A hydrodynamic model for silicon semiconductors including crystal heating

GIOVANNI MASCALI

Dipartimento di Matematica ed Informatica, Università della
Calabria and INFN-Gruppo c. Cosenza, 87036 Cosenza, Italy
email: g.mascali@unical.it

We present a macroscopic model for describing the electrical and thermal behaviour of silicon devices. The model makes use of a set of macroscopic state variables for phonons and electrons that are moments of their respective distribution functions. The evolution equations for these variables are obtained starting from the Bloch–Boltzmann–Peierls kinetic equations for the phonon and the electron distributions, and are closed by means of the maximum entropy principle. All the main interactions between electrons and phonons, the scattering of electrons with impurities, as well as the scattering of phonons among themselves are considered. In particular, we propose a treatment of the optical phonon decay directly based on the expression of its transition rate (Klemens 1966 *Phys. Rev.* **148** 845; Aksamija & Ravaioli 2010 *Appl. Phys. Lett.* **96**, 091911). As an application of the model, we evaluate the silicon thermopower.

1 Introduction

The influence of crystal heating on the performances of semiconductor devices and consequently of ultra-integrated chips [8] is becoming more and more relevant as mini-aturisation progresses and millions of transistors are assembled on chip areas of the order of square centimetres. In this paper, we propose a model which takes into account the presence of hot phonons, which can be reabsorbed by electrons, leading to a much slower relaxation of the whole system towards equilibrium [11]. So doing we consider thermal effects important for a correct description of the device and circuit behaviour.

At kinetic level, the energy transport by atomistic oscillations in crystalline solids can be described by means of a phonon gas which obeys a Boltzmann-like equation. As a consequence, a complete semi-classical description of device behaviour has to be based on a system of Boltzmann equations for electrons, holes, and phonons. Numerically solving the Boltzmann equations is computationally rather expensive [10], and this has spurred several authors to formulate reduced macroscopic models [30, 32]. As regards lattice energy transport, these models are usually based on a balance equation for the crystal lattice energy and differ for the proposed forms of the thermal conductivity and

the energy production. They are typically introduced by means of heuristic approaches and are based on ad hoc assumptions, which sometimes do not take into account all the main physical phenomena occurring in semiconductors. More systematic treatments based on extended thermodynamics have been given in [24, 25, 28]. The model for silicon that we propose is also based on extended thermodynamics, but it makes use of more accurate analytical approximations for the dispersion relationships of both electrons and phonons. Furthermore, the model takes into account all the main scattering mechanisms as necessary to describe well as possible the electrothermal properties of silicon devices. We assess the validity of the model by studying the silicon thermopower.

2 Electron and phonon dispersion relations

For the sake of simplicity, we will consider only cases in which the conductivity is essentially due to electrons, which happens for unipolar devices of n-type. Extensions to holes are straightforward [21]. Electrons which mainly contribute to the charge transport in semiconductors are those in the states in the neighbourhoods of the lowest conduction band minima, each neighbourhood being called a valley [15].

Here, for silicon, we will consider the six conduction band minima near the equivalent X symmetry points. In the Kane ellipsoidal approximation, in each valley the dependence of the electron energy $\mathscr{E}$ on the wave vector $\mathbf{k}$ is given by

$$\mathscr{E} = \frac{\hbar^2}{2} \gamma(\mathscr{E}) \sum_{i=1}^{3} \frac{(k_i - \kappa_{vi})^2}{m_i}, \qquad \gamma(\mathscr{E}) := \left(1 + \alpha\mathscr{E}\right)^{-1},$$

where the energy is referred to the minimum of the valley, κ_{vi}, $i = 1, 2, 3$, are the coordinates of the minimum, α is the non-parabolicity parameter, $\hbar$ is the reduced Planck constant, and m_i, $i = 1, 2, 3$, are the eigenvalues of the inverse effective valley mass tensor. Both the non-parabolicity parameter and the effective masses are temperature dependent [27]; moreover, the first Brillouin zone is usually extended to all $\mathbb{R}^3$.

As regards the phonon dispersion relations, the following isotropic quadratic approximations will be used

$$\epsilon_p = \epsilon_0^p + \hbar v_s^p \, |\mathbf{q}| + \hbar c^p \, |\mathbf{q}|^2, \quad |\mathbf{q}| \in \left[0, \frac{2\pi}{a}\right], \quad p = LA, \, TA, \, LO, \, TO, \qquad (2.1)$$

where ϵ and $\mathbf{q}$ are the phonon energy and wave vector, a is the silicon lattice constant, A, O, L, and T respectively stay for acoustic, optical, longitudinal, and transversal, and the coefficients in equation (2.1) can be found in [27].

Models based on such approximations give good results for electric fields less than 100 kV/cm. For higher fields, at which impact ionisation plays an important role, it is necessary to consider also the L-valleys [19], which implies a straightforward generalisation of the model presented in this paper. However, the above-written approximations have been used for models employed in the study of important phenomena which occur in devices operating at voltages below the silicon bandgap, such as those of future technologies [27, 29].

3 The Bloch–Boltzmann–Peierls kinetic system

Since the electrons in the valleys, which correspond to minima lying on the same principal axis, have the same mass tensor, they can be considered as a unique population. Therefore, there are three electron populations, depending on which axis the minimum of the valley, where the electrons live, belongs to. We will label the axes and the populations by x, y, z.

At kinetic level, the state of the electrons and the phonons can be described by their one-particle distribution functions, which we will indicate by f^e and g^p respectively, with $e = x, y, z$ and $p = LA, TA, LO, TO$. Their time evolution is determined by the Bloch–Boltzmann–Peierls system (see [6] and references therein)

$$
\frac{\partial f^e}{\partial t} + \mathbf{v}^e \cdot \nabla_{\mathbf{x}} f^e - \frac{q}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f^e = \mathscr{C}_{im}(f^e) + \sum_{\iota, e', p} \mathscr{C}_{\iota, p}^{ee'}(f^e, f^{e'}, g^p),
$$

$$
\frac{\partial g^p}{\partial t} + \mathbf{v}^p \cdot \nabla_{\mathbf{x}} g^p = \sum_{\iota, e, e'} \mathscr{C}_{\iota, e', e}^{p}(g^p, f^e, f^{e'}) + \sum_{\eta} \mathscr{C}_{\eta}^{p}(g^p), \tag{3.1}
$$

$$
\Delta(\varepsilon_s \phi) = q\left(n(\mathbf{x}, t) - N_D(\mathbf{x})\right),
$$

where $\mathbf{v}^e = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathscr{E}_e$ and $\mathbf{v}^p = \frac{1}{\hbar} \nabla_{\mathbf{q}} \epsilon_p$ are the electron and phonon group velocities, q is the absolute value of the electron charge, ε_s is the silicon permittivity, ϕ and $\mathbf{E}$ are the electric potential and field, ι and η label the type of scattering respectively between electrons and phonons and among phonons themselves (see below), N_D is the donor concentration, and n is the total electron density.

The electron collision operator due to the scattering with impurities, which is intra-valley and elastic, reads [15]

$$
\mathscr{C}_{im}(f^e) = \int_{\mathbb{R}^3} \left[P_{im}(\mathbf{k}', \mathbf{k}) f^e(\mathbf{k}') - P_{im}(\mathbf{k}, \mathbf{k}') f^e(\mathbf{k}) \right] d\mathbf{k}',
$$

the impurity scattering transition rate being given by

$$
P_{im}(\mathbf{k}, \mathbf{k}') = \mathscr{K}^{(im)} \frac{1}{\left[|\mathbf{k} - \mathbf{k}'|^2 + \lambda_D^2\right]^2} \delta(\mathscr{E}(\mathbf{k}') - \mathscr{E}(\mathbf{k})),
$$

with $\lambda_D = \sqrt{\frac{N_D q^2}{\varepsilon_s k_B T_L}}$ the inverse Debye length and $\mathscr{K}^{(im)} = \frac{Z^2 N_D q^4}{4\pi\hbar\varepsilon_s^2}$, where Z is the impurity charge number, T_L the lattice temperature and k_B the Boltzmann constant.

The electron collision operators due to scatterings with phonons read [6]

$$
\mathscr{C}_{\iota, p}^{e\,e'}(f^e, f^{e'}, g^p) = \int_{S_{\frac{2\pi}{d}}} \int_{\mathbb{R}^3} \left[w_{\iota, p}^{ee'+}(\mathbf{k}, \mathbf{k}', \mathbf{q}) \kappa_1(g^p, f^e, f^{e'}) \right.
$$

$$
\left. + w_{\iota, p}^{ee'-}(\mathbf{k}, \mathbf{k}', \mathbf{q}) \kappa_2(g^p, f^e, f^{e'}) \right] d\mathbf{k}' d\mathbf{q},
$$

where $S_{\frac{2\pi}{a}}$ is the sphere of radius $\frac{2\pi}{a}$ and

$$\kappa_1(g^p, f^e, f^{e'}) := \left(\frac{g^p}{y^p} + 1\right) f^{e'}(\mathbf{k}') - \frac{g^p}{y^p} f^e(\mathbf{k}),$$

$$\kappa_2(g^p, f^e, f^{e'}) := \frac{g^p}{y^p} f^{e'}(\mathbf{k}') - \left(\frac{g^p}{y^p} + 1\right) f^e(\mathbf{k}),$$

$$w_{\iota,p}^{ee'\pm}(\mathbf{k}, \mathbf{k}', \mathbf{q}) := s_{\iota,p}^{ee'}(\mathbf{q}) \delta\left(\mathscr{E}_{e'}(\mathbf{k}') - \mathscr{E}_e(\mathbf{k}) \mp \epsilon_p\right) \delta\left(\mathbf{k}' - \mathbf{k} \mp \mathbf{q} + \mathbf{G}\right),$$

