Nonlinear electronic transport in semiconductor systems with two types of carriers: Application to GaAs

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The balance-equation approach for hot-electron transport previously developed is extended to systems composed of two groups of carriers, each of different effective mass. This is the simplest model for a real band structure of a multivalley semiconductor. The separation of the center-of-mass (c.m.) motion from the relative motion of the electrons is incomplete due to the possibility of exchange of particle number between the two systems and thus is taken into account in the Liouville equation for the density matrix. General expressions for the rates of change of the c.m. momenta, electron system energies, and particle numbers are obtained. These equations in their classical forms are used for a model calculation for the high-field steady-state transport in GaAs and the calculated results show reasonably good agreement with experiments.

I. INTRODUCTION

Since the early successful experimental observations of high-field transport in n-type Ge (Ref. 1) and the later discovery of the Gunn effect in GaAs,[2] widespread experimental and theoretical interest has been focused on nonlinear transport in semiconductor materials for several decades. Interest intensified recently with the development of submicrometer semiconductor devices. Theoretical approaches to the problem, in addition to Monte Carlo simulations,[3] and with a few exceptions,[4] have been based on solving the semiphenomenological Boltzmann equation.[5–7] Recently an alternative attempt to solve this problem has been made by Lei and Ting[8] directly from the Liouville equation of motion for the density matrix of the system, based on a separation of the center-of-mass (c.m.) motion from the relative motion of the electrons. Concise balance equations are obtained by calculating the density matrix of the system to first order in the impurity and phonon scattering interaction. These equations, written in terms of the electron density correlation function, can describe the steady-state and transient transport beyond the Boltzmann approach.[9] This point has been clearly explained in Ref. 9. However, under a field strength $E < 10^5$ to 10^6 V/cm, it is generally believed[9,10] that the balance equations in their classical forms are valid for hot-electron transport. We wish to emphasize that the Lei-Ting balance equations are not equivalent to the Boltzmann equation, but do not go beyond the level of a semiclassical theory if only an electric field is applied, and the involved density correlation functions are evaluated in the random-phase approximation (RPA). These equations,[8] written in terms of an electron density correlation function, give a uniform description without and with a quantizing magnetic field.[11] For the latter case a semiclassical treatment is invalid. Even in the absence of a magnetic field, this theory[8] has the capacity to go beyond the semiclassical Boltzmann approach when the density correlation functions are also calculated beyond RPA.

The approach described in Ref. 8 is only for one type of carrier with parabolic band. However, semiconductors like GaAs and Si usually have more complicated band structures, and transitions between nonequivalent valleys may play an important role at room temperature or at high fields. The formulations presented in Ref. 8 are not applicable in that case. In this paper we try to go one step further in considering the complexity of the band structure by assuming that the system has two different nonequivalent isotropic valleys with different effective masses, i.e., a system composed of two types of carriers. The method shall be applied to study the steady-state transport in n-type GaAs. We shall limit the applied electric field $< 10^5$ V/cm for such a field strength, the validity of the semiclassical balance equations is expected.[9]

II. HAMILTONIAN

We can use this model to discuss the carrier transport along the crystal axes in GaAs systems. In n-type GaAs the center valley (Γ) has the lowest energy and is nearly

spherically symmetric with effective mass $m_1 \simeq 0.067 m_0$ (m_0 is the free-electron mass). The next lowest ones are four equivalent valleys at L points. They are energetically at $\epsilon_g = 0.27$ eV (Ref. 12) above the Γ valley and have elliptic symmetry with $\langle 111 \rangle$ (or $\langle \bar{1}11 \rangle$, etc.) as their symmetric axes. If we consider carrier transport along one of the crystal axes, any one of these valleys gives the same contribution. For simplicity, we will represent these valleys by spheres with effective mass $m_2 \simeq 0.23 m_0$. Neglecting the valleys of higher energy, we have a system composed of two types of carriers. The total number of these carriers $N = N_1 + N_2$ is assumed to be constant. However, the numbers of carrier particles of systems 1 and 2, N_1 and N_2, are variable since the carriers in systems 1 and 2 can exchange with each other. We introduce the coordinate $\mathbf{R}$ for the center of mass of the whole system, and $\mathbf{R}_1$ and $\mathbf{R}_2$ for systems 1 and 2:

$$\mathbf{R} = \frac{1}{N}\left[\sum_i^1 \mathbf{r}_{1i} + \sum_i^2 \mathbf{r}_{2i}\right] = (N_1/N)\mathbf{R}_1 + (N_2/N)\mathbf{R}_2 , \quad (1)$$

and momenta $\mathbf{P}_1$ and $\mathbf{P}_2$ for systems 1 and 2:

$$\mathbf{P}_1 = \sum_i^1 \mathbf{p}_{1i}, \quad \mathbf{p}_2 = \sum_i^2 \mathbf{p}_{2i} . \quad (2)$$

