Entropy **2015**, *17*, 528-538; doi:10.3390/e17020528

OPEN ACCESS
entropy
ISSN 1099-4300
www.mdpi.com/journal/entropy

Article

A New Telegrapher's-Poisson System in Semiconductor Theory: A Singular Perturbation Approach

Alberto Rossani

Dipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy; E-Mail: alberto.rossani@polito.it; Tel.: +39-011-0907369

Academic Editor: Giorgio Kaniadakis

Received: 3 December 2014 / Accepted: 21 January 2015 / Published: 29 January 2015

Abstract: In the theory of energy and momentum relaxation in semiconductor devices, the introduction of two temperatures and two mean velocities for electron and phonons is required. A new model, based on an asymptotic procedure for solving the kinetic equations of electrons and phonons is proposed, which naturally gives the displaced Maxwellian at the leading order. After that, balance equations for the electron number, energy densities and momentum densities are constructed, which constitute now a system of five equations for the chemical potential of electrons, the temperatures and the drift velocities. Moreover, Poisson's equation is coupled, in order to calculate the self-consistent electric field. In Bloch's approximation, we derive a telegrapher's-Poisson system for the electron number density and the electric potential, which could allow simple semiconductor calculations, but still including wave propagation effects.

Keywords: semiconductors; kinetic theory; telegrapher's equation

1. Introduction

In the past [1], a telegrapher's approach in semiconductor theory has already proposed, based on a stochastic model. Here, we resort strictly to the kinetic theory based on the Bloch–Boltzmann–Peierls (BBP) equations [2]. The telegrapher's equation we derive does not contain phenomenological constants, like relaxation times. Here, all of the coefficients are derived from the collision kernels of the electron-phonon, electron-electron and phonon-phonon interactions. Moreover, we introduce a self-consistent electric field by means of the coupled Poisson's equation.

In semiconductor modeling, three approaches are widely applied, according to the physical situation with which we deal. The microscopic approach is based on Monte Carlo simulations, which can account for as many aspects of semiconductor physics as we want. Nevertheless it is well known that these simulations are time consuming and therefore expensive.

The mesoscopic approach is based on the Boltzmann transport equation (BTE). Several numerical techniques are developed in order to face a numerical solution of the problem. The distribution function depends on seven variables (momentum, position, time), so that the task is quite formidable.

The macroscopic approaches are based on the weak form of the BTE, which give rise to a hierarchy of coupled equations for the moments of the distribution function. Such an approach requires a truncation at some order based on closure assumptions for the higher order fluxes and for the production terms for non-conservation equations.

Most of the semiconductor macroscopic models have in common the assumption, at the basis of the closure approximation, that some higher moments can be calculated by utilizing a displaced Maxwellian. This approach would be justified if one had a systematic approximation for solving the Boltzmann transport equations, asymptotic with respect to some parameters, whose leading terms would be displaced Maxwellians. Such an approximation (asymptotic expansion) is now available [3] and gives rise to a system of equations that recalls the extended thermodynamics model [4].

The thermalization, due to the electron-phonon interactions, of a non-equilibrium electron-phonon system occurs if electrons in metals or semiconductors are heated to a temperature T_e greater than the lattice temperature T_p. In [2], a homogeneous medium is considered. Here, more in general, we consider a non-uniform electron-phonon system. The result of [2] is recovered. Moreover, the momentum relaxation is accounted for.

We start from the Bloch–Boltzmann–Peierls (BBP) coupled equations for the distribution functions of electrons and phonons.

After that, by means of an expansion of both the unknowns and the interaction kernels with respect to a small parameter that accounts for the Umklapp processes (with no momentum conservation), the lowest order equations show that the displaced Maxwellian approximation is justified. A closed set of two-fluid equations is constructed for the chemical potential of electrons, the temperatures and the drift velocities. In Bloch's approximation, a telegrapher's-Poisson system can be derived for the electron number density and the electric potential. This result opens new possibilities for a simplified semiconductor modeling, which could include wave propagation effects [5].

We stress that in the present model:

(1) the displaced Maxwellian approximation is not an *ad hoc* assumption, but is justified by the expansion that we apply;

(2) phonons are treated as a participating species, which brings energy and momentum;

(3) the correct phonon-phonon, electron-phonon and electron-electron interaction kernels are utilized; we avoid the use of relaxation time approximations;

(4) a new telegrapher's-Poisson system is derived here, starting from kinetic theory.

