Maximum entropy principle within a total energy scheme: Application to hot-carrier transport in semiconductors

M. Trovato
Dipartimento di Matematica, Università di Catania, Viale A. Doria 6, 95125 Catania, Italy

L. Reggiani
Dipartimento di Ingegneria dell' Innovazione ed Istituto Nazionale di Fisica della Materia, Università di Lecce, Via Arnesano s/n, 73100 Lecce, Italy

(Received 1 November 1999)

The maximum entropy principle is applied to a conducting band with energy wave vector dispersion of general form and to an arbitrary number of generalized kinetic fields. By considering a linear expansion around a local Maxwellian, within a total average energy scheme, we obtain a closed system of hydrodynamic equations for a full band model in which all the unknown constitutive functions are completely determined. With this approach, under spatially homogeneous conditions we present a systematic study of the small-signal analysis for the most important response functions of the electron system in the general framework of the moments theory. The case of a n^+nn^+ nonhomogeneous structure is also considered. Numerical hydrodynamic calculations are validated by a comparison with Monte Carlo simulations performed for the case of *n*-type Si at 300 K.

I. INTRODUCTION

The field of hydrodynamic (HD) models was pioneered by Blotekjaer in 1970.[1] Since then, more or less refined HD approaches have been developed to describe the properties of hot carrier transport both in semiconductor materials and in submicron devices.[2–7] The popularity of the HD models stems from the computational efficiency and the practical flexibility of this approach that can be applied to different operation conditions and also to computer aided design simulators. However, it should be stressed that, in order to obtain a self-contained system of HD equations a variety of simplifying assumptions must be introduced. These assumptions leave a certain degree of freedom both in the *form* of the equations and in the determination of the *closure* for the usual HD system of equations (fluxes and collisional productions).

Recently the maximum entropy principle (MEP) has emerged as a powerful method to develop HD models starting from the moments of the Boltzmann transport equation (BTE)[8–14] and it has led to a renewed interest in the *construction* of self-consistent closure relations for semiconductor transport equations with higher-moment terms.[15–18] The MEP allows one to derive the macroequivalent distribution function under conditions very far from thermodynamic equilibrium, and to determine the microstate corresponding to the given macroscopic data. With this approach, the determination of the single-particle distribution function is obtained from the solution of the variational problem consisting in maximizing the *functional entropy* of the system under the constraint[14,19–22] that the macroscopic state could be described by a fixed number of *moments of the distribution function*. The basic limitations of existing MPE theories as applied to solid state physics are in (i) the use of parabolic energy dispersion for the single carrier and (ii) the use of a few number of macroscopic *moments* to be taken as constraints in the variational procedure. Both assumptions are dictated by the complexity of the analytical formulation.

The aim of this paper is to provide a general formulation of the MEP thus making it possible to overcome the two basic limitations adressed above. To this purpose, the theory is reformulated within a total-energy scheme described by a local and isotropic Maxwellian distribution in terms of an arbitrary number of generalized kinetic fields. In this context, it is further possible to reformulate, in more general terms the theory for small-signal analysis under spatial homogeneous conditions. As a matter of fact, by introducing a generalized relaxation matrix and generalized chord and differential mobilities for each moment of interest, we have succeeded in calculating the most relevant response functions of the electron system, thus extending previous results[23,24] where the time dependencies of the response functions were analyzed using the usual coupled HD equations for velocity and energy. The theory so developed is further applied to submicron n^+nn^+ structures and validated by comparison with full-band Monte Carlo (MC) simulations.

The layout of the paper is as follows. In Sec. II we introduce a brief kinetic description of the problem. Corresponding microscopic and macroscopic quantities are defined in the general framework of the moment theory using an energy dispersion of general form (full-band approach). In Sec. III we discuss the various concepts of thermodynamic equilibrium and, by taking an arbitrary number of macroscopic moments, the MEP is developed within a total average energy scheme. In Sec. IV, we start from a linear expansion around the local Maxwellian to obtain a closed system of extended balance equations in which all the unknown constitutive functions are completely determined. In Sec.V, by introducing an iterative procedure, we obtain the standard HD models with a general constitutive relation for the energy flux. In Sec. VI the general theory is applied to the case of electrons

in Si. Here, for the case of the bulk material, the linear response analysis for stationary conditions is developed and the closure condition for the energy flux is verified via MC simulations. For the case of submicron n^+nn^+ structures the spatial profiles of different kinetic moments are calculated and compared with MC simulations. Major conclusions are finally given in Sec. VII.

II. THE BTE AND MOMENT'S METHOD

Let us consider the BTE for the single carrier distribution function $\mathcal{F}(\vec{k},\vec{r},t)$ under nondegenerate conditions:

$$\frac{\partial \mathcal{F}}{\partial t}+u_i\frac{\partial \mathcal{F}}{\partial x_i}-\frac{e}{\hbar}E_i\frac{\partial \mathcal{F}}{\partial k_i}=Q(\mathcal{F}), \tag{1}$$

where u_i is the carrier group velocity, k_i the wave vector, E_i the external electric field, e the absolute value of the unit charge, $\hbar$ the reduced Planck constant and

$$Q(\mathcal{F})=\frac{V}{(2\pi)^3}\left\{\int d\vec{k}'S(\vec{k},\vec{k}')\mathcal{F}(\vec{k}',\vec{r},t) - \mathcal{F}(\vec{k},\vec{r},t)\int d\vec{k}'S(\vec{k}',\vec{k})\right\}, \tag{2}$$

the collision integral, being $S(\vec{k},\vec{k}')$ the total electron scattering rate from state $\vec{k}'$ to state $\vec{k}$, and V the crystal volume. Given the complexity of the problem, we will neglect two-particle interaction and assume that the phonons remain in thermal equilibrium.[25] Under these assumptions the BTE is linear and, neglecting the generation and recombination processes, we shall have only one conservation law (for the numerical density), moreover the collisional invariants can be classified and an *H-theorem* proved.[26,27] To pass from the kinetic level of the BTE to the HD level of the balance equations in the general framework of the moment theory, the following generalized kinetic fields must be considered:

$$\psi_A(\vec{k})=\{\varepsilon^m,\varepsilon^m u_{i_1},\ldots,\varepsilon^m u_{i_1}u_{i_2}\cdots u_{i_s},\ldots\}, \tag{3}$$

where $\varepsilon(\vec{k})$ is the single-particle band energy, $m=0,1,\ldots,N$, and $s=1,2,\ldots,M$ with arbitrary values for the integers N and M. Equation (3) is the key formula since it generalizes the kinetic fields to energy dispersions of general form. With this approach, if we consider the expectation values

$$F_A=\int \psi_A(\vec{k})\mathcal{F}(\vec{k},\vec{r},t)d\vec{k}, \tag{4}$$

then for $N=M=1$ we find the usual physical quantities such as *n (numerical density), W (total-energy density), nv_i (velocity flux density), and S_i (energy flux density)*. By contrast, for $N,M>1$ we obtain macroscopic additional variables, which in some cases correspond to fluxes of v_i and S_i.

The set of HD equations that are formally obtained within this scheme are[14,17,18]

$$\frac{\partial F_A}{\partial t}+\frac{\partial F_{Ak}}{\partial x_k}=-\frac{e}{\hbar}R_{Ai}E_i+P_A, \quad \text{with } A=1,\ldots,\mathcal{N}, \tag{5}$$

where $\mathcal{N}$ is the number of moments used, and F_{Ak}, R_{Ai}, P_A indicate, respectively, the fluxes, the external field productions, and the collisional productions defined as:

$$F_{Ak}=\int \psi_A(\vec{k})u_k\mathcal{F}(\vec{k},\vec{r},t)d\vec{k}, \tag{6}$$

$$R_{Ai}=\int \frac{\partial\psi_A(\vec{k})}{\partial k_i}\mathcal{F}(\vec{k},\vec{r},t)d\vec{k}, \tag{7}$$

$$P_A=\int \psi_A(\vec{k})Q(\mathcal{F})d\vec{k}. \tag{8}$$

With this procedure, we obtain a system of partial differential equations of finite order to be coupled with the Poisson equation. The flux of each equation of set (5) becomes the field variable (the moment) of the succesive equation. The structure of this system of equations shows that there are some unknown constitutive functions $H_A=\{F_{Ak},R_{Ai},P_A\}$ that must be determined, in a self-consistent way, in terms of the variables F_A. By following information theory, the MEP is introduced in terms of the generalized kinetic field given by Eq. (3). Accordingly, the unknown constitutive functions can be determined systematically together with the analytic expression for the nonequilibrium distribution function. Once the distribution function is so calculated, all the constitutive functions are determined from their kinetic expressions. In this way we obtain a closed system of balance equations for the expectation values F_A, and each solution of this set will be named *thermodynamic process*[14] for the hot carriers. The explicit HD expressions obtained from Eq. (5) will be explained in details in the following sections, where numerical results will be displayed with the purpose of validating this approach.

III. ENTROPY MAXIMIZATION WITHIN A TOTAL-ENERGY SCHEME

The MEP is based on the assumption that the least biased distribution function assigned to a physical system is that which maximizes the entropy under the constraints imposed by the available *information*. Therefore, we assume that the *information* expressed by a certain *fixed* number $\mathcal{N}$ of moments is sufficient to describe satisfactorily the thermodynamic state of hot carriers, and we look for the corresponding distribution function. Accordingly, the entropy is maximized under the constraints that the expectation values of the moments F_A are expressed by Eqs. (4). The method of Lagrange multipliers[14,17,19–22] proves to be the most efficient technique to include the constraints and solve this variational problem. A short calculation yields the distribution

$$\mathcal{F}=\exp(-\Pi), \quad \Pi=\sum_{A=1}^{\mathcal{N}}\psi_A\Lambda_A. \tag{9}$$

The Lagrange multipliers Λ_A can be obtained analytically, by considering a series expansion[12,14,17] of $\mathcal{F}$ around a suitable equilibrium configuration defined by a local Maxwellian $\mathcal{F}_M$ and by requiring that the expression of $\mathcal{F}$ satisfies the moment constraints. The choice of a local Maxwellian is

justified by the observation that, for most semiconductors,[6,23,24,28,29] the time scale of energy relaxation is much longer than that of any other moment relaxation. The presence of different scales of relaxation time implies that, during the process leading to termal equilibrium, there exists an intermediate state in which carriers are characterized by a specific *local equilibrium*. The usual way to define the local Maxwellian consists in introducing an equation of state that enables one to separate the drift from the heating effects associated with the average total energy of a single carrier $\tilde{W}=W/n$. Thus, a local electron-temperature concept[17] $T(\vec{r},t)$ can be defined.

Now we differ from this way of introducing a local temperature, typical for a parabolic band shape, by keeping the total average electron energy,[18] which is a well-defined quantity for any band shape.[30] To be consistent with this choice, the moments of the distribution function F_A cannot be separated into their convective and nonconvective parts and the local distribution function should be defined in terms of the total average energy of the single carrier as $\mathcal{F}_M=\gamma\exp[-\beta\varepsilon(\vec{k})]$ being $\gamma=\gamma(n,W)$ a normalization factor and $\beta^{-1}=\beta^{-1}(W/n)$ an appropriate average energy. By considering an explicit energy wave-vector relation $\varepsilon(\vec{k})$, the quantities $\{\gamma,\beta\}$, can be determined by means of the local equilibrium relationships

$$n(\vec{r},t)=\int \mathcal{F}_M d\vec{k}, \quad W(\vec{r},t)=\int \varepsilon(\vec{k})\mathcal{F}_M d\vec{k}. \tag{10}$$

Within this approach, the case of the parabolic band is recovered when

$$\gamma=n\left(\frac{\hbar^2}{\pi m^*}\frac{3}{4}\frac{n}{W}\right)^{3/2}, \quad \beta=\frac{3}{2}\frac{n}{W},$$

m^* being a constant effective mass.

