Comments

Comments are short papers which comment on papers of other authors previously published in the **Physical Review**. *Each Comment should state clearly to which paper it refers and must be accompanied by a brief abstract. The same publication schedule as for regular articles is followed, and page proofs are sent to authors.*

Equivalence of Lei and Ting balance equations for nonlinear electronic transport and a Boltzmann approach

M. C. Marchetti*
Department of Physics, University of Illinois at Chicago, Chicago, Illinois 60680

W. Cai
Department of Physics, City College of the City University of New York, New York, New York 10031
(Received 29 December 1986)

We discuss the connection between the Green's-function approach to nonlinear electronic transport in semiconductors proposed recently by Lei and Ting [Phys. Rev. B **32**, 1112 (1985)] and the description of high-field transport based on the familiar nonlinear Boltzmann equation. We show that their balance equations are identical to those one obtains from the Boltzmann equation by assuming that the carrier distribution function is a displaced Fermi-Dirac distribution at the electron temperature T_e.

Recently Lei and Ting (Ref. 1, hereafter referred to as I) proposed a description of steady-state high-field electronic transport in semiconductors. By separating the center-of-mass motion from the relative motion of the electrons and treating the electron-impurity and electron-phonon interactions to lowest order in perturbation theory, they obtained a set of macroscopic "balance equations" for the average carrier energy in the relative frame and the carrier drift velocity. The derivation is carried out in the framework of a Green's-function formalism. The authors refer to the resulting description of nonlinear transport as "non-Boltzmann" and argue that their approach contains no assumptions on the form of the carrier distribution function.

Here we discuss the connection between the method proposed in I and the description of high-field electronic transport based on the familiar nonlinear Boltzmann equation. We show that the approach of Lei and Ting is equivalent to a well-established semiphenomenological description of high-field transport, which is sometimes called in the literature the "drifted electron-temperature model."[2] This model is obtained from the nonlinear Boltzmann equation if one assumes that due to frequent electron-electron collisions the electrons thermalize and their distribution function is a displaced Fermi-Dirac function containing as parameters a drift velocity, $\mathbf{v}_d$, and an electron temperature, T_e. With this assumption on the form of the distribution function the balance equations of I are immediately obtained by taking the moments of the nonlinear Boltzmann equation in the usual way. To obtain the precise balance equations of I one needs to include wave-vector and frequency-dependent free carrier screening, computed in the random-phase approximation (RPA), of the relevant interactions appearing in the Boltzmann equation. In contrast to what was stated by Lei and Ting, their approach contains therefore assumptions that are equivalent to the introduction of a local equilibrium ansatz for the electron distribution function in the Boltzmann equation.

To see this connection in detail, we consider the Boltzmann equation for a gas of electrons interacting with impurities and phonons in an external static electric field, **E**. The notation of I is used here. Neglecting spatial inhomogeneities, the Boltzmann equation for the electron distribution function, $f(\mathbf{k},t)$, is given by,

$$\frac{\partial f(\mathbf{k},t)}{\partial t}-\frac{e}{\hbar}\mathbf{E}\cdot\frac{\partial f(\mathbf{k},t)}{\partial \mathbf{k}} = \left[\frac{\partial f(\mathbf{k},t)}{\partial t}\right]_{e\text{-ph}}+\left[\frac{\partial f(\mathbf{k},t)}{\partial t}\right]_{e\text{-}i}+\left[\frac{\partial f(\mathbf{k},t)}{\partial t}\right]_{e\text{-}e}. \tag{1}$$

