduction band is so simple that the relation between the energy, E, and the wave number, k, of a conduction electron is given by $E = \hbar^2k^2/2m$, where m is the effective mass of a conduction electron. The conduction electrons are scattered by the interaction with lattice vibrations of acoustic types. We introduce a parameter λ, which measures the strength of the interaction causing collisions. In the following we shall make two assumptions: one is that the interaction is so weak that we may

consider only the terms of the lowest order in λ; the other is that the lattice is always in thermal equilibrium with the outer world and the expectation value of phonon numbers is determined by the usual Planck law with temperature T. This assumption means that the amount of energy which is transferred to the lattice from the conduction electrons per unit time is quite small, so that the disturbance to the lattice through the interaction with the electrons is negligibly small. In fact, experiments on hot electrons are usually performed under conditions that keep the lattice temperature practically equal to the original one during the time of measurement.

3. MATHEMATICAL FORMULATION OF THE PROBLEM

The total Hamiltonian, H_t, for each electron in our problem may be written as

$$H_t = H_e+H_l+H_{\rm int}+H_F, \tag{1}$$

where H_e is the Hamiltonian of the free electron, H_l is the Hamiltonian of the lattice, $H_{\rm int}$ is the interaction with the lattice and H_F is the interaction with the external field. The explicit expressions are as follows:

$$H_e = p^2/2m, \tag{2}$$

$$H_l = \sum_q \left(-\frac{\hbar^2}{2M}\cdot\frac{\partial^2}{\partial X_q^2}+\frac{1}{2}M\omega_q^2 X_q^2\right) \tag{3}$$

and

$$H_{\rm int} = iC(\hbar/2MV)^{1/2}\sum_q \frac{q}{\sqrt{\omega_q}}[a_q\exp(iqr) - a_q^*\exp(-iqr)], \tag{4}$$

where C is the coupling constant between the conduction electron and the lattice vibration, M is the mass of the ion and ω_q is the angular frequency of the vibration of a wave vector q. Finally, H_F is given by

$$H_F = -eF_\alpha x_\alpha. \tag{5}$$

Following KOHN and LUTTINGER,[1] we assume that

$$F_\alpha = F_\alpha^0\exp(st), \tag{6}$$

where s is a very small parameter. In this approximation, we have

$$H_e\psi_k = E_k\psi_k, \tag{7}$$

where $E_k = \hbar^2k^2/2m$. Then the electron wave function ψ_k is determined as

$$\psi_k = \exp(ikr)/V^{1/2}, \tag{8}$$

where V is the volume of the crystal. Here, let us introduce the density matrix of the total system ρ_t, which varies with time according to

$$i\hbar(\partial\rho_t/\partial t) = [H_t,\rho_t]. \tag{9}$$

We shall choose the representation for which H_e+H_l is diagonal. In this representation the matrix element of ρ_t is expressed as

$$(k,N|\rho_t|k',N'), \tag{10}$$

where the N representation is used for the phonon system. For the sake of brevity, we shall use a simplified notation for a diagonal element of a matrix, for example,

$$\rho_t(kN) = (k,N|\rho_t|k,N). \tag{11}$$

We expand the density matrix by a power series of F:

$$\rho_t = \rho_0+\sum_{n=1}^{\infty}\rho_n, \tag{12}$$

where ρ_0 is a density matrix of the total system in thermal equilibrium when there is no external field, and ρ_n is a component of the density matrix of the system which is proportional to F^n. Inserting (12) into (9) we have:

$$-i\hbar\frac{\partial}{\partial t}(\rho_1+\rho_2+\ \ldots) = [\rho_0+\rho_1+\rho_2+\ \ldots, H+H_F], \tag{13}$$

where H is defined by

$$H = H_e+H_l+H_{\rm int}. \tag{14}$$

Equating the terms of the same power of F in both sides of (13) we have a set of coupled equations:

$$-i\hbar\partial\rho_1/\partial t = [\rho_0,H_F]+[\rho_1,H], \tag{15-1}$$

$$-i\hbar\partial\rho_2/\partial t = [\rho_1,H_F]+[\rho_2,H], \tag{15-2}$$

. . . . . .

$$-i\hbar\partial\rho_n/\partial t = [\rho_{n-1},H_F]+[\rho_n,H]. \tag{15-n}$$

In the following, we shall derive a set of equations which must be satisfied by the diagonal elements of the density matrix ρ_n, because only the diagonal elements are necessary for calculation of the electrical conductivity.