y^p being the phonon densities of states. The electron–phonon scatterings can be intra-valley ($\iota = sv$, $e = e'$, $p = LA, TA$)[1], which involve only acoustic phonons and conserve the total energy and momentum, or inter-valley [15]. These latter, which are due both to the acoustic and the optical phonons, in their turn can be distinguished in g-type ones ($\iota = dv$, $e = e'$, $p = LA, TA, LO$), which take electrons between equivalent valleys, that is valleys which have the transversal mass in the same direction, and f-type ones ($\iota = dv$, $e \neq e'$, $p = TA, LA/LO, TO$), taking electrons to non-equivalent valleys. Both of them are umklapp processes, which do not conserve the total momentum and involve a reciprocal lattice vector $\mathbf{G}$. The phonon wave vectors interested in the inter-valley transitions remain very close to the vector joining the minima of the initial and final valleys and therefore they are usually taken as constant and, after reduction to the first Brillouin zone, equal to $\frac{2\pi}{a}(1, 0.15, 0.15)$ for f-type scatterings and to $\frac{2\pi}{a}(0.3, 0, 0)$ for g-type scatterings. The scattering functions $s_{\iota,p}^{ee'}$ are given by [15]

$$s_{sv,LO}^{ee} = s_{sv,TO}^{ee} = 0, \quad s_{sv,p}^{ee'} = 0, \ e = x, y, z, \ e \neq e', \ p = LA, TA, LO, TO,$$

$$s_{sv,p}^{ee} = \frac{\hbar |\mathbf{q}|^2 D_{a,p}^2}{8 \pi^2 \rho \epsilon_p} I^2(|\mathbf{q}|), \ p = LA, TA, \ e = x, y, z,$$

$$s_{dv,p}^{ee} = \frac{\hbar (\Delta_p^{ee})^2}{8 \pi^2 \rho \, \bar{\epsilon}_p^{ee}}, \ p = LA, TA, LO, \ e = x, y, z,$$

$$s_{dv,p}^{ee'} = \frac{\hbar (\Delta_p^{ee'})^2}{4 \pi^2 \rho \, \bar{\epsilon}_p^{ee'}}, \ p = TA, LA/LO, TO, \qquad e \neq e', \ e, e' = x, y, z,$$

where $D_{a,p}$, $p = LA, TA$ are the acoustic deformation potentials, $I(|\mathbf{q}|)$ is the overlap integral, ρ is the material density, $\Delta_p^{ee'}$, $e, e' = x, y, z$, $p = LA, TA, LO, TO$, are the inter-valley deformation potentials, and $\bar{\epsilon}_p^{ee'}$, $e, e' = x, y, z$, $p = LA, TA, LO, TO$, are the phonon energies involved in the f-type and g-type transitions. The values of the various parameters and the expression of the overlap integral appearing in the above-written scattering functions can be found in [27].

The collision operators relative to the interactions of phonons with electrons read [6]

$$\mathscr{C}_{\iota, ee'}^p(g^p, f^e, f^{e'}) = \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \left[w_{\iota, p}^{ee'+}(\mathbf{k}, \mathbf{k}', \mathbf{q}) \kappa_1(g^p, f^e, f^{e'}) \right] d\mathbf{k}' d\mathbf{k}.$$

Phonons can also interact among themselves [13], these interaction processes can be distinguished into intrinsic ones, arising from the anharmonicity of the interatomic

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[1] sv and dv respectively stay for same valley and different valleys.

forces, and extrinsic ones, due to phonon scatterings at the boundaries of the crystal and at various types of crystal defects and imperfections. In their turn, the anharmonic scatterings can be normal processes (N-processes), in which the phonon total momentum after a collision is conserved, and umklapp processes (U-processes) for which the total momentum changes by a reciprocal lattice vector after a collision. On the other hand, all extrinsic processes do not conserve the total momentum after a collision and together with the umklapp ones are usually called resistive processes. For all of them, except the optical phonon decay, we will use a relaxation time approximation, paying attention to the phonon distribution function towards which each of these processes drive relaxation.

As regards the optical phonons, the most important process in which they are involved is their anharmonic decay into one trasversal acoustic phonon and one longitudinal phonon belonging either to the acoustic or to the optical branch [3]. The expression of the corresponding collision operator was first given by Klemens [17] and reads

$$\mathscr{C}^{p_o}_{p_o \leftrightarrow TA+p} = \frac{\gamma^2 y^{p_o}}{3\pi^2 \rho v_s^2} \int_0^{2\pi/a} \int_{S^2} |\mathbf{q}'|^2 \epsilon_{p_o} \omega'_p \omega_{TA}(\mathbf{q}'') \delta(\omega_{p_o} - \omega'_p - \omega_{TA}(\mathbf{q}'')) \left[\left(\frac{g^{p_o}(\mathbf{q})}{y^{p_o}} \right. \right.$$
$$\left. \left. +1 \right) \frac{g^p(\mathbf{q}')}{y^p} \frac{g^{TA}(\mathbf{q}'')}{y^{TA}} - \frac{g^{p_o}(\mathbf{q})}{y^{p_o}} \left(\frac{g^p(\mathbf{q}')}{y^p} + 1 \right) \left(\frac{g^{TA}(\mathbf{q}'')}{y^{TA}} + 1 \right) \right] d\Omega' \, d|\mathbf{q}'|,$$

where $p_o = LO, TO$, $p = LO, LA$, $\mathbf{q}'' = \mathbf{q} - \mathbf{q}' + \mathbf{G}$ (stemming from the generalised momentum conservation), S^2 is the unit sphere surface, γ is the Grüneisen parameter, and v_s is the sound velocity [3].

Analogous collision operators have to be taken into account in the right-hand sides of the Boltzmann equations relative to the transversal and longitudinal acoustic phonons which are also involved into the intra-branch transitions described by the following operators

$$\mathscr{C}^{p_A}_N = -\frac{g^{p_A} - g^{p_A}_{d-BE}(T_{p_A})}{\tau^{p_A}_N(\epsilon_{p_A}, T_{p_A})}, \qquad \text{normal processes,}$$

$$\mathscr{C}^{p_A}_U = -\frac{g^{p_A} - g^{p_A}_{BE}(T_{p_A})}{\tau^{p_A}_U(\epsilon_{p_A}, T_{p_A})}, \qquad \text{umpklapp processes,}$$

$$\mathscr{C}^{p_A}_{i-d} = -\frac{g^{p_A} - g^{p_A}_{BE}(T_{p_A})}{\tau^{p_A}_{i-d}(\epsilon_{p_A}, T_{p_A})}, \qquad \text{processes with impurities/defects,}$$

where

$$g^{p_A}_{BE}(\epsilon, T_{p_A}) = \frac{y^{p_A}}{\exp\left(\frac{\epsilon}{k_B T_{p_A}}\right) - 1},$$

$$g^{p_A}_{d-BE}(T_{p_A}) = \frac{y^{p_A}}{\exp\left(\frac{\epsilon_{p_A}}{k_B T_{p_A}}\right) - 1} \left(1 - \frac{\exp\left(\frac{\epsilon_{p_A}}{k_B T_{p_A}}\right)}{\exp\left(\frac{\epsilon_{p_A}}{k_B T_{p_A}}\right) - 1} \hbar \mathbf{q} \cdot \tilde{\Lambda}_{\mathbf{P}^{p_A}} \right),$$

respectively are the Bose–Einstein acoustic phonon distribution corresponding to their temperature T_{p_A}, and the drifted Bose–Einstein distribution [13, 29], with $\mathbf{P}^{p_A}$ the phonon momentum and $\tilde{\Lambda}_{\mathbf{P}^{p_A}}$, $p_A = LA, TA$, the related Lagrange multiplier such that the production of the corresponding momentum density is null. The latter statements will become

clearer in the next sections. The relaxation towards the drifted distribution in normal processes is due to the fact that they also conserve the total momentum. Often also the optical decay is included in the relaxations time approximation [14, 22, 29].

4 Macroscopic model

Macroscopic models can be constructed starting from the Bloch–Boltzmann–Peierls system by taking the moments of the distribution functions. In particular, we will consider the following functions of the electron and phonon wave vectors $\{\psi_e(\mathbf{k})\} := \{1, \mathbf{v}^e, \mathscr{E}_e, \mathscr{E}_e \mathbf{v}^e\}$ and $\{\psi_p(\mathbf{q})\} := \{\epsilon_p, \epsilon_p \mathbf{v}^p\}$, to which the following macroscopic state variables correspond:

$$\begin{pmatrix} n_e \\ W^e \end{pmatrix} = \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ \frac{\mathscr{E}_e}{n_e} \end{pmatrix} f^e d\mathbf{k}, \qquad \begin{pmatrix} \mathbf{V}^e \\ \mathbf{S}^e \end{pmatrix} = \frac{1}{n_e} \int_{\mathbb{R}^3} \begin{pmatrix} \mathbf{v}^e \\ \mathscr{E}_e \mathbf{v}^e \end{pmatrix} f^e d\mathbf{k}, \tag{4.1}$$

$$\begin{pmatrix} W^p \\ \mathbf{Q}^p \end{pmatrix} = \int_{S_{\frac{2\pi}{a}}} \begin{pmatrix} \epsilon_p \\ \epsilon_p \mathbf{v}^p \end{pmatrix} g^p d\mathbf{q}, \tag{4.2}$$

which respectively are the electron number densities, the average energies, the velocities, and the energy fluxes per electron, and the phonon average energies and energy fluxes. The phonon momentum densities are given by

$$\mathbf{P}^p = \int_{S_{\frac{2\pi}{a}}} \hbar \mathbf{q} \, g^p d\mathbf{q}, \quad p = LA, TA, LO, TO.$$

Here, we have chosen the minimal number of moments necessary for describing the thermal energy transport, but this number, if required by the physical problem under study, can be easily extended to cover, for example, an arbitrary number of scalar and vector moments both for electrons and phonons, by taking into account higher energy powers [13, 20, 31].

