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High-field balance equations for electronic transport in weakly nonuniform systems

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Balance equations for the spatial distribution of particle number density $n(\mathbf{R})$, drift velocity $\mathbf{v}(\mathbf{R})$, and internal energy $u(\mathbf{R})$ [or electron temperature $T_e(\mathbf{R})$] in high-field electronic transport of a weakly nonuniform electron-impurity-phonon system are derived using a model in which the dynamic interactions between different fluid elements are removed by a self-consistent mean-field approximation and thermodynamic forces are neglected. The resistive forces due to impurity and phonon scattering and the electron energy-loss rate to the phonon system have expressions similar to those in uniform case except that now the drift velocity and electron temperature are replaced by the corresponding spatially variable field parameters. Being a form of first-order space-time differential equation, the balance equations determine $\mathbf{v}(\mathbf{R})$ and $T_e(\mathbf{R})$ as well as the total electric potential if the initial and boundary conditions are given; thus they can easily be applied to the discussion of high electric field transport in weakly nonuniform systems.

I. INTRODUCTION

It has long been an unresolved problem to devise a tractable method of calculating high-field electronic transport in semiconductors.[1,2] Interest has recently been intensified with the development of submicron solid-state electronics. In addition to widely used Boltzmann-equation treatments and Monte Carlo simulations,[3] balance-equation analyses,[4,5] which eliminate the need for a distribution function and give rise to the most important transport information nearly analytically, have proven useful in practical calculation. Recently a balance-equation approach for high-field uniform systems was developed[5-7] on the basis of a separation of the center-of-mass degrees of freedom from the relative motion of electrons in the system. Besides its simplicity of mathematical structure, the advantages of this approach include its generality of description for nonlinear transport in the presence of both an electric field and a magnetic field of arbitrary strength, and its ease of treating dynamic, nonlocal intercarrier coupling. All the important transport properties are expressed in terms of carrier density-density correlation function in the absence of electric field without electron-impurity and electron-phonon scattering, but with magnetic field (if any) and full carrier-carrier interaction [in random-phase approximation (RPA) and beyond]. In this paper we extend this balance-equation method to a weakly nonuniform system as a step toward the need for the calculation of nonlinear transport in submicrometer devices, microstructures, etc.

II. HAMILTONIAN OF THE ELEMENTS

We consider an interacting electron system under the influence of an external field $\mathbf{E}_e(\mathbf{r})=-\nabla\phi_e(\mathbf{r})$. The Hamiltonian of the system is

$$H=\sum_i\left[\frac{p_i^2}{2m}+\frac{1}{2}\sum_{j(\neq i)}\frac{e^2}{4\pi\epsilon_0\,|\,\mathbf{r}_i-\mathbf{r}_j\,|}+e\phi_e(\mathbf{r}_i)+\Phi(\mathbf{r}_i)\right], \tag{1}$$

where e and m are particle charge and effective mass, $\mathbf{p}_i$ and $\mathbf{r}_i$ are the momentum and coordinate of the ith electron, and

$$\Phi(\mathbf{r}_i)=\sum_a u(\mathbf{r}_i-\mathbf{R}_a)+\sum_l \mathbf{u}_l\cdot\nabla v_l(\mathbf{r}_i-\mathbf{R}_l) \tag{2}$$

represents the scattering potential due to randomly distributed ($\mathbf{R}_a$) impurities and lattice vibrations ($\mathbf{R}_l$ stands for lattice sites). The whole system can be divided into many small subsystems. A subsystem is composed of electrons in a small volume $d\tau$ around a position $\mathbf{R}$. Macroscopically $d\tau$ is small over which all the expectations of physical quantities change little, whereas microscopically $d\tau$ is large enough that a great number of particles are within it. Such a subsystem is called a fluid element, or simply an element. The Hamiltonian of the element $d\tau$ can be written as

$$\delta H=\sum_i{}_{d\tau}\left[\frac{p_i^2}{2m}+\frac{1}{2}\sum_{j(\neq i)}\frac{e^2}{4\pi\epsilon_0\,|\,\mathbf{r}_i-\mathbf{r}_j\,|}+e\phi_e(\mathbf{r}_i)+\Phi(\mathbf{r}_i)\right]. \tag{3}$$