4. OHMIC CONDUCTIVITY

In this Section, we shall treat the equation of the lowest order of F. Following KOHN and LUTTINGER,[1] we put

$$\rho_1 = \xi_1 \exp(st), \tag{16}$$

and then we have

$$-i\hbar s\, \xi_1 = C^{(1)} + [\xi_1, H], \tag{17}$$

where

$$C^{(1)} = -eF_\alpha^0 [\rho_0, x_\alpha]. \tag{18}$$

After some elementary calculations, equation (17) is reduced to the following equations:

$$\begin{aligned}\hbar(\omega_{KK'} + \omega_{NN'} - is)(kN|\xi_1|k'N') &= (kN|C^{(1)}|k'N') \\ &+ \{\xi_1(kN) - \xi_1(k'N')\}(kN|H_{\text{int}}|k'N') \\ &+ \sum_{k''}{}' \sum_{N''}{}' \{(kN|\xi_1|k''N'')(k''N''|H_{\text{int}}|k'N') \\ &- (kN|H_{\text{int}}|k''N'')(k''N''|\xi_1|k'N')\},\end{aligned} \tag{19-1}$$

where $k \neq k'$ and $N \neq N'$. Here the prime in the summations means to exclude the cases $k = k''$, $k' = k''$, $N = N''$ and $N' = N''$, and further $\hbar\omega_{kk'} = E_k - E_{k'}$ and $\hbar\omega_{NN'} = E_N - E_{N'}$. On the other hand, the diagonal element of $\xi_1(kN)$ is given by

$$\begin{aligned}-i\hbar s\, \xi_1(kN) &= C^{(1)}(kN) \\ &+ \sum_{k'}{}' \sum_{N'}{}' \{(kN|\xi_1|k'N')(k'N'|H_{\text{int}}|kN) \\ &- (kN|H_{\text{int}}|k'N')(k'N'|\xi_1|kN)\}.\end{aligned} \tag{19-2}$$

Here we introduce approximations. Since the principle of the approximation is to retain only the terms of the lowest order in λ, we use the following approximate formula for $C^{(1)}$:

$$(kN|C^{(1)}|k'N') = ieF_\alpha^0 \frac{\partial}{\partial k_\alpha} (kN|\rho_0(H_e + H_l)|k'N')\delta_{kk'}\delta_{NN'}. \tag{20}$$

Further, the matrix element of ρ_0 is reduced to

$$(kN|\rho_0(H_e + H_l)|kN) = f_m(E_k) \cdot P(N) \tag{21}$$

because of the assumption that the lattice is always in thermal equilibrium. Here the function $f_m(E_k)$ is the Maxwell distribution function for electrons and $P(N)$ represents the probability that the lattice is in the state $|N)$:

$$P(N) = \exp(-E_N/kT) / \sum_{N'} \exp(-E_{N'}/kT). \tag{22}$$

In this approximation, $(kN|C^{(1)}|k'N')$ is given by

$$(kN|C^{(1)}|k'N') = ieF_\alpha^0 \frac{\partial f_m^{(k)}}{\partial k_\alpha} P(N) \cdot \delta_{kk'}\delta_{NN'}. \tag{23}$$

Following Kohn and Luttinger we estimate the order of the magnitude of the matrix elements as follows: $\xi_1(kN) \sim \lambda^{-2}$ and

$$(kN|\xi_1|k'N') = \frac{(kN|H_{\text{int}}|k'N')}{\hbar(\omega_{kk'} + \omega_{NN'} - is)} \{\xi_1(kN) - \xi_1(k'N')\} \sim \lambda^{-1}.$$

By using these relations we eliminate the non-diagonal matrix elements from (19-2) and then we have:

$$\begin{aligned}-i\hbar s \xi_1(kN) &= C^{(1)}(kN) \\ &+ \sum_{k'}{}' \sum_{N'}{}' |(kN|H_{\text{int}}|k'N')|^2 \{\xi_1(kN) - \xi_1(k'N')\} \\ &\times \left(\frac{1}{\hbar(\omega_{kk'} + \omega_{NN'} - is)} - \frac{1}{\hbar(\omega_{kk'} + \omega_{NN'} + is)} \right).\end{aligned} \tag{24}$$

Considering the limit of $s \to 0$ we have

$$\begin{aligned}C^{(1)}(kN) + 2\pi i \sum_{k'}{}' \sum_{k'}{}' &|(kN|H_{\text{int}}|k'N')|^2 \\ &\times \{\xi_1(kN) - \xi_1(k'N')\}\delta(\omega_{kk'} + \omega_{NN'}) = 0.\end{aligned} \tag{25}$$

