DISTRIBUTION FUNCTION FOR ELECTRONS IN A STRONG ELECTRIC FIELD

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We want to determine the expression for current density, or electron distribution function, obtainable by the method suggested in [1] in different approximations with regard to the magnitude of the parameter τ characterizing the interaction of the system with the environment. This parameter can also be interpreted as the energy-independent relaxation time of a process affecting the motion of electrons apart from their collisions with phonons. It was shown [2] that the effect of this interaction could be included by means of the additional term $\tau^{-1}(\varrho - \varrho_0)$ in the density matrix equation. In the presented paper, contrary to [1], the model is chosen in which ϱ_0 represents the Maxwell equilibrium density matrix $\varrho_0(H_0 + H_L)$ corresponding to the state realized in time $t = -\infty$. At this moment an electric field of the intensity E was applied in the x-direction and the system of dynamicaly independent electrons was exposed to the interaction with phonons.

We use the denotation in which $H_0 = p^2(2m)^{-1}$ represents the Hamiltonian of electron having the effective mass m. Phonon Hamiltonian H_L can be expressed by the sum of simple harmonic oscillator Hamiltonians. The interaction of an electron with a time independent electric field is represented by $H_F = -eEx$ and the electron-phonon interaction energy can be written in the form

$$H_i = \sum_{\vec{\sigma}} V_{\vec{\sigma}} a_{\vec{\sigma}} \exp(\mathrm{i}\,\vec{\sigma}\,.\,\vec{r}) + V^{*}_{\vec{\sigma}} a^{+}_{\vec{\sigma}} \exp(-\,\mathrm{i}\,\vec{\sigma}\,.\,\vec{r})$$

with $\vec{\sigma}$ signifying the phonon vector, $V_{\vec{\sigma}}$ characterizing the coupling and $a^{+}_{\vec{\sigma}}$, $a_{\vec{\sigma}}$ denoting the phonon creation and annihilation operators respectively.

The density matrix ϱ, necessary for the evaluation of current density, represents the solution of the equation

$$\frac{\partial \varrho}{\partial t} = \frac{\mathrm{i}}{\hbar}[\varrho, H_0 + H_L + H_F + H_i] - \frac{\varrho - \varrho_0}{\tau}$$

with the initial condition $\varrho(-\infty) = \varrho_0(H_0 + H_L)$. The formal solution of this equation can be written in the form

$$\varrho(t) = \varrho_0 + \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} \exp\left(\frac{t'-t}{\tau}\right)\exp\left\{\frac{\mathrm{i}}{\hbar}(H_0 + H_L + H_F)(t'-t)\right\}[\varrho(t'), H_t] \times$$

$$\times \exp\left\{-\frac{\mathrm{i}}{\hbar}(H_0 + H_L + H_F)(t'-t)\right\}\mathrm{d}t' + \tilde{\varrho}(t)$$

in which

$$\tilde{\varrho}(t) = \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{t} \exp\left(\frac{t'-t}{\tau}\right)\exp\left\{\frac{\mathrm{i}}{\hbar}(H_0 + H_L + H_F)(t'-t)\right\}[\varrho_0, H_F] \times$$

$$\times \exp\left\{-\frac{\mathrm{i}}{\hbar}(H_0 + H_L + H_F)(t'-t)\right\}\mathrm{d}t'.$$

This expression represents an integral equation which can be solved by iteration as long as the coupling parameter $V_{\vec{\sigma}}$ is a small quantity. When solving this equation we shall use the representation in which $H_0 + H_L$ is diagonal and we shall be interested in terms up to the second order in H_t.

The eigenvalues of H_0 will be denoted by $\varepsilon(\vec{k})$ and the corresponding eigenfunctions, which are normalized plane waves, will be denoted by $|\vec{k}\rangle$. The eigenfunctions of H_L will be denoted by $|N\rangle$ and the corresponding quantity for the Hamiltonian of the oscillator with frequency $\omega_{\vec{\sigma}}$ will be denoted by $|N_{\vec{\sigma}}\rangle$. The energy of this oscillator can be written in the form $E(N_{\vec{\sigma}}) = (N_{\vec{\sigma}} + 1/2)\hbar\omega_{\vec{\sigma}}$, with $N_{\vec{\sigma}}$ taking on all non-negative integral values.