Here the second term in the parentheses is the Coulomb interaction potential of the ith electron with all the other electrons. We can divide it into two parts: contribution from electrons inside $d\tau$ and those from outside $d\tau$. We will use a mean-field treatment for the latter. For small $d\tau$ it becomes the macroscopic induction potential $\phi_i(\mathbf{r}_i)$

caused by the electron charge distribution (plus positive charge background), such that

$$\delta H = \sum_i{}_{d\tau} \left[\frac{p_i^2}{2m} + \frac{1}{2} \sum_{j(\neq i)}{}_{d\tau} \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} + e\phi(\mathbf{r}_i) + \Phi(\mathbf{r}_i) \right] \tag{4}$$

with $\phi(r) = \phi_e(\mathbf{r}) + \phi_i(\mathbf{r})$ being the total potential. In the limit of small $d\tau$ the restricted sum $\sum_{d\tau}$ over the particles inside $d\tau$ around $\mathbf{R}$ can be conveniently represented by a δ function,

$$\sum_i{}_{d\tau} \sim d\tau \sum_i \delta(\mathbf{r}_i - \mathbf{R}) , \tag{5}$$

such that

$$\delta H = d\tau H(\mathbf{R}) \text{ and } H = \int d\tau H(\mathbf{R}) . \tag{6}$$

Here

$$H(\mathbf{R}) = H_e(\mathbf{R}) + \sum_i [e\phi(\mathbf{r}_i) + \Phi(\mathbf{r}_i)]\delta(\mathbf{r}_i - \mathbf{R}) , \tag{7}$$

and

$$H_e(\mathbf{R}) = \sum_i \left[\frac{p_i^2}{2m} + \frac{1}{2} \sum_{j(\neq i)}{}_{d\tau} \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_i - \mathbf{r}_j|} \right] \delta(\mathbf{r}_i - \mathbf{R}) \tag{8}$$

is the kinetic and Coulombic interacting energies of electrons in element $d\tau$. Note that, under the present approximation, different elements consist of different sets of electrons, and the Coulomb coupling between electrons in different elements has been included in the total potential $\phi(\mathbf{r})$, which is a parametrized variable to be determined self-consistently by the resulting equations. Therefore different subparts of H are independent and commutative. The number of electrons in element $d\tau$ is $\delta N = d\tau N(\mathbf{R})$ and

$$N(\mathbf{R}) = \sum_i \delta(\mathbf{r}_i - \mathbf{R}) \tag{9}$$

is the number density of electrons in the element around $\mathbf{R}$. It is convenient to identify $\mathbf{R}$ as the coordinate of the center of mass of the electrons in $d\tau$:

$$\mathbf{R} = \sum_i{}_{d\tau} \mathbf{r}_i / \delta N .$$

The total momentum of the electrons in element $d\tau$ is

$$\delta \mathbf{P} = \sum_i{}_{d\tau} \mathbf{P}_i = d\tau \mathbf{P}(\mathbf{R}) ,$$

with

$$\mathbf{P}(\mathbf{R}) = \sum_i \mathbf{p}_i \delta(\mathbf{r}_i - \mathbf{R}) \tag{10}$$

being the momentum density. Letting $\mathbf{v}(\mathbf{R})$ be the average velocity of the electrons in element $d\tau$, which is a parameter to be determined self-consistently by the resulting balance equations, we can write the statistical expectation of the momentum density as

$$\langle \mathbf{P}(\mathbf{R}) \rangle = mn(\mathbf{R})\mathbf{v}(\mathbf{R}) , \tag{11}$$

where $n(\mathbf{R}) = \langle N(\mathbf{R}) \rangle$ is the statistical average of the electron number density. It is convenient to use the relative electron variable $\mathbf{p}_i'$ and $\mathbf{r}_i'$, defined by

$$\mathbf{p}_i' = \mathbf{p}_i - m\mathbf{v}(\mathbf{R}), \quad \mathbf{r}_i' = \mathbf{r}_i - \mathbf{R} . \tag{12}$$

They are momentum and coordinate of the ith electron relative to the center of mass in element $d\tau$. With these relative electron variables the statistical average of $H_e(\mathbf{R})$ can be written as

$$\langle H_e(\mathbf{R}) \rangle = u(\mathbf{R}) + \tfrac{1}{2} mn(\mathbf{R}) v^2(\mathbf{R}) , \tag{13}$$

where

$$u(\mathbf{R}) = \left\langle \sum_i \frac{p_i'^2}{2m} \delta(\mathbf{r}_i - \mathbf{R}) \right\rangle \tag{14}$$

is the average of the kinetic energy of the relative electrons in $d\tau$. The interaction potential energy between electrons inside $d\tau$, which is a higher-order quantity in $d\tau$, has been neglected.

