

Generalized balance equations for an electron–phonon system

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys. A: Math. Theor. 43 165002

(<http://iopscience.iop.org/1751-8121/43/16/165002>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.157

The article was downloaded on 03/06/2010 at 08:44

Please note that [terms and conditions apply](#).

Generalized balance equations for an electron–phonon system

A Rossani

Dipartimento di Matematica, Politecnico di Torino, Corso Duca degli Abruzzi 24, 10129 Torino, Italy

E-mail: alberto.rossani@polito.it

Received 27 October 2009, in final form 24 February 2010

Published 1 April 2010

Online at stacks.iop.org/JPhysA/43/165002

Abstract

A new model, based on an asymptotic procedure for solving the generalized kinetic equations of electrons and phonons, is proposed, which gives naturally the displaced Maxwellian at the leading order. The balance equations for the electron number, total energy density and total momentum for the whole system constitute now, together with Poisson equation, a system of four equations for the electron chemical potential, the temperature of the system, the drift velocity and the electric potential. In the drift–diffusion approximation the constitutive laws are derived and the Onsager relations recovered.

PACS numbers: 63.20.kd, 41.20.Cv

1. Introduction

In semiconductor modeling three approaches are widely applied, according to the physical situation we deal with. 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. As observed in [1], presently such an approach does not seem to be available.

On the other hand, as pointed out in [2], fractal or power law distribution functions are of interest in solid state physics. An example, given in [2], is the thermalization of a non-equilibrium electron–phonon system. Only recently [3a–3d] a generalized kinetic theory of electrons and phonons (GKTEP) has been proposed, which accounts for non-Gibbsian statistics.

In the present paper we start from the generalized Bloch–Boltzmann–Peierls 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 which 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 equations for the chemical potential of electrons, the temperature of the mixture and the drift velocity can be constructed, which recalls the extended thermodynamics model [1].

In the drift–diffusion approximation the constitutive equations can be written and the Onsager symmetry relations are recovered.

We stress that in the present model

- (1) the displaced Maxwellian approximation is not an ad hoc assumption but is justified by the expansion we apply;
- (2) the statistics of both electrons and phonons is left general, in order to account for non-standard cases;
- (3) phonons are treated as a participating species, which brings energy and momentum;
- (4) the correct phonon–phonon and electron–phonon interaction kernels are utilized: we avoid the use of relaxation time approximations.

The most qualifying point is (3). In fact the usual assumption that the phonon field can be treated as a fixed background is dropped here, since ‘any thermal gradient gives rise to transport of heat by the phonons, whilst an electric current, though carried by electrons, cannot fail to transfer some of its momentum to the lattice vibrations, and drag them along with it’ (Ziman). Finally we can say that the present model can be seen as a generalization of previous ones like [4a, 4b], by means of the treatment of phonons.

2. The GKTEP 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. the 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 $\mathcal{E}_{\mathbf{p}}$). By neglecting e – e interactions, the GKTEP equations read

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

where

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

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.

Introduce now the non-negative functions Ψ , ψ and Φ , φ which represent the arrival and departure state availability (models can be found in [3d]). Moreover, we set

$$\begin{aligned}\Phi_g &= \Phi(N_g(\mathbf{k})), & \Psi_g &= \Psi(N_g(\mathbf{k})), \\ \varphi_{\mathbf{p}} &= \varphi(n_{\mathbf{p}}), & \psi_{\mathbf{p}} &= \psi(n_{\mathbf{p}}).\end{aligned}$$

In the non-generalized case

$$\begin{aligned}\Psi(N_g) &= 1 + N_g, & \Phi(N_g) &= N_g, \\ \psi(n_{\mathbf{p}}) &= 1 - n_{\mathbf{p}}, & \varphi(n_{\mathbf{p}}) &= n_{\mathbf{p}}.\end{aligned}$$

On the right-hand side of the GKTEP equations for phonons [3a] we have

$$\begin{aligned}(\partial N_g / \partial t)_{pp} &= \int \left[(1/2) \sum_{g_1 g_2} w_{pp}(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k}) (-\Phi_g \Psi_{g_1} \Psi_{g_2} + \Psi_g \Phi_{g_1} \Phi_{g_2}) \right. \\ &\quad \left. + \sum_{g_1 g_3} w_{pp}(\mathbf{k}, \mathbf{k}_1 \rightarrow \mathbf{k}_3) (\Psi_g \Psi_{g_1} \Phi_{g_3} - \Phi_g \Phi_{g_1} \Psi_{g_3}) \right] \frac{d\mathbf{k}_1}{8\pi^3},\end{aligned}$$

where

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

(\mathbf{b} is an appropriate vector belonging to the reciprocal lattice), which account for three-phonon processes:

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

Moreover,

$$(\partial N_g / \partial t)_{pe} = 2 \int w_{pe}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k}) (\varphi_{\mathbf{p}} \psi_{\mathbf{p}'} \Psi_g - \psi_{\mathbf{p}} \varphi_{\mathbf{p}'} \Phi_g) \frac{d\mathbf{p}}{8\pi^3},$$

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

For electrons we have

$$\begin{aligned}(\partial n_{\mathbf{p}} / \partial t)_{ep} &= \sum_g \int w_{ep}(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p}) (\varphi_{\mathbf{p}'} \psi_{\mathbf{p}} \Phi_g - \psi_{\mathbf{p}'} \varphi_{\mathbf{p}} \Psi_g) \\ &\quad + w_{ep}(\mathbf{p}'' \rightarrow \mathbf{p}, \mathbf{k}) (\varphi_{\mathbf{p}''} \psi_{\mathbf{p}} \Psi_g - \varphi_{\mathbf{p}} \psi_{\mathbf{p}''} \Phi_g) \frac{d\mathbf{k}}{8\pi^3},\end{aligned}$$

where

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

The first term corresponds to processes with 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 are transition probabilities which account for energy conservation and satisfy the following symmetry relations:

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

We consider now a system, exact but not closed, of three balance equations, to be utilized later. By projecting the electron equation over 1 we have (electron conservation)

$$\frac{\partial n}{\partial t} - (1/e) \nabla \cdot \mathbf{J}_e = 0,$$

where the electron number density (n) and the electric current \mathbf{J}_e are given by

$$n = 2 \int n_{\mathbf{p}} \frac{d\mathbf{p}}{8\pi^3}, \quad \mathbf{J}_e = -2e \int \mathbf{v} n_{\mathbf{p}} \frac{d\mathbf{p}}{8\pi^3}. \quad (1)$$

By projecting the electron equation over $2\mathbf{p}$ and the phonon ones on \mathbf{k} , summation gives the following balance equation for momentum:

$$\frac{\partial \mathbf{P}}{\partial t} + \nabla \cdot \mathbb{F}_{\mathbf{P}} = -e\mathbf{E}n + 2 \int \left(\frac{\partial n_{\mathbf{p}}}{\partial t} \right)_{ep} \frac{\mathbf{p} d\mathbf{p}}{8\pi^3} + \sum_g \int \left[\left(\frac{\partial N_g}{\partial t} \right)_{pp} + \int \left(\frac{\partial N_g}{\partial t} \right)_{pe} \right] \frac{\mathbf{k} d\mathbf{k}}{8\pi^3}, \quad (2)$$

where

$$\begin{aligned} \mathbf{P} &= 2 \int n_{\mathbf{p}} \frac{\mathbf{p} d\mathbf{p}}{8\pi^3} + \sum_g \int N_g \frac{\mathbf{k} d\mathbf{k}}{8\pi^3} \\ \mathbb{F}_{\mathbf{P}} &= 2 \int n_{\mathbf{p}} \mathbf{v} \otimes \mathbf{p} \frac{d\mathbf{p}}{8\pi^3} + \sum_g \int N_g \mathbf{u}_g \otimes \mathbf{k} \frac{d\mathbf{k}}{8\pi^3}. \end{aligned}$$

Finally, by projecting the electron equation over $2\mathcal{E}_{\mathbf{p}}$ and the phonon ones over ω_g , summation gives the following balance equation for energy (energy conservation):

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{F}_W = \mathbf{J}_e \cdot \mathbf{E}, \quad (3)$$

where the energy density W and the energy flux \mathbf{F}_W are given by

$$W = 2 \int \mathcal{E}_{\mathbf{p}} n_{\mathbf{p}} \frac{d\mathbf{p}}{8\pi^3} + \sum_g \int \omega_g N_g \frac{d\mathbf{k}}{8\pi^3}$$

and

$$\mathbf{F}_W = 2 \int \mathbf{v} \mathcal{E}_{\mathbf{p}} n_{\mathbf{p}} \frac{d\mathbf{p}}{8\pi^3} + \sum_g \int \mathbf{u}_g \omega_g N_g \frac{d\mathbf{k}}{8\pi^3}.$$

