SEVERAL KINETIC COEFFICIENTS AND THE RELATIONS BETWEEN THEM FOR ONE TYPE OF THE CHARGE CARRIER

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The results obtained in the present paper give for the kinetic coefficients expressions which are for a given type of scattering dependent on the chemical potential and temperature. This was possible by utilising the Lorentz solution of Boltzman's kinetic equation [2] introducing the free mean path in the form $l = l_0(T)e^r$ [3] and using the Fermi integrals. The analogical expressions known from the existing literature [4—8] are not suitable for further calculation.

I. THE BASIC RELATIONS

We use the results of the paper [1] giving for n-type circuit carriers the following relations for:

a. The density of the conventional electric current

$$j = \frac{16\pi e m^*}{3h^3} \, l_0(T)(r+1)(kT)^{r+1} F_r(\mu^*) \left[\frac{d\mu}{dx} + eE_x - \frac{\mu}{T} \frac{dT}{dx} + \right.$$
$$\left. + \frac{r+2}{r+1} k \frac{dT}{dx} \frac{F_{r+1}(\mu^*)}{F_r(\mu^*)} \right].$$

(1)

b. The thermoelectric voltage in a closed semi-conductive circuit

$$-\int_l^m dV = \int_l^m E_x dx = -\frac{1}{e} \int_l^m \left(\left(k \frac{r+2}{r+1} \frac{F_{r+1}(\mu^*)}{F_r(\mu^*)} - \frac{\mu}{T} \right) dT = \right.$$
$$= -\frac{1}{e} \int_l^m \frac{\beta_n}{T} dT = \frac{1}{e} \int_l^m \frac{T}{dx} \frac{d}{dx} \frac{\beta_n}{T} dx.$$

(2)

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c) The heat released in an element of an nonhomogeneous semiconductor of the length dx and the unit section during the unit time in the presence of a temperature gradient

$$dq_t = \frac{1}{e}\frac{1}{T}\frac{d}{dx}\frac{1}{T}\left(\frac{r+2}{r+1}kT\frac{F_{r+1}(\mu^*)}{F_r(\mu^*)} - \mu\right)dx = \frac{j}{e}\frac{d}{dx}\left(\frac{\beta_n}{T}\right)dx,$$ (3)

where $F_r(\mu^*)$ is the Fermi integral, μ is the chemical potential, $\mu^* = \mu/kT$: the free mean path is expressed by the relation $l = l_0(T)\varepsilon^r$, where ε is the energy of the electron relative to the bottom of the conduction band. The symbol β_n is defined by the relation (2). The same relations for a p-type of carriers are analogical.

II. THE EXPRESSIONS FOR THE COEFFICIENT OF DIFFUSION AND THE RELATION BETWEEN THE MOBILITY AND THE FREE MEAN PATH OF THE ELECTRON

In a inhomogenous sample the current of diffusion due to $\partial\mu/\partial x = 0$ at $dT/dx = 0$ is in equilibrium with that due to the electric field. Its value follows from the relation (1)

$$ja = \frac{j}{-e} = \frac{16\pi em*}{3h^3}l_0(T)(r+1)(kT)^{r+1}F_r(\mu^*)\frac{d\mu}{dx}\frac{1}{-e}$$ (4)

Neglecting the term $v_x q$ in the distribution function $f = f_0 - v_x q$ [1] we may write in the first approximation

$$n = 4\pi\left(\frac{2m*}{h^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{1/2}}{\exp\left(\frac{\varepsilon-\mu}{kT}\right)+1}d\varepsilon = 4\pi\left(\frac{2m*}{h^2}\right)^{3/2}(kT)^{3/2}F_{1/2}(\mu^*)$$ (5)

Putting $d\mu/dx = (d\mu/dn)(dn/dx)$ corresponding to $T = const.$ in the Eq. (4), we have

$$ja = \frac{-16\pi em*}{3h^3}l_0(T)(r+1)(kT)^{r+1}F_r(\mu^*)\frac{d\mu}{d\mu}$$

Putting

$$\frac{dn}{d\mu} = 4\pi\left(\frac{2m*}{h^2}\right)^{3/2}(kT)^{1/2}F_{-1/2}(\mu^*).$$ (6)

$$ja = \frac{\dfrac{-16\pi em*}{3h^3}l_0(T)(r+1)(kT)^{r+1}F_r(\mu^*)}{4\pi\left(\dfrac{2m*}{h^2}\right)^{3/2}(kT)^{1/2}F_{-1/2}(\mu^*)}\frac{dn}{dx} = -D\frac{dn}{dx}$$ (7)

and hence

$$D = \frac{l_0(T)(kT)^{r+1/2}}{3}\left(\frac{8}{m}\right)^{1/2}(r+1)\frac{F_r(\mu^*)}{F_{-1/2}(\mu^*)}.$$ (8)

For $dT/dx = 0$ and $j = 0$ we obtain from Eq. (1) $E = \frac{d\mu}{dx}\frac{1}{-e}$. Considering Eqs. (5) and (6) we may write for the density of the current carriers

$$ja = Ewn = -\frac{d\mu}{dx}\frac{w}{e}n = -\frac{2kT}{e}w\frac{F_{1/2}(\mu^*)}{F_{-1/2}(\mu^*)}\frac{dn}{dx} = -D\frac{dn}{dx},$$ (9)

where w is the mobility of electrons.