The evolution equations for the state variables (4.1), (4.2) can be obtained directly from the Boltzmann equations by integration:

$$\frac{\partial}{\partial t} \begin{pmatrix} n_e \\ n_e W^e \end{pmatrix} + \sum_j \frac{\partial}{\partial x_j} \left[n_e \begin{pmatrix} V_j^e \\ S_j^e \end{pmatrix} \right] + n_e q \begin{pmatrix} 0 \\ \sum_j E_j V_j^e \end{pmatrix} = n_e \begin{pmatrix} C_{n_e} \\ C_{W_e} \end{pmatrix}, \tag{4.3}$$

$$\frac{\partial}{\partial t} \left[n_e \begin{pmatrix} V_i^e \\ S_i^e \end{pmatrix} \right] + \sum_j \frac{\partial}{\partial x_j} \left[n_e \begin{pmatrix} F_{ij}^{e(0)} \\ F_{ij}^{e(1)} \end{pmatrix} \right]$$

$$+ n_e q \sum_j E_j \begin{pmatrix} G_{ij}^{e(0)} \\ G_{ij}^{e(1)} \end{pmatrix} = n_e \begin{pmatrix} C_{V_i^e} \\ C_{S_i^e} \end{pmatrix}, \qquad i = 1, 2, 3, \tag{4.4}$$

$$\frac{\partial}{\partial t} \begin{pmatrix} W^p \\ Q_i^p \end{pmatrix} + \sum_j \frac{\partial}{\partial x_j} \begin{pmatrix} Q_j^p \\ T_{ij}^p \end{pmatrix} = \begin{pmatrix} C_{W^p} \\ C_{Q_i^p} \end{pmatrix}, \qquad i = 1, 2, 3. \tag{4.5}$$

In the above equations, the extra-fluxes and production terms relative to electrons respectively read

$$
\begin{pmatrix} F_{ij}^{e(0)} \\ F_{ij}^{e(1)} \end{pmatrix} = \frac{1}{n_e} \int \begin{pmatrix} 1 \\ \mathscr{E}_e \end{pmatrix} v_i^e v_j^e f^e d\mathbf{k}, \quad \begin{pmatrix} \text{velocity flux,} \\ \text{flux of the energy flux} \end{pmatrix}
$$

$$
\begin{pmatrix} G_{ij}^{e(0)} \\ G_{ij}^{e(1)} \end{pmatrix} = \frac{1}{\hbar\, n_e} \int \begin{pmatrix} \frac{\partial v_i^e}{\partial k_j} \\ \frac{\partial \mathscr{E}_e v_i^e}{\partial k_j} \end{pmatrix} f^e d\mathbf{k},
$$

$$
n_e\, C_{M_{\psi_e}} = \int \psi_e(\mathbf{k}) \Big[\mathscr{C}_{im}(f^e) + \sum_{\iota,e',p} \mathscr{C}_{\iota,p}^{ee'}(f^e, f^{e'}, g^p) \Big] d\mathbf{k}, \quad M_{\psi_e}\text{-production,}
$$

with $\{M_{\psi_e}\} := \{n_e, \mathbf{V}_e, W_e, \mathbf{S}_e\}$, while for the phonons we have

$$
T_{ij}^p = \int \epsilon_p \mathbf{v}_i^p \, \mathbf{v}_j^p \, g^p(\mathbf{q}) d\mathbf{q}, \quad \text{flux of the energy flux,}
$$

$$
\begin{pmatrix} C_{W^p} \\ C_{Q_i^p} \end{pmatrix} = \int \begin{pmatrix} \epsilon_p \\ \epsilon_p \mathbf{v}_i^p \end{pmatrix} \Big[\sum_{\iota,e',e} \mathscr{C}_{\iota,e',e}^p + \sum_{\eta} \mathscr{C}_{\eta}^p \Big] d\mathbf{q}, \quad \begin{pmatrix} \text{energy production} \\ \text{energy flux production} \end{pmatrix}.
$$

In the evolution equations, the number of the unknowns is greater than that of the equations, therefore constitutive equations are needed for the extra-variables $F_{ij}^{e(0)}, G_{ij}^{e(0)}, F_{ij}^{e(1)}, G_{ij}^{e(1)}, T_{ij}^p, C_{n_e}, C_{W^e}, C_{\mathbf{V}^e}, C_{\mathbf{S}^e}, C_{W^p}, C_{\mathbf{Q}^p}$. A systematic way to find these relations is founded on a universal physical principle: the maximum entropy principle [16,23]. The maximum entropy principle states that, if a certain number of moments is known, then the least biased distribution functions, which can be used for evaluating the unknown moments, are those maximising the total entropy functional under the constraint that they reproduce the known moments. In the case under consideration, neglecting the mutual interactions among the subsystems, the total entropy is

$$
\mathscr{S} = -k_B \Bigg\{ \sum_e \int_{\mathbb{R}^3} \Big(f^e \ln \frac{f^e}{y^e} - f^e \Big) d\mathbf{k} + \sum_p \int_{S_{\frac{2\pi}{a}}} \Big[g^p \ln \frac{g^p}{y^p} - y^p
$$
$$
\times \Big(1 + \frac{g^p}{y^p} \Big) \ln \Big(1 + \frac{g^p}{y^p} \Big) \Big] d\mathbf{q} \Bigg\},
$$

with y^e the electron density of states, while the constraints are given by equations (4.1)–(4.2). The solution of this maximisation problem, linearised [1,2] with respect to the vector variables, is given by

$$
f_{ME}^e = \exp\big(-\Lambda^e - \Lambda_{W^e}\mathscr{E}_e\big)\big(1 - \mathbf{v}^e \cdot (\Lambda_{\mathbf{V}^e} + \mathscr{E}_e\Lambda_{\mathbf{S}^e})\big),
$$
$$
g_{ME}^p = \frac{y^p}{\exp(\epsilon_p \Lambda_{W^p}) - 1} - \frac{y^p \epsilon_p \exp(\epsilon_p \Lambda_{W^p})}{(\exp(\epsilon_p \Lambda_{W^p}) - 1)^2} \, \mathbf{v}^p \cdot \Lambda_{\mathbf{Q}^p},
$$

where the Λ's are Lagrange multipliers, related to the state variables by means of the constraint relations (4.1)–(4.2). Inverting these constraints, the dependence of the distribution functions on $(\mathbf{x}, t)$ will be only through the state variables, and substituting

the distributions into the integrals defining the extra-variables the needed closure relations can be obtained.

5 Inversion of the constraint relations and the phonon temperature

In this section, we will invert the constraint relations obtained by using the approximate maximum entropy distribution functions. From the scalar constraints, the densities and the energies are given by

$$
\begin{pmatrix} n_e \\ n_e \, W^e \end{pmatrix} = \frac{\sqrt{2m_0}\, m_0 \, J_0}{\hbar^3} \, e^{-\Lambda^e} \begin{pmatrix} d_0(\Lambda_{W^e}) \\ d_1(\Lambda_{W^e}) \end{pmatrix}, \qquad W^p = 4\pi y^p d_1^p(\Lambda_{W^p}),
$$

where

$$
d_n(x) := \int_0^\infty t^n \exp(-xt) \sqrt{\frac{t}{\gamma^5(t)}} \left(\gamma(t) - t\dot\gamma(t) \right) dt, \quad J_0 := \int_{S^2} \psi^{\frac{3}{2}} d\Omega,
$$

$$
\psi^{-1} := \sum_{i=1}^{3} \frac{m_0 k_i^2}{m_i |\mathbf{k}|^2}, \quad d_1^p(x) := \int_0^{\frac{2\pi}{a}} t^2 \frac{\epsilon_p(t)}{\exp(\epsilon_p(t)\, x) - 1} \, dt,
$$

m_0 being the free electron mass. Thus, one has

$$
\Lambda^e = -\log \left(\frac{\hbar^3 n_e}{\sqrt{2\, m_0}\, m_0 \, J_0 \, d_0} \right), \quad \Lambda_{W^e} = h_e^{-1}(W^e), \quad \Lambda_{W^p} = h_p^{-1}(W^p), \tag{5.1}
$$

h_e^{-1} and h_p^{-1} being the inverse functions of $h_e(x) := \frac{d_1(x)}{d_0(x)}$ and $h_p(x) := 4\pi y^p d_1^p(x)$ respectively. Hereafter, the Λ_W's will always be regarded as functions of the W's.

The vector Lagrange multipliers read

$$
\Lambda_{V_i^e} = \frac{b_{11}(W^e)}{J_{1,i}^e} V_i^e + \frac{b_{12}(W^e)}{J_{1,i}^e} S_i^e, \quad \Lambda_{S_i^e} = \frac{b_{12}(W^e)}{J_{1,i}^e} V_i^e + \frac{b_{22}(W^e)}{J_{1,i}^e} S_i^e, \tag{5.2}
$$

$$
\Lambda_{Q_i^p} = \frac{3}{4\pi y^p} \left(\frac{\partial}{\partial \Lambda_{W^p}} p_p^1(\Lambda_{W^p}) \right)^{-1} Q_i^p, \quad p_p^1(x) := \int_0^{\frac{2\pi}{a}} \frac{\epsilon_p(t)\, t^2 \, |\mathbf{v}^p(t)|^2}{\exp(\epsilon_p(t)x) - 1} dt. \tag{5.3}
$$

Here, $J_{1,i}^e := \int_{S^2} \frac{m_0^2}{(m_i^e)^2} \psi^{\frac{5}{2}} n_i^2 \, d\Omega$, and the b_{kl} are the elements of the matrix $\mathbf{B}$, which is the inverse of the symmetric matrix $\mathbf{A}$ of elements

$$
a_{kl} = -\frac{p^{k+l-2}}{m_0 \, J_0 \, d_0}, \; k, l = 1, 2, \; \text{with } p^n = p^n(x) := \int_0^\infty \frac{2t^{n+\frac{3}{2}} \gamma^{\frac{1}{2}}(t)}{\gamma(t) - t\dot\gamma(t)} \, e^{-xt} dt.
$$

We notice that the relations (5.2) depend on the direction, due to the presence of the $J_{1,i}$, which in the ellipsoidal approximation are different for different $i = 1, 2, 3$. Moreover, they also depend on the electron population, since the transversal mass of each population is differently directed.