The main differences with respect to [3] are:

(i) the electron-electron (e-e) collisional operator (w_{ee}) is now considered;

(ii) the asymptotic expansion is now singular for w_{ee} and regular for the electron-phonon collisional operator (w_{ep});

(iii) different temperatures and drift velocities for electrons and phonons now are taken into account.

With respect to [6], we observe that:

(iv) the generalization is dropped; here, we adopt Maxwell and Bose–Einstein statistics for electrons and phonons, respectively;

(v) the calculation is performed in the case of cubic symmetry;

(vi) a self-consistent electric field is accounted for.

2. The BBP Equations

Consider two interacting populations: electrons (e), with charge -e, and phonons (p). Let $N_g(\mathbf{k}, \mathbf{x}, t)$ be the distribution function of phonons (quasi-momentum $\mathbf{k}$, energy $\omega_g(\mathbf{k})$) of type g (*i.e.*, branch g of the phonon spectrum) and $n_{\mathbf{p}} = n_{\mathbf{p}}(\mathbf{p}, \mathbf{x}, t)$ the distribution function of electrons (quasi-momentum $\mathbf{p}$, energy $\mathcal{E}_{\mathbf{p}}$).

In the present paper, we utilize the same notation of [7], like in [3,6], to which the reader is referred. The BBP equations read:

$$\begin{aligned}\mathcal{S}_g N_g =& (\partial N_g/\partial t)_{pp} + (\partial N_g/\partial t)_{pe}\\ \mathcal{S}_{\mathbf{p}} n_{\mathbf{p}} =& (\partial n_{\mathbf{p}}/\partial t)_{ep}, \quad (\partial n_{\mathbf{p}}/\partial t)_{ee}\end{aligned}$$

where:

$$\begin{aligned}\mathcal{S}_g &= \partial/\partial t + \mathbf{u}_g \cdot \partial/\partial \mathbf{x}\\ \mathcal{S}_{\mathbf{p}} &= \partial/\partial t + \mathbf{v} \cdot \partial/\partial \mathbf{x} - e\mathbf{E} \cdot \partial/\partial \mathbf{p}\end{aligned}$$

with:

$$\mathbf{u}_g = \partial \omega_g/\partial \mathbf{k}, \quad \mathbf{v} = \partial \mathcal{E}_{\mathbf{p}}/\partial \mathbf{p}, \quad \mathbf{E} = -\partial \mathcal{P}/\partial \mathbf{x},$$

where $\mathcal{P}$ is the electric potential. Observe that, since ω_g and $\mathcal{E}_{\mathbf{p}}$ are even, $\mathbf{u}_g$ and $\mathbf{v}$ are odd.

At the right-hand sides of the BBP equations for phonons [8], we have:

$$\begin{aligned}(\partial N_g/\partial t)_{pp} = \int [(1/2) \sum_{g_1 g_2} w_{pp}(\mathbf{k}_1, \mathbf{k}_2 \to \mathbf{k})(-N_g(1+N_{g_1})(1+N_{g_2}) + (1+N_g)N_{g_1}N_{g_2}) +\\ + \sum_{g_1 g_3} w_{pp}(\mathbf{k}, \mathbf{k}_1 \to \mathbf{k}_3)[(1+N_g)(1+N_{g_1})N_{g_3} - N_g N_{g_1}(1+N_{g_3})]] \frac{d\mathbf{k}_1}{8\pi^3},\end{aligned}$$

where

$$\mathbf{k}_2 = \mathbf{k} - \mathbf{k}_1 + \mathbf{b}(\mathbf{k}_1, \mathbf{k}_2 \to \mathbf{k}), \quad \mathbf{k}_3 = \mathbf{k} + \mathbf{k}_1 + \mathbf{b}(\mathbf{k}, \mathbf{k}_1 \to \mathbf{k}_3),$$

which account for three-phonon processes:

$$(g, \mathbf{k}) \rightleftharpoons (g_1, \mathbf{k}_1) + (g_2, \mathbf{k}_2), \quad (g_3, \mathbf{k}_3) \rightleftharpoons (g, \mathbf{k}) + (g_1, \mathbf{k}_1).$$

In general, we must distinguish between normal processes (which conserve momentum) with $\mathbf{b} = \mathbf{0}$, and Umklapp processes (which do not conserve momentum) with $\mathbf{b} \neq \mathbf{0}$, where $\mathbf{b}$ is an appropriate vector of the reciprocal lattice [9].

