Coupled force-balance and particle-occupation rate equations for high-field electron transport

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It is pointed out that in the framework of balance-equation approach, the coupled force-balance and particle-occupation rate equations can be used as a complete set of equations to determine the high-field transport of semiconductors in both strong and weak electron-electron interaction limits. We call to attention that the occupation rate equation conserves the total particle number and maintains the energy balance of the relative electron system, and there is no need to introduce any other term in it. The addition of an energy-drift term in the particle-occupation rate equation [Phys. Rev. B **71**, 195205 (2005)] is physically inadequate for the violation of the total particle-number conservation and the energy balance. It may lead to a substantial unphysical increase of the total particle number by the application of a dc electric field.

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The balance-equation transport theory[1] treating the external (impurity and phonon) scatterings as small quantities, is a kind of perturbation theory.[2] The smallness of external scattering is in comparison with the effective interaction leading to the thermalization between carriers, and the perturbative expansion is essentially that in powers of the ratio of these two interactions.[3] The main formulation in the theory is derived by truncating the perturbation series at the lowest nonzero order, which corresponds to the limit of rapid thermalization or strong electron-electron (e-e) interaction. In a polar semiconductor such as n-GaAs with the electron density of the order of 10^{17} cm^{-3} at temperature around 100 K, the effective e-e scattering time or Coulomb lifetime, which is estimated of an order of 100 fs,[4–6] may not be short enough in comparison with the LO-phonon scattering time that it is desirable to go beyond the strong e-e scattering limit. A natural way along this direction seems to put the electron-impurity, electron-phonon, and electron-electron scatterings on an equal footing.[7]

If we deal with a system consisting of N interacting electrons subject to impurity and phonon scatterings under the influence of a spatially uniform electric field $\boldsymbol{E}$ (may be slowly time dependent), the total Hamiltonian of the electron and phonon system H is given by

$$H = \sum_i \frac{\boldsymbol{p}_i^2}{2m} + \frac{e^2}{4\pi\epsilon_0\kappa}\sum_{i<j}\frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} - e\sum_i \boldsymbol{r}_i\cdot\boldsymbol{E} + H_{\rm ph} + \sum_{i,a} u(\boldsymbol{r}_i - \boldsymbol{r}_a) - \sum_{i,l}\boldsymbol{u}_l\cdot\boldsymbol{\nabla}v_l(\boldsymbol{r}_i - \boldsymbol{R}_l). \quad (1)$$

Here, $\boldsymbol{r}_i$ and $\boldsymbol{p}_i = -i\boldsymbol{\nabla}_i$ $(i=1,2,\ldots,N)$ are the coordinate and momentum of the ith electron with effective mass m and charge e. The first term on the right-hand side of Eq. (1) is the kinetic energy of electrons; the second term is the electron-electron Coulomb interaction (κ is the dielectric constant of host material); the third term is the potential energy of electrons in the uniform electrical field $\boldsymbol{E}$; $u(\boldsymbol{r}-\boldsymbol{r}_a)$ is the scattering potential due to an impurity located at $\boldsymbol{r}_a$, which is assumed randomly distributed; $v_l(\boldsymbol{r}-\boldsymbol{R}_l)$ denotes the potential induced by the lth ion at lattice site $\boldsymbol{R}_l$, and $\boldsymbol{u}_l$ is its displacement from the regular (equilibrium) position; $H_{\rm ph}$ represents the lattice-ion vibration (phonon) Hamilitonian. In terms of the electron center-of-mass variables $\boldsymbol{P} = \Sigma_j^N \boldsymbol{p}_j$ and $\boldsymbol{R} = N^{-1}\Sigma_j^N \boldsymbol{r}_j$ and the relative-electron variables, the total Hamiltonian can be written in the form[1,8]

$$H = H_{\rm cm} + H_{e0} + H_{\rm ee} + H_{\rm ph} + H_{\rm ei} + H_{\rm ep}, \quad (2)$$

$$H_{\rm cm} = \frac{P^2}{2Nm} - Ne\boldsymbol{E}\cdot\boldsymbol{R}, \quad (3)$$

$$H_{e0} = \sum_{\boldsymbol{k},\sigma}\varepsilon_{\boldsymbol{k}} c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}, \quad (4)$$

