Semicond. Sci. Technol. 7 (1992) 1446–1452. Printed in the UK

Boltzmann kinetic equation with correction term for intracollisional field effect

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Received 18 November 1991, in final form 29 June 1992, accepted for publication 14 July 1992

Abstract. We have included a higher order term in the approximation of the electron density matrix used in deriving the Boltzmann kinetic equation from the Liouville–von Neumann equation by means of Kubo's formalism. This higher term has been added to the Boltzmann kinetic equation as the correction term. In a simplified case the field effect collision rate is introduced, representing the intracollisional field effect. The correction term gives a significant contribution to the Boltzmann kinetic equation for an electric field strength of 2.5 MV m^{-1}, which was determined by numerical calculation.

1. Introduction

The very small distances between elements produced by VLSI technology are responsible for high electric fields, and thus the motion of charge carriers needs a quantum-mechanical description. Transport processes in high electric fields were first investigated in bulk materials [1–4]. For a long time a method based on the expansion of the density matrix in the Liouville–von Neumann equation was used [5]. Another approach consisted in a generalization of the linear response method [6] to the case of strong electric fields by means of the resolvent superoperator technique [7]. The latest attempts at using non-equilibrium Green functions are described in [8, 9]. In our case [10–13] the integral transport equation [14–16] can be obtained by a set of approximations that can be solved only by numerical methods. Recently the Kubo formula for conductivity was derived exactly from the quantum Boltzmann equation [17].

This paper is based on the Liouville–von Neumann quantum-mechanical equation. By means of a method similar to that known as Kubo's formalism, which gives the transport equation [18, 19], we are able to find the equation valid for electrons in strong electric fields (section 2). In section 3 the Boltzmann kinetic equation with correction term is derived. Using approximations similar to those leading to the relaxation time approach in semiconductors, we are able to find the correction term in a form representing the intracollisional field effect (section 4). If we simplify the problem we are able to determine the magnitude of the electric field when the correction term contributes significantly to the Boltzmann equation (section 5).

2. Formulation of the problem and derivation of the scattering term

Let us consider a system in which electrons responsible for electric current interact weakly with lattice vibrations and let us ignore the electron–electron interaction.

We will introduce the Hamiltonian $H = H_e + H_L + H_F + H_i$, where H_e is the Hamiltonian of an electron with effective mass m, H_L is the Hamiltonian of lattice vibrations, the Hamiltonian H_F represents an interaction of electrons with the applied electric field of intensity $\boldsymbol{E}$ and H_i is a weak interaction of electrons with lattice vibrations. For the moment we will not discuss the magnitude of the electric field. The characteristic values and functions of H_e are denoted by $\varepsilon_{\boldsymbol{k}}$ and $|\boldsymbol{k}\rangle$, respectively, and in the case of operator H_L they are E_N and $|N\rangle$. We will use the interaction representation by introducing [5, 18].

We have already seen that the Boltzmann kinetic equation [18, 19] can be obtained in an approximation in which the drift term has its origin directly in the expression

$$\frac{i}{\hbar}\int_{t_0}^{t} [\rho'(t'), H'_F(t')]\,dt' \tag{1}$$

but the scattering term was obtained by approximating the expression

$$\frac{i}{\hbar}\int_{t_0}^{t} [\rho'(t'), H'_i(t')]\,dt' \tag{2}$$

where $\rho(t')$ is an electron density matrix and the comma indicates the interaction representation.

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That is why we will be interested in a change of situation when $\rho'(t')$ in (2) is approximated with accuracy up to the first order in H_F, because we are interested in linear effects of the electric field upon the interaction between electrons and phonons. The validity of the Boltzmann equation for strong electric fields will depend on the possibility or impossibility of neglecting in $\rho'(t')$ terms of higher order than zeroth order in H_F. Let $\rho'(t_0)$ be the density matrix of thermodynamic equilibrium. We will replace $\rho'(t')$ in (2) by an expression $\rho'(t_0)+\rho'_1(t_0,t')+\rho'_2(t_0,t')$ in which $\rho'_1(t_0,t')$ is of zeroth order in H'_F and first order in H'_i and $\rho'_2(t_0,t')$ is of first order in H'_F and in general of nth order in H'_i. We will not, however, deal with higher orders in H'_i than the second. In this way we will obtain

$$\begin{aligned}
&\frac{i}{\hbar}\int_0^{t-t_0}dt'\sum_N\langle \boldsymbol{k}N|[\rho'(t_0+t'),H'_i(t_0+t')]|\boldsymbol{k}N\rangle \\
&\longrightarrow \frac{i}{\hbar}\int_0^{t-t_0}dt'\sum_N\langle \boldsymbol{k}N|[\rho'(t_0)+\rho'_1(t_0,t_0+t') \\
&\quad +\rho'_2(t_0,t_0+t'),H'_i(t_0+t')|\boldsymbol{k}N\rangle \\
&=\frac{i}{\hbar}\int_0^{t-t_0}dt'\sum_N\langle \boldsymbol{k}N|[\rho'(t_0),H'_i(t_0+t')]|\boldsymbol{k}N\rangle \\
&\quad+\left(\frac{i}{\hbar}\right)^2\int_0^{t-t_0}dt'\int_0^{t'}dt''\sum_N\langle \boldsymbol{k}N|[[\rho'(t_0), \\
&\quad H'_i(t_0+t'')],H'_i(t_0+t')]|\boldsymbol{k}N\rangle \\
&\quad+\left(\frac{i}{\hbar}\right)^2\int_0^{t-t_0}dt'\int_0^{t'}dt''\sum_N\langle \boldsymbol{k}N|[[\rho'(t_0), \\
&\quad H'_\alpha(t_0+t'')],H'_\beta(t_0+t')]|\boldsymbol{k}N\rangle+\left(\frac{i}{\hbar}\right)^3 \\
&\quad\times\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''\sum_N\langle \boldsymbol{k}N|[[[\rho'(t_0), \\
&\quad H'_\alpha(t_0+t''')],H'_\beta(t_0+t'')],H'_\gamma(t_0+t')]|\boldsymbol{k}N\rangle .
\end{aligned} \tag{3}$$