For a general energy dispersion[31] $\{\gamma,\beta\}$ can be determined by solving numerically Eqs. (10). A fruitful way to introduce the total-energy scheme, is to consider a band energy represented in terms of an effective mass that depends on the average energy of the single carrier $m^*(\tilde{W})$. Accordingly, the energy and group-velocity relations can be written as

$$\varepsilon(\vec{k})=\frac{\hbar^2k^2}{2m^*(\tilde{W})}, \quad u_i=\frac{\hbar}{m^*(\tilde{W})}k_i. \tag{11}$$

As a consequence, the effective mass becomes a new constitutive function that should be independently determined from the fitting of experiments and/or MC calculations of the bulk material.[18] All other constitutive functions are implicitely determined by means of the MEP. We note that in this way the macroscopic dynamical properties of carriers are described by the same set of balance equations and of constitutive functions for both the parabolic (with m^* constant) and full-band cases [with $m^*=m^*(\tilde{W})$]. Additionally, by using Eq. (11), as generalized independent kinetic fields we have the unique quantities $\psi_A(\vec{k})=\{\varepsilon^p,\varepsilon^p u_{i_1},\varepsilon^p u_{\langle i_1}u_{i_2\rangle},\ldots,\varepsilon^p u_{\langle i_1}u_{i_2}\cdots u_{i_s\rangle},\ldots\}$ (where $u_{\langle i_1}u_{i_2}\cdots u_{i_s\rangle}$ is the traceless part of the tensor $u_{i_1}u_{i_2}\cdots u_{i_s}$) to which the

$$\mathcal{N}=(N+1)\left[\sum_{i=0}^{M}(2i+1)\right]$$

mean quantities correspond to

$$F_A=\{F_{(p)},F_{(p)|i_1},F_{(p)|\langle i_1i_2\rangle},\ldots,F_{(p)|\langle i_1\cdots i_s\rangle},\ldots\} \tag{12}$$

with $p=0,1,\ldots,N$ and $s=0,1,\ldots,M$.

All the scalar moments $F_{(p)}$ can be separated into a local equilibrium part and a nonequilibrium part with $\Delta_{(p)}=F_{(p)}-F_{(p)}|_E$ through the relationship

$$F_{(p)}=n\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^p+\Delta_{(p)} \tag{13}$$

with $\Delta_{(0)}=\Delta_{(1)}=0$.

The distribution function in Eq. (9) takes the explicit form

$$\mathcal{F}=\mathcal{F}_M\exp\left(-\sum_{s=0}^{M}\sum_{m=0}^{N}\hat{\Lambda}^{(m)}_{\langle i_1\cdots i_s\rangle}k^{2m}k_{\langle i_1}\cdots k_{i_s\rangle}\right) \tag{14}$$

with $\hat{\Lambda}_A$ the nonequilibrium part of the Lagrange multipliers and

$$\mathcal{F}|_E=\mathcal{F}_M=n\left(\frac{\hbar^2}{\pi m^*(\tilde{W})}\frac{3}{4\tilde{W}}\right)^{3/2}\exp\left(-\frac{3}{2}\frac{\varepsilon(\vec{k})}{\tilde{W}}\right). \tag{15}$$

Under thermodynamic equilibrium conditions it is $\tilde{W}=\tilde{W}_0=(3/2)K_BT_0$ and $\mathcal{F}_M$ becomes the Maxwellian distribution at the lattice temperature T_0. By expanding both the distribution function $\mathcal{F}$ and the constitutive functions H_A around the Maxwellian $\mathcal{F}_M$, these can be expressed as polynomials in the nonequilibrium variables $\{\Delta_p,F_{(p)|i_1},\ldots,F_{(p)|\langle i_1\cdots i_s\rangle},\cdots\}$, whose coefficients depend on the local equilibrium quantities $\{n(\vec{r},t),W(\vec{r},t)\}$. In the next sections we formally assume that the effective mass is a function of the total energy, i.e. $m^*=m^*(\tilde{W})$, also when, to simplify the notation, we omit the explicit dependence on $\tilde{W}$.

IV. BALANCE EQUATIONS AND CLOSURE RELATIONS

Let us consider an arbitraty number of moments F_A, defined by Eq. (12). The corresponding set of balance equations can be written in compact form

$$\frac{\partial F_{(p)|\langle i_1i_2\cdots i_s\rangle}}{\partial t}+\frac{s}{2s+1}\frac{\partial}{\partial x_{i_s\rangle}}\left\{\frac{2}{m^*}F_{(p+1)|\langle\langle i_1\cdots i_{s-1}\rangle}\right\}+\frac{\partial F_{(p)|\langle i_1\cdots i_sk}}{\partial x_k}$$
$$=-epF_{(p-1)|\langle i_1\cdots i_sk}E_k-\frac{e}{m^*}s\left[\frac{2(p+s)+1}{2s+1}\right]\times F_{(p)|\langle\langle i_1\cdots i_{s-1}\rangle}E_{i_s\rangle}+P_{(p)|\langle i_1\cdots i_s\rangle},$$
$$p=0,1,\ldots,N; \quad s=0,1,\ldots,M \tag{16}$$

where for $s=0$ we have the scalar moments $F_{(p)}$, for $s=1$ the vectorial moments $F_{(p)|i_1}$, and so on for the other

tensorial quantities. These equations contain unknown constitutive functions such as the collisional productions $P_{(p)|\langle i_1\cdots i_s\rangle}$, associated with intravalley and intervalley transitions, and the moments of higher order $G_A=\{F_{(N+1)|\langle i_1\cdots i_{r-1}\rangle},F_{(p)|\langle i_1\cdots i_M k\rangle}\}$ in the fluxes and in the external field productions, evaluated for $p=0,1,\ldots,N$; $s=0,1,\ldots,M$ and $r=1,\ldots,M$. To calculate these *constitutive relations* we consider a linear expansion of the distribution function in Eq. (14) around the Maxwellian $\mathcal{F}_M$ to obtain the nonequilibrium part of the Lagrange multipliers $\hat{\Lambda}_A$ from the solution (see Appendix A) of the linear system

$$F_A-F_A|_E=-\sum_{s=0}^{M}\sum_{m=0}^{N}\hat{\Lambda}^{(m)}_{\langle i_1 i_2\cdots i_s\rangle}\times\int\psi_A(k)k^{2m}k_{\langle i_1}k_{i_2}\cdots k_{i_s\rangle}d\vec{k}. \tag{17}$$

Once the distribution function is obtained, the constitutive functions $\{G_A,P_A\}$ can be determined through their kinetic expressions. As a matter of fact, by evaluating the integrals

$$F_{(N+1)|\langle i_1\cdots i_{r-1}\rangle}=\int\varepsilon^{N+1}u_{\langle i_1}\cdots u_{i_{r-1}\rangle}\mathcal{F}d\vec{k},$$

$$F_{(p)|\langle i_1\cdots i_M k\rangle}=\int\varepsilon^{p}u_{\langle i_1}\cdots u_{i_M}u_{k\rangle}\mathcal{F}d\vec{k},$$

to first order in the nonequilibrium variables $\{\Delta_{(p)},F_{(p)|\langle i_1\cdots i_n\rangle}\}$, for the G_A it is

$$F_{(N+1)}=n\frac{(2N+3)!!}{3^{N+1}}\left(\frac{W}{n}\right)^{N+1}+\sum_{l=2}^{N}\chi^{(1)}_{(N+1)l}\Delta_{(l)}, \tag{18}$$

$$F_{(N+1)|\langle i_1\cdots i_{r-1}\rangle}=\sum_{l=0}^{N}\chi^{(r)}_{(N+1)l}F_{(l)|\langle i_1\cdots i_{r-1}\rangle},\quad \text{for } r=2,\ldots,M \tag{19}$$

$$F_{(p)|\langle i_1\cdots i_M k\rangle}=0,\quad \text{for } p=0,\ldots,N, \tag{20}$$

where the coefficents $\chi^{(r)}_{(N+1)l}$ are functions of $\{n,W\}$ as reported in Appendix A.

To evaluate the collisional productions in Eq. (8) we use the collision rate for intravalley transitions with acoustic modes (within the elastic and energy-equipartition approximations)

$$S_{ac}(\vec{k},\vec{k}')=2\frac{\pi E_l^2K_BT_0}{\hbar V\rho U_l^2}\delta[\varepsilon(\vec{k}')-\varepsilon(\vec{k})], \tag{21}$$

and for intervalley transitions with acoustic and nonpolar optical modes

$$S_\eta(\vec{k},\vec{k}')=\frac{\pi\Delta_\eta^2}{V\rho\omega_\eta}\left[N_\eta+\frac{1}{2}\pm\frac{1}{2}\right]\delta\{\varepsilon(\vec{k}')-[\varepsilon(\vec{k})\pm\hbar\omega_\eta]\}, \tag{22}$$

where E_l is the acoustic deformation potential parameter, ρ the crystal density, U_l the longitudinal sound velocity, Δ_η the intervalley deformation potential, ω_η the phonon angular frequency, N_η the phonon distribution, with the $\pm$ options corresponding to emission and absorption processes, respectively. By using the linear expansion of the distribution function and inserting Eqs. (2), (21), and (22) in Eq. (8) we obtain

$$P_{(0)}=0,\quad P_{(p)}=-P^0_{(p)}-\sum_{l=2}^{N}\alpha^{(0)}_{pl}\Delta_{(l)}\ \text{ for }\ p=1,\ldots,N, \tag{23}$$

$$P_{(p)|\langle i_1\cdots i_s\rangle}=-\sum_{l=0}^{N}\alpha^{(s)}_{pl}F_{(l)|\langle i_1\cdots i_s\rangle}\ \text{ for }\ p=0,1,\ldots,N;\quad s=1,2,\ldots,M, \tag{24}$$

where $\{P^0_{(p)},\alpha^{(s)}_{pl}\}$ are functions of $\{n,W\}$ and of scattering parameters as reported in Appendix A. In closing we note that, the *linearized* maximum entropy approach used in this section is closely related to the Grad moment method,[32,33] where the nonequilibrium distribution function is expanded in terms of Hermite polynomials. By contrast, a higher-order expansion of Eq. (14) would clearly differ from the corresponding one in Grad's method. Nevertheless, within the present level of approximation, it is possible to proceed using directly a quadratic expansion of entropy, with the constraints (4), to obtain equivalent results (see, for example, Ref. 34).

V. TRANSITION TO STANDARD HD MODELS AND FOURIER LAW

In this section we show that, under appropriate conditions, the present HD approach recovers the standard nonequilibrium thermodynamic relations, characterized only by the first five moments of the distribution function $\{n,v_i,W\}$ and by the electric field E_i. Using these variables, as observable fields, it is possible to develop a reduction scheme in which all higher moments can be expressed in terms of the basic fields and their derivatives. Classical examples of reduction schemes, widely applied in literature, are the Chapman-Enskog expansion[35–37] and the Maxwellian iteration procedure.[17,33,36,38–40] Although there is no general convergence proof, here we use an iterative procedure analogous to the Maxwellian iteration because it can be easily implemented in a systematic way. As a simplified case, we start considering Eqs. (16), (18)–(20), and (23)–(24) calculated for $N=M=1$. In this way we obtain the usual balance equations for the quantities $\{n,W,v_i,S_i\}$, which together with Poisson's equation write:

$$\frac{\partial n}{\partial t}+\frac{\partial nv_k}{\partial x_k}=0, \tag{25}$$

$$\frac{\partial W}{\partial t}+\frac{\partial S_k}{\partial x_k}=-nev_lE_l-\nu_{\mathbf{w}}(W-W_0), \tag{26}$$

$$\frac{\partial nv_i}{\partial t}+\frac{\partial}{\partial x_i}\left\{\frac{2}{3}\frac{1}{m^*}W\right\}=-\frac{ne}{m^*}E_i-\alpha_{\mathbf{v}}nv_i-\beta_{\mathbf{v}}\frac{n}{W}S_i, \tag{27}$$

$$\frac{\partial S_i}{\partial t}+\frac{\partial}{\partial x_i}\left\{\frac{10}{9}\frac{n}{m^*}\left(\frac{W}{n}\right)^2\right\}=-\frac{5}{3}\frac{e}{m^*}WE_i-\alpha_{\mathbf{s}}Wv_i-\beta_{\mathbf{s}}S_i, \tag{28}$$

$$\varepsilon\Delta\phi=e(N_D-n), \tag{29}$$

where ϕ and N_D are the electrical potential and the fixed donor concentration, respectively, $\vec{E}=-\vec{\nabla}\phi$, the quantities $\{\nu_{\mathbf{w}},\alpha_{\mathbf{v}},\beta_{\mathbf{v}},\alpha_{\mathbf{s}},\beta_{\mathbf{s}}\}$ are average collision rates expressed as a function of electron energy whose explicit expressions are reported in Appendix A.