Because of the assumption mentioned previously we may write the function $\xi_1(kN)$ as a product

$$\xi_1(kN) = f_k^{(1)} P(N), \tag{26}$$

where $f_k^{(1)}$ is an abbreviation of the matrix element $(k|f^{(1)}|k)$. Inserting (23) and (26) into (25) we

have a following equation:

$$-\frac{eF_\alpha^0}{\hbar}\frac{\partial f_m(k)}{\partial k_\alpha}+L[f_k^{(1)}]=0, \tag{27}$$

where

$$L[f_k]\equiv\frac{2\pi}{\hbar}\sum_{k'}'\sum_{N,N'}\times|(kN|H_{\rm int}|k'N')|^2\delta(\omega_{kk'}+\omega_{NN'})\times\{f_{k'}P(N')-f_kP(N)\}. \tag{28}$$

Following the standard procedures we can easily evaluate the function $L[f_k^{(1)}]$ as follows:

$$L[f_k^{(1)}]=\frac{\pi C^2}{MV}\sum_{N_q}\sum_q\frac{q^2}{\omega_q}\times\{N_q[f_{k+q}^{(1)}P(N_q-1)-f_k^{(1)}P(N_q)]\delta(E_k-E_{k+q}+\hbar\omega_q)+(N_q+1)[f_{k-q}^{(1)}P(N_q+1)-f_k^{(1)}P(N_q)]\times\delta(E_k-E_{k-q}-\hbar\omega_q)\}. \tag{29}$$

Further, by using the relations

$$\sum(N_q+1)P(N_q)=n_q+1$$

and

$$\sum N_qP(N_q)=n_q,$$

where n_q is defined as $n_q=1/[\exp(\hbar\omega_q/kT)-1]$ we have a familiar expression:

$$L[f_k^{(1)}]=\frac{\pi C^2}{MV}\sum_q\frac{q^2}{\omega_q}\times\{f_{k+q}^{(1)}[(n_q+1)\delta(E_{k+q}-E_k+\hbar\omega_q)+n_q\delta(E_{k+q}-E_k-\hbar\omega_q)]-f_k^{(1)}[n_q\delta(E_{k+q}-E_k+\hbar\omega_q)+(n_q+1)\delta(E_{k+q}-E_k-\hbar\omega_q)]\}. \tag{30}$$

Thus, we see that equation (27) is identical to a usual Boltzmann transport equation.[2]

5. WARM ELECTRON

In this Section we shall solve equations (15–2) and (15–3) and discuss the warm-electron problem. As seen from equation (15), the structure of these two equations is the same as that of equation (15–1), so that we expect that we are able to derive the equations of the similar type as equation (27). First, we put

$$\rho_2=\xi_2\exp(2st) \tag{31}$$

and then equation (15–2) becomes

$$-i2s\hbar\xi_2=C^{(2)}+[\xi_2,H], \tag{32}$$

where

$$C^{(2)}=-eF_\alpha^0[\xi_1,\varkappa_\alpha]. \tag{33}$$

In the representation for which H_e+H_l is diagonal, the matrix element of $C^{(2)}$ is evaluated as

$$(kN|C^{(2)}|k'N')=ieF_\alpha^0\left(\frac{\partial}{\partial k_\alpha}+\frac{\partial}{\partial k_\alpha'}\right)(kN|\xi_1|k'N'), \tag{34}$$

and

$$C^{(2)}=ieF_\alpha^0\frac{\partial}{\partial k_\alpha}\xi_1(kN)=ieF_\alpha^0\frac{\partial f_k^{(1)}}{\partial k_\alpha}P(N). \tag{35}$$

Next, we must write down the equations which correspond to equations (19–1) and (19–2). These equations are easily obtained by replacing $i\hbar s$ in (19) by $2i\hbar s$ and ξ_1 by ξ_2. Since these equations are quite similar to equation (19), we write here only one of them explicitly:

$$-2i\hbar s\,\xi_2(kN)=C^{(2)}(kN)+\sum_{k'}'\sum_{N'}'\{(kN|\xi_2|k'N')(k'N'|H_{\rm int}|kN)-(kN|H_{\rm int}|k'N')(k'N'|\xi_2|kN)\}. \tag{36}$$