Here $\mathbf{r}_{1i}$, $\mathbf{p}_{1i}$ ($\mathbf{r}_{2i}$, $\mathbf{p}_{2i}$) are coordinates and momenta of the ith particle in system 1 (2), which satisfy the well-known commutation relation $[r_{1i}^{\alpha}, \mathbf{p}_{1j}^{\beta}] = i\delta_{ij}\delta_{\alpha\beta}$, $[r_{2i}^{\alpha}, \mathbf{p}_{2j}^{\beta}] = i\delta_{ij}\delta_{\alpha\beta}$. We also introduce the velocities $\mathbf{v}_1$ and $\mathbf{v}_2$ for the centers of mass of the systems 1 and 2:

$$\mathbf{P}_1 = N_1\mathbf{v}_1, \quad \mathbf{P}_2 = N_2\mathbf{v}_2 . \quad (3)$$

The relative coordinates and momenta for the carrier systems 1 and 2 are defined as

$$\mathbf{r}'_{1i} = \mathbf{r}_{1i} - \mathbf{R}_1, \quad \mathbf{r}'_{2i} = \mathbf{r}_{2i} - \mathbf{R}_2 , \quad (4)$$

$$\mathbf{p}'_{1i} = \mathbf{p}_{1i} - m_1\mathbf{v}_1, \quad \mathbf{p}'_{2i} = \mathbf{p}_{2i} - m_2\mathbf{v}_2 . \quad (5)$$

According to definitions (1) and (2), $[N_1 R_{1\alpha}, P_{1\beta}] = iN_1\delta_{\alpha\beta}$. Therefore it is consistent to consider $\mathbf{R}_1$, $\mathbf{P}_1$ as canonical variables of the center of mass satisfying

$$[R_{1\alpha}, P_{1\beta}] = i\delta_{\alpha\beta} , \quad (6)$$

and $\hat{N}_1$, the particle number of system 1, as a variable of the relative electron system 1, which commutes with c.m. variables. It is easily seen that to the order of $O(1/N)$ the relative electron variables $\mathbf{r}'_{1i}$ and $\mathbf{p}'_{ij}$ obey the canonical commutation relation

$$[r'^{\alpha}_{1i}, \mathbf{p}'^{\beta}_{1j}] = i\delta_{\alpha\beta}\left[\delta_{ij} + O\left[\frac{1}{N_1}\right]\right] . \quad (7)$$

Therefore, most of the discussions in Ref. 8 can still apply in the present case. In terms of these new variables the total Hamiltonian of the system in the presence of a uniform electric field $\mathbf{E}$ can be written as follows:

$$\begin{aligned} H &= H_{\text{c.m. }E} + H_{\text{c.m. }T} + H_{1e} + H_{2e} + H_{\text{ph}} + H_I , \\ H_I &= H_{12} + H_{1e\text{-}i} + H_{2e\text{-}i} + H_{1e\text{-ph}} + H_{2e\text{-ph}} . \end{aligned} \quad (8)$$

Here

$$H_{\text{c.m. }E} = -Ne\mathbf{E}\cdot\mathbf{R} , \quad (9)$$

and

$$H_{\text{c.m. }T} = \tfrac{1}{2}m_1\hat{N}_1\mathbf{v}_1^2 + \tfrac{1}{2}m_2\hat{N}_2\mathbf{v}_2^2 \quad (10)$$

are the center-of-mass part of the Hamiltonian. Particle numbers $\hat{N}_1$ and $\hat{N}_2$ can be expressed in the second quantization representation of the relative carrier systems 1 and 2 as