3. Asymptotic expansion and balance equations

By following Akhiezer and Peletminski [6] (see also [7]) 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 (which conserve momentum). 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

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

The singular expansion for w_{ep} reads

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

so that we can write

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

By collecting all these terms we have

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

At the orders -1 and 0 , we get

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

respectively. Analogously for phonons

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

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

$$\ln(\Phi_g^N / \Psi_g^N) = (\mathbf{V} \cdot \mathbf{k} - \omega_g) / T, \quad \ln(\varphi_{\mathbf{p}}^N / \psi_{\mathbf{p}}^N) = (\mu + \mathbf{V} \cdot \mathbf{p} - \mathcal{E}_{\mathbf{p}}) / T,$$

where $T = T(\mathbf{x}, t)$ is the absolute temperature of the mixture, $\mu = \mu(\mathbf{x}, t)$ is the chemical potential of the electron gas and $\mathbf{V} = \mathbf{V}(\mathbf{x}, t)$ is the drift velocity of the mixture. Thus, at the leading order of this expansion, we find the drifted (generalized) Bose–Einstein (BE) and Fermi–Dirac (FD) distribution functions. Let us define the functions \mathcal{B} and \mathcal{F} as follows:

$$N_g^N = \mathcal{B}[\beta(\omega_g - \mathbf{V} \cdot \mathbf{k})], \quad n_{\mathbf{p}}^N = \mathcal{F}[\beta(\mathcal{E}_{\mathbf{p}} - \mu - \mathbf{V} \cdot \mathbf{p})],$$

where $\beta = 1/T$. In the non-generalized case we have

$$\mathcal{B}(\zeta) = 1/(e^{\zeta} - 1), \quad \mathcal{F}(\zeta) = 1/(e^{\zeta} + 1),$$

that is the BE and FD distribution functions are recovered. Usually [5] N_g^N and $n_{\mathbf{p}}^N$ are factored into two components, a symmetric component (0) which is even in momentum and an anti-symmetric component (1) which is odd:

$$\begin{aligned} N_g^N &= \mathcal{B}(\beta\omega_g) - \beta \mathbf{V} \cdot \mathbf{k} \mathcal{B}'(\beta\omega_g) = N_g^0 + N_g^1, \\ n_{\mathbf{p}}^N &= \mathcal{F}[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] - \beta \mathbf{V} \cdot \mathbf{p} \mathcal{F}'[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] = n_{\mathbf{p}}^0 + n_{\mathbf{p}}^1. \end{aligned}$$

This simplification is valid when the drift energy is small compared to the thermal energy [4].

Under this assumption, after some calculations we find

$$\begin{aligned} (\partial N_g / \partial t)_{pp}^{NU} &= \beta \mathbf{V} \cdot \left\{ \int \left[(1/2) \sum_{g_1 g_2} \Psi_g^0 \Phi_{g_1}^0 \Phi_{g_2}^0 w_{pp}^U(\mathbf{k}_1, \mathbf{k}_2 \rightarrow \mathbf{k})(\mathbf{k}_2 + \mathbf{k}_1 - \mathbf{k}) \right. \right. \\ &\quad \left. \left. + \sum_{g_1 g_3} \Psi_g^0 \Phi_{g_3}^0 \Phi_{g_1}^0 w_{pp}^U(\mathbf{k}, \mathbf{k}_1 \rightarrow \mathbf{k}_3)(-\mathbf{k}_3 + \mathbf{k}_1 + \mathbf{k}) \right] \frac{d\mathbf{k}_1}{8\pi^3} \right\}, \\ (\partial N_g / \partial t)_{pe}^{NU} &= \beta \mathbf{V} \cdot \left\{ 2 \int \psi_{\mathbf{p}'}^0 \varphi_{\mathbf{p}}^0 \Psi_{g_1}^0 w_{pe}^U(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k})(\mathbf{p} - \mathbf{k} - \mathbf{p}') \frac{d\mathbf{p}}{8\pi^3} \right\} \end{aligned}$$