$$H_{\rm ee} = \sum_{\boldsymbol{q}}\frac{1}{2}v_c(q)(\rho_{\boldsymbol{q}}\rho_{-\boldsymbol{q}} - N), \quad (5)$$

$$H_{\rm ph} = \sum_{\boldsymbol{q},\lambda}\Omega_{\boldsymbol{q}\lambda} b_{\boldsymbol{q}\lambda}^\dagger b_{\boldsymbol{q}\lambda}, \quad (6)$$

$$H_{\rm ei} = \sum_{\boldsymbol{q},a} u(\boldsymbol{q}) e^{i\boldsymbol{q}\cdot(\boldsymbol{R}-\boldsymbol{r}_a)}\rho_{\boldsymbol{q}}, \quad (7)$$

$$H_{\rm ep} = \sum_{\boldsymbol{q},\lambda} M(\boldsymbol{q},\lambda)(b_{\boldsymbol{q}\lambda} + b_{-\boldsymbol{q}\lambda}^\dagger)e^{i\boldsymbol{q}\cdot\boldsymbol{R}}\rho_{\boldsymbol{q}}. \quad (8)$$

In this, we have assumed that the relative electron system consists of N independent particles described by means of the creation and annihilation operators $c_{\boldsymbol{k}\sigma}^\dagger$ and $c_{\boldsymbol{k}\sigma}$ with wave vector $\boldsymbol{k}$, spin σ, and energy $\varepsilon_{\boldsymbol{k}} = k^2/2m$. In these equations, $v_c(q) = e^2/\epsilon_0\kappa q^2$ is the Coulomb potential, $\rho_{\boldsymbol{q}} = \Sigma_{\boldsymbol{k},\sigma} c_{\boldsymbol{k}+\boldsymbol{q}\sigma}^\dagger c_{\boldsymbol{k}\sigma}$ is the density operator of the relative electrons, $b_{\boldsymbol{q}\lambda}^\dagger$ and $b_{\boldsymbol{q}\lambda}$ are creation and annihilation operators of phonon with wave vector $\boldsymbol{q}$ in branch λ having frequency $\Omega_{\boldsymbol{q}\lambda}$, $u(\boldsymbol{q})$ and $M(\boldsymbol{q},\lambda)$ are, respectively, the electron-impurity potential and the electron-phonon matrix element satisfying $u(\boldsymbol{q}) = u^*(-\boldsymbol{q})$ and $M(\boldsymbol{q},\lambda) = M^*(-\boldsymbol{q},\lambda)$.

We start from the Heisenberg equations for the rates of changes of the center-of-mass momentum $\boldsymbol{P}$ and relative-electron occupation number operator $\hat{n}_{\boldsymbol{k}} \equiv \Sigma_\sigma c_{\boldsymbol{k}\sigma}^\dagger c_{\boldsymbol{k}\sigma}$,

$$\dot{\boldsymbol{P}} = -i[\boldsymbol{P}, H], \quad (9)$$

$$\dot{\hat{n}}_{\boldsymbol{k}} = -i[\hat{n}_{\boldsymbol{k}}, H]. \tag{10}$$

The center-of-mass motion is treated classically and its fluctuation neglected that in the steady state $\boldsymbol{R}(t)-\boldsymbol{R}(t')=\boldsymbol{v}(t-t')$, $\boldsymbol{v}$ being the drift velocity of the electron system. For the statistical average we proceed in the interaction picture[1] to the lowest nonzero order in the perturbative scattering potential $H_I=H_{\mathrm{ei}}+H_{\mathrm{ep}}+H_{\mathrm{ee}}$, with an initial density matrix having the property that the statistical averages of multiple (relative-electron and phonon) single-particle operators with respect to it are reducible to the products of pair averages. The typical pair averages are the occupation number or the distribution function of relative electrons,

$$n_{\boldsymbol{k}} = \sum_{\sigma} \langle c^{\dagger}_{\boldsymbol{k}\sigma} c_{\boldsymbol{k}\sigma} \rangle, \tag{11}$$

and that of phonons,

$$N_{\boldsymbol{q}\lambda} = \sum_{\sigma} \langle b^{\dagger}_{\boldsymbol{q}\lambda} b_{\boldsymbol{q}\lambda} \rangle. \tag{12}$$