The first term on the right-hand side of (3) has its origin in $\rho'(t_0)$, the second one in $\rho'_1(t_0,t_0+t')$ and the rest in $\rho'_2(t_0,t_0+t')$. In the first term from $\rho'_2(t_0,t_0+t')$ the suffices α, β are unequal and may be F or i, in the second term the suffices α, β, γ may be F, i, i in a cyclic way.

The first term on the right-hand side of (3) is zero [18] and neither of the third terms contributes [18]. The scattering term of the Boltzmann equation $[df/dt]_S$ can be obtained [18, 20] from the second term. If the drift term is now expressed and the scattering term approximated in the way determined in (3) the term takes the form

$$\begin{aligned}
\langle\boldsymbol{k}|f'(t)|\boldsymbol{k}\rangle-\langle\boldsymbol{k}|f'(t_0)|\boldsymbol{k}\rangle &=\int_{t_0}^{t}\left(-\frac{e}{\hbar}\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k},t')\right)dt' \\
&\quad+(t-t_0)\left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_S+\sum_N\langle \boldsymbol{k}N|\Delta\rho'_I|\boldsymbol{k}N\rangle \\
&\quad+\sum_N\langle \boldsymbol{k}N|\Delta\rho'_{II}|\boldsymbol{k}N\rangle+\sum_N\langle \boldsymbol{k}N|\Delta\rho'_{III}|\boldsymbol{k}N\rangle
\end{aligned} \tag{4}$$

where f' is the diagonal operator and additional terms have the forms

$$\begin{aligned}
\Delta\rho'_I=\left(\frac{i}{\hbar}\right)^3\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''[[[\rho'(t_0), \\
H'_F(t_0+t''')],H'_i(t_0+t'')],H'_i(t_0+t')]
\end{aligned} \tag{5a}$$

$$\begin{aligned}
\Delta\rho'_{II}=\left(\frac{i}{\hbar}\right)^3\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''[[[\rho'(t_0), \\
H'_i(t_0+t''')],H'_F(t_0+t'')],H'_i(t_0+t')]
\end{aligned} \tag{5b}$$

$$\begin{aligned}
\Delta\rho'_{III}=\left(\frac{i}{\hbar}\right)^3\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''[[[\rho'(t_0), \\
H'_i(t_0+t''')],H'_i(t_0+t'')],H'_F(t_0+t')].
\end{aligned} \tag{5c}$$

The additional terms (5*a*)–(5*c*) were not included in the Boltzmann kinetic equation.

3. Derivation of Boltzmann kinetic equation with correction term

If we assume the thermal equilibrium of phonons then the matrix density satisfies the relation

$$\langle \boldsymbol{k}N|\rho(t)|\boldsymbol{k}'N'\rangle=\langle\boldsymbol{k}|f(t)|\boldsymbol{k}'\rangle P(N)\delta_{N,N'} \tag{6}$$

where $P(N)$ is the Boltzmann factor.

We will first analyse the contribution (5*a*). If we use the operator H_F in the form: $H_F=-e\boldsymbol{E}\cdot\boldsymbol{r}$, relation (6) is performed and the matrix elements of the commutator $[f,H_F]$ are performed then we obtain

$$\begin{aligned}
\langle \boldsymbol{k}N|\Delta\rho'_I|\boldsymbol{k}N\rangle &=\frac{2e}{\hbar^3}\sum_{\boldsymbol{k}'N'}\langle \boldsymbol{k}N|H_i|\boldsymbol{k}'N'\rangle\langle \boldsymbol{k}'N'|H_i|\boldsymbol{k}N\rangle \\
&\quad\times[\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k},t_0)P(N)-\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}'}f(\boldsymbol{k}',t_0)P(N')] \\
&\quad\times\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''\cos\left(\frac{1}{\hbar}(t'''+t''-t')\right. \\
&\quad\left.\times(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}'}+E_N-E_{N'})\right).
\end{aligned} \tag{7}$$

The three-fold time integral appearing in (7) can be expressed as

$$\begin{aligned}
I&=\int_0^{t-t_0}dt'\int_0^{t'}dt''\int_0^{t''}dt'''\cos\left[(t'''+t''-t')\omega\right] \\
&=\frac{t-t_0}{\omega^2}-\frac{t-t_0}{\omega^2}\frac{\sin[\omega(t-t_0)]}{\omega(t-t_0)}
\end{aligned} \tag{8}$$

in which

$$\omega=\frac{1}{\hbar}(\varepsilon_{\boldsymbol{k}}-\varepsilon_{\boldsymbol{k}'}+E_N-E_{N'}).$$