and

$$\begin{aligned} (\partial n_{\mathbf{p}} / \partial t)_{ep}^{NU} &= \beta \mathbf{V} \cdot \left\{ \sum_g \int \psi_{\mathbf{p}}^0 \varphi_{\mathbf{p}'}^0 \Phi_g^0 w_{ep}^U(\mathbf{p}', \mathbf{k} \rightarrow \mathbf{p})(\mathbf{k} + \mathbf{p}' - \mathbf{p}) \right. \\ &\quad \left. + \psi_{\mathbf{p}}^0 \varphi_{\mathbf{p}'}^0 \Psi_g^0 w_{ep}^U(\mathbf{p}' \rightarrow \mathbf{p}, \mathbf{k})(\mathbf{p}' - \mathbf{k} - \mathbf{p}) \right] \frac{d\mathbf{k}}{8\pi^3} \right\}. \end{aligned}$$

Since $w_{rs}^U = w_{rs} - w_{rs}^N$, in the last three equations w_{rs}^U can be substituted by w_{rs} due to momentum conservation for N -processes.

The equations of order 0 are the starting point of our macroscopic model. By projecting the electron one over 1 the continuity equation for electrons reads

$$\frac{\partial}{\partial t} \int n_{\mathbf{p}}^0 + \nabla \cdot \int \mathbf{v} n_{\mathbf{p}}^1 \, d\mathbf{p} = 0. \quad (4)$$

By projecting the electron equation over $2\mathbf{p}$ and the phonon ones on \mathbf{k} , summation gives the following balance equation for momentum:

$$\begin{aligned} & \frac{\partial}{\partial t} \left(2 \int n_{\mathbf{p}}^1 \mathbf{p} \, d\mathbf{p} + \int N_g^1 \mathbf{k} \, d\mathbf{k} \right) \\ & + \nabla \cdot \left(2 \int n_{\mathbf{p}}^0 \mathbf{v} \otimes \mathbf{p} \, d\mathbf{p} + \sum_g \int N_g^0 \mathbf{u}_g \otimes \mathbf{k} \, d\mathbf{k} \right) \\ & = -2e\mathbf{E} \int n_{\mathbf{p}}^0 \, d\mathbf{p} + 2 \int \left(\frac{\partial n_{\mathbf{p}}}{\partial t} \right)_{ep}^{NU} \mathbf{p} \, d\mathbf{p} \\ & + \int \left[\sum_g \left(\frac{\partial N_g}{\partial t} \right)_{pp}^{NU} + \int \left(\frac{\partial N_g}{\partial t} \right)_{pe}^{NU} \right] \mathbf{k} \, d\mathbf{k}, \end{aligned} \quad (5)$$

where we took advantage of

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

due to momentum conservation for N -processes.

Finally, by projecting the electron equation over $2\mathcal{E}_{\mathbf{p}}$ and the phonon ones over ω_g , summation gives the following balance equation for energy:

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

Equations (4)–(6) constitute now a closed set of equations for the unknowns μ , β , \mathbf{V} which recall the extended thermodynamical one [1].

4. Revised drift–diffusion approximation

In the drift–diffusion approximation we assume that the total momentum of the mixture does not vary appreciably over the momentum relaxation time [5]. Then the momentum balance equation reads

$$-2\beta\mathbb{R}_2 \cdot \nabla T - 2e\mathbb{R}_1 \cdot \mathbf{E}^* - \beta\mathbb{R}_3 \cdot \nabla T = \mathbb{B} \cdot \mathbf{V}, \quad (7)$$

which gives \mathbf{V} , where $\mathbf{E}^* = \mathbf{E} + (1/e)\nabla\mu$ and

$$\begin{aligned} \mathbb{R}_1 &= \int \mathcal{F}'[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] \mathbf{p} \otimes \mathbf{v} \, d\mathbf{p} \\ \mathbb{R}_2 &= \int \mathcal{F}'[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] (\mathcal{E}_{\mathbf{p}} - \mu) \mathbf{p} \otimes \mathbf{v} \, d\mathbf{p} = \mathbb{M}_2 - \mu\mathbb{R}_1 \\ \mathbb{R}_3 &= \sum_g \int \mathcal{B}'(\beta\omega_g) \omega_g \mathbf{k} \otimes \mathbf{u}_g \, d\mathbf{k}. \end{aligned}$$

