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Band-trap capture and emission in the generalized kinetic theory of electrons and holes

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Abstract

In this paper we propose a kinetic model which properly incorporates the band-trap capture and emission mechanism by including an evolution equation for the trapped electrons. Mathematical results on equilibrium and stability and their connections with thermodynamics are given. The recombination/generation rate is calculated and compared with the Shockley, Read and Hall model.

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1. Introduction

It is well known that, in bipolar devices, an interacting population of positively charged carriers (holes) must be taken into account, besides electrons and phonons. The hole–phonon interactions, similarly to electron–phonon, are emission/absorption phenomena. Another important effect to be accounted for, essential in driving the process, is generation/recombination of an electron–hole pair, which may occur in several ways.

There are different types of models in the physics of semiconductors [1] that describe the transport of conduction band (c.b.) electrons (distribution function n_e) and holes (distribution function n_h). The first one, i.e., the fluid model, relies on Shockley's equations [2]. It is based on the hypothesis that electrons and holes are drifted by the electric field and diffuse due to density gradients. Such a phenomenological approach, however, does not work in submicron devices. A more sophisticated approach, going deeper into the microscopic world, is provided by the kinetic model introduced by Poupaud [3], which relies on a system of nonlinear Boltzmann equations for electrons and holes and includes direct band–band recombination/generation processes.

It is well known, however, that other mechanisms may be much more effective in several meaningful physical situations [4]. For instance, if both the electron and hole densities are

large enough, the Auger recombination generation, which includes three-body interactions, cannot be neglected. On the other hand, if the electric field is high enough, impact ionization becomes significant. Moreover, when physical conditions are far from high density and high field regimes (and this is the scenario that is dealt with in this paper), the most important recombination–generation mechanism is the band-trap capture and emission. This effect is not included in the available models at a kinetic level [3]. In the literature one can find, to our knowledge, only the phenomenological derivation by Shockley and Read [5] and Hall [6] (SRH) of the recombination/generation rate at a macroscopic level. As is well known [4], such a derivation lacks a rigorous justification, although it is generally accepted. In our opinion, a full kinetic approach would be needed in order to investigate the whole process rigorously and to possibly justify, in some continuum limit, the usually adopted SRH model.

In the present work we propose a new kinetic model which properly incorporates the band-trap capture and emission mechanism by including an evolution equation for the trapped electrons (distribution function n_t). In particular we introduce the Boltzmann-like equations for such a kinetic model, including the possibility that also phonons (distribution function n_p) are not in local thermodynamical equilibrium, and behave then as a participating species. The analysis is performed in the spirit of the mathematical methods of kinetic theory [7], extended in order to deal with interactions which do not necessarily preserve momentum and kinetic energy [8–10]. For generality, particles or quasi-particles are allowed to obey general statistics, in order to possibly include non-standard or non-extensive effects [11]. We shall follow the lines of a recent paper [12], in which a generalized kinetic theory of electrons and phonons was proposed, reproducing the standard Fermi–Dirac and Bose–Einstein statistics as a particular case. The same formalism will be adopted here, extended to holes and trapped electrons. Collision integrals are represented in terms of suitable transition probabilities, and the investigation is based on their structure and general properties only. In fact, in this general approach, we are mainly interested in establishing fundamental results by exploiting the form of collision terms and the conservation of the proper physical quantities, without introducing explicit expressions or models for the microscopic collision probabilities. However, for further analysis or specific applications, useful transition probabilities are listed in the specialized literature (see for instance [1], as well as [13–15]). Our type of investigation leads to the determination of collision invariants and collision equilibria, and to the proof of an H-theorem [7]. The hydrodynamic limit is also studied by a preliminary asymptotic procedure with respect to the proper Knudsen numbers.

After introducing notation, physical framework and governing equations in section 2, mathematical results on equilibrium and stability and their connections with thermodynamics are given in section 3 for four interacting populations (c.b. electrons, holes, phonons and trapped electrons). Analogous steps are performed in section 4 for the similar but different case of an open system made up of three interacting species in a phonon background in local thermodynamical equilibrium, which is the most typical scenario for practical applications. Finally, in section 5 we develop a singular perturbation approach (zero-order Hilbert or Chapman–Enskog expansion [16]) aimed at deriving a hydrodynamic limit for the macroscopic recombination/generation rate, to be compared with the phenomenological SRH model [4].

2. Kinetic equations

Consider four populations: c.b. electrons (quasi-momentum (q.m.) \mathbf{p} , energy $\epsilon_e(\mathbf{p})$), trapped electrons (q.m. \mathbf{p} , energy $\epsilon_t(\mathbf{p})$), holes (q.m. \mathbf{p} , energy $\epsilon_h(\mathbf{p})$), phonons (q.m. \mathbf{k} , energy $\epsilon_p(\mathbf{k})$).

The distribution functions are normalized in such a way that the concentrations and the energy densities of electrons, trapped electrons, holes are given by

$$N_\alpha(\mathbf{x}, t) = \frac{1}{8\pi^3} \int n_\alpha(\mathbf{p}, \mathbf{x}, t) 2 d\mathbf{p} \quad E_\alpha(\mathbf{x}, t) = \frac{1}{8\pi^3} \int n_\alpha(\mathbf{p}, \mathbf{x}, t) \epsilon_\alpha(\mathbf{p}) 2 d\mathbf{p} \quad (1)$$

($\alpha = e, h, t$), respectively (the factor 2 inside these integrals accounts for degeneracy), while the thermal energy density of the crystal is given by

$$E_p(\mathbf{x}, t) = \frac{1}{8\pi^3} \int n_p(\mathbf{k}, \mathbf{x}, t) \epsilon_p(\mathbf{k}) d\mathbf{k}. \quad (2)$$

The recombination process that we are going to include occurs in two steps:

- (1) a conduction band electron is trapped by emission of a phonon,
- (2) a trapped electron fills a hole by emission of a phonon.

The generation process occurs correspondingly in two steps:

- (3) a valence band electron is trapped by absorption of a phonon: a hole appears,
- (4) a trapped electron moves to the conduction band by absorption of a phonon.

Processes (1) and (4) are obviously linked together and imply the gain (loss) of a phonon-trapped electrons accompanied by the loss (gain) of a c.b. electron. An analogous statement holds for processes (2) and (3), where a hole-trapped electron on one side, and a phonon on the other are involved. All other more standard, interaction mechanisms will be taken into account. They include the following processes [4]:

- (i) phonon–phonon interaction, with the creation of a single phonon, and its inverse,
- (ii) absorption and emission of a phonon by a c.b. electron,
- (iii) absorption and emission of a phonon by a hole.

As usual, in the last case, the phonon is actually absorbed or emitted by a v.b. electron, whose appearance (disappearance) corresponds of course to the loss (gain) of a hole.

All processes are assumed to satisfy microreversibility and to fulfil the laws of transformation between pre- and post-collisional momenta and energies which are in order for each specific mechanism. In particular, energy conservation holds for all interactions. For the sake of generality, all types of particles are allowed to obey a given statistics, defined by a pair of suitable smooth functions ($\varphi_\alpha, \psi_\alpha$), $\alpha = p, e, h, t$, describing saturation or enhancement effects in the departure/arrival state, respectively [12]. Quantities such as $\varphi_\alpha[n_\alpha(\mathbf{p})]$ will be written as $\varphi_\alpha(\mathbf{p})$ for brevity. By following [12], we assume that $\varphi_\alpha/\psi_\alpha$ is monotonically increasing as a function of n_α . Since the effects of quite cumbersome collision integrals are going to be stressed in this paper, only the space homogeneous version of the kinetic equations will be considered throughout. Also, to simplify notation, dependence on t will not be explicitly shown hereafter, unless strictly necessary.