Moreover, in the low density approximation,

$$(\partial N_g/\partial t)_{pe} = 2\int w_{pe}(\mathbf{p} \to \mathbf{p}', \mathbf{k})(n_{\mathbf{p}}(1+N_g) - n_{\mathbf{p}'}N_g)\frac{d\mathbf{p}}{8\pi^3},$$

where $\mathbf{p}' = \mathbf{p} - \mathbf{k} + \mathbf{b}(\mathbf{p} \to \mathbf{p}', \mathbf{k})$ is the difference between the number of phonons $\mathbf{k}$ emitted by electrons with any quasimomentum $\mathbf{p}$ and the number of phonons absorbed by electrons with any $\mathbf{p}'$.

For electrons, we have:

$$(\partial n_{\mathbf{p}}/\partial t)_{ep} = \sum_g \int [w_{ep}(\mathbf{p}', \mathbf{k} \to \mathbf{p})(n_{\mathbf{p}'}N_g - n_{\mathbf{p}}(1+N_g)) + w_{ep}(\mathbf{p}'' \to \mathbf{p}, \mathbf{k})(n_{\mathbf{p}''}(1+N_g) - n_{\mathbf{p}}N_g)]\frac{d\mathbf{k}}{8\pi^3},$$

where

$$\mathbf{p}' = \mathbf{p} - \mathbf{k} + \mathbf{b}(\mathbf{p}', \mathbf{k} \to \mathbf{p}), \quad \mathbf{p}'' = \mathbf{p} + \mathbf{k} + \mathbf{b}(\mathbf{p}'' \to \mathbf{p}, \mathbf{k}).$$

The first term corresponds to processes with the emission of a phonon having quasimomentum $\mathbf{k}$ by an electron having a given quasimomentum $\mathbf{p}$ and reverse processes. The second term corresponds to processes with absorption of a phonon by an electron with quasimomentum $\mathbf{p}$ and reverse processes.

The w's, which come from quantum mechanical calculations [9], are transition probabilities, which account for energy conservation, that is they contain a Dirac's delta function, which imposes such conservation. Moreover, the following symmetry relations are satisfied:

$$w_{pe}(\mathbf{p} \to \mathbf{p}', \mathbf{k}) = w_{ep}(\mathbf{p} \to \mathbf{p}', \mathbf{k}) = w_{ep}(\mathbf{p}', \mathbf{k} \to \mathbf{p}).$$

Furthermore, the e-e collision integral reads:

$$(\partial n_{\mathbf{p}}/\partial t)_{ee} = \int\int w_{ee}(\mathbf{p}, \mathbf{p}_1 \to \mathbf{p}', \mathbf{p}_1')(n_{\mathbf{p}'}n_{\mathbf{p}_1'} - n_{\mathbf{p}}n_{\mathbf{p}_1})\frac{d\mathbf{p}_1 d\mathbf{p}_1'}{64\pi^6}$$

3. Asymptotic Expansion and Balance Equations

By following [3], we expand the kernels and the unknowns with respect to a small parameter ϵ, which takes into account the effect of the Umklapp (U) processes in addition to the normal (N) ones. We start with electrons (the extension to phonons is trivial). The sought expansions for $n_{\mathbf{p}}$ and N_g read:

$$n_{\mathbf{p}} = n_{\mathbf{p}}^N + \epsilon n_{\mathbf{p}}^U, \quad N_g = N_g^N + \epsilon N_g^U.$$

Accordingly:

$$\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep} = \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^N + \epsilon\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^U,$$

where w_{ep} and w_{ee} read:

$$w_{ep} = w_{ep}^N + \epsilon w_{ep}^U, \quad w_{ee} = (1/\epsilon)w_{ee}^N + w_{ep}^U.$$

Observe that the expansion of w_{ee} is singular, since the relaxation due to e-e interactions is considered quicker with respect to the case of the e-p ones [2].

By introducing the expansions with respect to w_{ep} and w_{ee}, we can write:

$$\begin{aligned}
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{N} &= \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NN} + \epsilon \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NU}, \\
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{U} &= \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{UN} + \epsilon \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{UU}, \\
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{N} &= (1/\epsilon)\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NN} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NU}, \\
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{U} &= (1/\epsilon)\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UN} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UU}.
\end{aligned}$$

By collecting all of these terms and neglecting ϵ^{ℓ} with $\ell \geq 1$, we have:

$$\mathcal{S}_{\mathbf{p}} n_{\mathbf{p}}^{N} = (1/\epsilon)\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NN} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NU} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UN} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NN}.$$