The function $\sin[\omega(t-t_0)]/\omega$ behaves like $\pi\delta(\omega)$ for large $(t-t_0)$. It is more convenient to write the integral (8) in a different form. To do so we will express the second derivative of the function $\sin(\omega x)/\omega$ with $x = t - t_0$. We have

$$\left(\frac{\sin\omega x}{\omega}\right)'' = 2\frac{\sin\omega x}{\omega^3} - 2\frac{x\cos\omega x}{\omega^2} - \frac{x^2\sin\omega x}{\omega}. \quad (10)$$

If these terms appear in our physical problem then due to time averaging the second term on the right-hand side of (10) vanishes and the third term corresponds to non-Markovian processes having only a negligible effect. Then for sufficiently large $t - t_0$ integral I (8) can be replaced by the term

$$I = (t - t_0)\left(\frac{1}{\omega^2} - \frac{\pi}{2x}\delta''(\omega)\right) \quad (11)$$

in which the second derivative from the delta function appears and we use $x = t - t_0$.

For (5*a*) we then obtain

$$\langle \boldsymbol{k}N|\Delta\rho'_{\mathrm{I}}|\boldsymbol{k}N\rangle = \frac{2e}{\hbar^3}\sum_{\boldsymbol{k}'N'}\langle \boldsymbol{k}N|H_{\mathrm{i}}|\boldsymbol{k}'N'\rangle\langle \boldsymbol{k}'N'|H_{\mathrm{i}}|\boldsymbol{k}N\rangle$$
$$\times[\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k},t_0)P(N) - \boldsymbol{E}\cdot\nabla_{\boldsymbol{k}'}f(\boldsymbol{k}',t_0)P(N')]$$
$$\times(t - t_0)\left(\frac{1}{\omega^2} - \frac{\pi}{2x}\delta''(\omega)\right). \quad (12)$$

Now we will deal with the remaining contributions from equation (4). We use the electron–phonon interaction operator H_{i} in the form

$$H_{\mathrm{i}} = \sum_{\boldsymbol{q}}(V_{\boldsymbol{q}}\hat{a}_{\boldsymbol{q}}\mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} + V^*_{\boldsymbol{q}}\hat{a}^\dagger_{\boldsymbol{q}}\mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}})$$

in which $V_{\boldsymbol{q}}$ is a coupling parameter and $\hat{a}_{\boldsymbol{q}}$, $\hat{a}^\dagger_{\boldsymbol{q}}$ are respectively the annihilation and creation operators for a phonon with frequency $\omega_{\boldsymbol{q}}$. Summing up the contributions (5*b*) and (5*c*),

$$\langle \boldsymbol{k}N|\Delta\rho'_{\mathrm{II}}|\boldsymbol{k}N\rangle + \langle \boldsymbol{k}N|\Delta\rho'_{\mathrm{III}}|\boldsymbol{k}N\rangle$$

we obtain the same integral as (8) and (11). In conclusion we may express the summed terms as

$$\langle \boldsymbol{k}N|\Delta\rho'_{\mathrm{II}}|\boldsymbol{k}N\rangle + \langle \boldsymbol{k}N|\Delta\rho'_{\mathrm{III}}|\boldsymbol{k}N\rangle = 2\left(\frac{\mathrm{i}}{\hbar}\right)^3$$
$$\times\sum_{\boldsymbol{k}'N'}\left(\sum_{\boldsymbol{q}}D(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},N,N')[\langle \boldsymbol{k}N|H_{\mathrm{F}}|\boldsymbol{k}'N'\rangle\right.$$
$$\left.\times\langle \boldsymbol{k}'N'|H_{\mathrm{i}}|\boldsymbol{k}N\rangle + \langle \boldsymbol{k}N|H_{\mathrm{i}}|\boldsymbol{k}'N'\rangle\langle \boldsymbol{k}'N'|H_{\mathrm{F}}|\boldsymbol{k}N\rangle]\right)$$
$$\times(t - t_0)\left(\frac{1}{\omega^2} - \frac{\pi}{2x}\delta''(\omega)\right) \quad (13)$$

where

$$\sum_{\boldsymbol{q}}D(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},N,N') = V_{\boldsymbol{q}}\sqrt{N}P(N)\delta(\boldsymbol{k}' - \boldsymbol{k} + \boldsymbol{q})$$
$$+ V^*_{\boldsymbol{q}}\sqrt{N'}P(N')\delta(\boldsymbol{k}' - \boldsymbol{k} - \boldsymbol{q}). \quad (14)$$

From (12) and (13) it can be seen that the contributions (5*a*), (5*b*) and (5*c*) may be added to the Boltzmann kinetic equation and one can write

$$\int_{t_0}^{t}\mathrm{d}t'\left(\frac{\mathrm{d}f(\boldsymbol{k},t')}{\mathrm{d}t'} + \frac{e\boldsymbol{E}}{\hbar}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k}) - \left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_{\mathrm{S}}\right.$$
$$\left. - \left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_{\mathrm{SF}}\right) = 0. \quad (15)$$