Taking into account all processes in which a specific species may be gained or lost, the kinetic equations read

$$\begin{aligned} \frac{\partial n_p}{\partial t} &= I_{ppp}^p[n_p](\mathbf{k}) + I_{pee}^p[n_p, n_e](\mathbf{k}) + I_{phh}^p[n_p, n_h](\mathbf{k}) \\ &\quad + I_{pte}^p[n_p, n_t, n_e](\mathbf{k}) + I_{htp}^p[n_h, n_t, n_p](\mathbf{k}) = I^p(\mathbf{k}) \\ \frac{\partial n_e}{\partial t} &= I_{pee}^e[n_p, n_e](\mathbf{p}) + I_{pte}^e[n_p, n_t, n_e](\mathbf{p}) = I^e(\mathbf{p}) \\ \frac{\partial n_h}{\partial t} &= I_{phh}^h[n_p, n_h](\mathbf{p}) + I_{htp}^h[n_h, n_t, n_p](\mathbf{p}) = I^h(\mathbf{p}) \\ \frac{\partial n_t}{\partial t} &= I_{pte}^t[n_p, n_t, n_e](\mathbf{p}) + I_{htp}^t[n_h, n_t, n_p](\mathbf{p}) = I^t(\mathbf{p}). \end{aligned} \quad (3)$$

Here $I_{\alpha\beta\gamma}^{\delta}$ denotes the net collision contribution to the balance of species δ due to all interactions which involve the triple (α, β, γ) . Such contributions in turn will be expressed in terms of the appropriate scattering kernels $\mathcal{K}_{\alpha\beta\gamma}$, in the form

$$\begin{aligned}
I_{\text{ppp}}^{\text{p}}(\mathbf{k}) &= \frac{1}{16\pi^3} \iint [\mathcal{K}_{\text{ppp}}(\mathbf{k}', \mathbf{k}''; \mathbf{k}) - \mathcal{K}_{\text{ppp}}(\mathbf{k}, \mathbf{k}'; \mathbf{k}'')] d\mathbf{k}' d\mathbf{k}'' \\
I_{\alpha}^{\text{p}}(\mathbf{k}) &= -\frac{1}{4\pi^3} \iint \mathcal{K}_{\alpha}^{\text{p}}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) d\mathbf{p} d\mathbf{p}' \quad \alpha = \text{pee, phh, pte} \\
I_{\text{htp}}^{\text{p}}(\mathbf{k}) &= \frac{1}{4\pi^3} \iint \mathcal{K}_{\text{htp}}(\mathbf{p}, \mathbf{p}'; \mathbf{k}) d\mathbf{p} d\mathbf{p}' \\
I_{\text{p}\alpha\alpha}^{\alpha}(\mathbf{p}) &= \frac{1}{8\pi^3} \iint [\mathcal{K}_{\text{p}\alpha\alpha}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) - \mathcal{K}_{\text{p}\alpha\alpha}(\mathbf{k}, \mathbf{p}; \mathbf{p}')] d\mathbf{k} d\mathbf{p}' \quad \alpha = \text{e, h} \\
I_{\text{pte}}^{\text{e}}(\mathbf{p}) &= \frac{1}{4\pi^3} \iint \mathcal{K}_{\text{pte}}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) d\mathbf{k} d\mathbf{p}' \\
I_{\text{htp}}^{\text{h}}(\mathbf{p}) &= -\frac{1}{8\pi^3} \iint \mathcal{K}_{\text{htp}}(\mathbf{p}, \mathbf{p}'; \mathbf{k}) d\mathbf{k} d\mathbf{p}' \\
I_{\text{pte}}^{\text{t}}(\mathbf{p}) &= -\frac{1}{8\pi^3} \iint \mathcal{K}_{\text{pte}}(\mathbf{k}, \mathbf{p}; \mathbf{p}') d\mathbf{k} d\mathbf{p}' \\
I_{\text{htp}}^{\text{t}}(\mathbf{p}) &= -\frac{1}{8\pi^3} \iint \mathcal{K}_{\text{htp}}(\mathbf{p}', \mathbf{p}; \mathbf{k}) d\mathbf{k} d\mathbf{p}'.
\end{aligned} \tag{4}$$

The scattering kernels are given by

$$\mathcal{K}_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3) = G_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3)[\varphi_{\alpha}(\mathbf{v}_1)\varphi_{\beta}(\mathbf{v}_2)\psi_{\gamma}(\mathbf{v}_3) - \psi_{\alpha}(\mathbf{v}_1)\psi_{\beta}(\mathbf{v}_2)\varphi_{\gamma}(\mathbf{v}_3)] \tag{5}$$

where $G_{\alpha\beta\gamma}$ are the basic transition probabilities. The probability for phonon–phonon interaction, G_{ppp} , satisfies the obvious indistinguishability requirement $G_{\text{ppp}}(\mathbf{k}', \mathbf{k}''; \mathbf{k}) = G_{\text{ppp}}(\mathbf{k}'', \mathbf{k}'; \mathbf{k})$. All transition probabilities are to be understood in the sense of distributions, since they have to account for energy and momentum balance. If \mathbf{b} is an appropriate vector in the reciprocal lattice [12], they can be written as follows:

$$G_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3) = \mathcal{G}_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3)\delta(\mathbf{v}_3 - \mathbf{v}_1 - \mathbf{v}_2 + \mathbf{b})\delta[\epsilon_{\gamma}(\mathbf{v}_3) - \epsilon_{\alpha}(\mathbf{v}_1) - \epsilon_{\beta}(\mathbf{v}_2)] \tag{6}$$

where δ denotes Dirac's delta measure, and \mathcal{G} are positive smooth functions.

As usual in kinetic theory, the weak form of the kinetic equations (3) is essential for any further development. So, take a string of four smooth test functions

$$(\Phi_{\text{p}}(\mathbf{k}), \Phi_{\text{e}}(\mathbf{p}), \Phi_{\text{h}}(\mathbf{p}), \Phi_{\text{t}}(\mathbf{p})) \tag{7}$$

and multiply each of them by the corresponding collision operator appearing in (3), namely $I^{\text{p}}(\mathbf{k})$, $I^{\text{e}}(\mathbf{p})$, $I^{\text{h}}(\mathbf{p})$, $I^{\text{t}}(\mathbf{p})$, respectively. Then integrate each pair with respect to the relevant kinetic variable and sum up them, after multiplication by two when appropriate because of degeneracy, to get the functional

$$W(\Phi_{\text{p}}, \Phi_{\text{e}}, \Phi_{\text{h}}, \Phi_{\text{t}}) = \int \Phi_{\text{p}}(\mathbf{k})I^{\text{p}}(\mathbf{k}) d\mathbf{k} + 2 \sum_{\alpha} \int \Phi_{\alpha}(\mathbf{p})I^{\alpha}(\mathbf{p}) d\mathbf{p} \quad \alpha = \text{e, h, t.} \tag{8}$$