At the orders -1 and zero, we get:

$$\begin{aligned}
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NN} &= 0 \\
\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NU} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UN} + \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NN} &= \mathcal{S}_{\mathbf{p}} n_{\mathbf{p}}^{N},
\end{aligned} \tag{1}$$

respectively. Analogously, for phonons:

$$\begin{aligned}
\left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NN} &= 0 \\
\left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NU} + \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{UN} + \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NN} &= \mathcal{S}_g N_g^{N}.
\end{aligned} \tag{2}$$

The equations of order -1 for both phonons and electrons are solved (see the Appendix) by:

$$\ln[N_g^N/(1+N_g^N)] = (\mathbf{V}_p \cdot \mathbf{k} - \omega_g)/T_p, \;\; \ln n_{\mathbf{p}}^N = (\mu + \mathbf{V}_e \cdot \mathbf{p} - \mathcal{E}_{\mathbf{p}})/T_e$$

(with $\alpha = e, p$) where $T_\alpha = T_\alpha(\mathbf{x}, t)$ are the absolute temperatures, while $\mu = \mu(\mathbf{x}, t)$ is the chemical potential of the electron gas (the meaning of $\mathbf{V}_\alpha$ is discussed later). Thus, at the leading order of this expansion, we find the drifted Bose–Einstein (BE) and Maxwell–Boltzmann (MB) distribution functions:

$$N_g^N = \mathcal{B}[\beta_p(\omega_g - \mathbf{V}_p \cdot \mathbf{k})], \;\; n_{\mathbf{p}}^N = \mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}} - \mu - \mathbf{V}_e \cdot \mathbf{p})],$$

where $\beta_\ell = 1/T_\ell, \; \ell = e, p$:

$$\mathcal{B}(\zeta) = 1/(e^{\zeta} - 1), \;\; \mathcal{M}(\zeta) = e^{-\zeta},$$

that is, the BE and MB distribution functions are recovered. Usually [10], N_g^N and $n_{\mathbf{p}}^N$ are factored into two components, a symmetric component (zero), which is even in momentum, and an anti-symmetric component (one), which is odd, by expansion with respect to $\mathbf{V}_e$ and $\mathbf{V}_p$, respectively:

$$N_g^N = \mathcal{B}(\beta_p \omega_g) + \beta_p \mathbf{V}_p \cdot \mathbf{k} |\mathcal{B}'(\beta_p \omega_g)| = N_g^0 + N_g^1,$$

$$n^N_{\mathbf{p}} \;=\; \mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}}-\mu)]+\beta_e\mathbf{V}_e\cdot\mathbf{p}\mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}}-\mu)]=n^0_{\mathbf{p}}+n^1_{\mathbf{p}}$$

where $\mathcal{B}'(\zeta)=d\mathcal{B}/d\zeta=-\mathcal{B}^2(\zeta)e^{\zeta}$. This simplification is justified in the frame of the drift-diffusion approximation [10]. Observe that, under this assumption, the drift velocities $<\mathbf{v}>$ and $<\mathbf{u}_g>$ of electrons and phonons, respectively, are given by:

$$<\mathbf{v}>=\frac{\int n_{\mathbf{p}}\mathbf{v}d\mathbf{p}}{\int n_{\mathbf{p}}d\mathbf{p}}=\mathbf{V}_e,\;\; <\mathbf{u}_g>=\frac{\int N_g\mathbf{u}_g d\mathbf{p}}{\int N_g d\mathbf{p}}=\mathbf{V}_p.$$

In fact:

$$\int\mathbf{v}n_{\mathbf{p}}d\mathbf{p}=-\beta_e\int\mathbf{V}_e\cdot\mathbf{p}\mathcal{M}'(\beta_e\mathcal{E}_{\mathbf{p}})\mathbf{v}d\mathbf{p}=-\int\mathbf{V}_e\cdot\mathbf{p}\frac{\partial}{\partial\mathbf{p}}\mathcal{M}(\beta_e\mathcal{E}_{\mathbf{p}})d\mathbf{p}=\mathbf{V}_e\int\mathcal{M}(\beta_e\mathcal{E}_{\mathbf{p}})d\mathbf{p}$$

and analogously for $\int\mathbf{u}_gN_gd\mathbf{k}$. Moreover, by taking into account the MB and BE distribution functions, for electrons and phonons, respectively, after some calculations, we find, at the first order with respect to $\mathbf{V}_e$ and $\mathbf{V}_p$,