Hence

$$D = \frac{2kT}{e}w\frac{F_{1/2}(\mu^*)}{F_{-1/2}(\mu^*)} = -n\frac{du}{dn}.$$ (10)

Comparing Eqs. (8) and (10) we obtain the relation between the mobility and the free mean path of the electron

$$w = l\frac{e}{3}\left(\frac{2}{m*}\right)^{1/2}\frac{(kT)^{r-1/2}}{\varepsilon^r}(r+1)\frac{F_r(\mu^*)}{F_{1/2}(\mu^*)}.$$ (11)

From Eq. (10) the known expressions for the diffusion constant in the case of nondegenerate gas, when $F_r(x) \doteq \Gamma(r+1)\exp(x)$, and for the degenerate gas, when $F_r(x) \doteq x^{r+1}/(r+1)$, follow. With respect to the above mentioned fact we may write $D_{nondeg.} = kT/e$, which is the known Nernst-Townsend-Einstein relation. Analogically

$$D_{deg.} = \frac{2\mu}{3e}w.$$

By putting in this relation the corresponding expression for μ from Eq. (5) one obtains

$$D_{deg.} = \frac{1}{12}\frac{w}{m*}\frac{k^2}{e}\left(\frac{3n}{\pi}\right)^{2/3}.$$

Substituting ε into Eq. (11) by the mean value of the energy $\bar\varepsilon$, obtained under the same assumptions as in the case of deriving Eq. (5), i. e.

we obtain an expression for the mobility of the electron with a mean value of energy

$$\bar{\varepsilon} = \frac{1}{n}\frac{1}{4\pi}\left(\frac{2m^*}{h^2}\right)^{3/2}\int_0^\infty \frac{\varepsilon^{3/2}}{\exp\left(\frac{\varepsilon-\mu}{kT}\right)+1}\,d\varepsilon = kT\frac{F_{3/2}(\mu^*)}{F_{1/2}(\mu^*)},$$

In the degenerate case this expression becomes

$$\bar{w} = l\frac{e}{3}\left(\frac{2}{m^*kT}\right)^{1/2}(r+1)F_r(\mu^*)\frac{(F_{1/2}(\mu^*))^{r-1}}{(F_{3/2}(\mu^*))^r}. \qquad (11a)$$

and with regard to μ obtained from Eq. (5)

$$\bar{w} = l\frac{e}{2}\left(\frac{2}{m^*kT}\right)^{1/2}\left(\frac{5}{3}\right) \qquad (11b)$$

In the nondegenerate case Eq. (11a) becomes

$$\bar{w} = l\frac{e}{2}\left(\frac{\pi}{3n}\right)^{1/3}\left(\frac{5}{3}\right)^r. \qquad (11c)$$

$$\bar{w} = l\frac{e}{3}(m^*kT)^{1/2}T(r+2)\left(\frac{2}{3}\right)^r\frac{2}{\sqrt{\pi}}. \qquad (11d)$$

An advantage of the Eqs. (11c) and (11d) is that they contain besides the mean free path only the concentration of electrons or the effective mass. That fact enables an easy estimation of the mobility in any of the two above mentioned cases.

From Eq. (11) the particular expressions for the mobility for the different kinds of scattering in the nondegenerate and degenerate cases follow:

For $r = 0$ (atomic lattice)

a. in the nondeg. case

$$w = \frac{4el}{3(2\pi m^*kT)^{1/2}},$$

b. in the deg. case

$$w = \frac{le\sqrt{2}}{h}\left(\frac{\pi}{3m}\right)^{1/3}.$$

For $r = 1$ (ionic lattice at T) Debye temperature)

a. $$w = \left(\frac{2kT}{\pi m^*}\right)^{1/2}\frac{4le}{3\varepsilon},$$

b. $$w = \frac{leh}{9m^*\varepsilon}\left(\frac{3n}{\pi}\right)^{1/3}.$$

For $r = \frac{1}{2}$ (ionic lattice at $T <$ Debye temperature)

a. $$w = \frac{le}{\sqrt{2m^*\varepsilon}}$$

b. the same as under a.

The derived expressions are either in accordance with those mentioned in the literature [9] or the results following from these derived expressions agree with the results obtained in other ways [10].