By introducing the functions

$$\mathcal{L}_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3) = \mathcal{K}_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3)[\Phi_{\gamma}(\mathbf{v}_3) - \Phi_{\alpha}(\mathbf{v}_1) - \Phi_{\beta}(\mathbf{v}_2)] \tag{9}$$

and by inserting (4) into (8), it is possible to prove that the functional W can be written as

$$\begin{aligned}
 W(\Phi_p, \Phi_e, \Phi_h, \Phi_t) &= \frac{1}{16\pi^3} \iint \mathcal{L}_{\text{ppp}}(\mathbf{k}', \mathbf{k}''; \mathbf{k}) d\mathbf{k} d\mathbf{k}' d\mathbf{k}'' \\
 &+ \frac{1}{4\pi^3} \sum_{\alpha} \iint \mathcal{L}_{\alpha}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) d\mathbf{k} d\mathbf{p} d\mathbf{p}' + \frac{1}{4\pi^3} \iiint \mathcal{L}_{\text{htp}}(\mathbf{p}, \mathbf{p}'; \mathbf{k}) d\mathbf{p} d\mathbf{p}' d\mathbf{k}
 \end{aligned} \tag{10}$$

where $\alpha = \text{pee, phh, pte}$.

On physical grounds, W represents the net production by collisions of the molecular property defined by the string (7). It is clear that electric charge and energy are conserved in all interactions, and indeed it is easily seen by inspection that, irrespective of the distribution functions n_{α} , $W(0, -1, +1, -1) = 0$ and $W(\epsilon_p, \epsilon_e, \epsilon_h, \epsilon_t) = 0$ (the delta measures involved in (6) must be invoked for the latter, and the electron charge has been factored out for the former). The same does not occur for instance to the string (1, 1, 1, 1), representing particle number, which in fact is not conserved by collisions. Collision invariants in the spirit of kinetic theory [9] are defined as the strings Φ_{α} , $\alpha = p, e, h, t$, for which

$$\begin{aligned}
 \Phi_p(\mathbf{k}) &= \Phi_p(\mathbf{k}') + \Phi_p(\mathbf{k}'') & \forall \mathbf{k} &= \mathbf{k}' + \mathbf{k}'' - \mathbf{b}_1(\mathbf{k}', \mathbf{k}'', \mathbf{k}) & \epsilon_p(\mathbf{k}) &= \epsilon_p(\mathbf{k}') + \epsilon_p(\mathbf{k}'') \\
 \Phi_e(\mathbf{p}) &= \Phi_p(\mathbf{k}) + \Phi_e(\mathbf{p}') & \forall \mathbf{p} &= \mathbf{k} + \mathbf{p}' - \mathbf{b}_2(\mathbf{k}, \mathbf{p}', \mathbf{p}) & \epsilon_e(\mathbf{p}) &= \epsilon_p(\mathbf{k}) + \epsilon_e(\mathbf{p}') \\
 \Phi_h(\mathbf{p}) &= \Phi_p(\mathbf{k}) + \Phi_h(\mathbf{p}') & \forall \mathbf{p} &= \mathbf{k} + \mathbf{p}' - \mathbf{b}_3(\mathbf{k}, \mathbf{p}', \mathbf{p}) & \epsilon_h(\mathbf{p}) &= \epsilon_p(\mathbf{k}) + \epsilon_h(\mathbf{p}') \\
 \Phi_e(\mathbf{p}) &= \Phi_p(\mathbf{k}) + \Phi_t(\mathbf{p}') & \forall \mathbf{p} &= \mathbf{k} + \mathbf{p}' - \mathbf{b}_4(\mathbf{k}, \mathbf{p}', \mathbf{p}) & \epsilon_e(\mathbf{p}) &= \epsilon_p(\mathbf{k}) + \epsilon_t(\mathbf{p}') \\
 \Phi_p(\mathbf{k}) &= \Phi_h(\mathbf{p}) + \Phi_t(\mathbf{p}') & \forall \mathbf{k} &= \mathbf{p} + \mathbf{p}' - \mathbf{b}_5(\mathbf{p}, \mathbf{p}', \mathbf{k}) & \epsilon_p(\mathbf{k}) &= \epsilon_h(\mathbf{p}) + \epsilon_t(\mathbf{p}').
 \end{aligned} \tag{11}$$

Since energy is the only conserved quantity for phonons, $\Phi_p(\mathbf{k}) = \epsilon_p(\mathbf{k})$ is the unique solution to the first of conditions (11), apart from the trivial $\Phi_p(\mathbf{k}) = 0$ [12]. Then all other Φ defining collision invariants may be determined in cascade, under the usual continuity assumption. From $\Phi_p = \epsilon_p$ the same argument leads to $\Phi_e = \epsilon_e$, $\Phi_h = \epsilon_h$ and $\Phi_t = \epsilon_t$ (from both the fourth and fifth conditions). From $\Phi_p = 0$ there follow $\Phi_e = \text{constant} = c_2$, $\Phi_h = \text{constant} = c_3$, and simultaneously $\Phi_t = c_2$ and $\Phi_t = -c_3$, yielding the string (0, $-c$, c , $-c$), where multiplicative constants are not essential because of the linearity of conditions (11). This leads to the conclusion

Proposition 1. *Collisional invariants constitute a 2D linear space, generated by the strings of test functions*

$$(0, -1, 1, -1) \tag{12a}$$

and

$$(\epsilon_p(\mathbf{k}), \epsilon_e(\mathbf{p}), \epsilon_h(\mathbf{p}), \epsilon_t(\mathbf{p})). \tag{12b}$$

The first string represents the (dimensionless) electric charge and the second the energy.

3. Equilibrium and stability

The structure of (10) suggests that it is useful to introduce a new functional \mathcal{D}

$$\mathcal{D}(n_p, n_e, n_h, n_t) = W \left(\log \frac{\varphi_p}{\psi_p}, \log \frac{\varphi_e}{\psi_e}, \log \frac{\varphi_h}{\psi_h}, \log \frac{\varphi_t}{\psi_t} \right). \tag{13}$$

By using (5), (9) and (10), we see at once that \mathcal{D} is given by a sum of five integrals with integrands of type

$$\mathcal{G}_{\alpha\beta\gamma}(\mathbf{v}_1, \mathbf{v}_2; \mathbf{v}_3) [\varphi_{\alpha}(\mathbf{v}_1)\varphi_{\beta}(\mathbf{v}_2)\psi_{\gamma}(\mathbf{v}_3) - \psi_{\alpha}(\mathbf{v}_1)\psi_{\beta}(\mathbf{v}_2)\varphi_{\gamma}(\mathbf{v}_3)] \log \frac{\psi_{\alpha}(\mathbf{v}_1)\psi_{\beta}(\mathbf{v}_2)\varphi_{\gamma}(\mathbf{v}_3)}{\varphi_{\alpha}(\mathbf{v}_1)\varphi_{\beta}(\mathbf{v}_2)\psi_{\gamma}(\mathbf{v}_3)} \tag{14}$$

$\alpha\beta\gamma = \text{ppp, pee, phh, pte, htp}$. Here, \mathcal{G} , φ and ψ are positive functions. Since $(1-x)\log(x) \leq 0 \forall x \geq 0$, with equal sign only for $x = 1$, it follows that $\mathcal{D} \leq 0$. In addition, \mathcal{D} vanishes if and only if each of the kernels (14) vanishes, and this occurs, under the usual positivity and continuity assumptions, if the content of the relevant square bracket is identically zero. We have thus proved the pertinent version of the familiar Boltzmann inequality of kinetic theory, which may be stated as follows.