$$\begin{aligned}(\partial N_g/\partial t)^{NU}_{pp} =&\beta_p\mathbf{V}_p\cdot\{\int[(1/2)\sum_{g_1g_2}(1+N^0_gN^0_{g_1}N^0_{g_2}w^U_{pp}(\mathbf{k}_1,\mathbf{k}_2\to\mathbf{k})(\mathbf{k}_2+\mathbf{k}_1-\mathbf{k})+\\ &+\sum_{g_1g_3}(1+N^0_{g_3}N^0_gN^0_{g_1}w^U_{pp}(\mathbf{k},\mathbf{k}_1\to\mathbf{k}_3)(-\mathbf{k}_3+\mathbf{k}_1+\mathbf{k})]\frac{d\mathbf{k}_1}{8\pi^3}\},\\ (\partial n_{\mathbf{p}}/\partial t)^{NU}_{ee} =&\beta_e\mathbf{V}_e\cdot\int\int w^U_{ee}(\mathbf{p},\mathbf{p}_1\to\mathbf{p}',\mathbf{p}'_1)n^0_{\mathbf{p}}n^0_{\mathbf{p}_1}(\mathbf{p}+\mathbf{p}_1-\mathbf{p}'-\mathbf{p}'_1)\frac{d\mathbf{p}_1d\mathbf{p}'_1}{64\pi^6}\end{aligned}$$

Finally:

$$\begin{aligned}&(\partial N_g/\partial t)^{NN}_{pe}\\ =&4\sum_g\int w_{pe}(\mathbf{p}',\mathbf{k}\to\mathbf{p})(n'N_gn(1+N_g))^{1/2}\times\sinh\{[(\beta_e\mathbf{V}_e-\beta_p\mathbf{V}_p)\cdot\mathbf{k}+(\beta_p-\beta_e)\omega_g]/2\}\frac{d\mathbf{p}}{8\pi^3}\end{aligned}\tag{3}$$

and in the linear non-equilibrium thermodynamic approach,

$$\begin{aligned}&(\partial N_g/\partial t)^{NN}_{pe}\\ =&2(\beta_e\mathbf{V}_e-\beta_p\mathbf{V}_p)\cdot\sum_g\int w_{pe}(\mathbf{p}',\mathbf{k}\to\mathbf{p})n'^*N^*_g\mathbf{k}\frac{d\mathbf{p}}{8\pi^3}+2(\beta_p-\beta_e)\sum_g\int w_{pe}(\mathbf{p}',\mathbf{k}\to\mathbf{p})n'^*N^*_g\omega_g\frac{d\mathbf{p}}{8\pi^3},\end{aligned}$$

where $*$ stands for complete equilibrium (see the Appendix).

The equations of order zero are the starting point of our macroscopic model. By integrating (1), the continuity equation for electrons reads:

$$\frac{\partial}{\partial t}\int n^0_{\mathbf{p}}d\mathbf{p}+\nabla\cdot\int\mathbf{v}n^1_{\mathbf{p}}d\mathbf{p}=0\tag{4}$$

By projecting the (1) over $\mathbf{p}$ and (2) on $\mathbf{k}$, we get the following balance equations for momentum:

$$\begin{aligned}&\frac{\partial}{\partial t}\int n^1_{\mathbf{p}}\mathbf{p}d\mathbf{p}+\nabla\cdot\int n^0_{\mathbf{p}}\mathbf{v}\otimes\mathbf{p}d\mathbf{p}\\ =\;&-e\mathbf{E}\int n^0_{\mathbf{p}}d\mathbf{p}+\int\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)^{NN}_{ep}\mathbf{p}d\mathbf{p}+\int\left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)^{NU}_{ee}\mathbf{p}d\mathbf{p}\sum_g\left[\frac{\partial}{\partial t}\int N^1_g\mathbf{k}d\mathbf{k}+\nabla\cdot\sum_g\int N^0_g\mathbf{u}_g\otimes\mathbf{k}d\mathbf{k}\right]\\ =\;&+\sum_g\int\left[\left(\frac{\partial N_g}{\partial t}\right)^{NU}_{pp}+\left(\frac{\partial N_g}{\partial t}\right)^{NN}_{pe}\right]\mathbf{k}d\mathbf{k},\end{aligned}\tag{5}$$

where we took advantage of:

$$\int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UN} \mathbf{p}d\mathbf{p} = 0, \ \sum_g \int \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{UN} \mathbf{k}d\mathbf{k} = 0,$$

due to momentum conservation for N-processes. For the same reason, we have:

$$2\int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{pe}^{NN} \mathbf{p}d\mathbf{p} + \sum_g \int \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NN} \mathbf{k}d\mathbf{k} = 0,$$

where:

$$\sum_g \int (\partial N_g/\partial t)_{pe}^{NN} \mathbf{k}d\mathbf{k} = (\beta_e \mathbf{V}_e - \beta_p \mathbf{V}_p) \cdot \sum_g \int\int 2w_{pe}^N(\mathbf{p}', \mathbf{k} \to \mathbf{p}) n_{\mathbf{p}'}^* N_g^* \mathbf{k} \otimes \mathbf{k}d\mathbf{p}d\mathbf{k}/8\pi^3.$$