III. RATES OF CHANGE OF PARTICLE NUMBER, MOMENTUM, AND ENERGY

We now consider the rates of change of particle number, momentum, and energy. The rate of change of particle number density $\dot{N}(\mathbf{R}) = -i[N(\mathbf{R}), H]/\hbar$ can be easily calculated and this (after taking statistical average) results in the continuity equation:

$$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{v} n) = 0 . \tag{15}$$

Secondly, from Eq. (11),

$$\frac{\partial}{\partial t} \langle \mathbf{P}(\mathbf{R}) \rangle = m \frac{\partial n}{\partial t} \mathbf{v} + mn \frac{\partial \mathbf{v}}{\partial t} . \tag{16}$$

On the other hand, we can calculate $\dot{\mathbf{P}}(\mathbf{R})$ according to $\dot{\mathbf{P}}(\mathbf{R}) = -i[\mathbf{P}(\mathbf{R}), H]/\hbar$ to give

$$\dot{\mathbf{P}}(\mathbf{R}) = -\nabla_R \cdot \left[\sum_i \frac{\mathbf{p}_i \mathbf{p}_i}{m} \delta(\mathbf{r}_i - \mathbf{R}) \right] - \sum_i [\nabla \Phi(\mathbf{r}_i) + e\nabla\phi(\mathbf{r}_i)]\delta(\mathbf{r}_i - \mathbf{R}) . \tag{17}$$

Changing to relative electron variables and taking the statistical average we have

$$\langle \dot{\mathbf{P}}(\mathbf{R}) \rangle = -\nabla[\tfrac{2}{3} u(\mathbf{R})] - \nabla \cdot [mn(\mathbf{R})\mathbf{v}(\mathbf{R})\mathbf{v}(\mathbf{R})] + en(\mathbf{R})\mathbf{E}(\mathbf{R}) + \mathbf{f}(\mathbf{R}) , \tag{18}$$

where

$$\mathbf{f}(\mathbf{R}) = -\left\langle \sum_i \nabla \Phi(\mathbf{r}_i' + \mathbf{R}) \delta(\mathbf{r}_i') \right\rangle \tag{19}$$

is the resistive force experienced by the fluid element due to impurity and phonon scatterings. Equating Eq. (18) to Eq. (16) and making use of the continuity equation (15), we obtain an Euler-type momentum-balance equation:

$$\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}(\nabla\cdot\mathbf{v})=-\frac{2}{3}\frac{\nabla u}{mn}+\frac{e}{m}\mathbf{E}+\frac{1}{mn}\mathbf{f}\ . \tag{20}$$

Thirdly, the rate of change of $\langle H_e(R)\rangle$ is calculated from Eq. (13) to be

$$\frac{\partial}{\partial t}\langle H_e(\mathbf{R})\rangle=\frac{du}{dt}+\frac{m}{2}\frac{dn}{dt}v^2+mn\mathbf{v}\cdot\frac{d\mathbf{v}}{dt}\ , \tag{21}$$

which should be equated to that obtained averaging the expression

$$\dot{H}_e(\mathbf{R})=-i[H_e(\mathbf{R}),H]/\hbar\ :$$

$$\begin{aligned}\langle \dot{H}_e(\mathbf{R})\rangle=&-\nabla\cdot\mathbf{v}(\mathbf{R})\tfrac{5}{3}u(\mathbf{R})+\frac{m}{2}n(\mathbf{R})v^2(\mathbf{R})\\ &+en(\mathbf{R})\mathbf{v}(\mathbf{R})\cdot\mathbf{E}(\mathbf{R})-w(\mathbf{R})\ ,\end{aligned} \tag{22}$$

where

$$w(\mathbf{R})=\left\langle \sum_i \frac{\mathbf{p}_i'}{m}\cdot\nabla\Phi(\mathbf{r}_i'+\mathbf{R})\delta(\mathbf{r}_i')\right\rangle-\mathbf{v}(\mathbf{R})\cdot\mathbf{f}(\mathbf{R}) \tag{23}$$

is the electron energy-loss rate. Combining Eqs. (21) and (22) with considering Eqs. (15) and (20) we obtain an energy balance equation:

$$\frac{\partial u}{\partial t}+\mathbf{v}\cdot\nabla u=-\tfrac{5}{3}u(\nabla\cdot\mathbf{v})-w-\mathbf{v}\cdot\mathbf{f}\ . \tag{24}$$

IV. ELECTRON-TEMPERATURE FIELD

To calculate the resistive force f and the energy-loss rate w, we need the density matrix ρ, which can be obtained by solving the Liouville equation with the appropriate initial condition. In the present model the interactions between different fluid elements are included approximately in the total potential with mean-field treatment. Therefore different fluid elements, though geometrically correlative, are dynamically independent, and thus evolve separately from their own initial states.