Proposition 2. $\mathcal{D} \leq 0$ for any admissible distribution function (n_p, n_e, n_h, n_t) . In particular, $\mathcal{D} = 0$ if and only if the string

$$\left(\log \frac{\varphi_p}{\psi_p}, \log \frac{\varphi_e}{\psi_e}, \log \frac{\varphi_h}{\psi_h}, \log \frac{\varphi_t}{\psi_t} \right) \tag{15}$$

is a collision invariant.

The immediate consequence of this is that equilibria for the initial value problem (3), defined as the distribution functions for which

$$\begin{aligned} I_{\text{ppp}}^p + I_{\text{pee}}^p + I_{\text{phh}}^p + I_{\text{pte}}^p + I_{\text{htp}}^p &= 0 \quad \forall \mathbf{k} \\ I_{\text{pee}}^e + I_{\text{pte}}^e &= 0 \quad \forall \mathbf{p} \\ I_{\text{phh}}^h + I_{\text{htp}}^h &= 0 \quad \forall \mathbf{p} \\ I_{\text{pte}}^t + I_{\text{htp}}^t &= 0 \quad \forall \mathbf{p} \end{aligned} \tag{16}$$

are identified as those distributions for which the string (15) is a collision invariant (detailed balance principle). It is sufficient in fact to note that (16) implies $\mathcal{D} = 0$, which implies that (15) is a collision invariant, which finally leads back, by direct substitution, to (16).

Now proposition 1 applies, namely equilibria are determined from the fact that (15) must be a linear combination of the two invariants (12). Consequently, they constitute a two-parameter family of distribution functions. Explicitly, the infinitely many solutions to equation (16) are provided by the equations

$$\begin{aligned} \frac{\varphi_p[n_p]}{\psi_p[n_p]} &= \exp[b\epsilon_p(\mathbf{k})] & \frac{\varphi_e[n_e]}{\psi_e[n_e]} &= \exp[-a + b\epsilon_e(\mathbf{p})] \\ \frac{\varphi_h[n_h]}{\psi_h[n_h]} &= \exp[a + b\epsilon_h(\mathbf{p})] & \frac{\varphi_t[n_t]}{\psi_t[n_t]} &= \exp[-a + b\epsilon_t(\mathbf{p})] \end{aligned} \tag{17}$$

with arbitrary admissible real numbers a and $b < 0$. The usual condition that all $\varphi_\alpha/\psi_\alpha$ are monotonic functions of their argument [12] ensures unique solvability of equations (17) with respect to their unknowns n_α . Equilibrium solutions will be labelled by a star hereafter.

Concerning stability of the above equilibria, it is possible to establish an H-theorem, again along the lines of kinetic theory. Introduce the functional

$$\begin{aligned} H[n_p, n_e, n_h, n_t] &= \sum_\alpha H_\alpha[n_\alpha] \\ H_\alpha[n_\alpha] &= \int \mathcal{H}_\alpha[n_\alpha(\mathbf{p})] d\mathbf{p} \quad \alpha = e, h, t & H_p[n_p] &= \int \mathcal{H}_p[n_p(\mathbf{k})] d\mathbf{k} \end{aligned} \tag{18}$$

with the integrands \mathcal{H}_α defined by

$$\frac{d\mathcal{H}_p(x)}{dx} = \log \frac{\varphi_p(x)}{\psi_p(x)} \quad \frac{d\mathcal{H}_\alpha(x)}{dx} = 2 \log \frac{\varphi_\alpha(x)}{\psi_\alpha(x)} \quad \alpha = e, h, t. \tag{19}$$

Note that in our assumptions all \mathcal{H}_α are then convex functions of their argument. We can then prove

Proposition 3. *H is a strict Lyapunov functional for the initial value problem (3), in the sense that H and \dot{H} are positive and negative definite, respectively, with respect to equilibrium.*

In fact, following a solution of (3), the time derivative of H is in turn a functional, and coincides exactly with \mathcal{D} . Therefore $\dot{H} \leq 0$, and $\dot{H} = 0$ only at equilibrium. Moreover, it is not difficult to show, by convexity arguments, that

$$\int \left[\mathcal{H}_p - \mathcal{H}_p^* - \left(\frac{\partial \mathcal{H}_p}{\partial n_p} \right)^* (n_p - n_p^*) \right] (\mathbf{k}) d\mathbf{k} + \sum_{\alpha} \int \left[\mathcal{H}_{\alpha} - \mathcal{H}_{\alpha}^* - \left(\frac{\partial \mathcal{H}_{\alpha}}{\partial n_{\alpha}} \right)^* (n_{\alpha} - n_{\alpha}^*) \right] (\mathbf{p}) d\mathbf{p} \geq 0 \quad \alpha = e, h, t \quad (20)$$

where the equal sign holds if, and only if, the distribution function $\{n_{\alpha}\}$ equals the equilibrium $\{n_{\alpha}^*\}$. On the other hand, using the expressions of $(\log \varphi_{\alpha}/\psi_{\alpha})^*$ and resorting to both conservation laws, one can deduce

$$\int \left(\frac{\partial \mathcal{H}_p}{\partial n_p} \right)^* (n_p - n_p^*) (\mathbf{k}) d\mathbf{k} + \sum_{\alpha} \int \left(\frac{\partial \mathcal{H}_{\alpha}}{\partial n_{\alpha}} \right)^* (n_{\alpha} - n_{\alpha}^*) (\mathbf{p}) d\mathbf{p} = 0. \quad (21)$$

Finally, combination of (20) and (21) yields

$$H - H^* = \int (\mathcal{H}_p - \mathcal{H}_p^*) (\mathbf{k}) d\mathbf{k} + \sum_{\alpha} \int (\mathcal{H}_{\alpha} - \mathcal{H}_{\alpha}^*) (\mathbf{p}) d\mathbf{p} \geq 0 \quad \forall \{n_{\alpha}\} \quad (22)$$

with equal sign if and only if $\{n_{\alpha}\}$ coincides with $\{n_{\alpha}^*\}$, which completes the proof.

Of course, these mathematical results can be interpreted on physical grounds in terms of the second law of thermodynamics. By introducing in fact that entropy density $S = \sum_{\alpha} S_{\alpha}$, with $S_{\alpha} = -H_{\alpha}/(8\pi)^3$, it is apparent that proposition 3 is nothing but the entropy inequality $\dot{S} \geq 0$. In addition, equations (18) and (19), equipped with the equilibrium conditions (17), allow us to express all S_{α} and S at equilibrium. Moreover, it is possible to compute their derivatives with respect to any thermodynamical variable y . It is not difficult to verify that

$$\begin{aligned} \left(\frac{\partial S_p}{\partial y} \right)^* &= -\frac{\partial}{\partial y} (bE_p) & \left(\frac{\partial S_e}{\partial y} \right)^* &= \frac{\partial}{\partial y} (aN_e - bE_e) \\ \left(\frac{\partial S_h}{\partial y} \right)^* &= -\frac{\partial}{\partial y} (aN_h + bE_h) & \left(\frac{\partial S_t}{\partial y} \right)^* &= \frac{\partial}{\partial y} (aN_t - bE_t) \end{aligned} \quad (23)$$