This term is responsible for the momentum relaxation.

Finally, by projecting the electron equation over $\mathcal{E}_{\mathbf{p}}$ and the phonon ones over ω_g, we get the following balance equations for energy:

$$\begin{aligned} &\frac{\partial}{\partial t}\int \mathcal{E}_{\mathbf{p}} n_{\mathbf{p}}^0 d\mathbf{p} + \nabla \cdot \int \mathbf{v}\mathcal{E}_{\mathbf{p}} n_{\mathbf{p}}^1 d\mathbf{p} \\ &= -2e\mathbf{E} \cdot \int \mathbf{v} n_{\mathbf{p}}^1 d\mathbf{p} + \int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NN} \mathcal{E}_{\mathbf{p}} d\mathbf{p} \frac{\partial}{\partial t} \sum_g \int \omega_g N_g^0 d\mathbf{k} + \nabla \cdot \sum_g \int \mathbf{u}_g \omega_g N_g^1 d\mathbf{k} \\ &= + \int \sum_g \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NN} \omega_g d\mathbf{k}, \end{aligned} \tag{6}$$

where we took advantage of:

$$\int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{UN} \mathcal{E}_{\mathbf{p}} d\mathbf{p} = 0, \ \sum_g \int \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{UN} \omega_g d\mathbf{k} = 0,$$

$$\int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ee}^{NU} \mathcal{E}_{\mathbf{p}} d\mathbf{p} = 0, \ \sum_g \int \left(\frac{\partial N_g}{\partial t}\right)_{pp}^{NU} \omega_g d\mathbf{k} = 0,$$

due to energy conservation for N-processes. For the same reason, we have:

$$2\int \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)_{ep}^{NN} \mathcal{E}_{\mathbf{p}} d\mathbf{p} + \sum_g \int \left(\frac{\partial N_g}{\partial t}\right)_{pe}^{NN} \omega_g d\mathbf{k} = 0,$$

where:

$$\int (\partial N_g/\partial t)_{pe}^{NN} \omega_g d\mathbf{k} = 2\beta_e\beta_p(T_e - T_p) \sum_g \int\int w_{pe}(\mathbf{p}', \mathbf{k} \to \mathbf{p}) n_{\mathbf{p}'}^* N_g^* \omega_g^2 d\mathbf{p}d\mathbf{k}/8\pi^3.$$

This term, responsible for energy relaxation, is proportional to $T_e - T_p$, as in [2].

Equations (4), (5) and (6) constitute now a closed set of equations for the unknowns μ, β_α, $\mathbf{V}_\alpha$ ($\alpha = e, p$), which recall the extended thermodynamical one [4].

More explicitly, by inserting the expressions of $n^0_{\mathbf{p}}$ and $n^0_{\mathbf{p}}$ for electrons and N^0_g and N^1_g for phonons, as given in Section 3, Equation (5) can be rewritten as follows:

$$\begin{aligned}(\partial/\partial t)(L_p\hat{\mathbf{V}}_p)+\beta_p\mathbf{C}_p =&D(\hat{\mathbf{V}}_e-\hat{\mathbf{V}}_p)-B_p\hat{\mathbf{V}}_p\\ (\partial/\partial t)(L_e\hat{\mathbf{V}}_e)+\beta_e\mathbf{C}_e =&D(\hat{\mathbf{V}}_p-\hat{\mathbf{V}}_e)-B_e\hat{\mathbf{V}}_e,\end{aligned}\tag{7}$$

where $\hat{\mathbf{V}}_\alpha=\beta_\alpha\mathbf{V}_\alpha$ and:

$$\mathbf{C}_e=2\beta_eR_2\nabla T_e+2eR_1\mathbf{E}^*,\ \ \mathbf{C}_p=\beta_pR_3\nabla T_p,$$

with $\mathbf{E}^*=\mathbf{E}+(1/e)\nabla\mu$.