The set of Eqs. (25)–(27) and (29) correspond to the standard HD model that can be closed in a self-consistent way by determining an expression for the energy flux S_i as a function of the independent variables $\{n,v_i,W,E_i\}$. To obtain a constitutive relation for S_i we take the remaining Eq. (28) and, in the first iteration, we calculate at equilibrium the left-hand side of this equation. Then we get the first iterated values of S_i on the right-hand side of the same equation as

$$S_i=-\frac{10}{9}\frac{1}{\beta_{\mathbf{s}}}\frac{\partial}{\partial x_i}\left\{\frac{n}{m^*}\left(\frac{W}{n}\right)^2\right\}-\frac{5}{3}\frac{e}{m^*}\frac{W}{\beta_{\mathbf{s}}}E_i-\frac{\alpha_{\mathbf{s}}}{\beta_{\mathbf{s}}}Wv_i. \tag{30}$$

This procedure can be generalized (see Appendix B) by taking the complete set of tensorial equations (16) and by applying the above iterative method. If we know the variables $\{n,v_i,W,E_i\}$, then all the remaining $\mathcal{N}-5$ quantities $\{\Delta_{(l)}, F_{(r)|i},\ldots,F_{(p)|\langle i_1 i_2\ldots i_s\rangle}\}$ (with $l=2,\ldots,N$; $r=1,\ldots,N$, $p=0,\ldots,N$, and $s=2,\ldots,M$) can be expressed in terms of basic fields and their gradients. In this way, the first iterated values depends on $\{n,v_i, W, E_i, \partial n/\partial x_i, \partial W/\partial x_i\}$ while the second iterated values include terms in the second derivatives and so on. In particular, by considering the case $M=1$, it is possible to obtain a system of N equations [Eq. (B11)] for the N unknown vectorial variables $\{F_{(1)|i}=S_i,\ldots,F_{(r)|i},\ldots,F_{(N)|i}\}$ (see Appendix B)

$$\sum_{r=1}^{N}\alpha_{pr}^{(1)}F_{(r)|i}=-\alpha_{p0}^{(1)}nv_i-\frac{(2p+3)!!}{3^{p+1}}\times\left\{\frac{en}{m^*}\left(\frac{W}{n}\right)^p E_i+\frac{2}{3}\frac{\partial}{\partial x_i}\left[\frac{n}{m^*}\left(\frac{W}{n}\right)^{p+1}\right]\right\}, \tag{31}$$

with $p=1,2,\ldots N$.

By solving this system, each vectorial momentum (starting from the energy flux) can be expressed by a linear combination of: a diffusive term (which depends on $\vec{\nabla}W$ and on $\vec{\nabla}n$), a convective term (which is linear in v_i), and an electric-field term (which is linear in E_i), with the determination of successive approximations to all coefficents (functions of $\{n,W\}$) which depend on the given value of N.

A. Generalization of the Fourier law

An alternative method to obtain a constitutive expression for the energy flux consists in generalizing the standard Fourier equation. Accordingly, from the velocity balance equation we obtain the electric field, and after substitution into all other tensorial Eqs. (16), it is possible to generate a set of equations to which the above iterative procedure (as in Appendix B) can be applied. In this way the explicit dependence on $\vec{E}$ disappears in all the remaining equations and, analogously to the previous section, in the case $M=1$, we obtain a system of N equations for the single-particle variables $\tilde{F}_{(p)|i}=F_{(p)|i}/n$ (with $p=1,2,\ldots,N$)

$$\frac{(2p+3)!!}{3^{p+1}}\tilde{W}^p\sum_{r=0}^{N}\alpha_{0r}^{(1)}\tilde{F}_{(r)|i}-\sum_{r=0}^{N}\alpha_{pr}^{(1)}\tilde{F}_{(r)|i}=\frac{2p}{m^*}\frac{(2p+3)!!}{3^{p+2}}\tilde{W}^p\frac{\partial\tilde{W}}{\partial x_i}. \tag{32}$$

The solution of Eq. (32) enables all the vectorial moments $\tilde{F}_{(p)|i}$ (starting from $\tilde{S}_i$) to be expressed as the sum of a diffusive term (which is linear in $\vec{\nabla}\tilde{W}$) and of a convective term (which is linear in v_i) through relationships that formally resemble a generalized Fourier law[17,41]

$$\tilde{F}_{(p)|i}=-K_{(p,N)}\frac{\partial\tilde{W}}{\partial x_i}+\zeta_{(p,N)}\tilde{W}^p v_i, \quad \text{for } p=1,2,\ldots,N, \tag{33}$$

where the dimensionless quantities $\zeta_{(p,N)}$ and the coefficients $K_{(p,N)}$ depend on the scattering terms, the single-particle energy $\tilde{W}$, and the given number of vectorial moments N. In particular, by considering only the energy flux ($p=1$) we obtain a generalized Fourier law, where the diffusive term has the thermal conductivity $K_{(1,N)}$ as a coefficient. We notice that, by using the iterative procedure previously explained, the explicit dependence on the electric field is removed in all the equations. This allows one to solve the problem at a lower level with respect to the previous one and to obtain for the vectorial moments a Fourier-like law in which the transport coefficients $\{K_{(p,N)},\zeta_{(p,N)}\}$ do not depend explicitly on $\vec{E}$.

VI. APPLICATION TO *n* SILICON

In this section the theory of moments is applied to the case of n-Si. By considering the electric field applied along the $\langle 111\rangle$ crystallographic axes we keep the axial symmetry, and full-band effects are described by introducing an effective mass as a function of the electron total energy as recently reported.[18] Accordingly, we use the HD equations for the first eight moments of the distribution function $\{n,W,v_i,S_i\}$ (e.g., N=M=1) to fit the velocity-field characteristic obtained from MC full-band simulations. For the collisional processes, scattering with phonons of f and g type are considered with six possible transitions ($\eta=g_1,g_2,g_3,f_1,f_2,f_3$). The MC simulations have been performed using a full-band model[42] and analytic nonparabolic-band model.[43] The MC with analytic-band model and the HD calculations made use of the same physical scattering parameters.[43]

A. Homogeneous and stationary conditions

For space homogeneous and stationary conditions the set of Eqs. (16) consists of a system of algebrical equations for

the variables of single-particle $\tilde{F}_A = F_A/n$. When considering only the scalar and vectorial moments (e.g., $M=1$), due to the assumed axial symmetry, it is $\tilde{F}_{(p)|i} = \{\tilde{F}_{(p)|1}, 0, 0\}$, $E_i = \{E, 0, 0\}$, and the balance Eqs. (16) take the form

$$pe\tilde{F}_{(p-1)|1}E + \tilde{P}^0_{(p)} + \sum_{l=2}^{N} \alpha^{(0)}_{pl}\tilde{\Delta}_{(l)} = 0, \quad \text{for } p = 1, \ldots, N, \tag{34}$$

$$\frac{e}{m^*}\frac{2p+3}{3}\tilde{F}_{(p)}E + \sum_{l=0}^{N} \alpha^{(1)}_{pl}\tilde{F}_{(l)|1} = 0, \quad \text{for } p = 0, \ldots, N, \tag{35}$$

where use is made of the closure given in Eqs. (18)–(20) and (23) and (24). In general, the numerical solution of this system allows us to determine the moments as a function of the electric field E and, consequently, to define the *relaxation rates* ν_A associated with the corresponding variables $\tilde{F}_A$. For example, by considering only the quantities $\{\tilde{W}, v, \tilde{S}\}$ (i.e., $N=1$) the system can be solved analytically by means of the relations

$$v = \frac{eE}{m^*}\mathcal{G}(\tilde{W}),$$

$$\tilde{S} = -\frac{eE}{m^*}\frac{\tilde{W}}{\beta_{\mathbf{v}}}[\alpha_{\mathbf{v}}\mathcal{G}(\tilde{W}) + 1], \tag{36}$$

$$\frac{e^2E^2}{m^*}\mathcal{G}(\tilde{W}) + \nu_{\mathbf{w}}(\tilde{W} - \tilde{W}_0) = 0,$$

with

$$\mathcal{G}(\tilde{W}) = \left(\frac{\beta_{\mathbf{s}}}{\beta_{\mathbf{v}}} - \frac{5}{3}\right)\frac{\beta_{\mathbf{v}}}{\beta_{\mathbf{v}}\alpha_{\mathbf{s}} - \beta_{\mathbf{s}}\alpha_{\mathbf{v}}}.$$

These relations enables us to define explicitly the *relaxation rates* $\{\nu_{\mathbf{v}}, \nu_{\mathbf{s}}\}$ for the vectorial moments $\{v, \tilde{S}\}$,

$$\nu_{\mathbf{v}} = -\frac{1}{\mathcal{G}(\tilde{W})},$$

$$\nu_{\mathbf{s}} = \beta_{\mathbf{s}} - \alpha_{\mathbf{s}}\beta_{\mathbf{v}}\left[\frac{\mathcal{G}(\tilde{W})}{\alpha_{\mathbf{v}}\mathcal{G}(\tilde{W}) + 1}\right]. \tag{37}$$

The balance equation for $\{\tilde{W}, v, \tilde{S}\}$, can be rewritten in the standard form

$$evE + \nu_{\mathbf{w}}(\tilde{W} - \tilde{W}_0) = 0,$$

$$\frac{e}{m^*}E + \nu_{\mathbf{v}}v = 0, \tag{38}$$

$$\frac{5}{3}\tilde{W}\frac{e}{m^*}E + \nu_{\mathbf{s}}\tilde{S} = 0.$$

By increasing the number of scalar and vectorial moments (i.e., $N>1$) the system of Eqs. (34) and (35) should be solved numerically.

Figure 1 shows the HD values for $\{v, \tilde{W}, \tilde{S}\}$ as a function of the electric field, calculated by solving Eqs. (34) and (35) (for $N=1$, $N=3$, and $N=5$), both in the parabolic and full-band case. For the velocity, energy, and energy flux we report the MC values of full-band simulations[42] (open circles) and analytic nonparabolic-band simulations[43] (crosses); for the velocity we report also the experimental data, obtained with the microwave time-of-flight (MTOF) technique,[44,45] available up to 130 kV/cm. We note that the HD calculations exhibit small variations (at most within 10 %) from the number of moments used. In any case the numerical results converge for $N=5$ both in the parabolic and full-band case. The

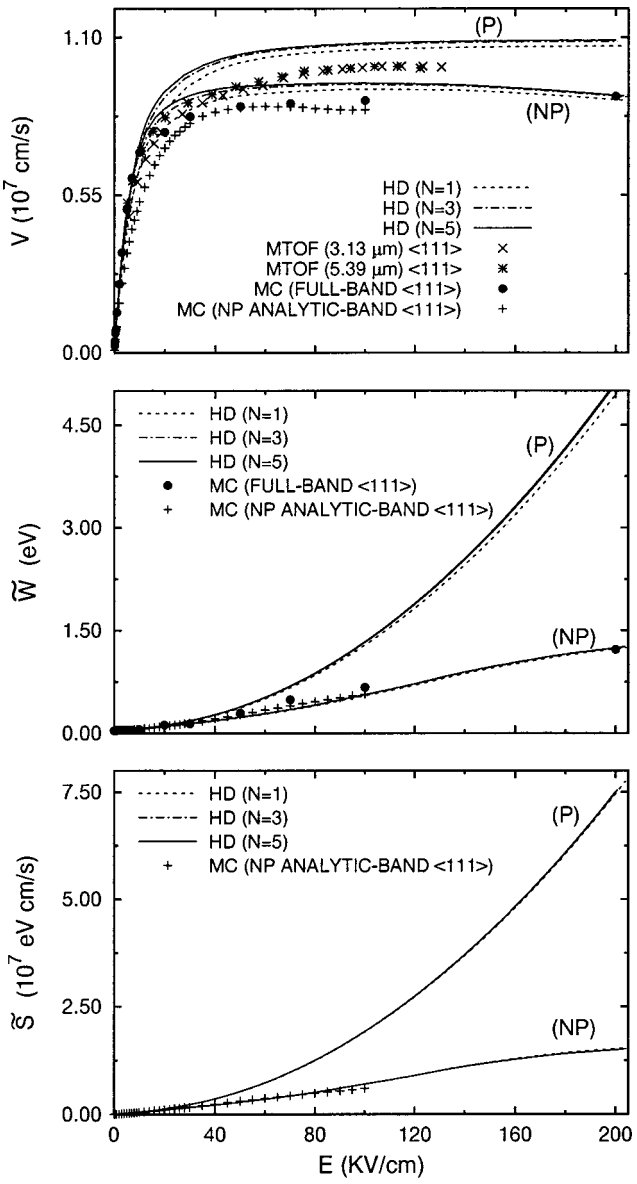

FIG. 1. Drift velocity v, average total-energy $\tilde{W}$, and energy flux $\tilde{S}$ vs electric field for electrons in Si at $T_0 = 300$ K. Lines refer to present parabolic (P) and nonparabolic (NP) HD calculations with $N=1$ (dashed lines), $N=3$ (dash-dotted lines) and $N=5$ (solid lines). Open circles refer to full-band MC simulations performed along $\langle 111\rangle$ crystallographic directions.[42] Crosses refer to analytical nonparabolic-band MC simulations performed along the $\langle 111\rangle$ crystallographic direction.[43] For the drift velocity we report also the experimental data obtained with the microwave time-of-flight technique along the $\langle 111\rangle$ crystallographic direction.[44]