where N_{α} and E_{α} are given by (1) and (2). Recalling the thermodynamical definitions of absolute temperatures T_{α} and chemical potentials μ_{α} as

$$\frac{1}{T_{\alpha}} = \left(\frac{\partial S_{\alpha}}{\partial E_{\alpha}} \right)^*_{N_{\alpha}} \quad \alpha = p, e, h, t \quad \mu_{\alpha} = -T_{\alpha} \left(\frac{\partial S_{\alpha}}{\partial N_{\alpha}} \right)^*_{E_{\alpha}} \quad \alpha = e, h, t \quad (24)$$

we realize that equilibrium is characterized by a common temperature $T_{\alpha} = T = -1/b, \forall \alpha$, while chemical potentials are related by $\mu_e = -\mu_h = \mu_t = \mu = -aT$, so that the parameters a and b have a clear interpretation as global thermodynamical properties of the mixture. Note that we have included the Boltzmann constant into our variables T , so that temperatures are measured in energy units in the present setting. Equilibria may then be rewritten as

$$\begin{aligned} \left(\frac{\varphi_p}{\psi_p} \right)^* (\mathbf{k}) &= \exp \left[-\frac{\epsilon_p(\mathbf{k})}{T} \right] & \left(\frac{\varphi_e}{\psi_e} \right)^* (\mathbf{p}) &= \exp \left[\frac{\mu - \epsilon_e(\mathbf{p})}{T} \right] \\ \left(\frac{\varphi_h}{\psi_h} \right)^* (\mathbf{p}) &= \exp \left[-\frac{\mu + \epsilon_h(\mathbf{p})}{T} \right] & \left(\frac{\varphi_t}{\psi_t} \right)^* (\mathbf{p}) &= \exp \left[\frac{\mu - \epsilon_t(\mathbf{p})}{T} \right] \end{aligned} \quad (25)$$

in terms of the free parameters $T > 0$ and $\mu \in \mathbb{R}$.

4. Electrons and holes in a phonon background

Since relaxation due to phonon–phonon processes is much faster than for all other interactions, phonons can be treated as a host medium in thermodynamical equilibrium at a fixed temperature T in most of the applications. These assumptions amount to discarding the kinetic equation for phonons, and to replacing n_p by the equilibrium distribution n_p^* in the kinetic equations for c.b. electrons, holes and trapped electrons. All previous steps may be adapted to the new scenario in a spontaneous way. The kinetic equations read

$$\begin{aligned}\frac{\partial n_e}{\partial t} &= \hat{I}_{ee}^e[n_e](\mathbf{p}) + \hat{I}_{te}^e[n_t, n_e](\mathbf{p}) = \hat{I}^e \\ \frac{\partial n_h}{\partial t} &= \hat{I}_{hh}^h[n_h](\mathbf{p}) + \hat{I}_{th}^h[n_t, n_h](\mathbf{p}) = \hat{I}^h \\ \frac{\partial n_t}{\partial t} &= \hat{I}_{et}^t[n_e, n_t](\mathbf{p}) + \hat{I}_{ht}^t[n_h, n_t](\mathbf{p}) = \hat{I}^t\end{aligned}\quad (26)$$

with

$$\begin{aligned}\hat{I}_{\alpha\alpha}^\alpha &= \frac{1}{4\pi^3} \int \hat{\mathcal{K}}_{\alpha\alpha}(\mathbf{p}', \mathbf{p}) d\mathbf{p}' & \alpha = e, h \\ \hat{I}_{\alpha\beta}^\beta &= \frac{1}{8\pi^3} \int \hat{\mathcal{K}}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) d\mathbf{p}' & \alpha\beta = et, te, ht, th.\end{aligned}\quad (27)$$

The scattering kernels are given by

$$\begin{aligned}\hat{\mathcal{K}}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) &= \hat{G}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) \left\{ \varphi_\alpha(\mathbf{p}') \psi_\beta(\mathbf{p}) - \exp\left[\frac{\epsilon_\beta(\mathbf{p}) - \epsilon_\alpha(\mathbf{p}')}{T}\right] \psi_\alpha(\mathbf{p}') \varphi_\beta(\mathbf{p}) \right\} \\ &\alpha\beta = ee, hh, et, te \\ \hat{\mathcal{K}}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) &= \hat{G}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) \left\{ \psi_\alpha(\mathbf{p}') \psi_\beta(\mathbf{p}) - \exp\left[\frac{\epsilon_\beta(\mathbf{p}) + \epsilon_\alpha(\mathbf{p}')}{T}\right] \varphi_\alpha(\mathbf{p}') \varphi_\beta(\mathbf{p}) \right\} \\ &\alpha\beta = ht, th\end{aligned}\quad (28)$$

with

$$\begin{aligned}\hat{G}_{\alpha\alpha}(\mathbf{p}', \mathbf{p}) &= \frac{1}{2} \int \left[G_{p\alpha\alpha}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) \varphi_p^*(\mathbf{k}) + G_{p\alpha\alpha}(\mathbf{k}, \mathbf{p}; \mathbf{p}') \psi_p^*(\mathbf{k}) \right] d\mathbf{k} & \alpha = e, h \\ \hat{G}_{te}(\mathbf{p}', \mathbf{p}) &= \int G_{pte}(\mathbf{k}, \mathbf{p}'; \mathbf{p}) \varphi_p^*(\mathbf{k}) d\mathbf{k} \\ \hat{G}_{et}(\mathbf{p}', \mathbf{p}) &= \int G_{pte}(\mathbf{k}, \mathbf{p}; \mathbf{p}') \psi_p^*(\mathbf{k}) d\mathbf{k} = \exp\left[-\frac{\epsilon_t(\mathbf{p}) - \epsilon_e(\mathbf{p}')}{T}\right] \hat{G}_{te}(\mathbf{p}, \mathbf{p}') \\ \hat{G}_{ht}(\mathbf{p}', \mathbf{p}) &= \int G_{htp}(\mathbf{p}', \mathbf{p}; \mathbf{k}) \varphi_p^*(\mathbf{k}) d\mathbf{k} = \hat{G}_{th}(\mathbf{p}, \mathbf{p}').\end{aligned}\quad (29)$$

The analogue of the functional W is

$$\hat{W}[\Phi_e, \Phi_h, \Phi_t] = 2 \sum_\alpha \int \Phi_\alpha(\mathbf{p}) \hat{I}^\alpha(\mathbf{p}) d\mathbf{p} \quad \alpha = e, h, t. \quad (30)$$

Again, by introducing the functions

$$\begin{aligned}\hat{\mathcal{L}}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) &= \hat{\mathcal{K}}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) [\Phi_\beta(\mathbf{p}) - \Phi_\alpha(\mathbf{p}')] & \alpha\beta = ee, hh, te \\ \hat{\mathcal{L}}_{th}(\mathbf{p}', \mathbf{p}) &= \hat{\mathcal{K}}_{th}(\mathbf{p}', \mathbf{p}) [\Phi_h(\mathbf{p}) + \Phi_t(\mathbf{p}')] \end{aligned}\quad (31)$$

it is possible to write \hat{W} as the sum

$$\hat{W}[\Phi_e, \Phi_h, \Phi_t] = \frac{1}{4\pi^3} \sum_\alpha \iint \hat{\mathcal{L}}_\alpha(\mathbf{p}', \mathbf{p}) d\mathbf{p} d\mathbf{p}' \quad \alpha = ee, hh, te, th. \quad (32)$$