By assuming a cubic symmetry, B_α can be written as follows:

$$\begin{aligned}B_p=&\frac{1}{6}\sum_{g_1g_2g_3}\int\!\!\int N^0_{g_2}N^0_{g_3}(1+N^0_{g_1})w_{pp}(\mathbf{k}_2,\mathbf{k}_3\to\mathbf{k}_1)(\mathbf{k}_1-\mathbf{k}_2-\mathbf{k}_3)^2d\mathbf{k}_1d\mathbf{k}_2=\\ B_e=&(1/6)\int\!\!\int\!\!\int w_{ee}(\mathbf{p},\mathbf{p}_1\to\mathbf{p}',\mathbf{p}'_1)n_{\mathbf{p}}n_{\mathbf{p}_1}(\mathbf{p}+\mathbf{p}_1-\mathbf{p}'-\mathbf{p}'_1)^2\frac{d\mathbf{p}d\mathbf{p}_1d\mathbf{p}'}{8\pi^3}\end{aligned}$$

while:

$$\begin{aligned}L_e=&(2/3)\int\mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}}-\mu)]|\mathbf{p}^2d\mathbf{p}\\ L_p=&(1/3)\sum_g\int|\mathcal{B}'(\beta_p\omega_g)|\mathbf{k}^2d\mathbf{k}.\end{aligned}$$

Moreover:

$$D=(2/3)\sum_g\int\!\!\int w_{pe}(\mathbf{p}',\mathbf{k}\to\mathbf{p})n'^*N^*_g\mathbf{k}^2d\mathbf{p}d\mathbf{k}$$

and:

$$\begin{aligned}R_1=&(1/3)\int\mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}}-\mu)]\mathbf{p}\cdot\mathbf{v}d\mathbf{p}\\ R_2=&(1/3)\int\mathcal{M}[\beta_e(\mathcal{E}_{\mathbf{p}}-\mu)]|(\mathcal{E}_{\mathbf{p}}-\mu)\mathbf{p}\cdot\mathbf{v}d\mathbf{p}\\ R_3=&(1/3)\sum_g\int|\mathcal{B}'(\beta_p\omega_g)|\omega_g\mathbf{k}\cdot\mathbf{u}_gd\mathbf{k}.\end{aligned}$$

4. The Telegrapher's-Poisson System

Consider now, according to Bloch (see [9]), the phonons as a fixed background. This means that we must set in Equation (7) $\mathbf{V}_p=\mathbf{0},\ \ T_e=T_p=T$:

$$(\partial/\partial t)(L_e\mathbf{V}_e)+\mathbf{C}_e=-D\mathbf{V}_e-B_e\mathbf{V}_e.$$

Now, since $\exp(\mu/T)=4\pi^3\mathtt{N}/\int\mathcal{M}(\beta\mathcal{E}_{\mathbf{p}})d\mathbf{p}$, we can write:

$$L^\bullet_e(\partial/\partial t)(\mathtt{N}\mathbf{V}_e)+\mathbf{C}^\bullet_e\mathtt{N}=-D^\bullet\mathbf{V}_e\mathtt{N}-Q\mathbf{V}_e\mathtt{N}^2,$$

where we have factored $\mathtt{N}$ and $\mathtt{N}^2$ as follows: $L_e = L_e^\bullet(T)\mathtt{N}$, $\mathbf{C}_e = \mathbf{C}_e^\bullet(T)\mathtt{N}$, $D = D^\bullet(T)\mathtt{N}$ and $B_e = Q(T)\mathtt{N}^2$. By inserting $\mathbf{J} = \mathtt{N}\mathbf{V}_e$ and $\mathbf{E}^*$, one obtains:

$$L_e^\bullet(\partial\mathbf{J}/\partial t) + 2R_1^\bullet(-e\mathtt{N}\nabla\mathcal{P} + \nabla\mathtt{N}) = -(D^\bullet + Q\mathtt{N})\mathbf{J}, \tag{8}$$

which, together with the continuity:

$$\partial\mathtt{N}/\partial t + \nabla\cdot\mathbf{J} = 0, \tag{9}$$

and Poisson equations:

$$\mathcal{D}\nabla^2\mathcal{P} = -e(\mathtt{N}_d - \mathtt{N}_a - \mathtt{N}) \tag{10}$$