The statistical average of operator equation (9) gives rise to the force-balance equation as follows:

$$\dot{\boldsymbol{P}} \equiv Nm\frac{d\boldsymbol{v}}{dt} = Ne\boldsymbol{E} + \boldsymbol{f}_i + \boldsymbol{f}_p, \tag{13}$$

with the frictional forces exerted on the center of mass, $\boldsymbol{f}_i$ and $\boldsymbol{f}_p$, given by

$$\boldsymbol{f}_i = 2\pi n_i \sum_{\boldsymbol{k},\boldsymbol{q}} |u(\boldsymbol{q})|^2 \boldsymbol{q}(n_{\boldsymbol{k}} - n_{\boldsymbol{k}+\boldsymbol{q}})\delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0), \tag{14}$$

$$\boldsymbol{f}_p = 4\pi \sum_{\boldsymbol{k},\boldsymbol{q},\lambda} |M(\boldsymbol{q},\lambda)|^2 \boldsymbol{q}[N_{\boldsymbol{q}\lambda}(n_{\boldsymbol{k}} - n_{\boldsymbol{k}+\boldsymbol{q}}) - n_{\boldsymbol{k}+\boldsymbol{q}}(1-n_{\boldsymbol{k}})] \times \delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0 - \Omega_{\boldsymbol{q}\lambda}), \tag{15}$$

where n_i is the impurity density and $\omega_0 \equiv \boldsymbol{q}\cdot v$. The statistical average of Eq. (10) yields the rate equations for the occupation number of relative electrons in state $\boldsymbol{k}$ as follows:

$$\frac{dn_{\boldsymbol{k}}}{dt} = \left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ei}} + \left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ep}} + \left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ee}}, \tag{16}$$

with

$$\left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ei}} = 4\pi n_i \sum_{\boldsymbol{q}} |u(\boldsymbol{q})|^2 (n_{\boldsymbol{k}+\boldsymbol{q}} - n_{\boldsymbol{k}})\delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0), \tag{17}$$

$$\left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ep}} = 4\pi \sum_{\boldsymbol{q},\lambda} |M(\boldsymbol{q},\lambda)|^2 \{[N_{\boldsymbol{q}\lambda}(n_{\boldsymbol{k}+\boldsymbol{q}} - n_{\boldsymbol{k}}) + n_{\boldsymbol{k}+\boldsymbol{q}}(1-n_{\boldsymbol{k}})]\delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0 - \Omega_{\boldsymbol{q}\lambda}) + [N_{\boldsymbol{q}\lambda}(n_{\boldsymbol{k}+\boldsymbol{q}} - n_{\boldsymbol{k}}) - n_{\boldsymbol{k}}(1-n_{\boldsymbol{k}+\boldsymbol{q}})] \times \delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0 + \Omega_{\boldsymbol{q}\lambda})\}, \tag{18}$$

$$\left[\frac{\partial n_{\boldsymbol{k}}}{\partial t}\right]_{\mathrm{ee}} = 2\pi n_i \sum_{\boldsymbol{q}} |\nu_{\mathrm{c}}(q)|^2 [(1-n_{\boldsymbol{k}})n_{\boldsymbol{k}-\boldsymbol{q}}(1-n_{\boldsymbol{k}'})n_{\boldsymbol{k}'+\boldsymbol{q}} - n_{\boldsymbol{k}}(1-n_{\boldsymbol{k}-\boldsymbol{q}})n_{\boldsymbol{k}'}(1-n_{\boldsymbol{k}'+\boldsymbol{q}})] \times \delta(\varepsilon_{\boldsymbol{k}} + \varepsilon_{\boldsymbol{k}'} - \varepsilon_{\boldsymbol{k}-\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}'+\boldsymbol{q}}). \tag{19}$$

One can directly verify that Eq. (16) obeys the sum rule to conserve the total number of relative electrons:

$$\sum_{\boldsymbol{k}} \frac{dn_{\boldsymbol{k}}}{dt} = 0. \tag{20}$$

This, of course, must be satisfied since the total number operator of relative electrons, $\Sigma_{\boldsymbol{k}}\hat{n}_{\boldsymbol{k}}$, is a conserved quantity in this system, $[\Sigma_{\boldsymbol{k}}\hat{n}_{\boldsymbol{k}}, H]=0$.