In order that equation (15) should always be satisfied the integrand must be zero. Since we are interested in a steady state this needs

$$\frac{e\boldsymbol{E}}{\hbar}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k}) = \left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_{\mathrm{S}} + \left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_{\mathrm{SF}} \quad (16)$$

where $f(\boldsymbol{k},t_0)$ is denoted simply by $f(\boldsymbol{k})$ and the last term on the right-hand side of (16) is given by

$$\left[\frac{\partial f(\boldsymbol{k},t_0)}{\partial t}\right]_{\mathrm{SF}} = \frac{2}{\hbar^3}\sum_{\boldsymbol{k}'N'}\left(e\langle \boldsymbol{k}N|H_{\mathrm{i}}|\boldsymbol{k}'N'\rangle\right.$$
$$\times\langle \boldsymbol{k}'N'|H_{\mathrm{i}}|\boldsymbol{k}N\rangle[\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k},t_0)P(N)$$
$$- \boldsymbol{E}\cdot\nabla_{\boldsymbol{k}'}f(\boldsymbol{k}',t_0)P(N')] + \mathrm{i}\Big[\langle \boldsymbol{k}N|H_{\mathrm{F}}|\boldsymbol{k}'N'\rangle$$
$$\times\langle \boldsymbol{k}'N'|H_{\mathrm{i}}|\boldsymbol{k}N\rangle + \langle \boldsymbol{k}N|H_{\mathrm{i}}|\boldsymbol{k}'N'\rangle\langle \boldsymbol{k}'N'|H_{\mathrm{F}}|\boldsymbol{k}N\rangle\Big]$$
$$\left.\times\sum_{\boldsymbol{q}}D(\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q},N,N')\right)\left(\frac{1}{\omega^2} - \frac{\pi}{2x}\delta''(\omega)\right).$$
$$(17)$$

This term includes effects appearing due to a strong electric field in the process of collision. As will be seen later the correction term (17) to the Boltzmann kinetic equation corresponds to an intracollisional field effect. Besides we will show that all three contributions (5*a*), (5*b*) and (5*c*) are in a certain approximation the same.

4. Term corresponding to the intracollisional field effect

We will first deal with the first contribution (12). We will assume that for large numbers of phonons N, N' the relation $P(N) = P(N')$ is approximately valid and we will use the relations

$$\sum_{\boldsymbol{q}}N'P(N) = \sum_{\boldsymbol{q}}(N_{\boldsymbol{q}} + 1)P(N) = \bar{N}_{\boldsymbol{q}} + 1$$

and

$$\sum_{\boldsymbol{q}}N\,P(N) = \sum_{\boldsymbol{q}}(N_{\boldsymbol{q}})P(N) = \bar{N}_{\boldsymbol{q}} \quad (18)$$

where $\bar{N}_{\boldsymbol{q}}$ is the distribution function for phonons.

Finally, with the use of (18), we will obtain for the first term (17) (or for term (12) in the Boltzmann equation) the expression

$$\left[\frac{\partial f(\mathbf{k},t_0)}{\partial t}\right]_{\rm (I)SF} = \frac{2e}{\hbar^3}\mathbf{E}\sum_q |V_q|^2\left[\frac{\pi}{2x}(\nabla_{\mathbf{k}'}f(\mathbf{k}'))\right.$$
$$\times[(\bar{N}_q+1)\delta''(\omega)+\bar{N}_q\delta''(\omega)]$$
$$-\frac{\pi}{2x}(\nabla_{\mathbf{k}}f(\mathbf{k}))[\bar{N}_q\delta''(\omega)+(\bar{N}_q+1)\delta''(\omega)]$$
$$-(\nabla_{\mathbf{k}'}f(\mathbf{k}'))\left((\bar{N}_q+1)\frac{1}{\omega^2}+\bar{N}_q\frac{1}{\omega^2}\right)$$
$$\left.+(\nabla_{\mathbf{k}}f(\mathbf{k}))\left(\bar{N}_q\frac{1}{\omega^2}+(\bar{N}_q+1)\frac{1}{\omega^2}\right)\right]. \tag{19}$$

where V_q is a parameter characterizing the type of electron–phonon interaction.

Now we will deal with the remaining terms of (17). We will again consider only the term having its origin in the contribution (5*b*) since the last term coming from the contribution (5*c*) can be dealt with in the same manner.

We will get

$$\mathrm{i}\langle \mathbf{k}N|H_{\rm F}|\mathbf{k}'N'\rangle\langle \mathbf{k}'N'|H_{\rm i}|\mathbf{k}N\rangle\sum_q D(\mathbf{k},\mathbf{k}',\mathbf{q},N,N')$$
$$\times\left(\frac{1}{\omega^2}-\frac{\pi}{2x}\delta''(\omega)\right)=e\mathbf{E}\cdot\nabla_{\mathbf{k}'}\delta(\mathbf{k}-\mathbf{k}')P(N_q)$$
$$\times\left(\sum_q[V_q\sqrt{N_q}\delta(\mathbf{k}'-\mathbf{k}+\mathbf{q})+V_q^*\sqrt{N_q+1}\,\delta\right.$$
$$\times(\mathbf{k}'-\mathbf{k}-\mathbf{q})]f(\mathbf{k}')\sum_q[V_q\sqrt{N_q}\delta(\mathbf{k}'-\mathbf{k}+\mathbf{q})$$
$$+V_q^*\sqrt{N_q+1}\,\delta(\mathbf{k}'-\mathbf{k}-\mathbf{q})]$$
$$-\sum_q[V_q\sqrt{N_q}\delta(\mathbf{k}'-\mathbf{k}+\mathbf{q})+V_q^*\sqrt{N_q+1}\,\delta$$
$$\left.\times(\mathbf{k}'-\mathbf{k}-\mathbf{q})]f(\mathbf{k})\right)\left(\frac{1}{\omega^2}-\frac{\pi}{2x}\delta''(\omega)\right). \tag{20}$$