$$\hat{N}_1 = \sum_{k,\sigma}^1 c^{\dagger}_{1\mathbf{k}\sigma}c_{1\mathbf{k}\sigma}, \quad \hat{N}_2 = \sum_{k,\sigma}^2 c^{\dagger}_{2\mathbf{k}\sigma}c_{2\mathbf{k}\sigma} , \quad (11)$$

where $c^{\dagger}_{i\mathbf{k}\sigma}$ ($c_{i\mathbf{k}\sigma}$) are creation (annihilation) operators of wave vector $\mathbf{k}$ for the ith ($i=1,2$) type of carriers relative to their respective center of mass. The summation over $\mathbf{k}$ is actually limited in the vicinity of Γ ($\mathbf{k}_1 = 0$) point (for type-1 carrier, or system 1) or those of all k_L points (for type-2 carriers, or system 2). H_{1e} and H_{2e} are the relative parts of the Hamiltonian for the first and the second carrier systems, including their ("intravalley") Coulomb interaction:

$$\begin{aligned} H_{1e} &= \sum_{\mathbf{k},\sigma}^1 \varepsilon_{1\mathbf{k}} c^{\dagger}_{1\mathbf{k}\sigma}c_{1\mathbf{k}\sigma} \\ &\quad + \tfrac{1}{2}\sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} \nu_c(q) c^{\dagger}_{1\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{1\mathbf{k}-\mathbf{q},\sigma'} c_{1\mathbf{k}'\sigma'} c_{1\mathbf{k}\sigma} , \end{aligned} \quad (12)$$

$$\begin{aligned} H_{2e} &= \sum_{\mathbf{k},\sigma}^2 \varepsilon_{2\mathbf{k}} c^{\dagger}_{2\mathbf{k}\sigma}c_{2\mathbf{k}\sigma} \\ &\quad + \tfrac{1}{2}\sum_{\substack{\mathbf{k},\mathbf{k}',q \\ \sigma,\sigma'}}^2 \nu_c(\mathbf{q}) c^{\dagger}_{2,\mathbf{k}+\mathbf{q},\sigma} c^{\dagger}_{2,\mathbf{k}'-\mathbf{q},\sigma'} c_{2\mathbf{k}'\sigma'} c_{2\mathbf{k}\sigma} , \end{aligned} \quad (13)$$

in which $\nu_c(\mathbf{q}) = e^2/\varepsilon_0\mathbf{q}^2$ is the Coulomb potential. For convenience we choose the band bottom of the Γ valley as the common zero for both systems, so that $\varepsilon_{1\mathbf{k}} = \mathbf{k}^2/2m_1$, and $\varepsilon_{2\mathbf{k}} = (\mathbf{k}-\mathbf{k}_L)^2/2m_2 + \epsilon_g$. In Eq. (1) $H_{1e\text{-}i}$, $H_{1e\text{-ph}}$, $H_{2\text{-}ei}$, and $H_{2\text{-ph}}$ are electron-impurity and electron-phonon couplings for type-1 and type-2 carriers, respectively:

$$H_{1e\text{-}i} = \sum_{\mathbf{q},a} u_1(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}_1 - \mathbf{R}_a)} \rho_{1\mathbf{q}} , \quad (14)$$

$$H_{2e\text{-}i} = \sum_{\mathbf{q},a} u_2(\mathbf{q}) e^{i\mathbf{q}\cdot(\mathbf{R}_2 - \mathbf{R}_a)} \rho_{2\mathbf{q}} , \quad (15)$$

$$H_{1e\text{-ph}} = \sum_{\mathbf{q},\lambda} M_1(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda} + b^{\dagger}_{-\mathbf{q}\lambda}) e^{i\mathbf{q}\cdot\mathbf{R}_1} \rho_{1\mathbf{q}} , \quad (16)$$

$$H_{2e\text{-ph}} = \sum_{\mathbf{q},\lambda} M_2(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda} + b^{\dagger}_{-\mathbf{q}\lambda}) e^{i\mathbf{q}\cdot\mathbf{R}_2} \rho_{2\mathbf{q}} , \quad (17)$$

in which

$$\rho_{1\mathbf{q}} = \sum_{\mathbf{k},\sigma}^1 c^{\dagger}_{1,\mathbf{k}+\mathbf{q}\sigma}c_{1,k\sigma} , \quad (18)$$