The rate equation (16) is exactly the same as Eq. (10) of Ref. 8 without "energy-drift" terms. It is similar to the Boltzmann equation for the single particle distribution function $n_{\boldsymbol{k}}$ of a nondrifting electron system but contains an extra parameter $\boldsymbol{v}$. By coupling Eqs. (16) and (13) one can obtain a complete set of equations to determine all the unknown parameters $n_{\boldsymbol{k}}$ and $\boldsymbol{v}$.

The appearance of the drift velocity $\boldsymbol{v}$ in $[\partial n_{\boldsymbol{k}}/\partial t]_{\mathrm{ei}}$ and $[\partial n_{\boldsymbol{k}}/\partial t]_{\mathrm{ep}}$ in Eq. (16) may result in an anisotropic distribution of $n_{\boldsymbol{k}}$. The $[\partial n_{\boldsymbol{k}}/\partial t]_{\mathrm{ee}}$ part, which contains no $\boldsymbol{v}$, however, always promotes an isotropic distribution and in the strong e-e scattering limit one expects to return to the results in Ref. 1. With the complete set of Eqs. (16) and (13) one can go beyond this limit.

An energy-balance equation for the relative electron system can be naturally derived by taking the statistical average of the Heisenberg equation for the rate of change of the relative-electron energy H_{e0},

$$\dot{H}_{e0} = -i[H_{e0}, H], \tag{21}$$

yielding

$$\langle \dot{H}_{e0} \rangle \equiv \frac{dU_e}{dt} = -\boldsymbol{v}\cdot(\boldsymbol{f}_i + \boldsymbol{f}_p) - w, \tag{22}$$

where $U_e=\langle H_{e0}\rangle=\Sigma_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}}n_{\boldsymbol{k}}$ is the average relative-electron energy, and $w=\langle \dot{H}_{\mathrm{ph}}\rangle=-i\langle[H_{\mathrm{ph}}, H]\rangle$ is the energy-transfer rate from the electron system to the phonon system, given by

$$w = 4\pi \sum_{\boldsymbol{k},\boldsymbol{q},\lambda} |M(\boldsymbol{q},\lambda)|^2 \Omega_{\boldsymbol{q}\lambda}[N_{\boldsymbol{q}\lambda}(n_{\boldsymbol{k}+\boldsymbol{q}} - n_{\boldsymbol{k}}) + n_{\boldsymbol{k}+\boldsymbol{q}}(1-n_{\boldsymbol{k}})]\delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0 - \Omega_{\boldsymbol{q}\lambda}). \tag{23}$$

Equation (22) states that the energy increase of the relative electron system equals the work done by the center of mass, $-\boldsymbol{v}\cdot(\boldsymbol{f}_i+\boldsymbol{f}_p)$, minus the energy transferred to the lattice, w. This energy-balance equation, however, has already been included in Eq. (16). In fact, multiplying Eq. (16) by $\varepsilon_{\boldsymbol{k}}$ and then summing over $\boldsymbol{k}$, one immediately gets[9]

$$\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} \frac{dn_{\boldsymbol{k}}}{dt} = -\boldsymbol{v}\cdot(\boldsymbol{f}_i + \boldsymbol{f}_p) - w, \tag{24}$$

i.e., the energy-balance equation (22). This indicates that the physical effects such as the work done by the center of mass

(through the antifrictional forces $-\boldsymbol{f}_i - \boldsymbol{f}_p$) on the relative electrons, and the energy transfer from the relative electron system to the phonon system, w, have already been contained in the rate equation (16) for the relative-electron occupation number, and that the erergy-balance equation (22) is no longer an independent equation. There is no need to introduce any other energy-related term into the rate equation (16).