When relation (18) is used the term (20) takes the same form as the term (19). Also the term (5*c*) leads finally to the form (19). Thus we have

$$\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\rm (I)SF}=\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\rm (II)SF}=\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\rm (III)SF} \tag{21}$$

where the terms express the corrections to the Boltzmann kinetic equation coming from the contributions (5*a*), (5*b*) and (5*c*).

For our further treatment it will be more convenient to utilize equation (21) and write the correction term to the Boltzmann equation in the form

$$\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\rm SF}=\frac{6e}{\hbar^3}\sum_{\mathbf{k}'N'}\langle \mathbf{k}N|H_{\rm i}|\mathbf{k}'N'\rangle\langle \mathbf{k}'N'|H_{\rm i}|\mathbf{k}N\rangle$$
$$\times\mathbf{E}\cdot P(N)\,[\nabla_{\mathbf{k}}f(\mathbf{k})-\nabla_{\mathbf{k}'}f(\mathbf{k}')]$$
$$\times\left(\frac{1}{\omega^2}-\frac{\pi}{2x}\delta''(\omega)\right). \tag{22}$$

The probability that inelastic scattering takes place is proportional to $1/\omega^2$ where the frequency ω is defined by (9).

5. Determination of the electric field strength

In order to find the magnitude of electric field in the correction term representing the significant term in the Boltzmann kinetic equation, we will use the simplest case (see appendix A), which can be used for heavily doped silicon. When further approximations are made we will get

$$\left[\frac{\partial f(\mathbf{k})}{\partial t}\right]_{\rm SF}=\nabla_{\mathbf{k}}[f(\mathbf{k})-f_0(\mathbf{k})]\,\Gamma_{\rm FR} \tag{23}$$

where f is the equilibrium distribution function and $\Gamma_{\rm FR}$ is a field scattering rate:

$$\Gamma_{\rm FR}=\frac{6e}{\hbar}\sum_{\mathbf{k}'N'}\langle \mathbf{k}N|H_{\rm i}|\mathbf{k}'N'\rangle\langle \mathbf{k}'N'|H_{\rm i}|\mathbf{k}N\rangle\cdot\mathbf{E}\cdot P(N)$$
$$\times\left(1-\frac{\nabla_{\mathbf{k}'_E}\left(\psi(\mathbf{k}')\frac{\partial f_0}{\partial\varepsilon'}\right)}{\nabla_{\mathbf{k}_E}\left(\psi(\mathbf{k})\frac{\partial f_0}{\partial\varepsilon}\right)}\right)\left(\frac{1}{\omega^2}-\frac{\pi}{2x}\delta''(\omega)\right) \tag{24}$$

where the same notation is used as in (9):

$$\omega=(1/\hbar)(\varepsilon_{\mathbf{k}}-\varepsilon_{\mathbf{k}'}+E_N-E_{N'})$$

and $\psi(\mathbf{k})$ in (24) is a linear function of the acting forces and $\varepsilon=\varepsilon_{\mathbf{k}}=\varepsilon(\mathbf{k})$, $\varepsilon'=\varepsilon_{\mathbf{k}'}=\varepsilon(\mathbf{k}')$.

If we assume elastic collisions of the conduction electrons with the scattering system and the validity of the parabolic dispersion law then for the field scattering rate (24) we obtain (see appendix B):

$$\Gamma_{\rm FR}=\frac{6\Omega m^2 e}{\pi^2\hbar^5}\frac{E}{k^2}\int_{q_{\rm min}}^{q_{\rm max}}\mathrm{d}q|V_q|^2(2\bar{N}_q+1)q$$
$$\times\left(\ln\left|\frac{q+2k}{q-2k}\right|-\frac{4kq}{q^2-4k^2}\right) \tag{25}$$

in which $q=k-k'$ is assumed due to the elastic electron–phonon scattering, the boundaries $q_{\rm min}$ and $q_{\rm max}$ of the integral (25) are determined by the laws of conservation of energy and momentum.

The function

$$\frac{f(q)}{q}=\ln\left|\frac{q+2k}{q-2k}\right|-\frac{4kq}{q^2-4k^2} \tag{26}$$

appearing in (25) plays a similar role in the field scattering rate to the delta function in the standard relaxation time. This exact result was given by a Bardeen self-consistent calculation for the free electron model [22], which is based on the scattering effect of a displacement of the bare ions. Its graphical form can be seen in figure 1.