When expressing the current density we must find the average value of the electron velocity operator which is diagonal in the representation chosen. We shall therefore be interested only in the diagonal matrix elements of ϱ. We shall not put down the direct expression for the current density since it can be easily expressed by means of the distribution function the derivation of which we are concentrated on.

From the character of H_t it is obvious that the diagonal matrix elements from those terms of ϱ which are of the first order in H_t are zero. Therefore only $\tilde{\varrho}$ and the second order term in H_t, namely ϱ_2, will contribute to the current. In order to express ϱ_2 we must know the non-diagonal matrix elements of the first order term in H_t, namely ϱ_1. Since the non-zero matrix elements of H_t are those of the type $\langle\vec{k}N|H_t|\vec{k}\pm\vec{\sigma}, \ldots N_{\vec{\sigma}} \mp 1 \ldots\rangle$ and the operator function $\exp\left\{\frac{\mathrm{i}}{\hbar}(H_0 + H_L + H_F)t\right\}$ can be written in the form (9)

from paper [1] and the diagonal matrix elements of $\tilde{\varrho}$ can be expressed by the relation

$$\langle\vec{k}N|\varrho|\vec{k}N\rangle = -\frac{eE\tau}{\hbar}\frac{\partial}{\partial k_x}\langle\vec{k}N|\varrho_0|\vec{k}N\rangle$$

we can obtain the following expression for ϱ_1:

$$\langle\vec{k}N|\varrho_1|\vec{k}\pm\vec{\sigma}\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle = \frac{\mathrm{i}}{\hbar}\int_{-\infty}^{0}\exp\left(\frac{t'}{\tau}\right)\exp\left\{\frac{\mathrm{i}}{\hbar}[\varepsilon(\vec{k}) - \varepsilon(\vec{k}\pm\vec{\sigma}) \pm \hbar\omega_{\vec{\sigma}}]t'\right\} \times$$

$$\times \exp\left\{\pm\frac{\mathrm{i}\, eE\sigma_x}{2m}t'^2\right\}\mathrm{d}t'\langle\vec{k}N|H_t|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}} \mp 1\ldots\rangle[\langle\vec{k}N|\varrho_0|\vec{k}N\rangle -$$

$$- \langle\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots|\varrho_0|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle - \frac{eE\tau}{\hbar}\frac{\partial}{\partial k_x}\langle\vec{k}N|\varrho_0|\vec{k}N\rangle +$$

$$+ \frac{eE\tau}{\hbar}\frac{\partial}{\partial(k_x \pm \sigma_x)}\langle\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots|\varrho_0|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle\Big].$$

Since $\langle\vec{k}N|\varrho_2|\vec{k}N\rangle$ can be written in the form

$$\langle\vec{k}N|\varrho_2|\vec{k}N\rangle = \frac{\mathrm{i}}{\hbar}\tau\sum_{\vec{\sigma}}\{\langle\vec{k}N|\varrho_1|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle\langle\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp$$

$$\mp 1\ldots|H_t|\vec{k}N\rangle - \langle\vec{k}N|H_t|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle\langle\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots|\varrho_1|\vec{k}N\rangle\}$$

and since

$$\langle\vec{k}N|H_t|\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots\rangle\langle\vec{k}\pm\vec{\sigma},\ldots N_{\vec{\sigma}}\mp 1\ldots|H_t|\vec{k}N\rangle = |V_{\vec{\sigma}}|^2\mathbf{N}(\pm\vec{\sigma})$$

with $\mathbf{N}(+\vec{\sigma}) = N_{\vec{\sigma}}$ and $\mathbf{N}(-\vec{\sigma}) = N_{\vec{\sigma}} + 1$, then after the transfer from the density matrix to the electron distribution function f consisting in the averaging over the lattice variables, we obtain the following expression for the part of the distribution function contributing to the current:

$$\sum_N\langle\vec{k}N|\Delta\varrho|\vec{k}N\rangle \equiv \langle\vec{k}|\Delta f|\vec{k}\rangle = -\frac{eE\tau}{\hbar}\frac{\partial}{\partial k_x}f_0(\vec{k}) +$$