Reference 8 introduces additional "energy-drift" terms $d_{\boldsymbol{k}}^{(i)}$ and $d_{\boldsymbol{k}}^{(p)}$ into the right-hand side of Eq. (16), referring to the work done by the impurity and phonon-related frictional forces "for increasing the thermal energy of electrons in the $\boldsymbol{k}$ state". The rate equation, Eq. (16), thus modified, which is called the energy-drift equation in Ref. 8, no longer conserves the total particle number of relative electrons and violates the energy balance as stated by Eq. (22) in the case of nonzero drift velocity. For instance, in the case of a small $\boldsymbol{v}$ one can write (see Ref. 8 for the details of $d_{\boldsymbol{k}}^{(i)}$ and $d_{\boldsymbol{k}}^{(p)}$)

$$\sum_{\boldsymbol{k}} d_{\boldsymbol{k}}^{(i)} = \pi n_i \sum_{\boldsymbol{k},\boldsymbol{q}} |u(\boldsymbol{q})|^2 \omega_0^2 \frac{\partial^2 n_{\boldsymbol{k}}}{\partial \varepsilon_{\boldsymbol{k}}^2} \delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0),$$

$$\sum_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} d_{\boldsymbol{k}}^{(i)} = \pi n_i \sum_{\boldsymbol{k},\boldsymbol{q}} |u(\boldsymbol{q})|^2 \omega_0^2 \varepsilon_{\boldsymbol{k}} \frac{\partial^2 n_{\boldsymbol{k}}}{\partial \varepsilon_{\boldsymbol{k}}^2} \delta(\varepsilon_{\boldsymbol{k}+\boldsymbol{q}} - \varepsilon_{\boldsymbol{k}} + \omega_0).$$

They are generally not zero unless for a very special form of $n_{\boldsymbol{k}}$. Therefore, the addition of these "energy-drift" terms into the rate equation, Eq. (16), for the electron-impurity-phonon system subject to a uniform electric field as described by the total Hamiltonian (1) or (2), is physically inadequate.

An example of the consequence of particle-number conservation violation in the energy-drift equation is provided directly by Fig. 8 of Ref. 8, where the distribution function $\bar{f}(\boldsymbol{k}) = (\varepsilon_F / k_F^3) f(\boldsymbol{k}) = (k/2\pi^2 k_F) n_{\boldsymbol{k}}$ (k_F and ε_F are zero-temperature Fermi wave vector and Fermi energy) for a GaAs semiconductor at $T=30$ K subjected to a dc field $E_{\mathrm{dc}}=0.75$ kV/cm (hot electrons) derived from solving the coupled energy-drift and force-balance equations and that without dc field (equilibrium electrons), are presented. Evaluating the total electron density $n_e = \Sigma_{\boldsymbol{k}} n_{\boldsymbol{k}}$ from these two distribution functions, one can clearly see that the electron density n_e for hot electrons would be at least 28% larger than that for equilibrium electrons. In the latter case n_e equals the given electron density $\sigma_{3\mathrm{D}} = 10^{18}$ cm^{-3}. This result for the hot electrons in Fig. 8 of Ref. 8 shows that if the energy-drift equation is used to describe the transport a substantial increase of the number of electrons may result merely due to the application of a dc field in a system which should physically conserve the particle number. Such a large unphysical change of the electron number is certainly intolerable. Furthermore, the effect of introducing these "energy drift" terms, which is considered in Ref. 8 as the major improvement over the previous equations, is to give rise to a decrease in the drift velocity and mobility around 11% (at $E_{\mathrm{dc}}=0.75$ kV/cm) in comparison with that obtained without "energy drift" terms (conserving the particle number) as shown in Fig. 9 of Ref. 8. An 11% decrease of drift velocity obtained at the cost of more than a 28% spurious increase of total particle number, is by no means a proper choice, and moreover, there is no experimental impetus for a prescription to reduce the high-field mobility.

It seems that the coupled force-balance and particle-occupation rate equations (13) and (16), are physically sound and sufficient for high-field electron transport in semiconductors in general cases. The equations proposed by Huang *et al.* in Ref. 7 without "energy-drift" terms, may provide a comparably rational base in the weak e-e scattering limit.

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[9] Note that $\Sigma_{\boldsymbol{k}} \varepsilon_{\boldsymbol{k}} [\partial n_{\boldsymbol{k}} / \partial t]_{\mathrm{ee}} = 0$, i.e., e-e interaction does not change the relative electron energy, as it should be.