and

$$\rho_{2\mathbf{q}} = \sum_{\mathbf{k},\sigma}^2 c^{\dagger}_{2,\mathbf{k}+\mathbf{q}\sigma}c_{2,\mathbf{k}\sigma} , \quad (19)$$

are density operators for type-1 and type-2 carriers, $u_j(\mathbf{q})$ and $M_j(\mathbf{q},\lambda)$ are intravalley electron-impurity potentials and electron-phonon matrix elements for system j ($j=1,2$), and $b^{\dagger}_{\mathbf{q}\lambda}$ ($b_{\mathbf{q}\lambda}$) are creation (annihilation) operators for phonons with wave vector $\mathbf{q}$ and frequency $\Omega_{\mathbf{q}\lambda}$. The phonon part of the Hamiltonian is

$$H_{\rm ph}=\sum_{\mathbf{q},\lambda}\Omega_{\mathbf{q}\lambda}b^{\dagger}_{\mathbf{q}\lambda}b_{\mathbf{q}\lambda}\ . \tag{20}$$

In Eq. (8) H_{12} stands for the Coulomb interaction between different types of carriers (intervalley Coulomb interaction):

$$H_{12}=\sum_{\mathbf{q}}v_c(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_2)}\rho_{1\mathbf{q}}\rho_{2-\mathbf{q}}\ . \tag{21}$$

Finally, $H^{12}_{e\text{-ph}}$ and $H^{21}_{e\text{-ph}}$ are intervalley electron-phonon interactions:

$$H^{12}_{e\text{-ph}}=\sum_{\mathbf{q},\lambda}M_{12}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_1}\times\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}(\mathbf{R}_1-\mathbf{R}_2)}c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{2\mathbf{k}\sigma}\ , \tag{22}$$

$$H^{21}_{e\text{-ph}}=\sum_{\mathbf{q},\lambda}M_{21}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_2}\times\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_2-\mathbf{R}_1)}c^{\dagger}_{2\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}\ , \tag{23}$$

with $M_{12}(\mathbf{q},\lambda)=M_{21}(\mathbf{q},\lambda)$ being matrix elements for intervalley electron-phonon scattering. Intervalley electron-impurity scattering is neglected.

Using Hamiltonian (8), the time derivative of center-of-mass momenta $\mathbf{P}_1$ and $\mathbf{P}_2$, the relative electron energies H_{1e} and H_{2e}, and the phonon energy $H_{\rm ph}$, can be obtained from the relation $\dot{O}=-i[O,H]$ (O stands for an arbitrary operator). The results are given in Appendix A.

III. BALANCE EQUATIONS FOR FORCES, ENERGIES, AND PARTICLE NUMBERS

The derivation of balance equations requires calculation of the statistical average of the time derivatives of the related quantities with respect to the appropriate density matrix of the system. This density matrix can be obtained by closely following the derivation in Ref. 8: i.e., treating the center of masses classically and treating H_I perturbatively to the lowest order. The coordinates and velocities of the center of masses enter the density matrix only through their time-dependent statistical averages. It should be noted, however, that there is an important difference in the present case of two types of carriers with different effective masses from that discussed in Ref. 8. The separation of center of masses from the relative degrees of freedom is incomplete in the sense that $H_{\rm c.m.\ }_T$ includes relative electron variable N_1 which does not commute with the interaction associated with particle exchange between these two systems. Therefore the Liouville equation for the statistical density matrix ρ of the relative electron-phonon system takes the form

$$i\frac{\partial\rho}{\partial t}=[H_{\rm c.m.\ }_T+H_{1e}+H_{2e}+H_I,\rho]\ . \tag{24}$$

To obtain an appropriate initial condition we imagine turning off all the electron-impurity, electron-phonon, and intersystem electron-electron Coulomb interactions, as well as the electric field, at time t_1. Then the two carrier systems, decoupled from each other, will approach their respective thermal equilibrium states with temperatures T_{1e} and T_{2e} and chemical potentials μ_1 and μ_2, which of course depend on the time t. The initial condition for the density matrix ρ is therefore chosen to be

$$\rho\,|_{\,t=-\infty}=\rho_0=\frac{1}{z_{\rm ph}}e^{-H_{\rm ph}/T}\frac{1}{z_1}e^{-(H_{1e}-\mu_1N_1)/T_{1e}}\times\frac{1}{z_2}e^{-(H_{2e}-\mu_2N_2)/T_{2e}}\ . \tag{25}$$