Next, let us estimate the order of the magnitude of various matrix elements in (36). From (35) and the knowledge about the order of the magnitude of the matrix elements of ξ_1 we can easily determine the order of the magnitude of the matrix elements of $C^{(2)}$:

$$C^{(2)}(kN)\sim\lambda^{-2}\text{ and }(kN|C^{(2)}|k'N')\sim\lambda^{-1}$$

If we assume that the order of the magnitude of $\xi_2(kN)$ is of λ^{-4}, then the order of the magnitude of $(kN|\xi_2|k'N')$ is estimated as λ^{-3}. Therefore, we may express the nondiagonal elements of ξ_2 by the diagonal elements of ξ_2 as in the case of ξ_1:

$$(kN|\xi_2|k'N')=\frac{(kN|H_{\rm int}|k'N')}{\hbar(\omega_{kk'}+\omega_{NN'}-2is)}\times\{\xi_2(kN)-\xi_2(k'N')\}. \tag{37}$$

We see that this matrix element has the same form as before.

Inserting (37) into (36) we have:

$$2i\hbar s\xi_2(kN) = C^{(2)}(kN) + \sum_{k'}{}' \sum_{N'}{}' |(kN|H_{\text{int}}|k'N')|^2 \times \{\xi_2(kN) - \xi_2(k'N')\} \times \left(\frac{1}{\hbar(\omega_{kk'} + \omega_{NN'} - 2is)} - \frac{1}{\hbar(\omega_{kk'} + \omega_{NN'} + 2is)}\right) \tag{38}$$

Since the matrix element $C^{(2)}(kN)$ has the order of the magnitude λ^{-2}, we justify the previous assumption that the order of the magnitude of $\xi_2(kN)$ is of λ^{-4}. Putting $\xi_2(kN) = f^{(2)}P(N)$ and after some elementary calculations, we have a following equation for $f_k^{(2)}$:

$$O = -\frac{eF_\alpha^0}{\hbar}\frac{\partial f_k^{(1)}}{\partial k_\alpha} + L[f_k^{(2)}], \tag{39}$$

where the operator L was defined by (28). Next, we proceed to the third-order equation. The method of deduction is quite similar as before. Putting $\rho_3 = \xi_3 \exp(3st)$ and defining $C^{(3)}$ by

$$C^{(3)} = -eF_\alpha^0[\xi_2, x_\alpha], \tag{40}$$

we see easily that the order of the magnitude of the matrix elements of $C^{(3)}$:

$$C^{(3)}(kN) = ieF_\alpha^0 \frac{\partial}{\partial k_\alpha}\xi_2(kN) \sim \lambda^{-4}$$

and

$$(kN|C^{(3)}|k'N') = ieF_\alpha^0\left(\frac{\partial}{\partial k_\alpha} + \frac{\partial}{\partial k_\alpha'}\right)(kN|\xi_2|k'N') \sim \lambda^{-3},$$

respectively. Further, if we assume that the order of the magnitude of ξ_3 is of λ^{-6} and repeat the similar calculation as before, we finally obtain the following equation which gives the distribution function $f_k^{(3)}$:

$$O = -\frac{eF_\alpha^0}{\hbar}\frac{\partial f_k^{(2)}}{\partial k_\alpha} + L[f_k^{(3)}], \tag{41}$$

where we put

$$\xi_3(kN) = f_k^{(3)}P(N). \tag{42}$$

Thus, we see that the quantum transport equation in the order of F^2 and F^3 are equivalent to the Boltzmann transport equation, as long as we consider only the lowest order of λ.

Let us investigate the general character of the distribution functions which are determined by the transport equations (27), (39) and (41), respectively. As is usually done, we expand each of the distribution functions by spherical harmonics:

$$f_k^{(i)} = \sum_n f_n^{(i)} P_n(\cos\theta).$$

Since $f_m(k)$ is spherically symmetric, equation (27) tells that $f_k^{(1)}$ is proportional to $P_1(\cos\theta)$. Then, from equation (39) we see that $f_k^{(2)}$ contains the terms which are proportional to $P_0(\theta)$ and $P_2(\theta)$, respectively. We see also that $f_k^{(3)}$ consists of terms which are proportional to $P_1(\theta)$ and $P_3(\theta)$, respectively. Therefore, if we can show that the term proportional to P_2 (or P_3) is very small as compared with the term proportional to P_0 (or P_1), then the correction to the spherically symmetric part of the distribution function is proportional to F^2, and the correction to the ohmic current is proportional to F^3. If the structure of the conduction band is complicated as in Ge and Si, the situation is not so simple as stated previously. The correction to the ohmic current is still proportional to F^3, but the non-ohmic current shows anisotropy.