The terms on the right-hand side represent the contribution from electron-phonon (*e*-ph), electron-impurity (*e*-*i*), and electron-electron (*e*-*e*) collisions. For instance, the rate of change of $f(\mathbf{k},t)$ due to *e*-ph collisions is given by

$$\left[\frac{\partial f}{\partial t}\right]_{e\text{-ph}}=-\sum_{\mathbf{k}_1}[W(\mathbf{k}_1,\mathbf{k})f(1-f_1) - W(\mathbf{k},\mathbf{k}_1)f_1(1-f)], \tag{2}$$

where f and f_1 denote the distribution function at $\mathbf{k}$ and $\mathbf{k}_1$, respectively. The rate for transitions from $\mathbf{k}$ to $\mathbf{k}_1$ is

$$W(\mathbf{k}_1,\mathbf{k})=\frac{2\pi}{\hbar}\sum_{\mathbf{q},\lambda}|\tilde{M}(\mathbf{q},\Omega_{q\lambda})|^2\sum_{\sigma=\pm1}\delta_{\mathbf{k}_1,\mathbf{k}+\sigma\mathbf{q}}\delta(\varepsilon_k-\varepsilon_{k_1}-\sigma\hbar\Omega_{q\lambda}[n(\Omega_{q\lambda}/T)+\tfrac{1}{2}+\sigma\tfrac{1}{2}] \ . \tag{3}$$

Here $\tilde{M}(\mathbf{q},\Omega_{q\lambda})$ is the matrix element of the e-ph interaction renormalized to include wave-vector and frequency-dependent screening in the RPA,[3]

$$\tilde{M}(\mathbf{q},\Omega_{q\lambda})=\frac{M(q,\lambda)}{\epsilon_{\mathrm{RPA}}(\mathbf{q},\Omega_{q\lambda})} \ . \tag{4}$$

The e-ph matrix element, $M(q,\lambda)$, depends on the specific interaction considered and can be found in I. Also, $\epsilon_{\mathrm{RPA}}(\mathbf{q},\omega)$ is the RPA for the dielectric function, given by

$$\epsilon_{\mathrm{RPA}}(\mathbf{q},\omega)=1-V_q\Pi_0(\mathbf{q},\omega) \ , \tag{5}$$

with V_q the Fourier transform of the Coulomb potential and $\Pi_0(\mathbf{q},\omega)$ the density-density correlation function of the free electron gas, given by

$$\Pi_0(\mathbf{q},\omega)=\lim_{\delta\to0^+}\frac{2}{V}\sum_{\mathbf{k}}\frac{f(\mathbf{k}+\mathbf{q},t)-f(\mathbf{k},t)}{\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}}+\hbar\omega+i\delta} \ . \tag{6}$$

with $\varepsilon_{\mathbf{k}}=\hbar^2k^2/2m$ and V the volume of the system. The average electron energy density, $\varepsilon_e(t)$, and the average drift velocity, $\mathbf{v}_d(t)$, are defined by[4]

$$\varepsilon_e(t)=\frac{2}{V}\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}f(\mathbf{k},t) \ , \tag{7a}$$

$$mn_e\mathbf{v}_d(t)=\frac{2}{V}\sum_{\mathbf{k}}\hbar\mathbf{k}f(\mathbf{k},t) \ . \tag{7b}$$

with n_e the electron density. Finally, we will need the average electron energy density in the relative frame, i.e., the average internal energy density, given by

$$\varepsilon_e'(t)=\frac{2}{V}\sum_{\mathbf{k}}\frac{\hbar^2}{2m}(\mathbf{k}-\mathbf{k}_d)^2f(\mathbf{k},t) \ , \tag{7c}$$

with $\mathbf{k}_d(t)=m\mathbf{v}_d(t)/\hbar$.