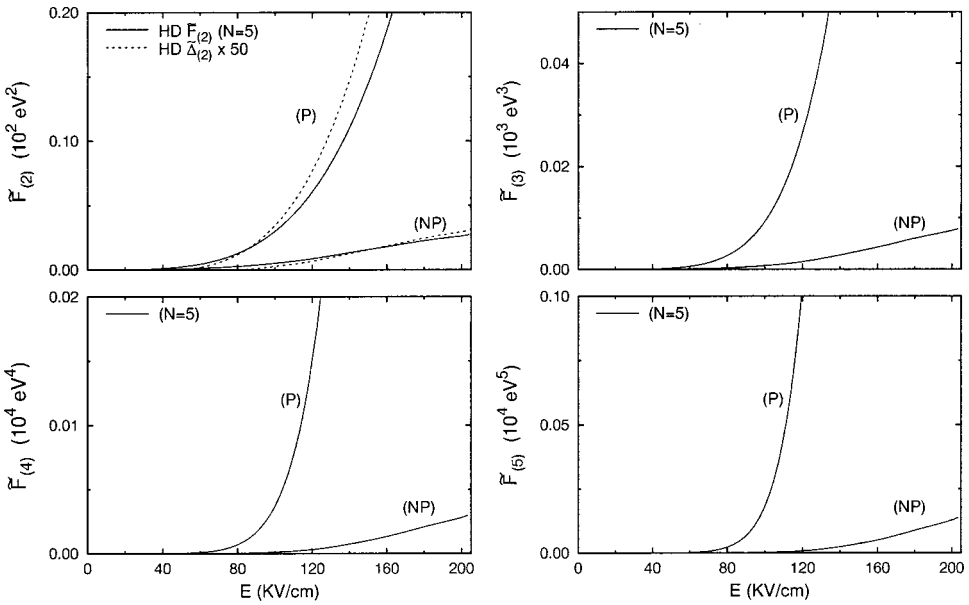

FIG. 2. Scalar moments $\tilde{F}_{(2)},\tilde{F}_{(3)},\tilde{F}_{(4)},\tilde{F}_{(5)}$ [with $\tilde{\Delta}_{(2)}$ the nonequilibrium part of $\tilde{F}_{(2)}$] vs electric field for electrons in Si in the case of parabolic (P) and nonparabolic (NP) band models at $T_0=300$ K.

convergence is particularly evident for the velocity-field curves that give values in close agreement with experimental data. The energy dependence of the effective mass obtained by fitting the velocity-field curve reproduces well the MC data of energy and energy flux, thus providing a valuable check of consistency of the present HD approach.

Figures 2 and 3 show the HD calculations for the remaining scalar $\{\tilde{F}_{(2)},\tilde{F}_{(3)},\tilde{F}_{(4)},\tilde{F}_{(5)}\}$ and vectorial $\{\tilde{F}_{(2)|1},\tilde{F}_{(3)|1},\tilde{F}_{(4)|1},\tilde{F}_{(5)|1}\}$ moments evaluated up to $N=5$ in the parabolic and nonparabolic case, respectively. Figure 2 reports also the $\tilde{\Delta}_{(2)}$ vs electric field to show, as an example, that the contribution of the nonequilibrium part of $\tilde{F}_{(p)}$ is negligible for the evaluation of the scalar moments.

Finally, we note that while the introduction of a greater number of moments yields small differences in the HD numerical results, by contrast the nonparabolicity provokes a strong suppression of all moments at increasing field value. Such a suppression is found to be more effective for higher moments as expected.

B. Linear analysis and response functions

To complete the study of the stationary state, we develop the small signal analysis over steady state for different moments. Being $\tilde{\Delta}_{(p)} \ll \tilde{F}_{(p)}|_E$, from a practical point of view, the scalar moments can be expressed in terms of energy powers [see Eq. (13)]. Accordingly, we will consider only the time evolution of a small perturbation of the average energy and of the vectorial moments $\{\tilde{W},\tilde{F}_{(p)|i}\}$. In this case the corresponding balance equations take the form:

$$\frac{d\tilde{W}}{dt} = -evE - \nu_{\mathrm{w}}(\tilde{W}-\tilde{W}_0), \tag{39}$$

$$\frac{d\tilde{F}_{(p)|1}}{dt} = -\frac{e}{m^*}\frac{(2p+3)!!}{3^{p+1}}\tilde{W}^p E - \sum_{r=0}^{N}\alpha_{pr}^{(1)}\tilde{F}_{(r)|1}, \quad \text{with } p=0,1,\ldots,N. \tag{40}$$

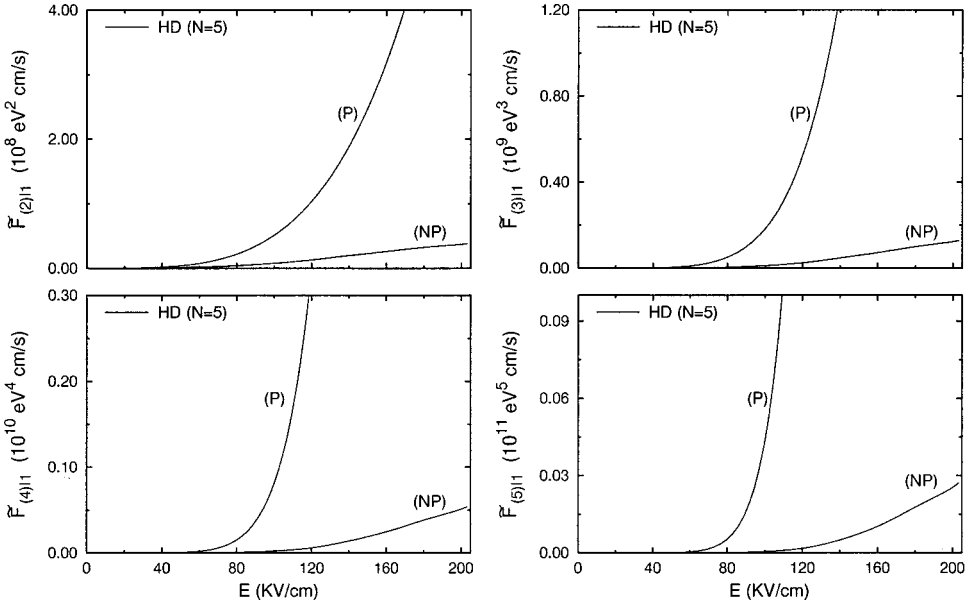

FIG. 3. Vectorial moments $\tilde{F}_{(2)|1},\tilde{F}_{(3)|1},\tilde{F}_{(4)|1},\tilde{F}_{(5)|1}$ vs electric field for electrons in Si in the case of parabolic (P) and nonparabolic (NP) band models at $T_0=300$ K.

By assuming that at the initial time the system of carriers is perturbed by an electric field $\delta E\xi(t)$ [where $\xi(t)$ is an arbitrary function of time satifying $|\xi(t)|\leqslant 1$], we will calculate the deviations from their average values of the energy and the vectorial moments denoted, respectively with $\delta\widetilde{W}(t)$ and $\delta\widetilde{F}_{(p)|1}$. After linearizing Eqs. (39) and (40) around the stationary state, we obtain a system of $N+2$ equations, which can be written in the form

$$\frac{d\Pi_\alpha(t)}{dt}=\Gamma_{\alpha\beta}\Pi_\beta(t)-e\,\delta E\,\xi(t)\Gamma_\alpha^{(E)}. \tag{41}$$

Where the vectors $\{\Pi_\alpha,\Gamma_\alpha^{(E)}\}$ express the quantities

$$\Pi_\alpha=\{\delta\widetilde{W}(t),\delta v(t),\delta\widetilde{S}(t),\delta\widetilde{F}_{(2)|1}(t),\ldots,\delta\widetilde{F}_{(p)|1}(t),\ldots,\delta\widetilde{F}_{(N)|1}(t)\}, \tag{42}$$

$$\Gamma_\alpha^{(E)}=\left\{v,\frac{1}{m^*},\frac{1}{m^*}\frac{5}{3}\widetilde{W},\ldots,\frac{1}{m^*}\frac{(2p+3)!!}{3^{p+1}}\times\widetilde{W}^p,\ldots,\frac{1}{m^*}\frac{(2N+3)!!}{3^{N+1}}\widetilde{W}^N\right\} \tag{43}$$

and with the response matrix $\Gamma_{\alpha\beta}$ given by

$$\Gamma_{\alpha\beta}=\begin{bmatrix}\Gamma_{ww} & -eE & 0 & \cdots & 0 & \cdots & 0\\ \Gamma_{0w} & -\alpha_{00}^{(1)} & -\alpha_{01}^{(1)} & \cdots & -\alpha_{0r}^{(1)} & \cdots & -\alpha_{0N}^{(1)}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ \Gamma_{pw} & -\alpha_{p0}^{(1)} & -\alpha_{p1}^{(1)} & \cdots & -\alpha_{pr}^{(1)} & \cdots & -\alpha_{pN}^{(1)}\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ \Gamma_{Nw} & -\alpha_{N0}^{(1)} & -\alpha_{N1}^{(1)} & \cdots & -\alpha_{Nr}^{(1)} & \cdots & -\alpha_{NN}^{(1)}\end{bmatrix} \tag{44}$$

being

$$\Gamma_{ww}=-\nu_{\mathbf{w}}-\frac{\partial\nu_{\mathbf{w}}}{\partial\widetilde{W}}(\widetilde{W}-\widetilde{W}_0), \tag{45}$$

$$\Gamma_{pw}=-\frac{(2p+3)!!}{3^{p+1}}\widetilde{W}^{p-1}eE\left(\frac{p}{m^*}+\widetilde{W}\frac{\partial(m^*)^{-1}}{\partial\widetilde{W}}\right)-\sum_{r=0}^{N}\frac{\partial\alpha_{pr}^{(1)}}{\partial\widetilde{W}}\widetilde{F}_{(r)|1} \tag{46}$$

with $p=0,1,\ldots,N$.

The relaxation of the system after the perturbation of the electric field is described by the *response matrix* $\Gamma_{\alpha\beta}$. Thus, introducing the standard chord mobility $\mu_0=v/E$, and differential mobility $\mu_0'=dv/dE$ and defining the *moment generalized chord mobility* $\{\mu_1=\widetilde{S}/E,\ \mu_2=\widetilde{F}_{(2)|1}/E,\ldots,\mu_N=\widetilde{F}_{(N)|1}/E\}$ and the *moment generalized differential mobility* $\{\mu_1'=d\widetilde{S}/dE,\ldots,\mu_N'=d\widetilde{F}_{(N)|1}/dE,\ \mu_w'=d\widetilde{W}/dE\}$ the diagonal and off-diagonal quantities of the matrix (44) Γ_{ww},Γ_{pw}, respectively, can be expressed in the form

$$\Gamma_{ww}=eE\frac{\mu_0'+\mu_0}{\mu_w'},\quad \Gamma_{pw}=\sum_{r=0}^{N}\alpha_{pr}^{(1)}\frac{\mu_r'-\mu_r}{\mu_w'}. \tag{47}$$

In this way, from the knowledge of the coefficients $\alpha_{pr}^{(1)}$ and from a numerical evaluation of the quantities μ_r and μ_r' all the elements of the matrix $\Gamma_{\alpha\beta}$ can be calculated. Let us assume that at the initial time $\mathbf{\Pi}(0)=0$. Then, Eq. (41) has the following formal solution[23,46]

$$\mathbf{\Pi}(t)=-e\,\delta E\int_0^t\mathbf{K}(s)\xi(t-s)ds, \tag{48}$$

with $\mathbf{K}(s)=\exp(\mathbf{\Gamma}s)\mathbf{\Gamma}^{(E)}$ that can be determined through the matrix

$$\exp(\mathbf{\Gamma}t)=\mathbf{\Phi}\mathrm{diag}\{\exp(\lambda_1 t),\ldots,\exp(\lambda_{N+2}t)\}\mathbf{\Phi}^{-1}, \tag{49}$$

where λ_α are the eigenvalues of $\Gamma_{\alpha\beta}$ and $\mathbf{\Phi}$ is the matrix of its eigenvectors.