$$+ \frac{eE\tau^2}{\hbar^3}\sum_{\vec{\sigma}}|V_{\vec{\sigma}}|^2\left\{\bar{N}_{\vec{\sigma}}\left(\frac{\partial}{\partial k_x}f_0(\vec{k}) - \exp\left(\frac{\hbar\omega_{\vec{\sigma}}}{k_0T}\right)\frac{\partial}{\partial(k_x+\sigma_x)}f_0(\vec{k}+\vec{\sigma})\right)\times\right.$$

$$\times (I_{+\vec{\sigma}} + I^*_{+\vec{\sigma}}) + (\bar{N}_{\vec{\sigma}} + 1)\left(\frac{\partial}{\partial k_x} f_0(\vec{k}) - \exp\left(-\frac{\hbar\omega_{\vec{\sigma}}}{k_0T}\right)\frac{\partial}{\partial(k-\sigma)} f_0(\vec{k}-\vec{\sigma})\right) \times$$

$$\times I_{-\vec{\sigma}} + I^*_{-\vec{\sigma}})\} - \frac{\tau}{\hbar^2}\sum_{\vec{\sigma}} |V_{\vec{\sigma}}|^2\{\bar{N}_{\vec{\sigma}}(f_0(\vec{k}) - \exp\left(\frac{\hbar\omega_{\vec{\sigma}}}{K_0T}\right) f_0(\vec{k}+\vec{\sigma})\right) \times$$

$$\times (I_{+\vec{\sigma}} + I^*_{+\vec{\sigma}}) + (\bar{N}_{\vec{\sigma}} + 1)\left(f_0(\vec{k}) - \exp\left(-\frac{\hbar\omega_{\vec{\sigma}}}{K_0T}\right) f_0(\vec{k}-\vec{\sigma})\,(I_{-\vec{\sigma}} + I^*_{-\vec{\sigma}})\right\}. \quad (+)$$

In this expression the denotation

$$I_{\pm\vec{\sigma}} = \int_{-\infty}^{0} \exp\left(\frac{t'}{\tau}\right) \exp\left\{\frac{i}{\hbar}[\varepsilon(\vec{k} \pm \vec{\sigma}) - \varepsilon(\vec{k}) \mp \hbar\omega_{\vec{\sigma}}]t'\right\} \exp\left\{\mp \frac{i\, eE\sigma_x}{2m} t'^2\right\} dt'$$

is introduced and under $\bar{N}_{\vec{\sigma}}$ the following is understood:

$$\bar{N}_{\vec{\sigma}} = \left[\sum_N \exp\left(-\frac{E_N}{K_0T}\right)\right]^{-1} \sum_N N_{\vec{\sigma}} \exp\left(-\frac{E_N}{K_0T}\right)$$

with E_N signifying the eigenvalues of H_L.

When phonons are assumed in the thermal equilibrium in spite of their being coupled to electrons obtaining energy from the electric field, we can write

$$\bar{N}_{\vec{\sigma}} = \left[\exp\left(\frac{\hbar\omega_{\vec{\sigma}}}{k_0T}\right) - 1\right]^{-1}.$$

This assumption is not valid at very low temperatures, since the effect of electrons on the phonon distribution cannot be neglected then [3].

The sums $I_{+\vec{\sigma}} + I^*_{+\vec{\sigma}}$ and $I_{-\vec{\sigma}} + I^*_{-\vec{\sigma}}$ represent the integrals of the type

$$2\int_{-\infty}^{0} \exp\left(\frac{t'}{\tau}\right) \cos(\Omega t'^2 + \omega t')\, dt'$$

in which

$$\omega = \begin{cases} \frac{1}{\hbar}[\varepsilon(\vec{k}+\vec{\sigma}) - \varepsilon(\vec{k}) - \hbar\omega_{\vec{\sigma}}] \\ \frac{1}{\hbar}[\varepsilon(\vec{k}-\vec{\sigma}) - \varepsilon(\vec{k}) + \hbar\omega_{\vec{\sigma}}] \end{cases} ; \quad \Omega = \begin{cases} -\frac{eE\sigma_x}{2m} \\ +\frac{eE\sigma_x}{2m} \end{cases}.$$