We now assume that due to frequent e-e collisions the electron gas thermalizes and that the electron distribution function is a drifted Fermi-Dirac function at the electron temperature T_e, different from the lattice temperature, T, i.e.,

$$f(\mathbf{k},t)=f(\varepsilon_{|\mathbf{k}-\mathbf{k}_d(t)|},T_e) \ , \tag{8}$$

where $f(\varepsilon_{\mathbf{k}},T_e)$ is the Fermi function given in Eq. (60) of I. The average energy density is then given by

$$\varepsilon_e(t)=\varepsilon_e'(t)+\tfrac{1}{2}mn_ev_d^2(t) \ . \tag{9}$$

By multiplying the Boltzmann equation with $\hbar\mathbf{k}$ and $\hbar^2(\mathbf{k}-\mathbf{k}_d)^2/2m$, respectively, and summing over $\mathbf{k}$, one obtains a set of two coupled nonlinear equations for the average internal energy density, $\varepsilon_e'(t)$, and the drift velocity, $\mathbf{v}_d(t)$, or equivalently for $T_e(t)$ and $\mathbf{v}_d(t)$. The resulting equations are

$$\frac{\partial}{\partial t}mn_e\mathbf{v}_d(t)+en_e\mathbf{E}=\frac{1}{V}\mathbf{F}(\mathbf{v}_d,T_e) \ , \tag{10a}$$

$$\frac{\partial}{\partial t}\varepsilon_e'(t)=-\mathbf{v}_d(t)\cdot\frac{1}{V}\mathbf{F}(\mathbf{v}_d,T_e)-\frac{1}{V}W(\mathbf{v}_d,T_e) \ , \tag{10b}$$

The right-hand side of Eqs. (10) represents the frictional forces and the energy dissipation due to e-ph and e-i collisions. The assumption on the form of $f(\mathbf{k},t)$ allows one to express these terms explicitly as nonlinear functions of $T_e(t)$ and $\mathbf{v}_d(t)$. The frictional force, $\mathbf{F}(v_d,T_e)$, is related to that introduced in I by $F(v_d)=\mathbf{v}_d\cdot\mathbf{F}(\mathbf{v}_d,T_e)$, where $\mathbf{v}_d$ is a unit vector in the direction of $\mathbf{v}_d$ and $F(v_d)$ is given in Eq. (64) of I. The rate of energy loss, W, is identical to that given in Eq. (67) of I. In a steady state Eqs. (10) reduce to the balance equations (65) and (68) of I.

The derivation of Eqs. (10) is straightforward. For instance, the rate of change of the electron momentum due to e-ph collisions in given by

$$\begin{aligned}\frac{2}{V}\sum_{\mathbf{k}}\hbar\mathbf{k}\left[\frac{\partial f}{\partial t}\right]_{e\text{-ph}}&=-2V\sum_{\mathbf{k}}\sum_{\mathbf{k}_1}\hbar\mathbf{k}\{W(\mathbf{k}_1,\mathbf{k})f(\varepsilon_{\mathbf{k}-\mathbf{k}_d})[1-f(\varepsilon_{\mathbf{k}_1-\mathbf{k}_d})]\\&\quad-W(\mathbf{k},\mathbf{k}_1)f(\varepsilon_{\mathbf{k}_1-\mathbf{k}_d})[1-f(\varepsilon_{\mathbf{k}-\mathbf{k}_d})]\} \ ,\end{aligned} \tag{11}$$

where to simplify the notation we have omitted the T_e dependence of the Fermi functions. By letting $\mathbf{k}'=\mathbf{k}-\mathbf{k}_d$ and $\mathbf{k}_1'=\mathbf{k}_1-\mathbf{k}_d$ and then dropping for simplicity the prime, after some straightforward algebra, Eq. (11) can be written as

$$\begin{aligned}\frac{2}{V}\sum_{\mathbf{k}}\hbar\mathbf{k}\left[\frac{\partial f}{\partial t}\right]_{e\text{-ph}}&=-\frac{2}{V}\sum_{\mathbf{k}}\sum_{\mathbf{k}_1}\frac{2\pi}{\hbar}\sum_{\mathbf{q},\lambda}\hbar\mathbf{q}\,|\tilde{M}(\mathbf{q},\Omega_{q\lambda})|^2\delta_{\mathbf{k}_1,\mathbf{k}+\mathbf{q}}\delta(\varepsilon_{k_1}-\varepsilon_k+\hbar\mathbf{q}\cdot\mathbf{v}_d+\hbar\Omega_{q\lambda})\\&\quad\times\{[n(\Omega_{q\lambda}/T)+1]f(\varepsilon_{\mathbf{k}})[1-f(\varepsilon_{\mathbf{k}_1})]-n(\Omega_{q\lambda}/T)f(\varepsilon_{\mathbf{k}_1})[1-f(\varepsilon_{\mathbf{k}})]\} \ .\end{aligned} \tag{12}$$