The vector function $\mathbf{K}(t)$ determines the linear response of the moments $\{\widetilde{W},\widetilde{F}_{(p)|i}\}$ to an arbitrary perturbation of the electric field and can be expressed in terms of its components in the form

$$K_\alpha(t)=\{K_w(t),K_v(t),K_s(t),K_2(t),\ldots,K_N(t)\}$$

where $K_w(t),K_v(t)$ and $K_s(t)$ are the *response functions*, respectively for the fluctuations of mean energy, velocity, and energy flux; the remaing components of $\mathbf{K}(t)$ refer to the fluctuations of other vectorial moments.

Since $\Gamma_{\alpha\beta}$ is a $(N+2)\times(N+2)$ not symmetric matrix, the eigenvalues are either real or complex conjugate values. These eigenvalues correspond[23,24] to the *generalized relaxation rate* $-\lambda_\alpha$, which determines the time behavior of the response functions. As a matter of fact, $-\lambda_\alpha$ can be considered as the analog of the energy and vectorial-moments relaxation rates, respectively, even if, strictly speaking, the correspondence between these generalized rates and the respective relaxation processes exist only in the absence of coupling among these variables.[47–49]

Figure 4 reports the generalized relaxation rates obtained using an increasing number of moments (i.e. $N=1,N=3,N$

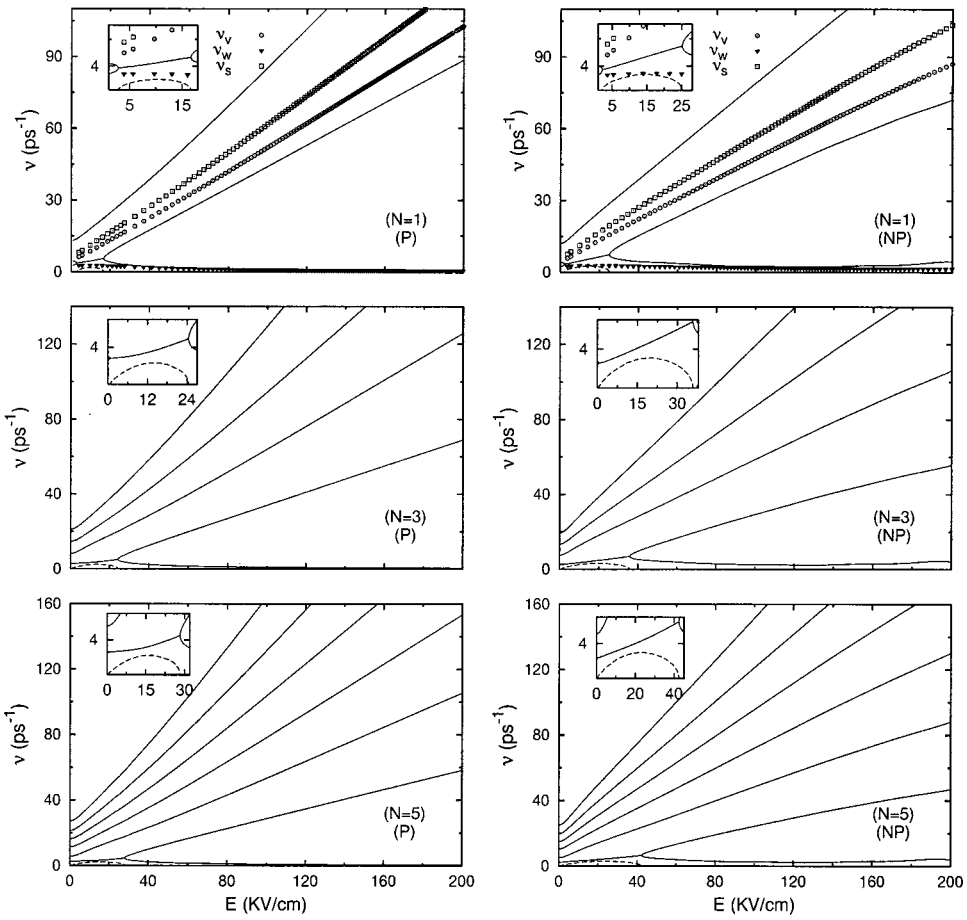

FIG. 4. Rates and eigenvalues of the relaxation matrix as a function of the electric field for electrons in Si in the case of parabolic (P) and nonparabolic (NP) band models at $T_0 = 300$ K. Symbols refer to the velocity $\nu_{\mathbf{v}}$, energy $\nu_{\mathbf{w}}$ and flux energy $\nu_{\mathbf{s}}$ relaxation rates (for $N=1$) respectively. The continuous and the dashed lines (better evidenced in the inserts) refer to the real part and the imaginary part of the eigenvalues evaluated for $N=1$, $N=3$, and $N=5$.

$=5$), both in the parabolic and nonparabolic case, respectively. As a general trend, the higher the moment the larger is the relaxation rate. Velocity and energy relaxation rates are coupled by the electric field and exhibit complex values in the low-field region. All rates, but energy, increase with increasing field, the steeper and the higher the moment is. The net effect of nonparabolicity is to systematically suppress the increase of all moments with field. These general behaviors are understood from a microscopic point of view by scattering processes that increase their efficiency at increasing carrier energy. The interesting feature of this approach is to provide an analytical theory able to simultaneously describe the response of all these moments under conditions very far from equilibrium. For the sake of comparison, in the case $N=1$, we report also the relaxation rates $\{\nu_{\mathbf{w}}, \nu_{\mathbf{v}}, \nu_{\mathbf{s}}\}$ calculated from Eqs. (37) and (A10)–(A14). The results show two distinct behaviors at increasing electric fields. A first one is associated with small and intermediate values of the electric field, in which there are a couple of complex conjugate eingenvalues due to the strong coupling between velocity and energy relaxation.[23,24] A complex eigenvalue indicates the presence of some kind of deterministic relaxation[48,49] in the system that can be attributed to a streaming character of the distribution function. In the present case, the joint action of electric field and emission of intervalley phonons is known to produce the condition of *streaming motion*.[45,50] A second region, corresponds to the highest electric field, where the eigenvalues become real. At these high fields, energy thermalization of the carrier system becomes so efficient that any deterministic character is washed out and the transport takes a full chaotic character attributed to a nearly isotropic (but heated) distribution function.

From Fig. 4 we note that the width of the region with complex values of the eigenvalues depends both on the increasing number of moments used and on the nonparabolicity. Indeed, in both cases we found that the eigenvalues are squeezed towards lower values with the consequent extension of the coupling region. For the time evolution of velocity and carrier energy, the eigenvalues of the relaxation matrix have been explicitly evaluated in analytical form,[23] using the MC data as input parameters. Therefore, by analyzing the extention of the region where the velocity and energy relaxations are strongly coupled, we observe that, in the nonparabolic case, the agreement between present results and those reported in Ref. 23 is within a factor of 2 for N=1 and improves significantly to within 20% for $N=5$.

Figure 5 reports the time dependence of the linear-response function, respectively, of velocity $K_v(t)$, energy $K_w(t)$, and energy flux $K_s(t)$ for $\{N=1, N=5\}$ at increasing electric fields. Values are calculated from Eqs. (43),(44),(47), and (49) and using the HD numerical results reported in Figs. 1–3. As a general trend, from Fig. 5 we notice that the increase in the number of moments yields small differences in the shape of the response function at any field value. By contrast, the nonparabolicity is responsible for a significant decrease of the response functions at short times; such a decrease becomes more pronounced at higher values of the electric field. This is particularly evident for $K_w(t)$ and $K_s(t)$

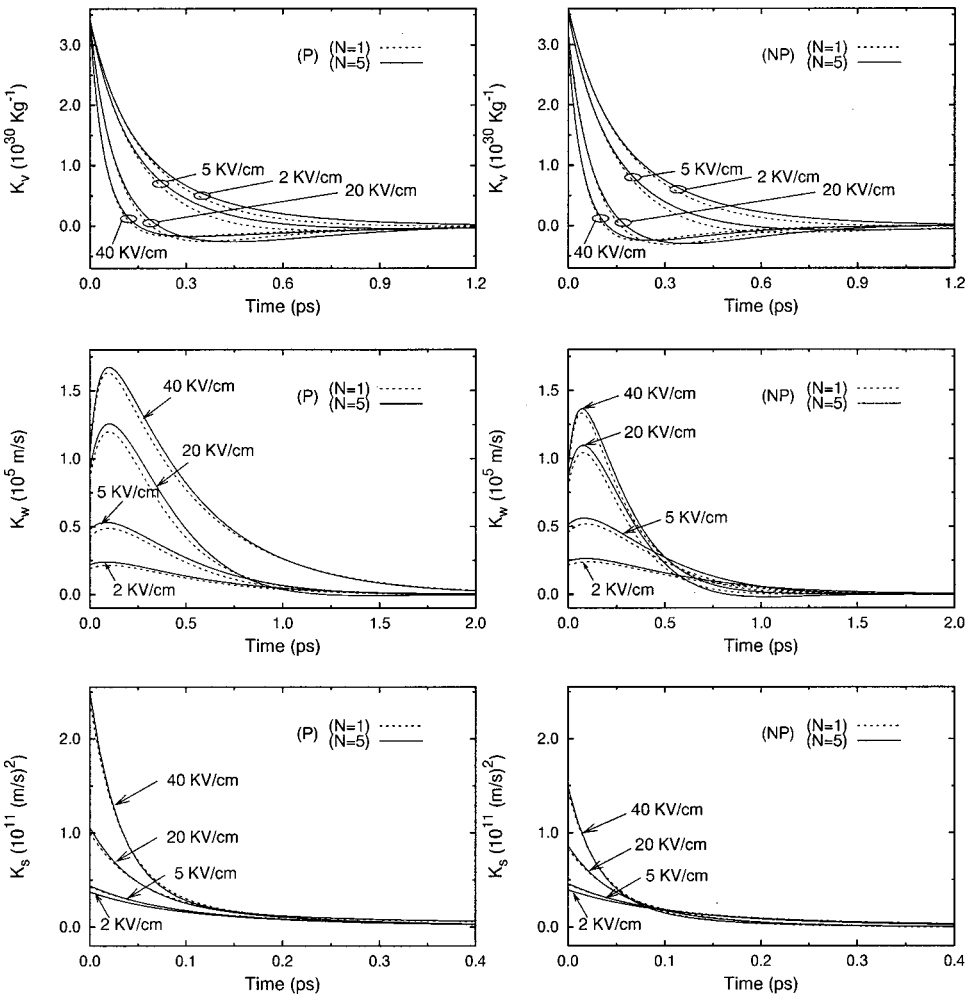

FIG. 5. Response functions $\{K_v, K_w, K_s\}$ vs time for electrons in Si in the case of parabolic (P) and nonparabolic (NP) band models at $T_0=300$ K and increasing electric fields $E=2$ kV/cm, $E=5$ kV/cm, $E=20$ kV/cm, and $E=40$ kV/cm. The dashed and the continuous lines refer to $N=1$ and to $N=5$, respectively.

at 20 kV/cm and 40 kV/cm and is associated with the fact that, with respect to the parabolic case, the nonparabolicity decreases the values of both the inverse effective mass and the average carrier energy (see Fig. 1 for $\tilde{W}$ and $\tilde{S}$), and thus reduces the value of the response function of the corresponding moment. The decay with time of the response functions is controlled essentially by the momentum and energy relaxation rates. The presence of the electric field couples the two relaxations processes, thus provoking a nonexponential shape of the decay. For the response function K_v, at the shortest times, a negative part is found at 20 and 40 kV/cm, which is associated with the above coupling between velocity and energy relaxation.[50] At increasing fields, the response function K_w clearly evidences the coupling between velocity and energy relaxation through a nonmonotonic behavior with a maximum that separates the velocity from the energy relaxation.[51] Finally, we note that K_s decays similarly but faster than K_v. A similar behavior is expected for all vectorial moments, with the natural tendency of a faster decrease the higher the order of the moment involved.