Due to the complicated form of these integrals we must use the approximations dependent on the magnitude of the parameter τ. One of them is convenient in case τ being sufficiently large in comparison with the relaxation time of the electron-phonon collisions. The fact that for small values of τ (interpreted as the relaxation time of certain scattering process) we could hardly involve such an interaction by means of the additional term $(\varrho - \varrho_0)/\tau$ in the density matrix equation, speaks in favour of the mentioned approximation. The effect of this additional term alone is equivalent with the treatment based on the solution of the Boltzmann equation with the scattering term expressed by means of the relaxation time τ and the substantiation of this equation is the better the larger the relaxation time of the corresponding scattering process is.

We shall evaluate separately the terms with $\sigma_x = 0$ and the terms with $\sigma_x \neq 0$. In the latter terms the factor $\exp(t/\tau)$, occuring in the mentioned integrals, can be considered approximately equal to unit. Since the integrals of the type $\int_{\infty}^{0} \cos(\Omega t^2 + \omega t)\, dt$ can be computed [4] we obtain:

$$(I_{+\vec{\sigma}} + I^*_{+\vec{\sigma}})_{\sigma_x \neq 0} = \sqrt{\frac{\pi}{2\Omega}}\left(\sin\frac{\omega_+^2}{4\Omega} - \cos\frac{\omega_+^2}{4\Omega}\right)$$

$$(I_{-\vec{\sigma}} + I^*_{-\vec{\sigma}})_{\sigma_x \neq 0} = \sqrt{\frac{\pi}{2\Omega}}\left(\sin\frac{\omega_-^2}{4\Omega} - \cos\frac{\omega_-^2}{4\Omega}\right)$$

where under Ω the expression $|\Omega_{\pm\vec{\sigma}}|$ is understood. For terms with $\sigma_x = 0$ we can write

$$(I_{+\vec{\sigma}} + I^*_{+\vec{\sigma}})_{\sigma_x = 0} = \frac{2\tau}{1 + \omega_+^2\tau^2}$$

$$(I_{-\vec{\sigma}} + I^*_{-\vec{\sigma}})_{\sigma_x = 0} = \frac{2\tau}{1 + \omega_-^2\tau^2}.$$

If these results are set into (+) and the definition of Ω is used, it can be seen that beside the terms linear in the applied field (coming from the first term of the right side of (+) and from the second term of the right side of (+) in case of $\sigma_x = 0$) there are in the expression for the distribution function the terms having the following dependence on the intensity of the applied field:

$$E^{1/2} \sum_{\substack{\vec{\sigma} \\ \sigma_x \neq 0}} \alpha_{\vec{\sigma}}[\sin(\gamma_{\vec{\sigma}} E^{-1}) - \cos(\gamma_{\vec{\sigma}} E^{-1})]$$

$$E^{-1/2} \sum_{\substack{\vec{\sigma} \\ (\sigma_x \neq 0)}} \mu_{\vec{\sigma}}[\sin(\gamma_{\vec{\sigma}} E^{-1}) - \cos(\gamma_{\vec{\sigma}} E^{-1})].$$

The first expression comes from the second term of the right side of (+) in case of $\sigma_x \neq 0$ and the second from the third term of the right side of (+) int he same case. The third term of the right side of (+) need not be considered in case of $\sigma_x = 0$ since it does not contribute to the current due to the symmetry of the Brillouin zone.

Since the assumption of τ large compared with the electron-phonon relaxation time (dependent on the intensity of the applied field), need not be fulfilled for sufficiently weak fields, we could hardly deduce the behaviour of the distribution function in case of a weak electric field. In case of a strong electric field the result obtained shows that besides the terms linear in E the terms with a slower increase of the type $\alpha E^{1/2}$ play a role in the distribution function. However, it must be stressed that the intensity of the applied field is limited by the effective mass approximation losing its substantiation in fields with the intensity of $10^7 - 10^9$ Vm^{-1} [5].*)

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