The points $q=+2k$ are its singular points and correspond to singular points of the delta function in the standard relaxation time. In the region $0<q<+2k$, which represents the first Brillouin zone, this function broadens the energetic spectrum of the electron. When the wavevector $q\to\pm\infty$ then (26) goes to 0.

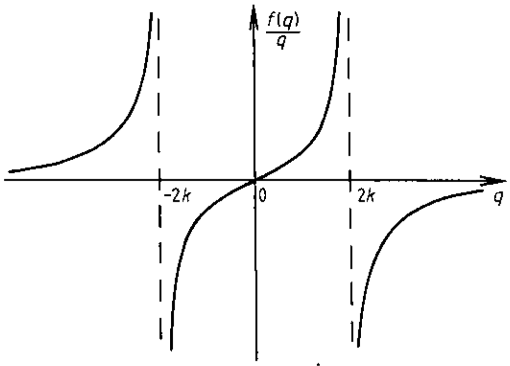

Figure 1. Graph of the function (29).

The influence of the correction term with field scattering rate (25) increases linearly from the electric field. Assuming the weak interactions of the electrons with phonons we obtain [25] for the scattering term (16):

$$\left[\frac{\partial f(k)}{\partial t}\right]_S = (f - f_0)\frac{\Omega m}{4\pi\hbar^3 k^3}\int_{q_{min}}^{q_{max}} dq |V_q|^2 (2\bar{N}_q + 1) q^3. \quad (27)$$

If the distribution functions f and f_0 in (23) and (27) are approximated by an arbitrary exponential function from k we are able to find the magnitude of the electric field for which the correction term gives a contribution comparable to the scattering term in (16). We found the value 2.49 MV m^{-1} by numerical calculation.

6. Conclusion

The Boltzmann kinetic equation has been generalized to describe transport in a strong electric field in semiconductors. The correction term involving the field effect scattering rate represents the intracollisional field effect [7, 24] which can be seen from the behaviour of the function (26) in figure 1. This behaviour indicates a certain quasielasticity (or inelasticity) of the electron–phonon collisions in the high electric field in spite of the fact that elastic collisions were assumed when deriving the field effect scattering rate.

We have succeeded in deriving a form of the field effect scattering rate which resembles that appearing in a standard relaxation time.

Using a numerical calculation we have succeeded in determining the electric field which gives a correction representing a significant term in the Boltzmann kinetic equation. Assuming convenience of the relaxation time of the electrons with phonons in the scattering term, we obtain the value 2.49 MV m^{-1} for this electric field. The contribution of our correction term from this value is of the same order as from the scattering term in the form (27).

This enables us to compare our result with those of Khan *et al* [14] and Barker and Ferry [25]. They claim that the Boltzmann equation fails in electric fields exceeding approximately a few MV m^{-1} in conventional semiconductors. Obviously, the validity of our Boltzmann kinetic equation with the correction term is restricted by the scattering of electrons on phonons.

Unfortunately, we cannot compare our result (26) with the important work of Chen and Su [17], but our result is certainly not a mere approximation (e.g. first order) of their result.

Acknowledgments

The author should like to thank Dr J Foltín and Dr V Čápek for their help and useful discussions.

Appendix A. Introduction of field effect scattering rate

We will assume that we know nothing about the magnitude of the electric field and that the electron distribution function $f(\boldsymbol{k})$ may be written in the form

$$f(\boldsymbol{k}) = f_0(\boldsymbol{k}) + f_1(\boldsymbol{k}) = f_0(\boldsymbol{k}) + \boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial \varepsilon} \quad (A.1)$$

where f_0 is the equilibrium distribution function, f_1 and ψ are a linear functions of the applied forces and the notation $\varepsilon = \varepsilon(\boldsymbol{k}), \varepsilon' = \varepsilon(\boldsymbol{k}')$ is introduced.

When the gradient of (A.1) is taken we get

$$\nabla_{\boldsymbol{k}} f(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} f_0(\boldsymbol{k}) + \nabla_{\boldsymbol{k}} f_1(\boldsymbol{k}) = \nabla_{\boldsymbol{k}} f_0(\boldsymbol{k}) + \nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial \varepsilon}\right) \quad (A.2)$$

Now we will take expression (12) and we will use the notation

$$\left[\frac{\partial f(\boldsymbol{k})}{\partial t}\right]_{(I)SF} = C(\boldsymbol{k}N)[\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}} f(\boldsymbol{k}) - \boldsymbol{E}\cdot\nabla_{\boldsymbol{k}'} f(\boldsymbol{k}')]P(N) \quad (A.3)$$

$$C(\boldsymbol{k}N) = \frac{6e}{\hbar^3}\sum_{\boldsymbol{k}'N'}\langle \boldsymbol{k}N|H_i|\boldsymbol{k}'N'\rangle\langle \boldsymbol{k}'N'|H_i|\boldsymbol{k}N\rangle \times\left(\frac{1}{\omega^2} - \frac{\pi}{2x}\delta''(\omega)\right). \quad (A.4)$$