For the results in this and in the following sections, we have used the following

Property 1 *If $\sigma(\mathbf{n})$ is any integrable even function of its argument, then*

$$\int_{S^2} \sigma(\mathbf{n})\, n_i \, d\Omega = 0, \quad \int_{S^2} \sigma(\mathbf{n})\, n_i \, n_j \, d\Omega = 0, \ \forall \, i \neq j \in \{1, 2, 3\},$$

$$\int_{S^2} \sigma(\mathbf{n})\, n_i \, n_j \, n_k \, d\Omega = 0, \ \forall \, i, j, k = 1, 2, 3.$$

We close this section by giving, in accordance with extended thermodynamics [23, 29], the following definition of the phonon temperature T:

Definition 1 $T := \frac{1}{k_B \Lambda_W}$, *where Λ_W is the Lagrange multiplier all phonon distributions would have if they were in the local thermodynamic equilibrium corresponding to the total energy density*

$$W(\Lambda_W) = \sum_p W^p(\Lambda_W) = \sum_p W^p(\Lambda_{W^p}).$$

Partial temperatures of one or more phonon branches are analogously defined.

6 Closure relations for the fluxes and the production terms

6.1 Fluxes

The above-written relations for the Lagrange multipliers allow us to find the constitutive equations for the fluxes. For the electrons, we obtain

$$\begin{pmatrix} F_{ij}^{e(0)} \\ F_{ij}^{e(1)} \end{pmatrix} = \frac{J_{1,i}^e}{m_0 J_0 \, d_0} \begin{pmatrix} p_0 \\ p_1 \end{pmatrix} \delta_{ij},$$

$$G_{ij}^{e(k)} = \Lambda_{W^e} \, F_{ij}^{e(k)}, \quad k = 0, 1,$$

the latter result can be immediately obtained by integration by parts. The phonon fluxes are given by

$$T_{ij}^p = \frac{4\pi y^p}{3} \, p_p^1(W^p)\delta_{ij},$$

where δ_{ij} is the Kronecker delta.

6.2 Electron production terms

As said, we consider both intra-valley and inter-valley scatterings of electrons with phonons. Unlike the traditional approach, for the intra-valley scattering we do not use the elastic approximation and treat the LA and TA modes separately, using equation (2.1) as dispersion relations [27]. We start from the density and energy productions, which, after integration with respect to $\mathbf{k}'$, a change of variables in the integral term containing $w_{sv,p}^{ee-}$,

and the Herring–Vogt transformation to the variables $q_i^* = \sqrt{\frac{m_0}{m_i}}\, q_i$, $k_i^* = \sqrt{\frac{m_0}{m_i}}\, k_i$, $i = 1, 2, 3$, become[2]

$$
n\begin{pmatrix} C_n \\ C_W \end{pmatrix} = \sum_p \left(\frac{m_d}{m_0}\right)^3 \int\!\!\int s_{sv,p}^{ee}(|\mathbf{q}^*|) \begin{pmatrix} 0 \\ \mathscr{E}(|\mathbf{k}^*|) - \mathscr{E}(|\mathbf{k}^* + \mathbf{q}^*|) \end{pmatrix} \delta(\mathscr{E}(|\mathbf{k}^* + \mathbf{q}^*|)
$$
$$
-\mathscr{E}(|\mathbf{k}^*|) - \epsilon_p) \left[\left(\frac{g^p(\mathbf{q}^*)}{y^p} + 1 \right) f^e(\mathbf{k}^* + \mathbf{q}^*) - \frac{g^p(\mathbf{q}^*)}{y^p} f^e(\mathbf{k}^*) \right] d\mathbf{q}^* \, d\mathbf{k}^*,
$$

with $m_d := (m_1 m_2 m_3)^{\frac{1}{3}}$ the density of states mass. If θ is the angle between $\mathbf{k}^*$ and $\mathbf{q}^*$, because of the momentum and the energy conservation [15], it can be expressed in terms of $|\mathbf{q}^*|$ and $\mathscr{E}$ as

$$
\cos\theta = \frac{m_0 \epsilon_p(|\mathbf{q}^*|)\left[1 + \alpha(\epsilon_p|\mathbf{q}^*| + 2\mathscr{E})\right] - \frac{\hbar^2 |\mathbf{q}^*|^2}{2}}{\hbar |\mathbf{q}^*| \sqrt{2 m_0 \mathscr{E}(1 + \alpha \mathscr{E})}} =: \bar{c}_p(\mathscr{E}, |\mathbf{q}^*|),
$$

where the Jacoboni–Reggiani approximation $|\mathbf{q}| \approx \sqrt{\frac{m_d}{m_0}}|\mathbf{q}^*|$ has been used [15]. Passing to polar coordinates and exploiting the properties of the delta function, one can perform integration first with respect to the phonon polar angle referred to $\mathbf{n}^* := \frac{\mathbf{k}^*}{|\mathbf{k}^*|}$ and then with respect to $\mathbf{n}^*$ itself, and obtain

$$
C_n = 0, \qquad C_W = \frac{8\pi^2 m_d^3}{\sqrt{2} m_0^{\frac{5}{2}} \hbar J_0 d_0} \sum_p \int \int_D s_{sv,p}^{ee}(|\mathbf{q}^*|)\gamma_1^{-1}(\mathscr{E})\gamma_1^{-1}(\mathscr{E}_p^+)
$$
$$
\times \frac{\epsilon_p(|\mathbf{q}^*|)e^{-\Lambda_W \mathscr{E}}}{e^{\epsilon_p \Lambda_{Wp}} - 1}\left[1 - e^{(\Lambda_{Wp} - \Lambda_W)\epsilon_p}\right]|\mathbf{q}^*|\, d\mathscr{E}\, d|\mathbf{q}^*|, \tag{6.1}
$$

where $D := \{(\mathscr{E}, |\mathbf{q}^*|) \in \mathbb{R}^+ \times [0, \frac{2\pi}{a}\sqrt{\frac{m_0}{m_d}}]: -1 \leqslant \bar{c}_p(\mathscr{E}, |\mathbf{q}^*|) \leqslant 1\}$, $\mathscr{E}_p^+ := \mathscr{E} + \epsilon_p$, and $\gamma_1 := \frac{\gamma^2}{\gamma - \mathscr{E}\dot{\gamma}} = (1 + 2\alpha\mathscr{E})^{-1}$. We notice that the energy production is null when $\Lambda_{Wp} = \Lambda_{We}$, as it has to be because of the energy conservation.

Similarly, one obtains

$$
C_{V_i}^e = \sum_p \left[(q_{sv,p}^{ee})_{11}\Lambda_{V_i^e} + (q_{sv,p}^{ee})_{12}\Lambda_{S_i^e} + (q_{sv,p}^{ee})_{13}\Lambda_{Q_i^p} \right]
$$
$$
= \sum_p \left[(c_{sv,p}^{ee})_{11}V_i^e + (c_{sv,p}^{ee})_{12}S_i^e + (c_{sv,p}^{ee})_{13}Q_i^p \right],
$$
$$
C_{S_i}^e = \sum_p \left[(q_{sv,p}^{ee})_{21}\Lambda_{V_i^e} + (q_{sv,p}^{ee})_{22}\Lambda_{S_i^e} + (q_{sv,p}^{ee})_{23}\Lambda_{Q_i^p} \right]
$$
$$
= \sum_p \left[(c_{sv,p}^{ee})_{21}V_i^e + (c_{sv,p}^{ee})_{22}S_i^e + (c_{sv,p}^{ee})_{23}Q_i^p \right],
$$

where the second equality is obtained by respectively expressing the $\Lambda_{V_i^e}$, $\Lambda_{S_i^e}$ in terms of the V_i^e, S_i^e by means of equation (5.2), and the $\Lambda_{Q_i^p}$ in terms of the Q_i^p by means of

---

[2] Here and whenever there is no possibility of confusion, we omit the electron population index. Moreover, with a slight abuse of notation we indicate with the same letter the functions depending on the starred quantities.

equation (5.3), and

$$
(q_{sv,p}^{ee})_{ij} = \frac{4\sqrt{2}\pi^2 m_d^3}{3m_0^3 m_i J_0 d_0} \int \int_D \frac{s_{sv,p}^{ee}(|\mathbf{q}^*|)e^{-\Lambda_W \mathscr{E}}}{e^{\Lambda_{Wp}\epsilon_p} - 1} \gamma_1^{-1}(\mathscr{E}_p^+)\gamma_1^{-1}(\mathscr{E})|\mathbf{q}^*|
$$

$$
\times \left\{ \left(\frac{\sqrt{2m_0}}{\hbar}\gamma_2(\mathscr{E})(\mathscr{E}^{i-1}\gamma_1(\mathscr{E}) - (\mathscr{E}_p^+)^{i-1}\gamma_1(\mathscr{E}_p^+)) - (\mathscr{E}_p^+)^{i-1}\bar{c}_p(\mathscr{E},|\mathbf{q}^*|)\gamma_1(\mathscr{E}_p^+)|\mathbf{q}^*| \right) \right.
$$

$$
\times \sqrt{2}\left(\mathscr{E}^{j-1}\gamma_1(\mathscr{E})\gamma_2(\mathscr{E}) - e^{(\Lambda_{Wp} - \Lambda_W)\epsilon_p}(\mathscr{E}_p^+)^{j-1}\gamma_1(\mathscr{E}_p^+)\gamma_2(\mathscr{E}) \right)
$$

$$
- \left(\frac{\sqrt{2m_0}}{\hbar}\gamma_2(\mathscr{E})\bar{c}_p(\mathscr{E},|\mathbf{q}^*|)(\mathscr{E}^{i-1}\gamma_1(\mathscr{E}) - (\mathscr{E}_p^+)^{i-1}\gamma_1(\mathscr{E}_p^+)) - (\mathscr{E}_p^+)^{i-1}\gamma_1(\mathscr{E}_p^+)|\mathbf{q}^*| \right)
$$

$$
\left. \times \frac{\hbar}{\sqrt{m_0}}e^{(\Lambda_{Wp} - \Lambda_W)\epsilon_p}(\mathscr{E}_p^+)^{j-1}\gamma_1(\mathscr{E}_p^+)|\mathbf{q}^*| \right\} d\mathscr{E}d|\mathbf{q}^*|, \quad i,j = 1,2,
$$