III. THE EXPRESSIONS FOR THE THERMOELECTRIC COEFFICIENTS AND THE RELATIONS BETWEEN THEM

From the modification of Eq. (2), i. e.

$$V_m - V_l = \frac{1}{e}\int_l^m \frac{\beta_n}{T}\,dT = \int_l^m \alpha_n\,dT,$$

follows

$$\alpha_n = \frac{1}{e}\frac{\beta_n}{T}. \qquad (12)$$

In the general case $\mu = \mu(x,T)$ and $T = T(x)$. If $r = const.$ along the sample we may write

$$\frac{d}{dx} = \frac{d\mu}{dx}\frac{\partial}{\partial\mu} + \frac{dT}{dx}\frac{\partial}{\partial T} = \left(\frac{\partial\mu}{\partial x} + \frac{\partial\mu}{\partial T}\frac{dT}{dx}\right)\frac{\partial}{\partial\mu} + \frac{dT}{dx}\frac{\partial}{\partial T}.$$

From Eq. (3) with regard to Eq. (13) it follows for the Peltier heat in the case of grad $T = 0$ (13)

$$dq_P = \frac{j}{e}T\frac{\partial\mu}{\partial x}\frac{\partial}{\partial\mu}\left(\frac{\beta_n}{T}\right)dx = \pi j dx,$$

hence

$$\pi = \frac{T}{e}\frac{\partial\mu}{\partial x}\frac{\partial}{\partial\mu}\left(\frac{\beta_n}{T}\right) = \frac{1}{e}\frac{d}{dx}(\beta_n). \qquad (14)$$

The Peltier heat, released in an arbitrary section 1—2 which can be composed from different nonhomogenous parts, can be written as

$$q_{JP} = j \int_1^2 \frac{T}{e} \frac{d}{dx} \frac{\beta_n}{T} dx = j \frac{T}{e} \left[\left(\frac{\beta_n}{T}\right)_2 - \left(\frac{\beta_n}{T}\right)_1 \right] = j(\Pi_2 - \Pi_1) =$$

$$= jT(\alpha_2 - \alpha_1) = j\pi_{1-2}. \qquad (16)$$

Eq. (16) determines the Peltier heat in a general case contrary to the existing literature in which only the Peltier heat is considered released upon the contact of different materials or volume and contact contributions are considered separately. Eq. (16) expresses the relations between the introduced quantities

$$\Pi = T\alpha \, (16a), \quad \varkappa = \frac{d(\pi_{1-2})}{dx} \, (16b), \quad \pi_{1-2} = T(\alpha_2 - \alpha_1). \qquad (16c)$$

Analogically from Eq. (3) with respect to Eq. (13) the expression for the Thomson heat in the case when $\partial \mu/\partial x = 0$ and $dT/dx \neq 0$, can be written

$$dq_{JT} = \frac{j}{e} T \frac{dT}{dx} \left(\frac{\partial \mu}{\partial T} \frac{\partial}{\partial \mu} + \frac{\partial}{\partial T} \right) \left(\frac{\beta_n}{T} \right) dx = \varkappa j \frac{dT}{dx} \qquad (17)$$

hence

$$\tau = \frac{T}{e} \left(\frac{\partial \mu}{\partial T} \frac{\partial}{\partial \mu} + \frac{\partial}{\partial T} \right) \left(\frac{\beta_n}{T} \right) = \frac{T}{e} \frac{d}{dT} \left(\frac{\beta_n}{T} \right). \qquad (18)$$

From Eqs. (12) and (18) one obtains

$$\alpha_{T2} - \alpha_{T1} = \int_{T_1}^{T_2} \frac{1}{e} \frac{d}{dT} \left(\frac{\beta_n}{T} \right) dT = \int_{T_1}^{T_2} \frac{\tau}{T} dT, \qquad (19)$$

wherefrom in the limiting case when $T_1 \to T_2$ it follows that

$$\frac{d\alpha}{dT} = \frac{\tau}{T}. \qquad (20)$$

Eq. (16c) becomes in the limiting case with regard to Eq. (16b)

$$\frac{d\varkappa}{dx} = \frac{\pi}{T}. \qquad (21)$$

From the foregoing it is evident that the whole Peltier heat released in a closed circuit equals zero. The same is valid also for the Thomson heat. In both cases the corresponding integrands are total differentials. For a further modification

of the expressions which contain the derivatives of β_n introduced in Eq. (2) it is possible to use the relation

$$\frac{d}{dx} F_r(x) = r F_{r-1}(x) \text{ for } r > 0.$$

By comparing Eq. (2) and Eq. (3) for a closed circuit it follows that the whole heat released in a unit time is equal to the product of the current and the thermoelectric voltage, which expresses the first law of thermodynamics for this case. From Eq. (3) it follows that

$$\oint \frac{dq_J}{T} = 0,$$

this is the expression for the second law of thermodynamics. Thus the obtained results satisfy the first and second laws of thermodynamics identically- which follows from the quantum-mechanical method of their derivations. The derivation of the relations between the thermoelectric coefficients is only a formal modification without the application of further laws. The corresponding relations in the phenomenological theory are derived [9], [11] by means of the first and second laws of thermodynamics.

IV. CONCLUSION

Using the Lorentz solution of Boltzman's kinetic equation several kinetic coefficients and relations between them for different kinds of scattering — not mentioned so far in the existing literature — are obtained. They do not contain symbols for complicated integrals which would not be applicable for the calculations, but they contain only Fermi integrals $F_r(\mu^*)$, which depend only on the mechanism of the scattering (which is represented by the value of r), the chemical potential and the temperature, respectively.

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