When (A.2) is inserted into (A.3) we get

$$C(\boldsymbol{k}N)\boldsymbol{E}\cdot[\nabla_{\boldsymbol{k}} f(\boldsymbol{k}) - \nabla_{\boldsymbol{k}'} f(\boldsymbol{k}')]P(N) = C(\boldsymbol{k}N)\boldsymbol{E}\cdot\left[\nabla_{\boldsymbol{k}} f_0(\boldsymbol{k}) + \nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial \varepsilon}\right) - \nabla_{\boldsymbol{k}'} f_0(\boldsymbol{k}') - \nabla_{\boldsymbol{k}'}\left(\boldsymbol{v}'\cdot\psi(\boldsymbol{k}')\frac{\partial f_0}{\partial \varepsilon'}\right)\right]P(N). \quad (A.5)$$

(A.2) can be written in the form

$$\nabla_{\boldsymbol{k}}[f(\boldsymbol{k}) - f_0(\boldsymbol{k})] = \nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial \varepsilon}\right). \quad (A.6)$$

In order to be able to further modify (A.4) we will assume that $\nabla_{\boldsymbol{k}} f_0(\boldsymbol{k}) \simeq \nabla_{\boldsymbol{k}'} f_0(\boldsymbol{k}')$, i.e. the gradients of the equilibrium distribution functions are approximately equal. Using these assumptions and inserting (A.5) into (A.4) we obtain

$$\begin{aligned}
&C(\boldsymbol{k}N)\boldsymbol{E}\cdot[\nabla_{\boldsymbol{k}} f(\boldsymbol{k}) - \nabla_{\boldsymbol{k}'} f(\boldsymbol{k}')]P(N)\\
&= C(\boldsymbol{k}N)\boldsymbol{E}\left[\nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial\varepsilon}\right) - \nabla_{\boldsymbol{k}'}\left(\boldsymbol{v}'\cdot\psi(\boldsymbol{k}')\frac{\partial f_0}{\partial\varepsilon'}\right)\right]P(N)\\
&= C(\boldsymbol{k}N)\boldsymbol{E}\left[\nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial\varepsilon}\right) \times\left(1-\frac{\nabla_{\boldsymbol{k}'}\left(\boldsymbol{v}'\cdot\psi(\boldsymbol{k}')\frac{\partial f_0}{\partial\varepsilon'}\right)}{\nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial\varepsilon}\right)}\right)\right]P(N)\\
&= \nabla_{\boldsymbol{k}}[f(\boldsymbol{k}) - f_0(\boldsymbol{k})]\Gamma_{\mathrm{FR}}
\end{aligned}$$

and

$$\Gamma_{\mathrm{FR}} = C(\boldsymbol{k}N)\boldsymbol{E}\cdot\left(1-\frac{\nabla_{\boldsymbol{k}'}\left(\boldsymbol{v}'\cdot\psi(\boldsymbol{k}')\frac{\partial f_0}{\partial\varepsilon'}\right)}{\nabla_{\boldsymbol{k}}\left(\boldsymbol{v}\cdot\psi(\boldsymbol{k})\frac{\partial f_0}{\partial\varepsilon}\right)}\right)P(N). \tag{A.7}$$

Appendix B. Further approximations of field effect scattering rate

We will start from the field effect scattering rate and we will further assume: (i) validity of the parabolic dispersion law and (ii) elasticity of the electron–phonon collisions. Then (A.7) can be written as

$$\Gamma_{\mathrm{FR}} = C(\boldsymbol{k}N)\boldsymbol{E}\left(1-\frac{\frac{\hbar^2}{m}k'_E\nabla_{\varepsilon'}\left(\psi(\boldsymbol{k}')\frac{\partial f_0}{\partial\varepsilon'}\right)}{\frac{\hbar^2}{m}k_E\nabla_{\varepsilon}\left(\psi(\boldsymbol{k})\frac{\partial f_0}{\partial\varepsilon}\right)}\right)P(N) \tag{B.1}$$

in which $C(\boldsymbol{k}N)$ is defined by (A.4) and the linear function ψ of an applied force depends directly on ε as a consequence of the assumptions (i) and (ii). (B.1) can be written in the following way:

$$\begin{aligned}
\Gamma_{\mathrm{FR}} &= C(\boldsymbol{k}N)\boldsymbol{E}\frac{k_E-k'_E}{k_E}P(N)\\
&= \frac{2e}{\hbar^3}\sum_{\boldsymbol{k}'N'}\langle\boldsymbol{k}N|H_{\mathrm{i}}|\boldsymbol{k}'N'\rangle\langle\boldsymbol{k}'N'|H_{\mathrm{i}}|\boldsymbol{k}N\rangle\\
&\quad\times\boldsymbol{E}\frac{k_E-k'_E}{k_E}P(N)\left(\frac{1}{\omega^2}-\frac{\pi}{2x}\delta''(\omega)\right)
\end{aligned} \tag{B.2}$$

where k_E and k'_E are particular components of the electron wavevector in the direction of the applied electric field and ω is defined by (9).

Assumption (ii) means that the phonon wavevector satisfies the relation $q_E = k_E - k'_E$ and for (B.2) we obtain

$$\begin{aligned}
\Gamma_{\mathrm{FR}} = \frac{6e}{\hbar^2}\sum_{q}|V_q|^2\boldsymbol{E}\frac{q_E}{k_E}&\left[\bar{N}_q\frac{\hbar}{(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})^2} - (\bar{N}_q+1)\frac{\hbar}{(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})^2} - \left(\frac{\pi}{2x}\bar{N}_q\delta''(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})\right.\right.\\
&\left.\left.+\frac{\pi}{2x}(\bar{N}_q+1)\delta''(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})\right)\right].
\end{aligned} \tag{B.3}$$

In (B.3) V_q is a characteristic parameter of the electron–phonon interaction and $\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} = \varepsilon(\boldsymbol{k}+\boldsymbol{q})$ etc.