$$
(q_{sv,p}^{ee})_{ij} = \frac{4\sqrt{2}\pi^2 m_d^3}{3m_0^3 J_0 d_0} \int \int_D \frac{s_{sv,p}^{ee}(|\mathbf{q}^*|)e^{-\Lambda_W \mathscr{E}}}{e^{\Lambda_{Wp}\epsilon_p} - 1} \gamma_1^{-1}(\mathscr{E}_p^+)\gamma_1^{-1}(\mathscr{E})|\mathbf{q}^*|
$$

$$
\left(\frac{\sqrt{2m_0}}{\hbar}\gamma_2(\mathscr{E})\bar{c}_p(\mathscr{E},|\mathbf{q}^*|)(\mathscr{E}^{i-1}\gamma_1(\mathscr{E}) - (\mathscr{E}_p^+)^{i-1}\gamma_1(\mathscr{E}_p^+)) - (\mathscr{E}_p^+)^{i-1}\gamma_1(\mathscr{E}_p^+)|\mathbf{q}^*|) \right)
$$

$$
\times \sqrt{\frac{1}{m_d}}\frac{\epsilon_p}{e^{\Lambda_{Wp}\epsilon_p} - 1}|\mathbf{v}^p(|\mathbf{q}^*|)|\left(e^{\Lambda_{Wp}\epsilon_p} - e^{\epsilon_p(\Lambda_{Wp} - \Lambda_W)} \right) \right\} d\mathscr{E}d|\mathbf{q}^*|, \quad i = 1,2, j = 3,
$$

with $\gamma_2(x) := \sqrt{\frac{x}{\gamma(x)}} = \sqrt{x(1 + \alpha x)}$.

As regards the inter-valley scatterings, one finds

$$
n_e \begin{pmatrix} C_{n^e} \\ C_{W^e} \end{pmatrix} = \frac{\sqrt{2m_0^3}J_0}{\hbar^3}\sum_{e',p} s_{dv,p}^{ee'}(|\bar{\mathbf{q}}_{ee'}|) \left\{ -\frac{n_e}{d_0(W^e)}\int_0^\infty \zeta_0(\mathscr{E},\mathscr{E} + \bar{\epsilon}_p^{ee'})e^{-\Lambda_{We}\mathscr{E}} \right.
$$

$$
\times \left[e^{-\Lambda_{We}\bar{\epsilon}_p^{ee'}}\left(\frac{g_0^p(\bar{\epsilon}_p^{ee'})}{y^p} + 1 \right) \begin{pmatrix} 1 \\ \mathscr{E} + \bar{\epsilon}_p^{ee'} \end{pmatrix} + \frac{g_0^p(\bar{\epsilon}_p^{ee'})}{y^p} \begin{pmatrix} 1 \\ \mathscr{E} \end{pmatrix} \right] d\mathscr{E} + \frac{n_{e'}}{d_0(W^{e'})}
$$

$$
\times \int_0^\infty \zeta_0(\mathscr{E},\mathscr{E} + \bar{\epsilon}_p^{ee'})e^{-\Lambda_{We'}\mathscr{E}}\left[\left(\frac{g_0^p(\bar{\mathbf{q}}_p^{ee'})}{y^p} + 1 \right)e^{-\Lambda_{We'}\bar{\epsilon}_p^{ee'}}\begin{pmatrix} 1 \\ \mathscr{E} \end{pmatrix} \right.
$$

$$
\left. + \frac{g_0^p(-\bar{\mathbf{q}}_p^{ee'})}{y^p}\begin{pmatrix} 1 \\ \mathscr{E} + \bar{\epsilon}_p^{ee'} \end{pmatrix} \right] d\mathscr{E} \right\},
$$

$$
C_{V_i}^e = \sum_{p,e'} \left[(q_{dv,p}^{ee'})_{11}\Lambda_{V_i^e} + (q_{dv,p}^{ee'})_{12}\Lambda_{S_i^e} \right] = \sum_{p,e'} \left[(c_{dv,p}^{ee'})_{11}V_i^e + (c_{dv,p}^{ee'})_{12}S_i^e \right],
$$

$$
C_{S_i}^e = \sum_{p,e'} \left[(q_{dv,p}^{ee'})_{21}\Lambda_{V_i^e} + (q_{dv,p}^{ee'})_{22}\Lambda_{S_i^e} \right] = \sum_{p,e'} \left[(c_{dv,p}^{ee'})_{21}V_i^e + (c_{dv,p}^{ee'})_{22}S_i^e \right],
$$

where

$$
(q_{dv,p}^{ee'})_{ij} = \frac{2\sqrt{2m_0}J_{1,i}}{\hbar^3 d_0(W^e)}s_{dv,p}^{ee'}(|\bar{\mathbf{q}}_{ee'}|)\left\{ \frac{g_0^p(\bar{\epsilon}_p^{ee'})}{y^p}\int_0^\infty \mathscr{E}^{i+j-2}\zeta_1(\mathscr{E},\mathscr{E} + \bar{\epsilon}_p^{ee'})e^{-\Lambda_{We}\mathscr{E}}d\mathscr{E} \right.
$$

$$
\left. + \left(\frac{g_0^p(\bar{\epsilon}_p^{ee'})}{y^p} + 1 \right)\int_0^\infty (\mathscr{E} + \bar{\epsilon}_p^{ee'})^{i+j-2}\zeta_1(\mathscr{E} + \bar{\epsilon}_p^{ee'},\mathscr{E})e^{-\Lambda_{We'}(\mathscr{E} + \bar{\epsilon}_p^{ee'})}d\mathscr{E} \right\}, \quad i,j = 1,2,
$$

with g_0^p the isotropic part of the phonon distribution functions, $\zeta_0(x, y) :=$ $\gamma_1^{-1}(x)\gamma_1^{-1}(y)\gamma_2(x)\gamma_2(y)$, and $\zeta_1(x, y) := \gamma_1(x)\gamma_1^{-1}(y)\gamma_2^3(x)\gamma_2(y)$.

6.3 Phonon production terms

It is easy to check that for the intra-valley scattering with electrons, the contribution to the energy production terms C_{W^p}, $p = LA, TA$, due to the electrons belonging to a certain population $e \in \{x, y, z\}$ is equal to the opposite of the corresponding addend of the sum in equation (6.1), multiplied by n_e, as it has to be due to the energy conservation. While, as regards the energy flux production terms, one has

$$C_{Q^p} = \sum_e n_e \left[(q_{sv,ee}^p)_{11} \Lambda_{Q_i^p} + (q_{sv,ee}^p)_{12} \Lambda_{V_i^e} + (q_{sv,ee}^p)_{13} \Lambda_{S_i^e} \right]$$

$$= \sum_e n_e \left[(c_{sv,ee}^p)_{11} Q_i^p + (c_{sv,ee}^p)_{12} V_i^e + (c_{sv,ee}^p)_{13} S_i^e \right],$$

where

$$(q_{sv,ee}^p)_{ij} = \frac{8\pi^2\, m_d^2\, m_i}{3\hbar\sqrt{2m_0^5 J_0 d_0}} \int \int_D \epsilon_p(|\mathbf{q}^*|)\, |\mathbf{v}_p(\mathbf{q}^*)|^2 s_{sv,p}^{ee}(|\mathbf{q}^*|) \gamma_1^{-1}(\mathscr{E}_p^+)\gamma_1^{-1}(\mathscr{E})$$

$$\times \frac{\epsilon_p e^{-\Lambda_{We}\mathscr{E}}}{(e^{\Lambda_{Wp}\epsilon_p} - 1)^2} \left(e^{\Lambda_{Wp}\epsilon_p} - e^{(\Lambda_{Wp}-\Lambda_{We})\epsilon_p} \right) |\mathbf{q}^*|\, d|\mathbf{q}^*|\, d\mathscr{E}, \quad i, j = 1,$$

$$(q_{sv,ee}^p)_{ij} = \frac{8\pi^2\, m_d^{\frac{5}{2}}}{3\hbar\sqrt{2m_0^5 J_0 d_0}} \int \int_D \epsilon_p(|\mathbf{q}^*|)\, |\mathbf{v}_p(\mathbf{q}^*)|\, s_{sv,p}^{ee}(|\mathbf{q}^*|) \gamma_1^{-1}(\mathscr{E}_p^+)\gamma_1^{-1}(\mathscr{E})$$

$$\times \frac{e^{-\Lambda_{We}\mathscr{E}}}{e^{\Lambda_{Wp}\epsilon_p} - 1} \left\{ -\frac{\hbar}{\sqrt{m_0}} e^{(\Lambda_{Wp}-\Lambda_{We})\epsilon_p} (\mathscr{E}_p^+)^{j-2} \gamma_1(\mathscr{E}_p^+)\left(\frac{\sqrt{2m_0}}{\hbar}\gamma_2(\mathscr{E})\bar{c}_p(\mathscr{E}, |\mathbf{q}^*|) + |\mathbf{q}^*| \right) \right.$$

$$\left. + \sqrt{2}\,\mathscr{E}^{j-2}\gamma_1(\mathscr{E})\gamma_2(\mathscr{E})\bar{c}_p(\mathscr{E}, |\mathbf{q}^*|) \right\} |\mathbf{q}^*|\, d|\mathbf{q}^*|\, d\mathscr{E} \quad i = 1, j = 2, 3.$$

For the inter-valley scattering with electrons, one finds

$$\begin{pmatrix} C_{W^p} \\ C_{Q_i^p} \end{pmatrix} = \frac{\sqrt{2}m_0^{\frac{3}{2}} J_0}{\hbar^3} \sum_{e_a, e_b'} \begin{pmatrix} \bar{\epsilon}_p^{ee'} \\ \bar{\epsilon}_p^{ee'}\, v_i^p(\bar{\mathbf{q}}_{e_a e_b'}) \end{pmatrix} s_{dv,p}^{ee'}(|\bar{\mathbf{q}}_{e_a e_b'}|) \int_0^\infty \zeta_0(\mathscr{E}, \mathscr{E} + \bar{\epsilon}_p^{ee'})$$

$$\left[\frac{n_{e'}}{d_0(\Lambda_{W^{e'}})} e^{-\Lambda_{We'}(\mathscr{E}+\bar{\epsilon}_p^{ee'})} \left(\frac{g^p(\bar{\mathbf{q}}_{e_a e_b'})}{y^p} + 1 \right) - \frac{n_e}{d_0(\Lambda_{We})} e^{-\Lambda_{We}\mathscr{E}} \frac{g^p(\bar{\mathbf{q}}_{e_a e_b'})}{y^p} \right] d\mathscr{E},$$

where $a, b = +, -, x_+, x_-, y_+, y_-, z_+, z_-$ refer to the valley centred in the positive x-semi-axis and so on, and $\bar{\mathbf{q}}_{e_a e_b'}$ is the wave vector going from the centre of the valley e_a to that of the valley e_b', reduced to the first Brillouin zone.