C. Energy flux in nonhomogeneous conditions

As a test to validate the constitutive relations, expressed through the Eqs. (31) and Eq. (33), obtained in Sec. V for the energy flux, we apply the present theory to a one-dimensional 0.1-0.4-0.1 μm n^+nn^+ Si structure with doping levels $n^+=5\times10^{17}$ cm^{-3} and $n=2\times10^{15}$ cm^{-3}, $T_0=300$ K, applied voltage respectively of 0.5 V, 1 V, and 1.5 V. The analytical results are then compared with MC simulations performed with nonparabolic models.[41,52] By using the spatial profiles of $\{n, W, v, E\}$ obtained from MC simulations, for $N=1$ we have calculated the energy flux from Eq. (30); while for $N>1$ the energy flux $\tilde{S}$ is determined by resolving the system of Eqs. (31). Starting from the above relations, the energy flux can be conveniently decomposed, respectively, in a diffusive term, a convective term, and an electric-field term. To analyze the contribution due to each term, Fig. 6 reports their spatial profiles calculated for $N=1$ and $N=5$. The contribution of the diffusive term is maximum near the cathode homojunctions, where it compensates the spike of the electric-field term. In the *n* region the main contributions are due to the convective and field terms, whose values, even if they separately depend on *N*, keep their sum practically constant in the *n*-region. Near the anode homojunction, at the highest voltage considered of 1.5 V, the diffusive term exhibits a spike that leads to overestimate the total-energy flux. As a matter of fact, in this region the constitutive relations obtained for $\tilde{S}$ give values greater than those directly calculated by MC simulations. The total constitutive relation for the energy flux is thus well verified in all points of the structure except for the region strictly adjacent to the anode junction where both the electric field and its gradient exhibit very high values. Here the energy flux shows a peak that

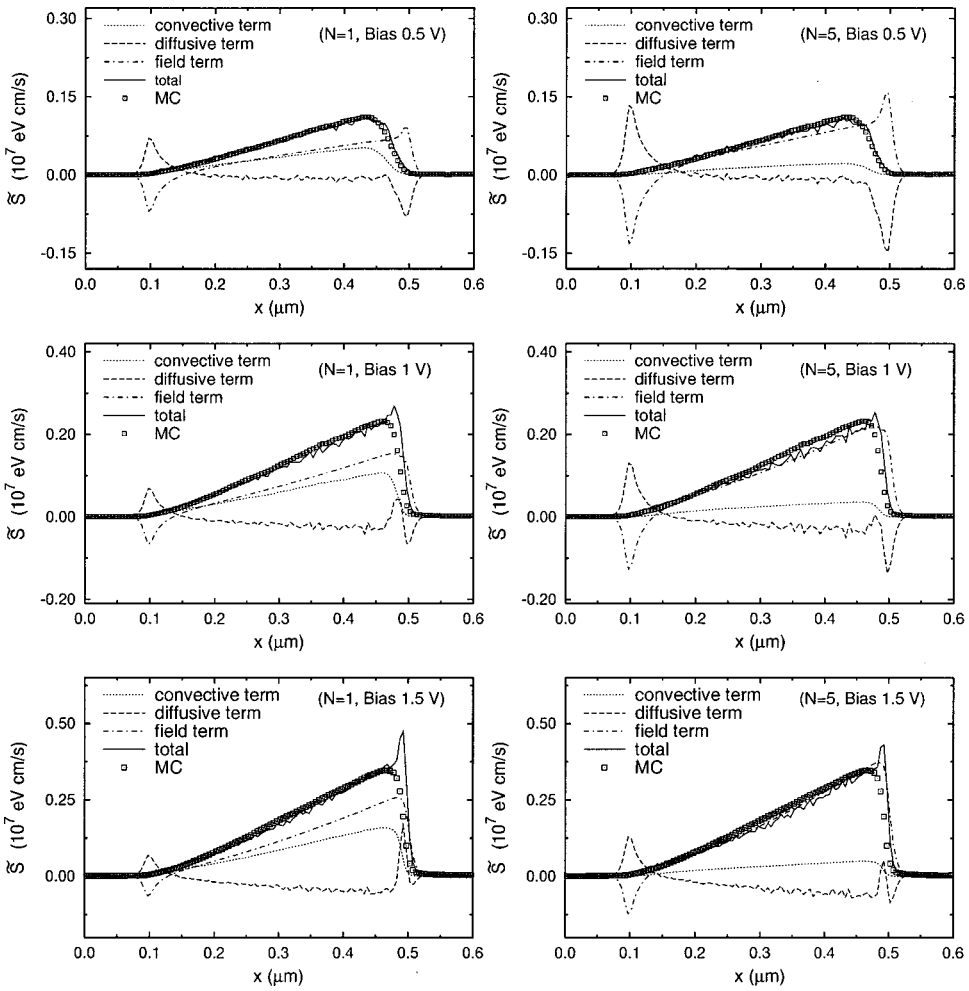

FIG. 6. Spatial profile of energy flux $\tilde{S}$ for a n^+nn^+ Si structure with a channel length of 0.4 μm, $n^+=5\times10^{17}$ cm^{-3}, $n=2\times10^{15}$ cm^{-3} and applied voltages of, respectively, 0.5 V, 1 V, and 1.5 V. Symbols refer to an explicit evaluation of the energy flux making use of data obtained from nonparabolic MC simulations.[41,52] Curves refer to results obtained from the constitutive functions (dotted lines for the convective term, dashed lines for the diffusive term, dash-dotted lines for the field term and continuous lines for the total) by substituting in Eq. (30) (for $N=1$) and in Eq. (31) (for $N=5$) the values of $\{n,W,v,E\}$ obtained from MC data.

tends to reduce by increasing the number of moments N [see Fig. 7(a)]. We remark, that for a more rigorous approach, it is necessary to implement a nonlinear theory for the constitutive relations. Indeed, the present approach is based on a linearization of the distribution function that implies a modellization of constitutive relations strictly valid only in the limit of small gradients. From HD calculations it was observed[15–18] that only with a nonlinear description of the distribution function it is possible to improve significantly the agreement with MC simulations even in proximity of the critical regions adiacent to the homojunctions. Overall, the agreement between the HD and MC results is considered to be satisfactory, thus validating the constitutive relations presented here within the limits described above.

Finally, Fig. 7(b) reports the spatial profile of the energy flux for the device with the highest bias of 1.5 V, calculated with the generalized Fourier law given in Eq. (33), for $N=1$ and $N=5$, respectively. We have found that the agreement between HD and MC results near the anode homojunction becomes less satisfactory when compared to similar results in Fig. 7(a). As a matter of fact, a very high spike is observed in the spatial profile of $\tilde{S}$ that, contrary to expectations, further increases by increasing the number of moments. These unexpected results are due to the fact that, fol-

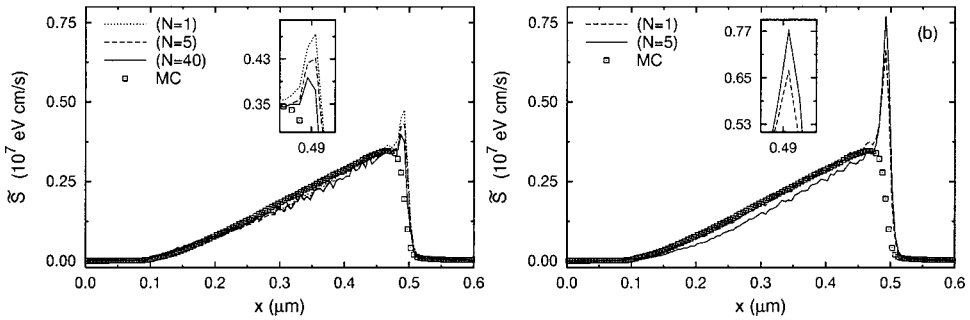

FIG. 7. Spatial profile of the energy flux $\tilde{S}$ as in Fig. (6) for an applied voltage of 1.5 V. Symbols refer to an explicit evaluation of the energy flux directly obtained from MC simulations. Curves refer to results obtained from the constitutive functions obtained using Eqs. (31) (on the left) with $N=1$, $N=5$, and $N=40$ and using the generalized Fourier law of Eq. (33) (on the right) with $p=1$, $N=1$, and $N=5$.

lowing the iterative procedure described in Sec. V A, the explicit dependence on the electric field has been removed in the balance equation for the vectorial moments. This further approximation allows us to solve the problem at a low level and to obtain a Fourier-like law with a diffusive term in which the thermal conductivity (not depending explicitely from the electric field) is overestimated in the *n* region near the anode homojunction. This drawback is already known in the literature and has been recently considered in Ref. 53. Here, the presence of different time scales for the velocity, energy, and energy fluxes all depending on the local-field strength, was proved to be of major importance in trying to generalize the thermal conductivity under hot-carrier conditions.

VII. CONCLUSIONS

By means of generalized kinetic fields we have developed a general formulation of the maximum entropy principle within a total energy scheme and including the contribution of higher moments of the distribution function. A new system of generalized hydrodynamic equations is derived with the full complexity of the band modeled in terms of a single particle with an effective mass that is a function of the average total energy. From the knowledge of the effective mass, which becomes a new constitutive function, and of the physical constants of the bulk materials all other constitutive functions are determined. Present hydrodynamic theory thus does not need other adjustable parameters but, for a kinetic level, the knowledge of the elementary microscopic interactions. The set of equations so introduced is proven to be sufficient to describe the relevant transport properties of electrons in the bulk material. Accordingly, stationary and small signal kinetic coefficients are consistently obtained as a function of the external electric field. In the context of the small signal analysis we have introduced a generalized *response matrix* and evaluated numerically the linear *response functions* of the different moments in the time domain. The validity of this approach has been confirmed by the satisfactory agreement with the numerical results of full-band Monte Carlo simulations and available experimental data for the case of electrons in Si (bulk and n^+nn^+ structures) at $T_0=300$ K. In particular, we have provided a generalization of the Fourier law for the thermal conductivity of hot carriers in the small gradient limit, indicating the possibility for a further extension within a nonlinear expansion of the distribution function. We notice that, although the general closure scheme (with an arbitrary number of moments) is obtained using a linearized maximum entropy method, the maximum entropy formalism can be developed also in a nonlinear context using both the collision integral [Eqs. (21)–(22)] and the fixed most important macroscopic variables $\{n, W, v_i, S_i, F_{(0)|\langle ij\rangle}\}$.[15–18] We believe that the present hydrodynamic method can be fruitfully applied to describe transport properties of hot carriers having the relevant advantage of providing a closed analytical approach and a reduced computational effort with respect to other competitive numerical methods at a kinetic level.

ACKNOWLEDGMENTS

Dr. M. V. Fischetti, Dr. T. Gonzalez, and Dr. M. J. Martin are thanked for providing the MC data. Partial support from MADESS II project of the Italian National Research Council (CNR) is gratefully acknowledged.