To simplify the computation of (B.3) we will introduce the notation:

$$\Gamma_{\mathrm{FR}} = T_{\mathrm{I}} - T_{\mathrm{II}} \tag{B.4}$$

$$T_{\mathrm{I}} = \frac{6e}{\hbar^2}\sum_{q}|V_q|^2\boldsymbol{E}\frac{q_E}{k_E}\left(\bar{N}_q\frac{\hbar}{(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})^2} - (\bar{N}_q+1)\frac{\hbar}{(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})^2}\right)$$

$$T_{\mathrm{II}} = \frac{3e\pi}{\hbar^2 x}\sum_{q}|V_q|^2\boldsymbol{E}\frac{q_E}{k_E}\left[\bar{N}_q\delta''(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}}) - (\bar{N}_q+1)\delta''(\varepsilon_{\boldsymbol{k}-\boldsymbol{q}}-\varepsilon_{\boldsymbol{k}})\right].$$

First we will evaluate the expression T_{II}. Instead of the sum we will compute an integral:

$$\sum_{q}\longrightarrow\frac{\Omega}{(2\pi)^3}\int \mathrm{d}^3q \tag{B.5}$$

where Ω is the volume of the crystal. Then on the right-hand side of (B.5) we will use the parabolic dispersion law:

$$\begin{aligned}
T_{\mathrm{II}} = \frac{3e\Omega}{8\pi^2\hbar^2 x}\int \mathrm{d}^3q|V_q|^2\boldsymbol{E}\frac{q_E}{k_E}
&\times\left[\bar{N}_q\delta''\left(\frac{\hbar^2}{2m}(q^2+2\boldsymbol{k}\cdot\boldsymbol{q})\right)\right.\\
&\left.-(\bar{N}_q+1)\delta''\left(\frac{\hbar^2}{2m}(q^2-2\boldsymbol{k}\cdot\boldsymbol{q})\right)\right].
\end{aligned} \tag{B.6}$$

After introducing spherical coordinates we obtain

$$\begin{aligned}
T_{\mathrm{II}} = \frac{3em\Omega\boldsymbol{E}}{4\pi\hbar^4k^2x}\int_0^\infty \mathrm{d}q\int_{-1}^{1}\mathrm{d}z|V_q|^2q^2z
&\times\left[\bar{N}_q\delta''\left(\frac{q}{2k}+z\right)-(\bar{N}_q+1)\delta''\left(\frac{q}{2k}-z\right)\right]=0.
\end{aligned} \tag{B.7}$$

From the properties of the second derivative of the delta function we can say that T_{II} does not contribute.

Now we turn back to (B.4) and again replace the sum by an integral and use the parabolic dispersion law. Then we arrive at

$$T_{\rm I} = \frac{3e\Omega m^2 \boldsymbol{E}}{\pi^3 \hbar^5} \int \mathrm{d}^3 q |V_{\boldsymbol{q}}|^2 \frac{q_E}{k_E} \times \left(\frac{\bar{N}_{\boldsymbol{q}}}{(q^2 + 2\boldsymbol{k}\cdot\boldsymbol{q})^2} - \frac{\bar{N}_{\boldsymbol{q}} + 1}{(q^2 - 2\boldsymbol{k}\cdot\boldsymbol{q})^2} \right). \tag{B.8}$$

In analogy with (B.7) we introduce spherical coordinates and the vectors k_E, q_E. After substituting $\cos\vartheta = z$ we get

$$\begin{aligned} T_{\rm I} &= \frac{6e\Omega m^2 \boldsymbol{E}}{\pi^2 \hbar^5 k} \int_0^\infty \mathrm{d}q \int_{-1}^{1} \mathrm{d}z |V_{\boldsymbol{q}}|^2 q^3 z \times \left(\frac{\bar{N}_{\boldsymbol{q}}}{(q^2 + 2kqz)^2} - \frac{\bar{N}_{\boldsymbol{q}} + 1}{(q^2 - 2kqz)^2} \right) \\ &= \frac{6e\Omega m^2 \boldsymbol{E}}{\pi^2 b \hbar^5 k^2} \int_0^\infty \mathrm{d}q |V_{\boldsymbol{q}}|^2 (2\bar{N}_q + 1) \times q \frac{\mathrm{d}}{\mathrm{d}q} \left(q \ln\left| \frac{q+2k}{q-2k} \right| - \frac{4kq}{q^2 - 4k^2} \right) \end{aligned} \tag{B.9}$$

or

$$T_{\rm I} = \frac{6e\Omega m^2 \boldsymbol{E}}{\pi^2 \hbar^5 k^2} \int_0^\infty \mathrm{d}q |V_{\boldsymbol{q}}|^2 (2\bar{N}_q + 1) q \times \left(\ln\left| \frac{q+2k}{q-2k} \right| - \frac{4kq}{q^2 - 4k^2} \right). \tag{B.10}$$

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