It is worth saying more about the optical decay. In this process, energy and crystal momentum are conserved

$$\hbar\omega^{p_o} = \hbar\omega_p' + \hbar\omega_{TA}(\mathbf{q}''), \quad p_o = LO, TO, \quad p = LA, LO,$$

$$\hbar\mathbf{q} + \hbar\mathbf{G} = \hbar\mathbf{q}' + \hbar\mathbf{q}'',$$

where $\mathbf{G}$ is a vector of the reciprocal lattice different from zero if $\mathbf{q} - \mathbf{q}'$ exceeds the first Brillouin zone (umklapp processes). Exploiting these conservation laws, where the linear approximation $\epsilon_{TA} \approx v_{ts}|\mathbf{q}|$ is used for the transversal acoustic phonon energy, with v_{ts} transverse sound velocity, it is possible to express the angle θ' between $\mathbf{q}$ and $\mathbf{q}'$ by means of the relation

$$
\cos\theta' = \begin{cases}
\dfrac{|\mathbf{q}|^2 + |\mathbf{q}'|^2 - \frac{(\omega_{p_O} - \omega_p')^2}{v_{ts}^2}}{2|\mathbf{q}||\mathbf{q}'|} =: \bar{c}_{p_O p}^1(|\mathbf{q}|, |\mathbf{q}'|), & \text{if } \mathbf{q} - \mathbf{q}' \in \mathscr{B}, \\[3mm]
\dfrac{|\mathbf{q}|^2 + |\mathbf{q}'|^2 - \frac{(\omega_{p_O} - \omega_p' + \frac{2\pi}{a} v_{ts})^2}{v_{ts}^2}}{2|\mathbf{q}||\mathbf{q}'|} =: \bar{c}_{p_O p}^2(|\mathbf{q}|, |\mathbf{q}'|), & \text{if } \mathbf{q} - \mathbf{q}' \notin \mathscr{B},
\end{cases}
$$

being, in the spherical approximation used for $\mathscr{B}$ in the case of phonons,

$$
\mathbf{G} = \begin{cases}
0, & \text{if } \mathbf{q} - \mathbf{q}' \in \mathscr{B}, \\[3mm]
-\dfrac{2\pi}{a} \dfrac{\mathbf{q} - \mathbf{q}'}{|\mathbf{q} - \mathbf{q}'|}, & \text{if } \mathbf{q} - \mathbf{q}' \notin \mathscr{B}.
\end{cases}
$$

In this way, passing to polar coordinates, $d\mathbf{q}' = |\mathbf{q}'|^2 d\Omega' d|\mathbf{q}'| = |\mathbf{q}'|^2 \sin\theta' d\varphi' d\theta' d|\mathbf{q}'|$, where $d\Omega'$ is the solid angle element and θ' the polar angle, and exploiting the properties of the delta function, angular integration can be performed analytically for the production terms. For example, the production terms relative to the transversal optical phonons can be expressed as follows:

$$
C_{W^{TO}}^{TO \leftrightarrow TA+p} = \int_{\mathscr{B}} \epsilon_{TO}(|\mathbf{q}|) \mathscr{C}_{TO \leftrightarrow TA+p}^{TO} d\mathbf{q}
$$

$$
= \frac{8\gamma^2 y^{TO}}{3\rho v_s^2} \int_0^{\frac{2\pi}{a}} \int_0^{\frac{2\pi}{a}} \epsilon_{TO}^2(|\mathbf{q}|) \omega_p(|\mathbf{q}'|)(\omega_{p_O} - \omega_p')|\mathbf{q}|^2 |\mathbf{q}'|^2 g_{BE}^{TO}(\epsilon_{TO}, \Lambda_{W^{TO}}) g_{BE}^p(\epsilon_p', \Lambda_{W^p})
$$

$$
\times g_{BE}^{TA}(\epsilon_{TO} - \epsilon_p', \Lambda_{W^{TA}}) \left(\chi_1^{TO,p} + \chi_2^{TO,p}\right)(|\mathbf{q}|, |\mathbf{q}'|) \left(e^{\epsilon_{TO}\Lambda_{W^{TO}}} - e^{\epsilon_p'\Lambda_{W^p} + (\epsilon_{TO} - \epsilon_p')\Lambda_{W^{TA}}}\right) d|\mathbf{q}| \, d|\mathbf{q}'|,
$$

$$
C_{\mathbf{Q}^{TO}}^{TO \leftrightarrow TA+p} = \int_{\mathscr{B}} \epsilon_{TO}(|\mathbf{q}|) \mathbf{v}_{TO}(\mathbf{q}) \mathscr{C}_{TO \leftrightarrow TA+p}^{TO} d\mathbf{q}
$$

$$
= \frac{8\gamma^2 y^{TO}}{9\rho v_s^2} \int_0^{\frac{2\pi}{a}} \int_0^{\frac{2\pi}{a}} \epsilon_{TO}^2(|\mathbf{q}|) |\mathbf{v}^{TO}(|\mathbf{q}|)| \omega_p(|\mathbf{q}'|)(\omega_{p_O} - \omega_p')|\mathbf{q}|^2 |\mathbf{q}'|^2 g_{BE}^{TO}(\epsilon_{TO}, \Lambda_{W^{TO}})
$$

$$
\times g_{BE}^p(\epsilon_p', \Lambda_{W^p}) g_{BE}^{TA}(\epsilon_{TO} - \epsilon_p', \Lambda_{W^{TA}})
$$

$$
\times \left\{ |\mathbf{v}^{TO}(|\mathbf{q}|)| g_{BE}^{TO} e^{\epsilon_{TO}\Lambda_{W^{TO}}} \left(e^{\epsilon_p'\Lambda_{W^p} + (\epsilon_{TO} - \epsilon_p')\Lambda_{W^{TA}}} - 1\right) \left(\chi_1^{TO,p} + \chi_2^{TO,p}\right) \right.
$$

$$
\times \Lambda_{\mathbf{Q}^{TO}} + |\mathbf{v}^p(|\mathbf{q}'|)| g_{BE}^p \left(e^{\epsilon_p'\Lambda_{W^p} + (\epsilon_{TO} - \epsilon_p')\Lambda_{W^{TA}}} - e^{\epsilon_{TO}\Lambda_{W^{TO}} + \epsilon_p'\Lambda_{W^p}}\right) \left(\sum_{k=1}^2 \bar{c}_{TO,p}^k \chi_k^{TO,p}\right) \Lambda_{\mathbf{Q}^p}
$$

$$
+ \frac{\left|\mathbf{v}^{TA}\left(\frac{\omega_{TO} - \omega_p'}{v_{ts}}\right)\right|}{\frac{\omega_{TO} - \omega_p'}{v_{ts}}} g_{BE}^{TA} \left(e^{\epsilon_p'\Lambda_{W^p} + (\epsilon_{TO} - \epsilon_p')\Lambda_{W^{TA}}} - e^{\epsilon_{TO}\Lambda_{W^{TO}} + (\epsilon_{TO} - \epsilon_p')\Lambda_{W^{TA}}}\right) \left[|\mathbf{q}|\left(\chi_1^{TO,p} + \chi_2^{TO,p}\right)\right.
$$

$$
\left. - |\mathbf{q}'|\left(\bar{c}_{TO,p}^1 \chi_1^{TO,p} + \bar{c}_{TO,p}^2 \chi_2^{TO,p}\right) - \frac{\frac{2\pi}{a} v_{ts}}{\omega_{TO} - \omega_p' + \frac{2\pi}{a} v_{ts}} (|\mathbf{q}| - \bar{c}_{TO,p}^2 |\mathbf{q}'|) \chi_2^{TO,p}\right] \Lambda_{\mathbf{Q}^{TA}} \right\} d|\mathbf{q}| \, d|\mathbf{q}'|,
$$

where $p = LO, LA$, and

$$\chi_1^{pp'}(|\mathbf{q}|, |\mathbf{q}'|) := \frac{\omega_p(|\mathbf{q}|) - \omega_p'(|\mathbf{q}'|)}{v_{ts}^2 |\mathbf{q}||\mathbf{q}'|} \mathbb{1}_{D_1^{pp'}}(|\mathbf{q}|, |\mathbf{q}'|),$$

$$\chi_2^{pp'}(|\mathbf{q}|, |\mathbf{q}'|) := \frac{\omega_p(|\mathbf{q}|) - \omega_p'(|\mathbf{q}'|) + \frac{2\pi}{a} v_{ts}}{v_{ts}^2 |\mathbf{q}||\mathbf{q}'|} \mathbb{1}_{D_2^{pp}}(|\mathbf{q}|, |\mathbf{q}'|),$$

with $\mathbb{1}$ the characteristic function and

$$D_1^{pp'} := \left\{ (|\mathbf{q}|, |\mathbf{q}'|) \in \mathscr{B} \times \mathscr{B} : \bar{c}_{pp'}^1 \geqslant \frac{|\mathbf{q}|^2 + |\mathbf{q}'|^2 - \frac{4\pi^2}{a^2}}{2|\mathbf{q}||\mathbf{q}'|} \vee \omega_p - \omega_p' > 0 \vee -1 \leqslant \bar{c}_{pp'}^1 \leqslant 1 \right\},$$

$$D_2^{pp'} := \left\{ (|\mathbf{q}|, |\mathbf{q}'|) \in \mathscr{B} \times \mathscr{B} : \bar{c}_{pp'}^1, \bar{c}_{pp'}^2 \leqslant \frac{|\mathbf{q}|^2 + |\mathbf{q}'|^2 - \frac{4\pi^2}{a^2}}{2|\mathbf{q}||\mathbf{q}'|} \vee \omega_p - \omega_p' > 0 \vee -1 \leqslant \bar{c}_{pp'}^2 \leqslant 1 \right\}.$$

The production terms for the longitudinal optical phonons and for the acoustic phonons, relative to the decay processes mentioned in Section 3, have analogous expressions. Also all the other phonon anharmonic third-order processes, which however are less important, could be treated similarly.