APPENDIX A

By resolving the system of Eqs. (17) and defining the elements of matrix $A_{ml}^{(s)}$ through the relation

$$(A_{ml}^{(s)})^{-1}=\frac{[2(m+l+s)+1]!!}{2^{m+l+s+1}}, \tag{A1}$$

we obtain the general expressions for the scalars $\hat{\Lambda}^{(m)}$ and the tensorial $\hat{\Lambda}^{(m)}_{\langle i_1 i_2 \cdots i_s\rangle}$ Lagrange multipliers

$$\hat{\Lambda}^{(m)}=-\frac{1}{2n}\left(\frac{\hbar}{m^*}\right)^{2m}\left(\frac{3}{4}\frac{nm^*}{W}\right)^m\sum_{l=2}^{N}A_{ml}^{(0)}\left(\frac{3}{2}\frac{n}{W}\right)^l\Delta_{(l)}, \tag{A2}$$

$$\hat{\Lambda}^{(m)}_{\langle i_1 i_2 \cdots i_s\rangle}=-\frac{1}{2n}\frac{(2s+1)!!}{s!}\left(\frac{\hbar}{m^*}\right)^{2m+s}\left(\frac{3}{4}\frac{nm^*}{W}\right)^{m+s}\times\sum_{l=0}^{N}A_{ml}^{(s)}\left(\frac{3}{2}\frac{n}{W}\right)^l F_{(l)|\langle i_1 i_2 \cdots i_s\rangle}, \tag{A3}$$

$$\text{for } m=0,1,\ldots,N \text{ and } s=1,2,\ldots,M.$$

The coefficents $\chi^{(r)}_{(N+1)l}$ entering the constitutive relations given by Eqs. (18) and (19) are

$$\chi^{(r)}_{(N+1)l}=\sum_{m=0}^{N}\frac{[2(N+m+r)+1]!!}{2^{N+m+r+1}}A_{ml}^{(r-1)}\left(\frac{2}{3}\frac{W}{n}\right)^{N+1-l}, \tag{A4}$$

$$\text{for } r=1,2,\ldots,M.$$

The quantities $\{P^0_{(p)},\alpha^{(s)}_{pl}\}$ entering the collisional productions of Eqs. (23) and (24) are

$$P^0_{(p)}=4\left(\frac{2}{3}\frac{W}{n}\right)^{p+2}\sum_{\eta}\mathcal{A}_\eta\sum_{k=0}^{p-1}\binom{p}{k}(2X_\eta)^{p-k}\times[N_\eta H^-_{2k+1}+(-1)^{p-k}(N_\eta+1)H^+_{2k+1}], \tag{A5}$$

$$\alpha^{(0)}_{pl}=\frac{2}{n}\left(\frac{2}{3}\frac{W}{n}\right)^{p-l+2}\sum_{\eta}\mathcal{A}_\eta\sum_{m=0}^{N}A_{ml}^{(0)}\sum_{k=0}^{p-1}\binom{p}{k}(2X_\eta)^{p-k}\times[N_\eta H^-_{2(k+m)+1}+(-1)^{p-k}(N_\eta+1)H^+_{2(k+m)+1}] \tag{A6}$$

$$\alpha^{(s)}_{pl}=-\frac{2}{n}\left(\frac{2}{3}\frac{W}{n}\right)^{p-l+2}\sum_{\eta}\mathcal{A}_\eta\sum_{m=0}^{N}A_{ml}^{(s)}\times[(N_\eta+1)H^+_{2(m+p+s)+1}+N_\eta H^-_{2(m+p+s)+1}]+\frac{1}{2}\left(\frac{2}{3}\frac{W}{n}\right)^{p-l-1}\xi\sum_{m=0}^{N}(m+p+s+1)!A_{ml}^{(s)}, \tag{A7}$$

$$\text{for } s=1,2,\ldots,M$$

with

$$A_\eta=-\frac{n}{\hbar^3}\left(\frac{3}{4}\frac{m^*}{\pi}\frac{n}{W}\right)^{3/2}\frac{\Delta_\eta^2}{\rho\omega_\eta}Z_\eta X_\eta,\quad X_\eta=\frac{3}{4}\hbar\omega_\eta\frac{n}{W},$$

$$\xi=\frac{E_l^2K_BT_0}{\hbar^4\rho U_l^2}\left(\frac{4}{3}\frac{m^*}{\pi}\frac{W}{n}\right)^{3/2},$$

where Z_η is the number of equivalent valleys that are possible final states and the dimensionless quantities $H_{2r+1}^{\pm}$ are expressed through the modified Bessel functions of second kind K_1 and K_2. By defining $G^{\pm}=X_\eta\exp(\mp X_\eta)K_2(X_\eta)$ and $H_1^{\pm}=\exp(\mp X_\eta)K_1(X_\eta)$ we have, in general, that

$$H_3^{\pm}=\pm X_\eta H_1^{\pm}+G^{\pm}, \tag{A8}$$

$$H_{2r+1}^{\pm}=\pm 2X_\eta H_{2r-1}^{\pm}\pm(r+1)!\times\left[\sum_{n=1}^{r-2}\frac{3X_\eta H_{2n+1}^{\pm}}{(n+3)!}\pm\frac{G^{\pm}}{2}\right]\ \text{with}\ r\geqslant 2. \tag{A9}$$

We note that the collisions with intravalley acoustic phonon, being considered as elastic processes, lead the scalar moments to relax more slowly than other dynamical variables $\{F_{(p)|\langle i_1\cdots i_n\rangle}\}$. In this way, in local thermodynamic equilibrium all collisional productions vanish except the quantities $P_{(p)}|_E=-P_{(p)}^0$. By using Eq. (A5) it is possible to verify, also that the production $P_{(p)}$ cancels out only when thermal equilibrium condition is achieved (i.e., $\Delta_{(p)}=F_{(p)|\langle i_1\cdots i_s\rangle}=0$ and $W=3/2nK_BT_0$).

The average collision rates $\{\nu_{\mathbf{w}},\alpha_{\mathbf{v}},\beta_{\mathbf{v}},\alpha_{\mathbf{s}},\beta_{\mathbf{s}}\}$ entering the relations (25)–(30) and (36)–(37) are

$$\alpha_{\mathbf{v}}=-\frac{16}{27}\sum_\eta\tilde{\mathcal{A}}_\eta\{7[(N_\eta+1)H_3^+ +N_\eta H_3^-]-2[(N_\eta+1)H_5^+ +N_\eta H_5^-]\}+\tilde{\xi}, \tag{A10}$$

$$\beta_{\mathbf{v}}=-\frac{16}{9}\sum_\eta\tilde{\mathcal{A}}_\eta\left\{-[(N_\eta+1)H_3^+ +N_\eta H_3^-]+\frac{2}{5}[(N_\eta+1)H_5^+ +N_\eta H_5^-]\right\}+\frac{3}{5}\tilde{\xi}, \tag{A11}$$

$$\nu_{\mathbf{w}}=-\frac{64}{27}\frac{W}{W-W_0}\sum_\eta\tilde{\mathcal{A}}_\eta X_\eta[(N_\eta+1)H_1^+ -N_\eta H_1^-], \tag{A12}$$

$$\alpha_{\mathbf{s}}=-\frac{32}{81}\sum_\eta\tilde{\mathcal{A}}_\eta\{7[(N_\eta+1)H_5^+ +N_\eta H_5^-]-2[(N_\eta+1)H_7^+ +N_\eta H_7^-]\}-2\tilde{\xi}, \tag{A13}$$

$$\beta_{\mathbf{s}}=-\frac{32}{27}\sum_\eta\tilde{\mathcal{A}}_\eta\left\{-[(N_\eta+1)H_5^+ +N_\eta H_5^-]+\frac{2}{5}[(N_\eta+1)H_7^+ +N_\eta H_7^-]\right\}+\frac{18}{5}\tilde{\xi}, \tag{A14}$$

with

$$\tilde{\mathcal{A}}_\eta=-\frac{(m^*)^{3/2}\tilde{W}^{1/2}}{\hbar^3}\left(\frac{3}{4\pi}\right)^{3/2}\frac{\Delta_\eta^2}{\rho\omega_\eta}Z_\eta X_\eta,$$

$$\tilde{\xi}=(m^*)^{3/2}\tilde{W}^{1/2}\frac{E_l^2K_BT_0}{\hbar^4\rho U_l^2}\left(\frac{4}{3\pi}\right)^{3/2}.$$

APPENDIX B

From the knowledge of the constitutive relations (18)–(20), (23)–(24), and (A5)–(A7), we can separate the closed system of field Eqs. (16) in two sets. The first set represents the usual balance equations for the variables $\{n,W,v_i\}$ coupled with Poisson's equation for the electric field E_i

$$\frac{\partial n}{\partial t}+\frac{\partial nv_k}{\partial x_k}=0, \tag{B1}$$

$$\frac{\partial W}{\partial t}+\frac{\partial F_{(1)|k}}{\partial x_k}=-nev_lE_l-P_{(1)}^0-\sum_{l=2}^{N}\alpha_{1l}^{(0)}\Delta_{(l)}, \tag{B2}$$

$$\frac{\partial nv_i}{\partial t}+\frac{\partial}{\partial x_i}\left\{\frac{2}{3}\frac{1}{m^*}W\right\}+\frac{\partial F_{(0)|\langle ik\rangle}}{\partial x_k}=-\frac{ne}{m^*}E_i-\alpha_{00}^{(1)}nv_i-\sum_{l=1}^{N}\alpha_{0l}^{(1)}F_{(l)|i}, \tag{B3}$$

$$\varepsilon\Delta\phi=e(N_D-n). \tag{B4}$$

The second set represents the balance equations for the remaining

$$(N+1)\left[\sum_{i=0}^{M}(2i+1)\right]-5$$

higher moments $\{\Delta_{(l)},F_{(r)|i},\ldots,F_{(p)|\langle i_1i_2\ldots i_s\rangle}\}$

$$\frac{\partial\Delta_{(p)}}{\partial t}+\frac{\partial F_{(p)|k}}{\partial x_k}+\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}\times\left\{(p-1)\left(\frac{W}{n}\right)\frac{\partial nv_k}{\partial x_k}-p\frac{\partial F_{(1)|k}}{\partial x_k}\right\}=-ep\left\{F_{(p-1)|k}-\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}nv_k\right\}E_k+p\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}P_{(1)}^0-P_{(p)}^0+\sum_{l=2}^{N}\left\{p\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}\alpha_{1l}^{(0)}-\alpha_{pl}^{(0)}\right\}\Delta_{(l)},$$

$$\text{for}\ \ p=2,\ldots,N, \tag{B5}$$

$$\frac{\partial F_{(p)|i}}{\partial t}+\frac{1}{3}\frac{\partial}{\partial x_i}\left\{\frac{2}{m^*}F_{(p+1)}\right\}+\frac{\partial F_{(p)|\langle ik\rangle}}{\partial x_k}$$
$$=-epF_{(p-1)|\langle ik\rangle}E_k-\frac{e}{m^*}\frac{2p+3}{3}F_{(p)}E_i$$
$$-\sum_{l=0}^{N}\alpha_{pl}^{(1)}F_{(l)|i},\quad \text{for } p=1,\ldots,N \tag{B6}$$

$$\frac{\partial F_{(p)|\langle i_1 i_2\cdots i_s\rangle}}{\partial t}+\frac{s}{2s+1}\frac{\partial}{\partial x_{i_s\rangle}}\left\{\frac{2}{m^*}F_{(p+1)|\langle\langle i_1\cdots i_{s-1}\rangle}\right\}$$
$$+\frac{\partial F_{(p)|\langle i_1\cdots i_s k\rangle}}{\partial x_k}$$
$$=-epF_{(p-1)|\langle i_1\cdots i_s k\rangle}E_k-\frac{e}{m^*}s\left[\frac{2(p+s)+1}{2s+1}\right]$$
$$\times F_{(p)|\langle\langle i_1\cdots i_{s-1}\rangle}E_{i_s\rangle}-\sum_{l=0}^{N}\alpha_{pl}^{(s)}F_{(l)|\langle i_1 i_2\cdots i_s\rangle},$$
$$\text{for } s=2,\ldots,M;\quad p=0,\ldots,N, \tag{B7}$$

where, the time derivates of the density and of the energy have been eliminated from the scalar Eqs. (B5) through the use of Eqs. (B1)–(B2), and the constitutive relations $G_A=\{F_{(N+1)|\langle i_1\cdots i_{r-1}\rangle},\ F_{(p)|\langle i_1\cdots i_M k\rangle}\}$ is expressed by Eqs. (18)–(20).