The same change of variable in the wave-vector sum can be used in Eq. (6) to show that

$$\Pi_0(\mathbf{q},\Omega_{q\lambda})=\Pi_1(\mathbf{q},\Omega_{q\lambda}+\mathbf{q}\cdot\mathbf{v}_d)+i\Pi_2(\mathbf{q},\Omega_{q\lambda}+\mathbf{q}\cdot\mathbf{v}_d) \ , \tag{13}$$

where Π_1 and Π_2 are given in Eqs. (58) and (59) of I. Finally, by inserting Eq. (13) in Eqs. (4) and (5), making use of Eq. (59) of I, and noticing that, in virtue of the energy-conserving δ function, the term in curly brackets in Eq. (12) can be written as

$$\{[n(\Omega_{q\lambda}/T)-n((\Omega_{q\lambda}+\mathbf{q}\cdot\mathbf{v}_d)/T_e)][f(\varepsilon_{\mathbf{k}})-f(\varepsilon_{\mathbf{k}_1})]\} ,$$

it is easy to show that the right-hand side of Eq. (12) is identical to the frictional force due to e-ph collisions, as given by the second term in Eq. (64) of I, per unit volume.

The equivalence of the present result and the approach of Lei and Ting is due to two assumptions that are made in their derivation: (1) The approximation contained in Eq. (36) of I replaces the microscopic center-of-mass displacement of the electrons, $\Delta\mathbf{R}$, with its macroscopic average value, $\mathbf{v}_d(t)\Delta t$. (2) The balance equations of I are obtained by assuming that at $t=-\infty$ the electrons and phonons are described by equilibrium density matrices at the temperatures T_e and T, respectively, neglecting then all e-e and ph-ph interactions and treating the e-ph interaction in perturbation theory. It can be shown that if the same procedure is used to derive a kinetic equation for the electrons one obtains the familiar Boltzmann equation, with the electron distribution function everywhere replaced by a (drifted) Fermi-Dirac distribution at T_e.

While we do not dispute the value of the explicit calculation of electron temperature and electron resistivity in strong fields carried out in I, we think it is important to clarify the connection of the work of Lei and Ting to others and to emphasize that their results can be obtained from the Boltzmann equation in a straightforward way. The idea of separating center-of-mass motion and relative motion of the carriers is certainly a useful one and it can also be employed in the analysis of the Boltzmann equation.

Finally, it was found in I that under certain conditions the electron temperature T_e can be lower than the lattice or bath temperature, T. The same result is obtained when the set of Eqs. (10) obtained from the Boltzmann equation are solved for the case of a nonequilibrium steady state.[5] It is, however, important to emphasize that the fact that $T_e<T$ does not imply that energy is transferred from the bath to the carriers, since the total average energy density of the electrons, ε_e, is always larger than the thermal energy of the bath.

This work was supported in part by the Army Research Office and the Department of Energy.

---

*Present address: Physics Department, Syracuse University, Syracuse, NY 13244.

[1]X. L. Lei and C. S. Ting, Phys. Rev. B **32**, 1112 (1985).

[2]See, for instance, E. M. Conwell, *High Field Transport in Semiconductors* (Academic, New York, 1967).

[3]See, for instance, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971).

[4]In contrast with I, we prefer to use intensive quantities, e.g., energy density instead of total energy. Since the total number of electrons is assumed constant, our results only differ for a factor of volume from those of I.

[5]W. Cai and M. C. Marchetti (unpublished).