The tensor \mathbb{B} can be written in the following symmetric form:

$$\mathbb{B} = -\frac{1}{2} \sum_{g_1 g_2 g_3} \iint \Phi_{g_2}^0 \Phi_{g_3}^0 \Psi_{g_1}^0 w_{pp}(\mathbf{k}_2, \mathbf{k}_3 \rightarrow \mathbf{k}_1) (\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \otimes (\mathbf{k}_1 - \mathbf{k}_2 - \mathbf{k}_3) \frac{d\mathbf{k}_1 d\mathbf{k}_2}{8\pi^3} \\ - 2 \sum_g \iint \varphi_{\mathbf{p}}^0 \psi_{\mathbf{p}'}^0 \Psi_g^0 w_{ep}(\mathbf{p} \rightarrow \mathbf{p}', \mathbf{k}) (\mathbf{p} - \mathbf{k} - \mathbf{p}') \otimes (\mathbf{p} - \mathbf{k} - \mathbf{p}') \frac{d\mathbf{p} d\mathbf{k}}{8\pi^3}.$$

Since in the present approximation all the moments are calculated by means of drifted (generalized) FD or BE distribution functions, the electrical (\mathbf{J}_e) and thermal ($\mathbf{U}_e, \mathbf{U}_p$) currents are given by [8]

$$\mathbf{J}_e = -\frac{e}{4\pi^3} \int \mathbf{v} n_{\mathbf{p}} d\mathbf{p} = \frac{e\beta}{4\pi^3} \int \mathbf{v} \mathbf{V} \cdot \mathbf{p} \mathcal{F}'[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] d\mathbf{p} \\ \mathbf{U}_e = \frac{1}{4\pi^3} \int \mathbf{v} (\mathcal{E}_{\mathbf{p}} - \mu) n_{\mathbf{p}} d\mathbf{p} = -\frac{\beta}{4\pi^3} \int \mathbf{v} \mathbf{V} \cdot \mathbf{p} \mathcal{F}'[\beta(\mathcal{E}_{\mathbf{p}} - \mu)] (\mathcal{E}_{\mathbf{p}} - \mu) d\mathbf{p} \\ \mathbf{U}_p = \frac{1}{8\pi^3} \sum_g \int \omega_g \mathbf{u}_g N_g d\mathbf{k} = -\frac{\beta}{8\pi^3} \sum_g \int \omega_g \mathbf{u}_g \mathbf{V} \cdot \mathbf{k} \mathcal{B}'(\beta\omega_g) d\mathbf{k}.$$

By introducing \mathbf{V} from equation (7) we obtain

$$\mathbf{J}_e = -\frac{e\beta}{4\pi^3} [2e\mathbb{K}_{11} \cdot \mathbf{E}^* + \beta(2\mathbb{K}_{12} + \mathbb{K}_{13}) \cdot \nabla T] \\ \mathbf{U}_e = \frac{\beta}{4\pi^3} [2e\mathbb{K}_{21} \cdot \mathbf{E}^* + \beta(2\mathbb{K}_{22} + \mathbb{K}_{23}) \cdot \nabla T] \\ \mathbf{U}_p = \frac{\beta}{8\pi^3} [2e\mathbb{K}_{31} \cdot \mathbf{E}^* + \beta(2\mathbb{K}_{32} + \mathbb{K}_{33}) \cdot \nabla T],$$

where $\mathbb{K}_{lm} = \tilde{\mathbb{R}}_l \cdot \mathbb{B}^{-1} \cdot \mathbb{R}_m$ (\sim means transpose). The tensors \mathbb{K}_{h_2} and \mathbb{K}_{h_3} account for the presence of electrons and phonons, respectively. Since $\mathbb{B} = \tilde{\mathbb{B}}$ the following Onsager symmetry relation is in order:

$$\mathbb{K}_{lm} = \tilde{\mathbb{K}}_{ml}.$$

Consider now the electron number and energy balance equations (the momentum balance equation has been already accounted for). By means of their definitions we can write