For a given element $d\tau$ we can separate the electron Hamiltonian δH into a center-of-mass part δH_c and a relative motion part δH_e by making the transformation (12): $\delta H=\delta H_c+\delta H_e+\delta H_I$, with

$$\delta H_c=(\tfrac{1}{2}mnv^2+en\phi)d\tau\ , \tag{25}$$

$$\delta H_e=\sum_i{}_{d\tau}\left[\frac{p_i'^2}{2m}+\frac{1}{2}\sum_{j(\neq i)}{}_{d\tau}\frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i'-\mathbf{r}_j'|}\right]\ , \tag{26}$$

$$\delta H_I=\sum_i{}_{d\tau}\Phi(\mathbf{r}_i'+R)\ . \tag{27}$$

δH_I denotes impurity and phonon scattering interactions. Numerous relative electrons in $d\tau$ can be treated as an ordinary many-particle system with volume $d\tau$. According to Eqs. (25)–(27), they are coupled with the center of mass and the electric field only by way of impurity and phonon scatterings. We will include the scattering interaction to lowest order in terms of linear response of the system, choosing the unperturbed state (a state in the absence of δH_I) as follows. We imagine turning off the scattering interaction at some time in the transport process, and note that the decoupled relative electrons and phonons will separately approach quasiequilibrium states, in which electrons have a temperature $T_e(\mathbf{R})$ and phonons have a lattice temperature T (assumed mode and space independent, thus the nonequilibrium phonon effect is neglected). Accordingly the unperturbed state is chosen to be described by a density matrix ρ_0 of the local equilibrium form,

$$\begin{aligned}\rho_0=&\frac{1}{Z}\exp\left[-\int[\delta H-\mu(\mathbf{R})\delta N]/k_BT_e(\mathbf{R})\right]\\ &\times\exp(-H_{\mathrm{ph}}/k_BT)\ ,\end{aligned} \tag{28}$$

where electron-temperature field $T_e(\mathbf{R})$ and chemical potential field $\mu(\mathbf{R})$ are parameters to be determined self-consistently by the resulting balance equations, and H_{ph} is the phonon Hamiltonian.

The process to derive the perturbed density matrix $\rho=\rho_0+\rho_1$ to linear order of δH_I and the calculation of statistical expectations exactly follow those in Ref. (5). To lowest nonzero order the average local kinetic energy density of the relative electrons is determined by ρ_0 only:

$$u=2\sum_{\mathbf{k}}\epsilon_k f[(\epsilon_k-\mu)/k_BT_e]\ , \tag{29}$$

and the local chemical potential $\mu(\mathbf{R})$ is related to the local density $n(\mathbf{R})$ of electrons via the relation

$$n=2\sum_{\mathbf{k}}f[(\epsilon_k-\mu)/k_BT_e]\ . \tag{30}$$

Here $\epsilon_{\mathbf{k}}=\hbar^2k^2/2m$ and $f(x)=(e^x+1)^{-1}$. The resistive force density $\mathbf{f}(\mathbf{R})$ and energy loss rate $w(\mathbf{R})$ are found to be

$$\begin{aligned}\mathbf{f}=\mathbf{f}(n(\mathbf{R}),T_e(\mathbf{R}),\mathbf{v}(\mathbf{R}))=&\,n_I\int\frac{d\mathbf{q}}{(2\pi)^3}|u(q)|^2q_x\Pi_2(\mathbf{q},\omega_0)\\ &+2\int\frac{d\mathbf{q}}{(2\pi)^3}q_x\sum_\lambda|M(\mathbf{q},\lambda)|^2\Pi_2(\mathbf{q},\omega_0+\Omega_{\mathbf{q}\lambda})\left[N\left[\frac{\hbar\Omega_{\mathbf{q}\lambda}}{k_BT}\right]-N\left[\frac{\hbar(\Omega_{\mathbf{q}\lambda}+\omega_0)}{k_BT_e}\right]\right]\ ,\end{aligned} \tag{31}$$