The usual definition of collision invariant yields a unique linearly independent invariant, namely the string $(-1, 1, -1)$, representing (dimensionless) electric charge. Of course, energy is no longer an invariant, since it is exchanged with the background lattice by collisions. Furthermore, the quantity (see also [17])

$$\hat{D}[n_e, n_h, n_t] = \hat{W} \left[\log \left(\frac{\varphi_e}{\psi_e} e^{\epsilon_e/T} \right), \log \left(\frac{\varphi_h}{\psi_h} e^{\epsilon_h/T} \right), \log \left(\frac{\varphi_t}{\psi_t} e^{\epsilon_t/T} \right) \right]$$

is given by a sum of four integrals with integrands of types

$$\begin{aligned} \hat{G}_{\alpha\beta}(\mathbf{p}', \mathbf{p}) & \left\{ \varphi_\alpha(\mathbf{p}')\psi_\beta(\mathbf{p}) - \exp \left[\frac{\epsilon_\beta(\mathbf{p}) - \epsilon_\alpha(\mathbf{p}')}{T} \right] \psi_\alpha(\mathbf{p}')\varphi_\beta(\mathbf{p}) \right\} \\ & \times \log \left\{ \frac{\varphi_\alpha(\mathbf{p}')\psi_\beta(\mathbf{p})}{\psi_\alpha(\mathbf{p}')\varphi_\beta(\mathbf{p})} \exp \left[-\frac{\epsilon_\beta(\mathbf{p}) - \epsilon_\alpha(\mathbf{p}')}{T} \right] \right\} \\ \hat{G}_{th}(\mathbf{p}', \mathbf{p}) & \left\{ \psi_t(\mathbf{p}')\psi_h(\mathbf{p}) - \exp \left[\frac{\epsilon_h(\mathbf{p}) + \epsilon_t(\mathbf{p}')}{T} \right] \varphi_t(\mathbf{p}')\varphi_h(\mathbf{p}) \right\} \\ & \times \log \left\{ \frac{\psi_t(\mathbf{p}')\psi_h(\mathbf{p})}{\varphi_t(\mathbf{p}')\varphi_h(\mathbf{p})} \exp \left[-\frac{\epsilon_h(\mathbf{p}) + \epsilon_t(\mathbf{p}')}{T} \right] \right\} \end{aligned} \tag{33}$$

$\alpha\beta = ee, hh, te$. Therefore, by the same arguments leading to proposition 2, we may conclude that $\hat{D} \leq 0$ for any admissible distribution function (n_e, n_h, n_t) , and that $\hat{D} = 0$ if and only if the string

$$\log \left[\frac{\varphi_\alpha(\mathbf{p})}{\psi_\alpha(\mathbf{p})} \exp^{\epsilon_\alpha(\mathbf{p})/T} \right] \quad \alpha = e, h, t \tag{34}$$

is a collision invariant. Since this last requirement implies $\hat{I}^e = \hat{I}^h = \hat{I}^t = 0 \forall \mathbf{p}$, which in turn implies $\hat{D} = 0$, the detailed balance principle is again established, and consequently we have (in obvious agreement with equation (25)).

Proposition 4. *The equilibrium condition*

$$\hat{I}^e = \hat{I}^h = \hat{I}^t = 0 \quad \forall \mathbf{p} \tag{35}$$

admits exactly a one-parameter family of solutions, namely

$$\begin{aligned} \left(\frac{\varphi_e}{\psi_e} \right)^* (\mathbf{p}) & = \exp \left[\frac{\mu - \epsilon_e(\mathbf{p})}{T} \right] & \left(\frac{\varphi_h}{\psi_h} \right)^* (\mathbf{p}) & = \exp \left[-\frac{\mu + \epsilon_h(\mathbf{p})}{T} \right] \\ \left(\frac{\varphi_t}{\psi_t} \right)^* (\mathbf{p}) & = \exp \left[\frac{\mu - \epsilon_t(\mathbf{p})}{T} \right] \end{aligned} \tag{36}$$

with $\mu \in \mathbb{R}$, where T is the background temperature.

It is also possible to prove an H theorem for the study of stability by introducing the functional

$$\hat{H}[n_e, n_h, n_t] = \sum_\alpha H_\alpha[n_\alpha] + \frac{2}{T} \sum_\alpha \int \epsilon_\alpha(\mathbf{p})n_\alpha(\mathbf{p}) d\mathbf{p} \tag{37}$$

where α takes the values e, h, t, and H_α is defined by (18) and (19). We have

Proposition 5. \hat{H} is a strict Lyapunov functional for the initial value problem (26).

For a sketch of the proof (which closely resembles that of proposition 3), it is first easily verified that $\dot{\hat{H}} = \hat{D}$, which ensures the proper definiteness in sign for $\dot{\hat{H}}$ itself. Then, for

any distribution function different from equilibrium, equation (20) holds by convexity, even without the integral with respect to \mathbf{k} . Now charge conservation during the evolution reads

$$\sum_{\alpha} \int \left[\left(\frac{\partial \mathcal{H}_{\alpha}}{\partial n_{\alpha}} \right)^* + \frac{2}{T} \epsilon_{\alpha} \right] (n_{\alpha} - n_{\alpha}^*) d\mathbf{p} = 0 \quad (38)$$

and therefore it is easy to check that, for $\{n_{\alpha}\} \neq \{n_{\alpha}^*\}$,

$$\hat{H} - \hat{H}^* = \sum_{\alpha} \int \left[\mathcal{H}_{\alpha} - \mathcal{H}_{\alpha}^* + \frac{2}{T} \epsilon_{\alpha} (n_{\alpha} - n_{\alpha}^*) \right] (\mathbf{p}) d\mathbf{p} > 0 \quad (39)$$

which completes the proof.

Again, previous results have a clear physical interpretation. Bearing the definition of the single entropies S_{α} and of the total entropy $S = \sum_{\alpha} S_{\alpha}$ in mind, one can define temperature and chemical potential for each species, and realize that equilibrium is characterized by $T_e = T_h = T_t = T$ and by $\mu_e = -\mu_h = \mu_t = \mu$, where T is the phonon temperature and μ a free parameter. Moreover, setting

$$E = E_e + E_h + E_t \quad (40)$$

for the total energy, it is easily realized that the irreversibility condition $\dot{\hat{H}} \leq 0$ for the open system of the three-species mixture in the lattice is nothing but the well-known Clausius inequality $\dot{S} \geq \dot{E}/T$.