Eventually, for the acoustical normal and resistive scatterings, since they conserve the energy of the acoustic phonons the energy productions are null, while for the energy flux productions each process gives the contribution

$$C_{Q_i^{p_A}}^{\eta} = \frac{4\pi y^{p_A}}{3} \left(\int_0^{\frac{2\pi}{a}} \frac{\epsilon_{p_A}^2 |\mathbf{v}^{p_A}|^2 |\mathbf{q}|^2 e^{\epsilon_{p_A} \Lambda_{W^{p_A}}}}{(e^{\epsilon_{p_A} \Lambda_{W^{p_A}}} - 1)^2 \tau_\eta^{p_A}(\epsilon_{p_A}, T_{p_A})} d|\mathbf{q}| - \delta_{N\eta} \frac{(I_{2,p_A}^N)^2}{I_{1,p_A}^N} \right) \Lambda_{Q_i^{p_A}}, \quad \eta = N, U, i-d,$$

with

$$I_{1,p_A}^N = \int_0^{\frac{2\pi}{a}} \frac{|\mathbf{q}|^4 e^{\epsilon_{p_A} \Lambda_{W^{p_A}}}}{(e^{\epsilon_{p_A} \Lambda_{W^{p_A}}} - 1)^2 \tau_\eta^{p_A}(\epsilon_{p_A}, T_{p_A})} d|\mathbf{q}|, \quad I_{2,p_A}^N = \int_0^{\frac{2\pi}{a}} \frac{\epsilon_{p_A} |\mathbf{v}^{p_A}| |\mathbf{q}|^3 e^{\epsilon_{p_A} \Lambda_{W^{p_A}}}}{(e^{\epsilon_{p_A} \Lambda_{W^{p_A}}} - 1)^2 \tau_\eta^{p_A}(\epsilon_{p_A}, T_{p_A})} d|\mathbf{q}|,$$

being $\tilde{\Lambda}_{\mathbf{P}^{p_A}} = \frac{I_{2,p_A}^N}{\hbar I_{1,p_A}^N} \Lambda_{\mathbf{Q}^{p_A}}$.

7 Thermoelectric power

In this section, as a first validation of the proposed model, we investigate the thermoelectric power S, which is a measure of the magnitude of a thermoelectric voltage induced by a temperature difference across the material, and is defined as

$$S := \frac{\Delta \hat{\phi}_e}{\Delta T_L} |_{\mathbf{J}=0},$$

where $\hat{\phi}_e = -\mu_e + q\phi$ is the electrochemical potential, with μ_e the electron chemical potential, T_L is the lattice temperature, and $\mathbf{J} = n\mathbf{V}$ is the electron flow density. The thermopower is the sum of a diffusion part S_d and a phonon drag part S_g. The diffusion part results from the spatial variation of the electron distribution due to the temperature gradient along the material sample, while the drag part is caused by the momentum

transfer from the phonon system to the electron one due to the phonon–electron scattering. In order to find an expression of the thermopower starting from our model, we have therefore to look for stationary solutions of the system of equations (4.3)–(4.5), under the presence of a small lattice temperature gradient in a direction which we call x and under the hypothesis that the circuit is open ($\mathbf{V} = 0$). For simplicity, we consider the case of an isotropic electron dispersion relation ($m_1 = m_2 = m_3 = m_d$), in such a way that the x, y, and z electron populations can be considered as equivalent. First of all, we rewrite the equations of the model in a form in which the electrochemical potential explicitly appears. For this purpose, it is convenient to reformulate the model in the framework of linear extended thermodynamics as already has been done in [4, 26]. Here, we use a slightly different approach which allows us to avoid the introduction of integral functions. By differentiating the kinetic expression of the electron entropy density and the expressions (4.1)$_1$ for the electron and energy densities, where the maximum entropy distribution function is substituted, we find[3]

$$d\mathscr{S}_e = -k_B\left[\left(\Lambda^e + \ln y^e\right)n_e d\Lambda^e + n_e W^e d\left(\left(\Lambda^e + \ln y^e\right)\Lambda_{W^e}\right) + n_e W_2^e \Lambda_{W^e} d\Lambda_{W^e}\right],$$

$$dn_e = -n_e d\Lambda^e - n_e W^e d\Lambda_{W^e},$$

$$d(n_e W^e) = -n_e W^e d\Lambda^e - n_e W_2^e d\Lambda_{W^e},$$

where $n_e W_2^e = \int_{\mathbb{R}^3} \mathscr{E}^2 f^e d\mathbf{k}$. From the latter differentials, it is easy to obtain

$$d\mathscr{S}_e = k_B\left(\Lambda^e + \ln y^e\right)dn_e + k_B \Lambda_{W^e} d(n_e W^e),$$

which compared with the Gibbs relation for the electrons

$$T_e d\mathscr{S}_e = d(n_e W^e) - \mu_e dn_e$$

allows us the following identifications

$$\Lambda_{W_e} = \frac{1}{k_B T_e}, \qquad \mu_e = -k_B T_e\left(\Lambda^e + \ln y^e\right).$$

Using the closure relation (5.1)$_1$, the chemical potential can be rewritten as

$$\mu_e = k_B T_e \ln\left(\frac{\hbar^3}{\sqrt{2}\, y^e m_0^{\frac{3}{2}} J_0}\frac{n_e}{d_0(\Lambda_{W^e})}\right),$$

from which, by differentiation, we get

$$dn_e = -\left[\frac{n_e}{T_e}\ln\left(\frac{\hbar^3}{\sqrt{2}\, y^e m_0^{\frac{3}{2}} J_0}\frac{n_e}{d_0(\Lambda_{W^e})}\right) - \frac{n_e W^e}{k_B T_e^2}\right]dT_e + \frac{n_e}{k_B T_e}d\mu_e. \tag{7.1}$$

Moreover, from the definition of the electrochemical potential we have

$$q\, d\phi = d\hat{\phi}_e + d\mu_e. \tag{7.2}$$

---

[3] Here and in the following, the index e stays for electrons.

Now we substitute the latter two expressions in the equations for the *x*-components of the electron velocity and the energy flux, written in the stationary case, and we obtain

$$\left[\frac{n_e}{k_B T_e^2}F_{xx}^{e(1)}+F_{xx}^{e(0)}\left(\frac{n_e W^e}{k_B T_e^2}-\frac{n_e}{T_e}\ln\left(\frac{\hbar^3}{\sqrt{2}\,y^e m_0^{\frac{3}{2}}J_0}\frac{n_e}{d_0(\Lambda_{W^e})}\right)\right)\right]\frac{\partial T_e}{\partial x}-n_e\Lambda_{W^e}F_{xx}^{e(0)}\frac{\partial\hat\phi_e}{\partial x}$$
$$=n_e\left(c_{11}^e V_x^e+c_{12}^e S_x^e+c_{13}^{e,LA}Q_x^{LA}+c_{13}^{e,TA}Q_x^{TA}\right), \tag{7.3}$$

$$\left[\frac{n_e}{k_B T_e^2}F_{xx}^{e(2)}+F_{xx}^{e(1)}\left(\frac{n_e W^e}{k_B T_e^2}-\frac{n_e}{T_e}\ln\left(\frac{\hbar^3}{\sqrt{2}\,y^e m_0^{\frac{3}{2}}J_0}\frac{n_e}{d_0(\Lambda_{W^e})}\right)\right)\right]\frac{\partial T_e}{\partial x}-n_e\Lambda_{W^e}F_{xx}^{e(1)}\frac{\partial\hat\phi_e}{\partial x}$$
$$=n_e\left(c_{21}^e V_x^e+c_{22}^e S_x^e+c_{23}^{e,LA}Q_x^{LA}+c_{23}^{e,TA}Q_x^{TA}\right), \tag{7.4}$$

where the *c*'s coefficients at the right-hand sides are the sums of the *c*'s coefficients relative to the various electron-phonon scatterings taken into account. Equations (7.3)–(7.4) have to be completed with equation $(4.5)_2$ relative to the energy fluxes of the acoustic phonons which are those responsible of the thermal energy transport [29]. These equations, in the stationary case, can be rewritten as follows:

$$-\frac{4\pi y^{LA}}{3k_B T_L^2}\left(\frac{\partial}{\partial\Lambda_{W^{LA}}}p_p^1(\Lambda_{W^{LA}})\right)\frac{\partial T_L}{\partial x}=n_e\left(c_{12}^{LA,e}V_x^e+c_{13}^{LA,e}S_x^e\right)+c_{11}^{LA}Q_x^{LA}, \tag{7.5}$$

$$-\frac{4\pi y^{TA}}{3k_B T_L^2}\left(\frac{\partial}{\partial\Lambda_{W^{TA}}}p_p^1(\Lambda_{W^{TA}})\right)\frac{\partial T_L}{\partial x}=n_e\left(c_{12}^{TA,e}V_x^e+c_{13}^{TA,e}S_x^e\right)+c_{11}^{TA}Q_x^{TA}, \tag{7.6}$$

where T_L is the lattice temperature, we recall that in the case under study the temperatures of all the subsystems (electrons and phonons) are the same. Here, as regards the scatterings involving the acoustic phonons, we use the approximations which can be found in [29], according to which the forms for normal (*N*) and umklapp (*U*) phonon–phonon as well as phonon-impurity/defect (p-i) scattering rates are taken to be of the relaxation type with

$$\frac{1}{\tau_{p-p,N}^{LA}}=A_{N,LA}\omega_{LA}^2 T_L^3,$$

$$\frac{1}{\tau_{p-p,N}^{LA}}=A_{N,TA}\omega_{TA}T_L^4,$$

$$\frac{1}{\tau_{p-p,U}^{TA}}=\begin{cases}A_{U,TA}/\sinh\left(\frac{\epsilon_{TA}}{k_B T_L}\right), & \omega_1<\omega_{TA}<\omega_2,\\ 0, & \text{otherwise},\end{cases}$$

$$\frac{1}{\tau_{p-i}}=(A_{\delta M}+A_{\delta R})\omega^4,$$

where the set of *A* coefficients are given in Table 1 of [29].