$$\mathbf{J}_e = \mathbb{H}^{11}(\mu, T) \cdot \nabla(\mu/e - \mathcal{P}) + \mathbb{H}^{12}(\mu, T) \cdot \nabla T \\ \mathbf{F}_W = \mathbb{H}^{21}(\mu, T) \cdot \nabla(\mu/e - \mathcal{P}) + \mathbb{H}^{22}(\mu, T) \cdot \nabla T,$$

where

$$\mathbb{H}^{21} = \frac{\beta}{4\pi^3} (2\tilde{\mathbb{M}}_2 + \tilde{\mathbb{R}}_3) \cdot \mathbb{B}^{-1} \cdot \mathbb{R}_1, \quad \mathbb{H}^{22} = \frac{\beta^2}{8\pi^3} (2\tilde{\mathbb{M}}_2 + \tilde{\mathbb{R}}_3) \cdot \mathbb{B}^{-1} \cdot (2\mathbb{R}_2 + \mathbb{R}_3).$$

The balance equations now read

$$\frac{\partial n}{\partial \mu} \frac{\partial \mu}{\partial t} + \frac{\partial n}{\partial T} \frac{\partial T}{\partial t} - \frac{1}{e} \left[H_{ij}^{11} \frac{\partial^2}{\partial x_i \partial x_j} \left(\frac{\mu}{e} - \mathcal{P} \right) + H_{ij}^{12} \frac{\partial^2 T}{\partial x_i \partial x_j} \right. \\ \left. + \left(\frac{\partial H_{ij}^{11}}{\partial \mu} \frac{\partial \mu}{\partial x_i} + \frac{\partial H_{ij}^{11}}{\partial T} \frac{\partial T}{\partial x_i} \right) \frac{\partial}{\partial x_j} \left(\frac{\mu}{e} - \mathcal{P} \right) \right. \\ \left. + \left(\frac{\partial H_{ij}^{12}}{\partial \mu} \frac{\partial \mu}{\partial x_i} + \frac{\partial H_{ij}^{12}}{\partial T} \frac{\partial T}{\partial x_i} \right) \frac{\partial T}{\partial x_j} \right] = 0,$$

$$\begin{aligned}
& \frac{\partial W}{\partial \mu} \frac{\partial \mu}{\partial t} + \frac{\partial W}{\partial T} \frac{\partial T}{\partial t} + H_{ij}^{21} \frac{\partial^2}{\partial x_i \partial x_j} \left(\frac{\mu}{e} - \mathcal{P} \right) + H_{ij}^{22} \frac{\partial^2 T}{\partial x_i \partial x_j} \\
& + \left(\frac{\partial H_{ij}^{21}}{\partial \mu} \frac{\partial \mu}{\partial x_i} + \frac{\partial H_{ij}^{21}}{\partial T} \frac{\partial T}{\partial x_i} \right) \frac{\partial}{\partial x_j} \left(\frac{\mu}{e} - \mathcal{P} \right) + \left(\frac{\partial H_{ij}^{22}}{\partial \mu} \frac{\partial \mu}{\partial x_i} + \frac{\partial H_{ij}^{22}}{\partial T} \frac{\partial T}{\partial x_i} \right) \frac{\partial T}{\partial x_j} \\
& = - \frac{\partial \mathcal{P}}{\partial x_i} \left(H_{ij}^{11} \frac{\partial}{\partial x_j} (\mu/e - \mathcal{P}) + H_{ij}^{12} \frac{\partial T}{\partial x_j} \right),
\end{aligned}$$

which together with the Poisson equation

$$\nabla \cdot (\mathbb{D} \cdot \nabla \mathcal{P}) = -e(N_D - N_A - n)$$

(\mathbb{D} is the dielectric tensor, N_A and N_B are the number densities of acceptors and donors, respectively) constitute a system of three PDEs for the three unknowns μ , T , \mathcal{P} whose coefficients are expressed by means of integrals.

5. Conclusions

A new hydrodynamical model for the electron–phonon system has been proposed which is certainly related to the extended thermodynamical one [1]. However, the treatment resorts here strictly to kinetic theory so that the model is closed. This means that we do not need adjustment of some free parameters (namely the relaxation times) by means of comparisons with Monte Carlo calculations. A revised drift–diffusion approximation has been derived. An obvious improvement with respect to the classical drift–diffusion model is constituted by the introduction of an energy balance equation. The fulfilment of the symmetry Onsager relations is not trivial, since it cannot be taken for granted in many macroscopic models.