5. Recombination/generation rate

As usual in kinetic theory it is convenient to introduce an appropriate scaling in equation (26). Then, macroscopic equations at a hydrodynamic level can be derived by an asymptotic procedure. The scaling is performed according to the typical values of the various characteristic times, which are the macroscopic time and the relaxation times of the four interaction mechanisms taken into account, namely those involving the pairs ee, hh, te, th. The ratio of a microscopic mean free path to a typical macroscopic length is usually referred to as a Knudsen number [9], and it coincides with the ratio between the corresponding time scales, when, as typical in kinetic theory, macroscopic and microscopic speeds are assumed to be of the same order of magnitude [7]. All relaxation times are typically very short on the macroscopic scale, and, in the physical applications we are interested in, the generation/recombination processes, te and th, which involve trapped electrons, are much slower than the usual electron-phonon interactions affecting only electrons within the separate conduction and valence bands (ee and hh) [4]. Therefore, the Knudsen numbers relevant to ee and hh processes are much smaller than the other two. These facts define the level of importance of the various collision terms in (26) and their influence on the overall time evolution. It is then always possible, upon a suitable scaling of the kinetic equations, to introduce a smallness parameter ε in such a way that the initial value problem takes the singular perturbation form

$$\begin{aligned} \frac{\partial n_e}{\partial t} &= \frac{1}{\varepsilon^2} \hat{I}_{ee}^e[n_e] + \frac{1}{\varepsilon} \hat{I}_{te}^e[n_t, n_e] \\ \frac{\partial n_h}{\partial t} &= \frac{1}{\varepsilon^2} \hat{I}_{hh}^h[n_h] + \frac{1}{\varepsilon} \hat{I}_{th}^h[n_h, n_t] \\ \frac{\partial n_t}{\partial t} &= \frac{1}{\varepsilon} \hat{I}_{et}^t[n_e, n_t] + \frac{1}{\varepsilon} \hat{I}_{ht}^t[n_h, n_t]. \end{aligned} \quad (41)$$

We shall perform a preliminary asymptotic analysis, to leading order only, valid of course only in the bulk region after the initial layer. All distributions should then be expanded in asymptotic series

$$n_\alpha = \sum_{j=0}^{\infty} \varepsilon^j n_\alpha^{(j)} \tag{42}$$

and equal powers of ε should be equated in each equation. For that purpose, explicit knowledge of the functions φ_α and ψ_α is needed. We shall then take

$$\varphi_\alpha(n_\alpha) = n_\alpha \quad \psi_\alpha(n_\alpha) = 1 - n_\alpha \quad \alpha = e, h, t \tag{43a}$$

while in the integrals defining the kernels, one should use

$$\varphi_p(n_p) = n_p \quad \psi_p(n_p) = 1 + n_p. \tag{43b}$$

Equilibria n_α^* ($\alpha = e, h, t$) are then defined by (36), with given T . Of course, this is in agreement with (25), which also includes n_p^* . The relevant equations can now be solved explicitly. The well-known Fermi–Dirac and Bose–Einstein distributions, for gas particles and phonons, respectively, are recovered.

The first step in the asymptotic algorithm, however, relevant to the $O(\varepsilon^{-2})$ terms, is independent of the chosen statistics, and reads

$$\hat{I}_{ee}^e[n_e^{(0)}](\mathbf{p}) = 0 \quad \hat{I}_{hh}^h[n_h^{(0)}](\mathbf{p}) = 0 \tag{44}$$

namely two nonlinear integral equations for $n_e^{(0)}$ and $n_h^{(0)}$. It is remarkable that these equations can be solved explicitly, which at least allows initialization of the procedure. We have in fact

$$\begin{aligned} \int \log \left(\frac{\varphi_e}{\psi_e} e^{\epsilon_e/T} \right) \hat{I}_{ee}^e[n_e] d\mathbf{p} &= \frac{1}{8\pi^3} \iint \hat{G}_{ee}(\mathbf{p}', \mathbf{p}) \left\{ \varphi_e(\mathbf{p}') \psi_e(\mathbf{p}) \right. \\ &\quad \left. - \exp \left[\frac{\epsilon_e(\mathbf{p}) - \epsilon_e(\mathbf{p}')}{T} \right] \psi_e(\mathbf{p}') \varphi_e(\mathbf{p}) \right\} \log \left\{ \frac{\varphi_e(\mathbf{p}) \psi_e(\mathbf{p}')}{\psi_e(\mathbf{p}) \varphi_e(\mathbf{p}')} \right. \\ &\quad \left. \times \exp \left[\frac{\epsilon_e(\mathbf{p}) - \epsilon_e(\mathbf{p}')}{T} \right] \right\} d\mathbf{p} d\mathbf{p}' \leq 0 \end{aligned} \tag{45}$$

with an equal sign only if the curly bracket vanishes identically. This establishes a sort of Boltzmann inequality for the collision operator \hat{I}_{ee}^e alone, which from a physical point of view corresponds to considering the c.b. electrons in the phonon background separated from the rest of the system, coherently with this approximation order. From this inequality it is possible to show, by usual argument, that the first of (44) is equivalent to

$$\frac{\varphi_e(\mathbf{p})}{\psi_e(\mathbf{p})} e^{\epsilon_e(\mathbf{p})/T} = \frac{\varphi_e(\mathbf{p}')}{\psi_e(\mathbf{p}')} e^{\epsilon_e(\mathbf{p}')/T} \quad \forall \mathbf{p}, \mathbf{p}'. \tag{46}$$

The function singled out in this way must then be a constant with respect to \mathbf{p} , that we may label as $e^{\mu_e/T}$, and this determines the solution, up to an arbitrary time dependent parameter μ_e . Repeating the same reasoning for the second of (44) and for the relevant operator \hat{I}_{hh}^h , we end up with the explicit expressions for $n_e^{(0)}$ and $n_h^{(0)}$,

$$\frac{\varphi_e[n_e^{(0)}]}{\psi_e[n_e^{(0)}]}(\mathbf{p}) = \exp \left[\frac{\mu_e - \epsilon_e(\mathbf{p})}{T} \right] \quad \frac{\varphi_h[n_h^{(0)}]}{\psi_h[n_h^{(0)}]}(\mathbf{p}) = \exp \left[\frac{\mu_h - \epsilon_h(\mathbf{p})}{T} \right]. \tag{47}$$

For the statistics given in (43a) they result in non-stationary Fermi–Dirac distributions. In fact, chemical potentials are in general time-dependent and different for electrons and holes.

Passing to the $O(\varepsilon^{-1})$ terms, all three equations (41) get involved, which implies that electrons and phonons get coupled, and new unknowns $n_e^{(1)}, n_h^{(1)}, n_t^{(0)}$ come in. The third equation is still independent of the statistics used, and reads

$$\hat{I}_{\text{et}}^t[n_e^{(0)}, n_t^{(0)}] + \hat{I}_{\text{ht}}^t[n_h^{(0)}, n_t^{(0)}](\mathbf{p}) = 0. \quad (48)$$

It is seen by inspection from (27) that the unknown $n_t^{(0)}$ is always evaluated at \mathbf{p} . Therefore, the integral equation (48) collapses to an algebraic equation and can be solved explicitly. More precisely

$$\frac{\varphi_t[n_t^{(0)}]}{\psi_t[n_t^{(0)}]}(\mathbf{p}) = \exp\left[-\frac{\epsilon_t(\mathbf{p})}{T}\right] \frac{A_{\text{ht}}(\mathbf{p}) + e^{\mu_e/T} A_{\text{et}}(\mathbf{p})}{A_{\text{et}}(\mathbf{p}) + e^{\mu_h/T} A_{\text{ht}}(\mathbf{p})} \quad (49)$$

where

$$\begin{aligned} A_{\text{et}}(\mathbf{p}) &= \int \hat{G}_{\text{et}}(\mathbf{p}', \mathbf{p}) \psi_e[n_e^{(0)}](\mathbf{p}') \exp\left[-\frac{\epsilon_e(\mathbf{p}')}{T}\right] d\mathbf{p}' \\ &= \exp\left[-\frac{\epsilon_t(\mathbf{p})}{T}\right] \int \hat{G}_{\text{te}}(\mathbf{p}, \mathbf{p}') \psi_e[n_e^{(0)}](\mathbf{p}') d\mathbf{p}' \\ A_{\text{ht}}(\mathbf{p}) &= \int \hat{G}_{\text{ht}}(\mathbf{p}', \mathbf{p}) \psi_h[n_h^{(0)}](\mathbf{p}') d\mathbf{p}' = \int \hat{G}_{\text{th}}(\mathbf{p}, \mathbf{p}') \psi_h[n_h^{(0)}](\mathbf{p}') d\mathbf{p}'. \end{aligned} \quad (50)$$