The expressions for the statistical average of the rates of change of the particle number, the center-of-mass momentum, and the relative electron energy of each type of carrier can be calculated to the lowest order of the interaction at time t as

$$\langle d\hat{N}_1/dt\rangle=N(v_1,v_2)\ , \tag{26}$$

$$\langle\dot{P}_{1x}\rangle=N_1eE+F_1(v_1)+F_p^{12}(v_1,v_2)+F_{12}(v_1-v_2)\ , \tag{27}$$

$$\langle\dot{P}_{2x}\rangle=N_2eE+F_2(v_2)+F_p^{21}(v_1,v_2)-F_{12}(v_1-v_2)\ , \tag{28}$$

$$-\langle\dot{H}_{1e}\rangle=v_1F_1(v_1)+W_1(v_1)+W_p^{12}(v_1,v_2)+W_{12}(v_1-v_2)\ , \tag{29}$$

$$-\langle\dot{H}_{2e}\rangle=v_2F_2(v_2)+(v_1-v_2)F_{12}(v_1-v_2)-W_{12}(v_1-v_2)+W_2(v_2)+W_p^{21}(v_2,v_1)\ . \tag{30}$$

Here N_1 and N_2 are the average particle numbers of carrier systems 1 and 2, v_1 and v_2 are the average velocities of the c.m. particle 1 and c.m. particle 2; i.e., the average drift velocities of the type-1 and type-2 carriers. The total current J is due to both types of carriers:

$$J=N_1ev_1+N_2ev_2\ , \tag{31}$$

the average drift velocity of the total system should be

$$v=(N_1v_1+N_2v_2)/(N_1+N_2)\ . \tag{32}$$

The expression for N, F, and W functions in Eqs. (26)–(30) are given in Appendix B. They include electron temperatures T_{1e} and T_{2e}, as well as the chemical potentials μ_1 and μ_2, as parameters. Since after turning off the interaction the two carrier systems cannot exchange particles and energy with each other, nor with phonons, the particle numbers and the internal energies of the two systems at time t can be calculated by means of the initial density matrix relevant to time t. Whence we have

$$N_1=\sum_{\mathbf{k},\sigma}^{1} f((\varepsilon_{1k}-\mu_1)/T_{1e}) , \tag{33}$$

$$N_2=N-N_1=\sum_{\mathbf{k},\sigma}^{2} f((\varepsilon_{2k}-\mu_2)/T_{2e}) , \tag{34}$$

and

$$E_1=\sum_{\mathbf{k},\sigma}^{1} \varepsilon_{1\mathbf{k}} f((\varepsilon_{1k}-\mu_1)/T_{1e}) , \tag{35}$$

$$E_2=\sum_{\mathbf{k},\sigma}^{2} \varepsilon_{2\mathbf{k}} f((\varepsilon_{2k}-\mu_2)/T_{2e}) , \tag{36}$$

in which $f((\varepsilon-\mu)/T)=1/\{\exp[(\varepsilon-\mu)/T]+1\}$ is the Fermi function.

In Eqs. (27) and (28) $F_{12}(v_1-v_2)$ is the force exerted on the center-of-mass particle 1, resulting from intervalley Coulomb interaction. It has nonzero value only when two center of masses move at different velocities. This is in agreement with the fact that there is no momentum exchange during the process of Coulomb interaction. However, the energy-loss rate of the relative system 1 due to intervalley Coulomb interaction could be nonzero even when $v_1=v_2$, unless $T_{1e}=T_{2e}$. This means that if the electron temperatures of the two relative carrier systems are different there may be an energy exchange between them due to intervalley Coulomb interaction. When $v_1=v_2$, it is easily seen from the expression of $W_{12}(v_1-v_2)$ that energy always transfers from the system with higher temperature to that with lower temperature, in agreement with the conventional heat transfer idea. However, this conclusion might not be valid when $v_1\neq v_2$.