Observe that the asymptotic expansion we introduce is valid ($\epsilon \ll 1$) when the room temperature is much lower than the Debye temperature (in silicon, for example). A subject for future works is the extension to a system which includes holes, in order to allow a numerical treatment of silicon devices.

Appendix

Consider the equations at order -1 :

$$\begin{aligned}
& \left(\frac{\partial n_{\mathbf{p}}}{\partial t} \right)_{ep}^{NN} = 0 \\
& \left(\frac{\partial N_g}{\partial t} \right)_{pp}^{NN} + \left(\frac{\partial N_g}{\partial t} \right)_{pe}^{NN} = 0.
\end{aligned}$$

By following the same approach as in [3a] it can be shown that these conditions are equivalent to

$$\Phi_g^N \Phi_{g_1}^N \Phi_{g_2}^N = \Phi_g^N \Phi_{g_1}^N \Psi_{g_2}^N \quad \forall \mathbf{k}, \mathbf{k}_1 \quad (\text{A.1})$$

$$\varphi_{\mathbf{p}}^N \psi_{\mathbf{p}}^N \Psi_g^N = \varphi_{\mathbf{p}}^N \psi_{\mathbf{p}}^N \Phi_g^N \quad \forall \mathbf{p}, \mathbf{k}. \quad (\text{A.2})$$

Condition (A.1) shows that $\ln(\Phi_g^N / \Psi_g^N)$ is a collisional invariant for phonons. In the case of N -processes

$$\ln(\Phi_g^N / \Psi_g^N) = (\mathbf{V} \cdot \mathbf{k} - \omega_g) / T. \quad (\text{A.3})$$

By inserting (A.3) into (A.2) and taking into account that

$$\mathbf{p} = \mathbf{p}' + \mathbf{k}, \quad \mathcal{E}_{\mathbf{p}} = \mathcal{E}_{\mathbf{p}'} + \omega_{\mathbf{g}},$$

we find that $\ln(\varphi_{\mathbf{p}}^N/\psi_{\mathbf{p}}^N) + (\mathcal{E}_{\mathbf{p}} - \mathbf{V} \cdot \mathbf{p})/T$ is a collisional invariant for electrons:

$$\ln(\varphi_{\mathbf{p}}^N/\psi_{\mathbf{p}}^N) = (-\mathcal{E}_{\mathbf{p}} + \mathbf{V} \cdot \mathbf{p} + \mu)/T.$$

Observe that at equilibrium, if the phonon distribution function is drifted, then the electron distribution function is drifted with the same \mathbf{V} .

References

- [1] Anile A M and Pennisi S 1992 Thermodynamic derivation of the hydrodynamical model for charge transport in semiconductors *Phys. Rev. B* **46** 13186
- [2] Koponen I 1997 Thermalization of an electron–phonon system in a non-equilibrium state characterized by fractal distribution of phonon excitations *Phys. Rev. E* **55** 349
- [3a] Rossani A 2002 Generalized kinetic theory of electrons and phonons *Physica A* **305** 323
- [3b] Rossani A, Spiga G and Domaingo A 2003 Band-trap capture and emission in the generalized kinetic theory of electrons and holes *J. Phys. A* **36** 1195
- [3c] Rossani A and Spiga G 2006 Auger effect in the generalized kinetic theory of electrons and holes *J. Math. Phys.* **47** 013301
- [3d] Rossani A and Scarfone A M 2003 Generalized kinetic theory of electrons and phonons: models, equilibrium, stability *Physica B* **334** 292
- [4a] Ben Abdallah N, Degond P and Genyeis S 1996 An energy-transport model for semiconductors derived from the Boltzmann equation *J. Stat. Phys.* **84** 205
- [4b] Ben Abdallah N and Degond P 1996 On a hierarchy of macroscopic models for semiconductors *J. Math. Phys.* **37** 3306
- [5] Lundstrom M 2000 *Fundamentals of Carrier Transport* (Cambridge: Cambridge University Press)
- [6] Akhiezer A and Peletminski S 1980 *Les Methodes de la Physique Statistique* (Moscow: Mir)
- [7] Lifshitz E M and Pitaevskii L P 1981 *Physical Kinetics* (Oxford: Pergamon)
- [8] Ziman J M 1960 *Electrons and Phonons* (Oxford: Clarendon)