($\mathtt{N}_d$ and $\mathtt{N}_a$ are the number densities of acceptors and donors, respectively, while $\mathcal{D}$ is the dielectric constant) constitute a system of three equations for three unknowns: $\mathtt{N}$, $\mathbf{J}$, $\mathcal{P}$. Observe that, by neglecting the product $\mathtt{N}\mathbf{J}$ (low-density and weak current) from (8) and (9), we can derive an equation for $\mathtt{N}$ and $\mathcal{P}$ only:

$$\partial\mathtt{N}/\partial t + (1/D^\bullet)[L_e^\bullet(\partial^2\mathtt{N}/\partial t^2) + 2R_1^\bullet(e\nabla\cdot(\mathtt{N}\nabla\mathcal{P}) - \nabla^2\mathtt{N})] = 0. \tag{11}$$

Equations (10) and (11) constitute the sought telegrapher's-Poisson system for $\mathtt{N}$ and $\mathcal{P}$. With respect to [5], this model is much more simplified, but still, it is able to describe wave propagation phenomena. The present model is an improvement of the drift-diffusion approach; therefore, it is applicable whenever the drift-diffusion approach is applicable.

5. Conclusions

A new two-fluid model for an electron-phonon system has been proposed, which is certainly related to the extended thermodynamical one [4], for the purpose of the next calculations of energy and momentum relaxation, which generalize the results available in the literature [2]. The treatment resorts here strictly to kinetic theory, so that the model is closed. This means that we do not need the adjustment of some free parameters (namely the relaxation times) by means of comparisons with Monte Carlo calculations. Bloch's approximation leads to a telegrapher's-Poisson system, suitable for simplified calculations in semiconductor modeling, with the capability to study wave propagation phenomena in semiconductors [5].

Let us summarize the main hypotheses, which lead to the telegrapher's-Poisson system that we propose:

(1) The ee and pp collisions are active for driving the distribution functions of electrons and phonons, respectively, towards the Maxwell–Boltzmann (by neglecting Pauli's exclusion principle) and Bose–Einstein distribution functions; [2]

(2) In the philosophy of the drift-diffusion approximation, we expand the distribution functions up to the first order with respect to the mean velocities [10];

(3) A cubic symmetry of the lattice is adopted;

(4) In Bloch's approximation [9], we consider finally electrons in a phonon background;

(5) Low-density and weak current are assumed for electrons.

Appendix

Consider the equations at order -1:

$$\left(\frac{\partial N_g}{\partial t}\right)^{NN}_{pp} = 0, \quad \left(\frac{\partial n_{\mathbf{p}}}{\partial t}\right)^{NN}_{ee} = 0.$$

By means of the usual methods of kinetic theory, it can be shown that these conditions are equivalent to:

$$N_g^N(1+N_{g_1}^N)(1+N_{g_2}^N) = (1+N_g^N)N_{g_1}^N N_{g_2}^N \ \ \forall \mathbf{k}, \mathbf{k}_1 \qquad (A1)$$

$$n_{\mathbf{p}'} n_{\mathbf{p}'_1} = n_{\mathbf{p}} n_{\mathbf{p}_1} \ \ \forall \mathbf{p}, \mathbf{p}_1. \qquad (A2)$$

Condition (A1) shows that $\ln(N_g^N/(1+N_g^N))$ is collisional invariant for phonons. In the case of N-processes:

$$\ln(N_g^N/(1+N_g^N)) = (\mathbf{V}_p \cdot \mathbf{k} - \omega_g)/T_p.$$

Condition (A2) shows that $\ln n_{\mathbf{p}}^N$ is collisional invariant for electrons. In the case of N-processes:

$$\ln n_{\mathbf{p}}^N = (\mathbf{V}_e \cdot \mathbf{k} - \mathcal{E}_{\mathbf{p}} + \mu)/T_e.$$

Moreover, the complete equilibrium condition requires also:

$$n_{\mathbf{p}}^N(1+N_g^N) = n_{\mathbf{p}'}^N N_g^N \ \ \forall \mathbf{p}, \mathbf{k}$$

which gives:

$$(\beta_e \mathbf{V}_e - \beta_p \mathbf{V}_p) \cdot \mathbf{k} + \omega_g(\beta_p - \beta_e) = 0$$

or:

$$-(\beta_e \mathbf{V}_e - \beta_p \mathbf{V}_p) \cdot \mathbf{k} + \omega_g(\beta_p - \beta_e) = 0,$$

since ω_g is even. From the last two equations, we get:

$$\mathbf{V}_e = \mathbf{V}_p, \ \ \beta_e = \beta_p.$$

Conflicts of Interest

The author declares no conflict of interest.

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