$$\begin{aligned}w=&\,w(n(\mathbf{R}),T_e(\mathbf{R}),\mathbf{v}(\mathbf{R}))\\ =&\,2\int\frac{d\mathbf{q}}{(2\pi)^3}\sum_\lambda|M(\mathbf{q},\lambda)|^2\Omega_{\mathbf{q}\lambda}\Pi_2(\mathbf{q},\,\omega_0+\Omega_{\mathbf{q}\lambda})\left[N\left[\frac{\hbar\Omega_{\mathbf{q}\lambda}}{k_BT}\right]-N\left[\frac{\hbar(\Omega_{\mathbf{q}\lambda}+\omega_0)}{k_BT_e}\right]\right]\ .\end{aligned} \tag{32}$$

Here $\omega_0 \equiv \mathbf{q}\cdot\mathbf{v}(\mathbf{R})$, $N(x) \equiv (e^x - 1)^{-1}$ denotes the Bose function, n_I is the impurity density around $\mathbf{R}$, $\Omega_{\mathbf{q}\lambda}$ is the phonon frequency and, $\Pi_2(\mathbf{q},\omega)$ is the density-density correlation function of relative electrons in unit volume with density $n(\mathbf{R})$ at temperature $T_e(\mathbf{R})$ including the effect of Coulomb interaction between carriers, which can be treated in RPA or beyond. We see that although the intercarrier Coulomb coupling inside the element gives a vanishing contribution to the average energy of relative electron system of the element, it plays an important role in screening.

V. EQUATIONS FOR WEAKLY NONUNIFORM TRANSPORT

In the present description the velocity field $\mathbf{v}(\mathbf{R})$ and electron temperature field $T_e(\mathbf{R})$ are fundamental parametric variables; besides, we have $u(\mathbf{R})$, $n(\mathbf{R})$, $\mu(\mathbf{R})$, as well as the total electric potential $\phi(\mathbf{R})$ or field $\mathbf{E}(\mathbf{R})$. They apparently can give most of the important information of a nonuniform transport system. These variables may be time dependent on a macroscopic timescale to describe time-dependent process. We now have three hydrodynamic-type equations: continuity equation (15), momentum-balance equation (20), and energy-balance equation (24), supplemented by two relations (29) and (30) plus the Poisson equation relating electric charge density and potential (n^+ denotes the density of positive charge background):

$$\nabla^2\phi = -\frac{e}{\epsilon_0}[n(\mathbf{R}) - n^+] \ . \tag{33}$$

All the space-time field variables can be determined for the given initial and boundary conditions.

In the case of a uniform transport system, these equations immediately reduce to those discussed in Ref. (7). For steady state, they simply become

$$en\mathbf{E} + \mathbf{f} = 0$$

and

$$w + \mathbf{n}\cdot\mathbf{f} = 0 \ ,$$

which are force- and energy-balance equations obtained in Ref. (5) for steady-state uniform transport.

In the present model the dynamic interaction between different elements is removed by a self-consistent mean-field approximation; thus heat conduction, diffusion, and viscosity are neglected. This is justified for a weakly nonuniform system since all the contributions of these thermodynamic forces to balance equations are in higher order of the gradients of parametric fields. Furthermore, in the high-field regime impurity and phonon scatterings are major dissipative processes of the electronic transport. Because of this the balance equations obtained are essentially hydrodynamic type of an ideal fluid. These equations can be conveniently applied to discuss the high-field transport in metal-semiconductor contacts, p-n junctions, interfaces and heterostructures.

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[1] E. M. Conwell, *High Field Transport in Semiconductors* (Academic, New York, 1967).

[2] L. Reggiani, in *Hot Electron Transport in Semiconductors*, edited by L. Regianni (Springer-Verlag, Berlin, 1985).

[3] C. Jacoboni and L. Reggiani, Rev. Mod. Phys. **55**, 645 (1983).

[4] K. K. Thornber and R. P. Feynman, Phys. Rev. B **1**, 4099 (1970).

[5] X. L. Lei and C. S. Ting, Phys. Rev. B **32**, 1112 (1985); X. L. Lei, W. Cai, and C. S. Ting, J. Phys. C **18**, 4315 (1985).

[6] D. Y. Xing, and C. S. Ting, Phys. Rev. B **34**, 7003 (1986).

[7] X. L. Lei and N. J. M. Horing, Phys. Rev. B **35**, 6281 (1987); X. L. Lei, H. L. Cui, and N. J. M. Horing, J. Phys. C **20**, L287 (1987).