Now, we look for solutions of equaions (7.3)–(7.6) with $V_x^e=0$. We solve equations (7.4)–(7.6) with respect to the unknowns S_x^e,Q_x^{LA},Q_x^{TA}, by writing $(M_{ij}^{th})_{i,j=1}^3$ as the matrix

of the coefficients of these unknowns which has elements

$$
\begin{aligned}
M_{11}^{th} &= n_e c_{22}^e, & M_{12}^{th} &= n_e c_{23}^{e,LA}, & M_{13}^{th} &= n_e c_{23}^{e,TA}, \\
M_{21}^{th} &= n_e c_{13}^{LA,e}, & M_{22}^{th} &= c_{11}^{LA}, & M_{23}^{th} &= 0, \\
M_{31}^{th} &= n_e c_{13}^{e,TA}, & M_{32}^{th} &= 0, & M_{33}^{th} &= c_{11}^{TA}.
\end{aligned}
$$

Substituting this solution into equation (7.3), we obtain the following compatibility condition

$$
D_{\hat{\phi}_e}(n_e, T_e, T_L) \frac{\partial \hat{\phi}_e}{\partial x} = D_{T_e}(n_e, T_e, T_L) \frac{\partial T_e}{\partial x} - D_{T_L}(n_e, T_e, T_L) \frac{\partial T_L}{\partial x},
$$

where

$$
D_{\hat{\phi}_e} = n_e \Lambda_{W^e} F_{xx}^{e(0)} - n_e^2 \Lambda_{W^e} F_{xx}^{e(1)} \left(c_{12}^e M_{11}^{th-1} + c_{13}^{e,LA} M_{21}^{th-1} + c_{13}^{e,TA} M_{31}^{th-1} \right),
$$

$$
\begin{aligned}
D_{T_e} =\ & \frac{n_e}{k_B T_e^2} F_{xx}^{e(1)} + F_{xx}^{e(0)} \left(\frac{n_e W^e}{k_B T_e^2} - \frac{n_e}{T_e} \ln \left(\frac{\hbar^3}{\sqrt{2}\, y^e m_0^{\frac{3}{2}} J_0} \frac{n_e}{d_0(\Lambda_{W^e})} \right) \right) \\
& - \left[\frac{n_e^2}{k_B T_e^2} F_{xx}^{e(2)} + n_e F_{xx}^{e(1)} \left(\frac{n_e W^e}{k_B T_e^2} - \frac{n_e}{T_e} \ln \left(\frac{\hbar^3}{\sqrt{2}\, y^e m_0^{\frac{3}{2}} J_0} \frac{n_e}{d_0(\Lambda_{W^e})} \right) \right) \right] \left(c_{12}^e M_{11}^{th-1} \right. \\
& \left. + c_{13}^{e,LA} M_{21}^{th-1} + c_{13}^{e,TA} M_{31}^{th-1} \right),
\end{aligned}
$$

$$
\begin{aligned}
D_{T_L} =\ & -\frac{4\pi n_e y^{LA}}{3 k_B T_L^2} \left(\frac{\partial}{\partial \Lambda_{W^{LA}}} p_p^1(\Lambda_{W^{LA}}) \right) \left(c_{12}^e M_{12}^{th-1} + c_{13}^{e,LA} M_{22}^{th-1} + c_{13}^{e,TA} M_{32}^{th-1} \right) \\
& -\frac{4\pi n_e y^{TA}}{3 k_B T_L^2} \left(\frac{\partial}{\partial \Lambda_{W^{TA}}} p_p^1(\Lambda_{W^{TA}}) \right) \left(c_{12}^e M_{13}^{th-1} + c_{13}^{e,LA} M_{23}^{th-1} + c_{13}^{e,TA} M_{33}^{th-1} \right).
\end{aligned}
$$

From the compatibility condition, it is easy to obtain

$$
\begin{aligned}
S &= \frac{\Delta \hat{\phi}_e}{\Delta T_L} = S_d(n_e(N_D, T_L), T_L, T_L) + S_g(n_e(N_D, T_L), T_L, T_L) \\
&= \frac{D_{T_e}(n_e(N_D, T_L), T_L, T_L)}{D_{\hat{\phi}_e}(n_e(N_D, T_L), T_L, T_L)} - \frac{D_{T_L}(n_e(N_D, T_L), T_L, T_L)}{D_{\hat{\phi}_e}(n_e(N_D, T_L), T_L, T_L)}.
\end{aligned}
$$

It remains to express n_e as a function of the temperature and the doping concentration. From equation $(5.1)_1$, we have

$$
n_e = \frac{\exp(-\Lambda^e)}{y^e} \frac{m_0 \sqrt{2 m_0}\, y^e}{\hbar^3} J_0 \, d_0(\Lambda_{W^e}),
$$

which compared with equation (6) of [33] allows us the identifications

$$
n_0 = \frac{m_0 \sqrt{2 m_0}\, y^e}{\hbar^3} J_0 \, d_0(\Lambda_{W^e}), \qquad \frac{\exp(-\Lambda^e)}{y^e} = \exp \left(\frac{\mathscr{E}_F - \mathscr{E}_C}{k_B T_L} \right),
$$

with n_0 the effective density of states in the conduction band, $\mathscr{E}_F$ the Fermi energy, and $\mathscr{E}_C$
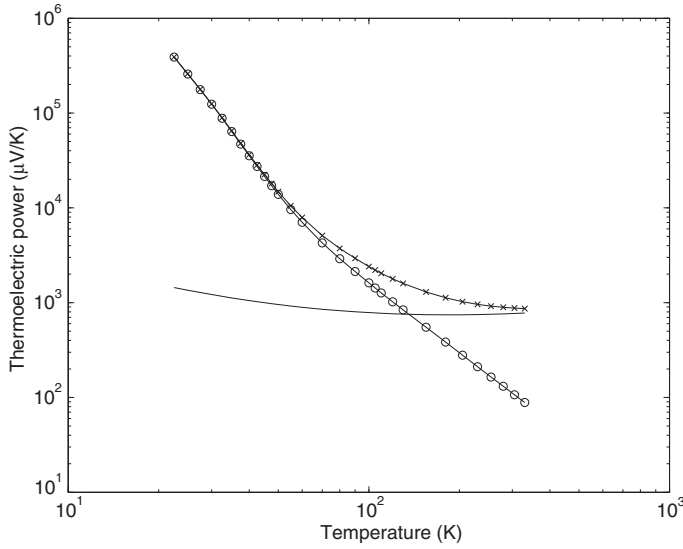
FIGURE 1. Thermoelectric power S as a function of temperature. The continuous line, the line with circles, and the line with crosses respectively represent the diffusion part, the drag part, and the total thermopower.

the edge of the conduction band. The Fermi energy can be determined from the neutrality condition, which implies that the number of ionised donors must be equal to the electron concentration [33]

$$N_D\left\{1 - \left[\frac{1}{2}\exp\left(\frac{\mathscr{E}_i - \mathscr{E}_C}{k_B T_L}\right) + 1\right]\right\} = n_0\exp\left(\frac{\mathscr{E}_F - \mathscr{E}_C}{k_B T_L}\right),$$

where $\mathscr{E}_i$ is the ionisation energy, which in silicon doped with phosphorus is equal to $\mathscr{E}_C - 0.044$ eV [5]. Eventually, we obtain

$$n_e = \frac{1}{2}\left[\sqrt{\frac{n_0^2}{4}\exp\left(2\frac{\mathscr{E}_i - \mathscr{E}_C}{k_B T_L}\right) + 2n_0 N_D\exp\left(\frac{\mathscr{E}_i - \mathscr{E}_C}{k_B T_L}\right)} - \frac{n_0}{2}\exp\left(\frac{\mathscr{E}_i - \mathscr{E}_C}{k_B T_L}\right)\right].$$

At this point, we can compute the coefficients $D_{\hat{\phi}_e}, D_{T_e}, D_{T_L}$ by numerically evaluating all the integrals which appear in the production terms and in the extra-fluxes. These integrals have been computed once and for all for suitable values of the temperatures on which they depend and the results have been stored to be used in future numerical simulations of silicon devices. The two contributions to the thermoelectric power are shown in Figure 1, in the case $N_D = 2.8 \times 10^{16}$ cm^{-3}. The total thermopower is in good agreement with the experimental results which can be found in Figure 4 of [33].

Conclusions

The formal model presented in this paper can be considered as a first step towards a consistent model of charge transport and heat effects in a semiconductor, phenomena

which have generally been treated separately. Analytical approximations, valid in a certain range of the electric field, have been taken for the dispersion relations both of electrons and phonons, moreover all the main scattering mechanisms between electrons and phonons and among phonons have been considered. As a first application, the silicon thermopower has been investigated. Further applications of this model (possibly introducing sub-bands where required by confined dimensions [7,9]) to the simulation of benchmark devices are under current investigation and will be presented in future works. The present model can also be applied in the analysis of anomalous temperature rises due to ballistic phonon transport near the heat source in a transistor as well as in the study of the time and dynamical behaviours of the thermal conductivity of semiconductor crystals [14].

Acknowledgement

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