The resulting zeroth-order distribution functions only depend on two free parameters, μ_e and μ_h . Note that the trapped distribution function does not have the time-dependent Fermi–Dirac structure of the other two species. However the ratio on the right-hand side of (49) always belongs to a kind of time-dependent Fermi–Dirac strip ($e^{\mu_{\min}/T}, e^{\mu_{\max}/T}$), with $\mu_{\min} = \min(\mu_e, -\mu_h)$ and $\mu_{\max} = \max(\mu_e, -\mu_h)$. In particular, at equilibrium we have $\mu_e = -\mu_h = \mu$, so that we recover, also for trapped electrons, a stationary Fermi–Dirac distribution with chemical potential μ .

By introducing now the low-density approximation $\psi_e = \psi_h \simeq 1$, we have explicitly

$$n_\alpha^0(\mathbf{p}) = c_\alpha(T) N_\alpha \exp\left[-\frac{\epsilon_\alpha(\mathbf{p})}{T}\right] \quad \alpha = e, h \quad (51)$$

where

$$c_\alpha(T) = \left\{ \frac{1}{8\pi^3} \int \exp\left[-\frac{\epsilon_\alpha(\mathbf{p})}{T}\right] 2 d\mathbf{p} \right\}^{-1}. \quad (52)$$

Macroscopic equations are obtained from (26) by integration with respect to \mathbf{p} . These equations for the particle densities N_α are exact, but not closed, due to the presence of the distribution functions in the collision integrals on the right-hand side. In particular, they include as first integral the particle conservation law $N_e - N_h + N_t = \text{constant}$. The sought zero-order asymptotic closure is achieved by substituting the leading order approximations $n_\alpha^{(0)}$ for n_α in those integrals. This leads to the dynamical system for N_e and N_h

$$\dot{N}_e = \frac{1}{32\pi^6} \int A_{\text{et}}(\mathbf{p}) \exp\left[\frac{\epsilon_t(\mathbf{p})}{T}\right] n_t^0(\mathbf{p}) \left[1 - \frac{A_{\text{et}}(\mathbf{p}) + c_h(T) N_h A_{\text{ht}}(\mathbf{p})}{A_{\text{ht}}(\mathbf{p}) + c_e(T) N_e A_{\text{et}}(\mathbf{p})} c_e(T) N_e \right] d\mathbf{p} \quad (53)$$

$$\dot{N}_h = \frac{1}{32\pi^6} \int A_{\text{ht}}(\mathbf{p}) \exp\left[\frac{\epsilon_t(\mathbf{p})}{T}\right] n_t^0(\mathbf{p}) \left[\frac{A_{\text{et}}(\mathbf{p}) + c_h(T) N_h A_{\text{ht}}(\mathbf{p})}{A_{\text{ht}}(\mathbf{p}) + c_e(T) N_e A_{\text{et}}(\mathbf{p})} - c_h(T) N_h \right] d\mathbf{p} \quad (54)$$

with

$$n_t^0(\mathbf{p}) = \left\{ 1 + \frac{A_{\text{et}}(\mathbf{p}) + c_h(T) N_h A_{\text{ht}}(\mathbf{p})}{A_{\text{ht}}(\mathbf{p}) + c_e(T) N_e A_{\text{et}}(\mathbf{p})} \exp\left[\frac{\epsilon_t(\mathbf{p})}{T}\right] \right\}^{-1}. \quad (55)$$

From (53) and (54), by introducing (55), we finally get

$$\dot{N}_e = \dot{N}_h = \frac{1}{32\pi^6} \int \frac{A_{et}(\mathbf{p})A_{ht}(\mathbf{p})(1 - c_e c_h N_e N_h) \exp[\epsilon_t(\mathbf{p})/T]}{[A_{et}(\mathbf{p}) + c_h N_h A_{ht}(\mathbf{p})] \exp[\epsilon_t(\mathbf{p})/T] + A_{ht}(\mathbf{p}) + c_e N_e A_{et}(\mathbf{p})} d\mathbf{p}. \quad (56)$$

Now we have for the zeroth-order approximation $\dot{N}_e = \dot{N}_h$. This is in agreement with the conservation law and with the fact that $\dot{N}_t = 0$ at such a level of approximation, as predicted by (48). By the way, the latter is one of the basic assumptions in order to derive the SRH recombination/generation rate. Actually, equation (56) may be rewritten in standard notation [4] as $\dot{N}_e = \dot{N}_h = -R$, where

$$R = \frac{1}{32\pi^6} \int \frac{N_e N_h - N_e^\# N_h^\#}{\tau_h(N_e + N_e^\#) + \tau_e(N_h + N_h^\#)} d\mathbf{p} = R(N_e, N_h) \quad (57)$$

with

$$N_e^\# = \frac{A_{ht}}{c_e A_{et}} \quad N_h^\# = \frac{A_{et}}{c_h A_{ht}} \quad \tau_h = \frac{e^{-\epsilon_t/T}}{c_h A_{ht}} \quad \tau_e = \frac{1}{c_e A_{et}}. \quad (58)$$

Although, in general, without further assumptions on the transition probabilities \mathcal{G} , we are not able to ‘extract’ the explicit dependence of the recombination/generation rate on N_e and N_h , we remark that our consistent kinetic approach leads to an integrand which has the typical form of the phenomenological SRH model [4].

6. Conclusions

In this paper we have presented two improved kinetic models for the description of electron–phonon interaction in semiconductors. The generalization concerns inclusion of band-trap capture and emission, and is motivated by the fact that this is the most important recombination/generation mechanism in physical conditions which are interesting for applications. With respect to previous literature, we consider then explicitly an evolution equation for the population of trapped electrons, and their collision effects on the evolution of the other species. The interacting populations in the first model are conduction band electrons, trapped electrons, holes and phonons. In the second model the phonon population is supposed to constitute a fixed background in local thermodynamical equilibrium, which represents a very reasonable, and generally adopted, physical approximation. We have tried to keep our developments as general as possible by allowing each species to obey a general, even non-extensive, statistics. Typical methods from kinetic theory are applied in order to derive the basic mathematical properties of the relevant nonlinear integrodifferential Boltzmann-type equations, such as characterization of collision invariants, collision equilibria, stability and H-theorem. These results follow from the general properties of the underlying transition probabilities, without requiring their explicit detailed knowledge. We have also presented preliminary results on the asymptotic analysis with respect to an appropriate small parameter arising after a suitable scaling of the kinetic equations. Such an analysis should lead eventually to the determination of fluid-dynamic equations at a macroscopic level. Our first results allow us to derive, to leading order, a crucial quantity for application, namely the recombination/generation rate for electrons and holes. The form obtained here resembles, and, in some sense, generalizes, the well-known macroscopic SRH formula, which is generally accepted on phenomenological grounds, but still lacks a rigorous derivation based on kinetic theory.

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