We are interested in a theory characterized by the first five moments $\{n,v_i,W\}$ and by the electric field E_i. In this case the quantities $L_A=\{\Delta_{(l)},F_{(r)|i},F_{(0)|\langle ij\rangle}\}$, (with $l=2,\ldots,N$, $r=1,\ldots,N$) present in the balance Eqs. (B2)–(B3) must be expressed in terms of the independent variables $\{n,v_i,W,E_i\}$. In order to get the constitutive relations for the quantities L_A we take the remaining Eqs. (B5)–(B7) and use a method akin to the Maxwellian iteration procedure.[17,33,36,38,39] The first iteration is obtained by inserting the equilibrium values

$$\overset{[0]}{\Delta}_{(l)}=\overset{[0]}{F}_{(r)|i}=\cdots=\overset{[0]}{F}_{(p)|\langle i_1 i_2\cdots i_s\rangle}=0$$

and

$$\overset{[0]}{G}_A=0$$

in the left-hand side of Eqs. (B5)–(B7). In this way, from the right-hand side of Eqs. (B5)–(B7), we obtain a set of equations for the first iterated values $\{\overset{[1]}{\Delta}_{(l)},\overset{[1]}{F}_{(r)|i},\ldots,\overset{[1]}{F}_{(p)|\langle i_1 i_2\cdots i_M\rangle}\}$:

$$\sum_{l=2}^{N}\left\{p\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}\alpha_{1l}^{(0)}-\alpha_{pl}^{(0)}\right\}\overset{[1]}{\Delta}_{(l)}$$
$$+ep\left\{\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}nv_k-\overset{[1]}{F}_{(p-1)|k}\right\}E_k$$
$$+p\frac{(2p+1)!!}{3^p}\left(\frac{W}{n}\right)^{p-1}P_{(1)}^0-P_{(p)}^0=0,$$
$$\text{for } p=2,\ldots,N, \tag{B8}$$

$$\sum_{l=1}^{N}\alpha_{pl}^{(1)}\overset{[1]}{F}_{(l)|i}+\alpha_{p0}^{(1)}nv_i+ep\overset{[1]}{F}_{(p-1)|\langle ik\rangle}E_k+\frac{e}{m^*}\frac{2p+3}{3}$$
$$\times[F_{(p)}|_E+\overset{[1]}{\Delta}_{(p)}]E_i+\frac{1}{3}\frac{\partial}{\partial x_i}\left\{\frac{2}{m^*}F_{(p+1)}\Big|_E\right\}=0,$$
$$\text{for } p=1,\ldots,N, \tag{B9}$$

$$\sum_{l=0}^{N}\alpha_{pl}^{(s)}\overset{[1]}{F}_{(l)|\langle i_1 i_2\cdots i_s\rangle}+\frac{e}{m^*}s\left[\frac{2(p+s)+1}{2s+1}\right]$$
$$\times\overset{[1]}{F}_{(p)|\langle\langle i_1\cdots i_{s-1}\rangle}E_{i_s\rangle}+ep\overset{[1]}{F}_{(p-1)|\langle i_1\cdots i_s k\rangle}E_k=0$$
$$\text{for } s=2,\ldots,M;p=0,\ldots,N \tag{B10}$$

with $F_{(p)|\langle i_1\cdots i_M k\rangle}=0$ for $p=0,\ldots,N$.

We note that, for fixed values of the basic fields $\{n,W,v_i,E_i\}$ and of the gradients $\{\partial n/\partial x_i,\ \partial W/\partial x_i\}$, the set of Eqs. (B8)–(B10) is a linear system of algebrical equations for the first iteration of the remaining variables. Analogously, in the second iteration we substitute into the left-hand side of Eqs. (B5)–(B7) the linear expressions for the G_A describing the quantities $\{\Delta_{(l)},F_{(r)|i},\ldots,F_{(p)|\langle i_1 i_2\cdots i_s\rangle}\}$ by means of the first iteration. In this way, from the right-hand side of Eqs. (B5)–(B7), one obtains a system of equations for the second iterated values $\{\overset{[2]}{\Delta}_{(l)},\overset{[2]}{F}_{(r)|i},\ldots,\overset{[2]}{F}_{(p)|\langle i_1 i_2\cdots i_M\rangle}\}$. With this procedure, the values of the second iteration are more complex than those of the first since the former depend on the second derivatives of the basic fields, but here we consider only the values of the first iteration.

When considering the scalar and vectorial moments (e.g. M=1) we have only the two Eqs. (B8) and (B9) with the constraints $F_{(p)|\langle i_1\cdots i_s\rangle}=0$ for all the tensorial moments. In this case, by assuming that $\Delta_{(p)}\ll F_{(p)}|_E$ (see, for example, the numerical results for the bulk), from the vectorial Eq. (B9) we obtain:

$$\sum_{r=1}^{N}\alpha_{pr}^{(1)}\overset{[1]}{F}_{(r)|i}=-\alpha_{p0}^{(1)}nv_i-\frac{e}{m^*}\frac{2p+3}{3}F_{(p)}|_E E_i$$
$$-\frac{1}{3}\frac{\partial}{\partial x_i}\left\{\frac{2}{m^*}F_{(p+1)}\Big|_E\right\}, \tag{B11}$$

where, in general, the solution of this system suffices to determine *explicitly* the first iteration for all the vectorial moments as functions of the basic fields $\{n,W,v_i,E_i\}$.

[1] K. Blotekjaer, IEEE Trans. Electron Devices **17**, 38 (1970).
[2] A. Forghieri, R. Guerrieri, P. Ciampolini, A. Gnudi, M. Rudan, and G. Baccarani, IEEE Trans. Comput.-Aided Des. **7**, 231 (1988).
[3] R. A. Stewart and J. N. Churchill, Solid-State Electron. **33**, 819 (1990).
[4] D. L. Woolard, H. Tian, R. J. Trew, M. A. Littlejohn, and W. Kim, Phys. Rev. B **44**, 11 119 (1991).
[5] R. Thoma, A. Emunds, B. Meinerzhagen, H. J. Peifer, and W. L. Engl, IEEE Trans. Electron Devices **38**, 13434 (1991).
[6] A. M. Anile and O. Muscato, Phys. Rev. B **51**, 16 728 (1995).
[7] M. Rudan, M. Vecchi, and D. Ventura, in *Mathematical Problems in Semiconductor Physics*, Mathematical Series Pitman research notes, 186 edited by P. Marcati, P. Markowich, and R. Natalini (Longman, 1995).
[8] S. A. Trugman, Phys. Rev. Lett. **57**, 607 (1986).
[9] A. E. Carlsson, Phys. Rev. Lett. **59**, 1108 (1987).
[10] W. Dreyer, H. Struchtrup, Continuum Mech. Thermodyn. **5**, 3 (1993).
[11] H. Struchtrup, Ann. Phys. **257**, 111 (1997).
[12] A. M. Anile and M. Trovato, Phys. Lett. A **230**, 387 (1997).
[13] I. V. Karlin, A. N. Gorban, S. Succi, and V. Boffi, Phys. Rev. Lett. **81**, 6 (1998).
[14] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics*, Springer Tracts in Natural Philosophy, Vol. 37 (Springer-Verlag, New York, 1998).
[15] P. Falsaperla and M. Trovato, VLSI Design **8**, 527 (1998).
[16] M. Trovato and P. Falsaperla, Phys. Rev. B **57**, 4456 (1998); and erratum in *ibid.* **57**, 12 617 (1998).
[17] M. Trovato and L. Reggiani, J. Appl. Phys. **85**, 4050 (1999).
[18] M. Trovato, P. Falsaperla, and L. Reggiani, J. Appl. Phys. **86**, 5906 (1999).
[19] E. T. Jaynes, Phys. Rev. **106**, 620 (1957).
[20] D. N. Zubarev, *Non-equilibrium Statistical Mechanics* (Consultants Bureau, London, 1974).
[21] E. T. Jaynes, in *Papers on Probability, Statistics, and Statistical Physics*, edited by R. D. Rosenkrantz (Reidel, Dordrecht, 1983), pp. 39 and 211.
[22] D. Jou, J. Casas-Vasquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer-Verlag, Berlin, 1996).
[23] V. Gruzhinskis, E. Starikov, P. Shiktorov, L. Reggiani, M. Saranniti, and L. Varani, Semicond. Sci. Technol. **8**, 1283 (1993).
[24] L. Reggiani, E. Starikov, P. Shiktorov, V. Gruzhinskis, and L. Varani, Semicond. Sci. Technol. **12**, 141 (1997).
[25] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. **55**, 645 (1983).
[26] A. Majorana, Transp. Theory Stat. Phys. **20**, 261 (1991).
[27] A. Majorana, Nuovo Cimento Soc. Ital. Fis., B **108**, 871 (1993).
[28] K. Tomizava, *Numerical Simulation of Submicron Semiconductor Devices* (Artech Hous, Boston, 1993).
[29] O. Muscato, in *Progress in Industrial Mathematics at ECMI 96*, 192, edited by M. Brøns, M. P. Bendøe, and M. P. Sørensen (B. G. Teubner, Stuttgart, 1997).
[30] H. M. J. Boots, Phys. Rev. B **46**, 9428 (1992).
[31] For example, introducing the nonparabolicity with the analytic energy-wave-vector relation of kane $\varepsilon(\vec{k})[1+\alpha\varepsilon(\vec{k})] = \hbar k^2/2m^*$ we obtain $\{\gamma,\beta\}$ as numerical solutions of the system

$$\frac{W}{n} = \frac{(24\alpha^2+\beta^2-4\alpha\beta)K_1+(6\alpha\beta-\beta^2)K_0}{(8\alpha^2\beta)K_1+(2\alpha\beta^2)K_0},$$

$$\gamma = \frac{n}{4\pi}\left(\frac{2\alpha\hbar^2}{m^*}\right)^{3/2}\frac{\beta^2}{2\alpha}\frac{exp(-\beta/2\alpha)}{(4\alpha K_1+\beta K_0)},$$

where $K_1(\beta/2\alpha)$, $K_0(\beta/2\alpha)$ are the modified Bessel functions.
[32] H. Grad, *Principles of the Kinetic Theory of Gases*, Handbuch der Physik XII, edited by S. Flugge (Springer-Verlag, Berlin, 1958).
[33] S. Reinecke and G.M. Kremer, Phys. Rev. A **42**, 815 (1990).
[34] A. N. Gorban and I. V. Karlin, Phys. Rev. E **54**, R3109 (1996).
[35] S. Chapman and Cowling, *Mathematical Theory of Non-Uniform Gases* (Cambridge University Press, Cambridge, 1970).
[36] S. Reinecke and G.M. Kremer, Continuum Mech. Thermodyn. **3**, 155 (1991).
[37] I. V. Karlin, Phys. Rev. B **55**, 6324 (1997).
[38] C. Truesdell and R. G. Muncaster, *Fundamentals of Maxwell's Kinetic Theory of a Simple Monoatomic Gas*, edited by S. Eilenberg and H. Bass (Academic Press, New York, 1980).
[39] G.M. Kremer, Int. J. Eng. Sci. **25**, 95 (1987).
[40] In particular, starting from a $(13+9N)$-field theory based on the method of Grad, Ref. 36 showed (in the case of a monatomic gas), that the transition to a five-field theory by the Maxwellian iteration leads to the same results of the Chapman-Enskog approach when considering successive approximations of the transport coefficents.
[41] P. Golinelli, R. Brunetti, L. Varani, J. C. Vaissiere, J. P. Nougier, L. Reggiani, E. Starikov, P. Shiktorov, V. Gruzhinskis, T. Gonzalez, M. J. Martin, and D. Pardo, Semicond. Sci. Technol. **12**, 1511 (1997).
[42] M. Fischetti, IEEE Trans. Electron Devices **38**, 634 (1991).
[43] M. J. Martin, T. Gonzalez, J. E. Velasquez, and D. Pardo, Semicond. Sci. Technol. **8**, 1291 (1993).
[44] P. M. Smith, M. Inoue, and Jeffrey Frey, Appl. Phys. Lett. **37**, 797 (1980).
[45] L. Reggiani, *Hot-Electron Transport In Semiconductors*, Topics in Applied Physics, Vol. 58 (Springer-Verlag, Berlin, 1985).
[46] P. J. Price, J. Appl. Phys. **53**, 8805 (1982).
[47] T. Kuhn, L. Reggiani, and L. Varani, in *Proceedings 4th International Conference on Simulation of Semiconductors Devices and Processes*, edited by W. Fichtner and D. Aemmer (Hartung-Gorre, Zurich, 1991), Vol. 4, p. 115.
[48] T. Kuhn, L. Reggiani, and L. Varani, Phys. Rev. B **42**, 11 133 (1992).
[49] T. Kuhn, L. Reggiani, and L. Varani, Phys. Rev. B **45**, 1903 (1992).
[50] P. Lugli, L. Reggiani, and J. J. Niez, Phys. Rev. B **40**, 12 382 (1989).
[51] Similar results have been recently found (with MC method) by M. Nedjalkov, H. Kosina, and S. Selberherr, in *Proceedings of the International Conference on Simulation of Semiconductor Processes and Devices SISPAD'99*, edited by K. Taniguchi and N. Nakayama (Business Center for Academic Societies, Kyoto, 1999), p. 155.
[52] E. Starikov, P. Shiktorov, V. Gruzhinskis, T. Gonzalez, M. J. Martin, D. Pardo, L. Reggiani, and L. Varani, Semicond. Sci. Technol. **11**, 865 (1996).
[53] R. Brunetti, P. Golinelli, M. Rudan, and L. Reggiani, J. Appl. Phys. **85**, 1572 (1999).