From the theory developed previously, we find that the distribution function $f_k^{(n)}$ is proportional to $(\lambda^{-2}F)^n$. The parameter λ has been assumed to be infinitesimally small in order that only the terms of the lowest order of λ are taken into account. In practice, however, we may choose some quantity of real importance as a parameter, although it is not always very small. Since the mobility of the conduction electron is proportional to λ^{-2}, we may say that $f_k^{(n)}$ is proportional to $(\mu F)^n$. In the previous paper,[3] we developed a theory of hot electrons in semiconductors on the basis of the Boltzmann approach. We introduced there a non-dimensional parameter which is defined by $p = 3\pi\mu^2F^2/16c^2$, where c is the velocity of sound and μ is the mobility, and we found that $f_k^{(n)}$ is proportional to $p^{n/2}$. Thus, we see that the parameter p may be regarded as a parameter which is used here instead of $(\lambda^{-2}F)^2$. When p is much

smaller than 1, the correction to the ohmic conductivity is sufficiently small and we are able to disregard the terms higher than F^4. Then, we conclude that the usual transport equation is applicable to the warm electron problem, just as the usual transport equation is applicable to the ohmic conductivity in semiconductors.

6. HOT ELECTRON

In this Section we shall treat the equations

$$-i\hbar\frac{\partial\rho_n}{\partial t}=[\rho_{n-1},H_F]+[\rho_n,H]$$

for any n. From the discussions mentioned in the previous Sections, the general characters of the equations are almost certain. Following the method developed in the previous Sections we may prove that $f_k^{(n)}$ is proportional to $(\lambda^{-2}F)^n$. Therefore, we may determine the distribution function by solving these equations successively. There remains, however, a question concerning convergence of the series

$$f(k)=\sum_n f_k^{(n)},$$

because the value of the parameter p is usually much larger than 1 in hot-electron problems. Unfortunately, it is very difficult to test the convergence of the series in general. We have, however, a special example which may be mentioned. In the previous paper,[3] we showed that, when the scattering of conduction electrons is caused only by the interaction with the acoustic vibration, the transport equation was solved with good accuracy and the convergence of the series was easily proved. Here we mention only the main results. If we expand the distribution function by a power series of F

$$f(k)=f_0(E)+kg(E)\cos\theta+k^2h(E)P_2(\theta)+\ldots, \quad (44)$$

where

$$f_0(E)=\sum\alpha_n(E)F^n \quad (45)$$

and

$$g(E)=\sum\beta_n(E)F^n,\ h(E)=\sum\gamma_n(E)F^n,\ldots \quad (46)$$

The coefficient $\alpha_{2l}(E)$ is determined as

$$\alpha_{2l}(E)F^{2l}=\frac{1}{(l!)}p^l\left[\ln\left(\frac{E}{kT}+p\right)\right]^l\alpha_0(E). \quad (47)$$

Thus, the distribution function $f_0(E)$ is

$$f_0(E)=\sum_{l=0}^{\infty}\alpha_{2l}(E)F^{2l}=\left(\frac{E}{kT}+p\right)^p\exp\left(-\frac{E}{kT}\right). \quad (48)$$

Since $\beta_{2l+1}(E)$ is connected with $\alpha_{2l}(E)$ by a relation

$$\beta_{2l+1}(E)F=(\text{const})F\frac{1}{\sqrt{E}}\frac{d\alpha_{2l}}{dE}, \quad (49)$$

the distribution function $g(E)$ is determined as

$$g(E)=(\text{const})F\frac{1}{\sqrt{E}}\frac{d}{dE}\sum_{n=\text{even}}\alpha_nF^n$$

$$=(\text{const})F\frac{1}{\sqrt{E}}\frac{df_0}{dE}. \quad (50)$$

Further, we are able to show that $h(E)$ terms are quite small as compared with $f_0(E)$. Thus, we see that we have a distribution function as a closed form in this simple example. In fact, we have derived a differential equation which is satisfied by the function (48) in a previous paper.[4] The differential equation was, however, derived from the transport equation by a rather intuitive procedure. In the present paper we have justified such a procedure from a more fundamental point of view.

The theoretical treatment developed here will be extended to the case in which the conduction electron is scattered by a set of fixed impurities distributed at random throughout the lattice. In other cases we have not yet succeeded to prove the convergence of the series

$$\sum f_k^n.$$

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