It is straightforward to generalize the theoretical approach to transient hot-electron transport[9] to the system with two types of carriers. If the memory effect on the drift velocity and electron temperature is neglected, the evolution equations for the average particle number, forces, and energies can be obtained:

$$\frac{dN_1}{dt}=\langle d\hat{N}_1/dt\rangle , \tag{37}$$

$$m_1N_1\frac{dv_1}{dt}=\langle \dot{P}_{1x}\rangle , \tag{38}$$

$$m_2(N-N_1)\frac{dv_2}{dt}=\langle \dot{P}_{2x}\rangle , \tag{39}$$

$$C_1\frac{dT_{1e}}{dt}+\lambda_1\frac{dN_1}{dt}=\langle \dot{H}_{1e}\rangle , \tag{40}$$

$$C_2\frac{dT_{2e}}{dt}-\lambda_2\frac{dN_1}{dt}=\langle \dot{H}_{2e}\rangle , \tag{41}$$

in which $C_1=(\partial E_1/\partial T_{1e})_{N_1}$, $C_2=(\partial E_2/\partial T_{2e})_{N_2}$, $\lambda_1=(\partial E_2/\partial N_1)_{T_{1e}}$, and $\lambda_2=(\partial E_2/\partial N_2)_{T_{2e}}$ are to be determined by the relations (33)–(36).

Now we have a set of five differential equations for five variables: N_1, v_1, v_2, T_{1e}, and T_{2e}, and two parameters μ_1 and μ_2, supplemented by the two relations (33) and (34) valid at any time t. The time-dependent solution can be obtained uniquely for given lattice temperature T, electric field E as a function of t, and for given initial values of N_1, v_1, v_2, T_{1e}, and T_{2e}.

In the steady state the time derivatives of all the variables N_1, v_1, v_2, T_{1e}, and T_{2e} vanish. The equations $\langle d\hat{N}_1/dt\rangle=0$, $\langle \dot{P}_{1x}\rangle=0$, $\langle \dot{P}_{2x}\rangle=0$, $\langle \dot{H}_{1e}\rangle=0$, and $\langle \dot{H}_{2e}\rangle=0$, together with relations (33) and (34) form a complete set of equations to determine the steady-state values of N_1, v_1, v_2, T_{1e}, and T_{2e} at given T and E.

IV. NUMERICAL RESULTS FOR GaAs

We have performed numerical calculation for GaAs to obtain high-field steady-state transport for electric fields less than 50 kV/cm at lattice temperatures $T=150$, 200, 300, and 350 K, using the Γ-valley plus four L-valleys model discussed in the preceding sections. At electron temperatures higher than these T's, a nondegenerate distribution is assumed for the Fermi function in all the equations. As most other authors did in these kinds of studies, intravalley Coulomb interactions between carriers are considered only in a constant screening approximation, and intervalley (between Γ and L valleys) Coulomb interaction effects are neglected for simplicity.

For Γ valley (system 1) we include (1) acoustic-phonon deformation potential scattering with

$$|M_1(\mathbf{q},\lambda_1)|^2=\frac{\hbar E_1^2 q}{2Vdv_s} , \tag{42}$$

and (2) polar-optic-phonon scattering with

$$|M_1(\mathbf{q},\lambda_2)|^2=\frac{e^2\hbar\Omega_{\mathrm{LO}}}{2V\epsilon_0 q^2}\left[\frac{1}{\kappa_\infty}-\frac{1}{\kappa}\right] . \tag{43}$$

Here the GaAs mass density $d=5.36$ g/cm^3, acoustic-phonon deformation potential $E_1=7.0$ eV, longitudinal sound velocity $v_s=5.24\times10^5$ cm/sec, static dielectric constant $\kappa=12.9$, high-frequency dielectric constant $\kappa_\infty=10.9$, and longitudinal-optic-phonon energy $\hbar\Omega_{\mathrm{LO}}=35.4$ meV.

Four equivalent L valleys comprise system 2. For them we consider (1) acoustic-phonon intravalley scattering with matrix element having the same form as (42) but with $E_1=9.2$ eV, and (2) optical-phonon deformation potential intravalley scattering with

$$|M_2(\mathbf{q},\lambda_2)|^2=\frac{\hbar D^2}{2Vd\Omega_L} . \tag{44}$$

Here optic-phonon energy $\hbar\Omega_L=34.3$ meV, optical-phonon deformation potential $D=3.0\times10^8$ eV/cm. Besides there are intervalley electron-optical phonon scattering, having

$$|M_2(\mathbf{q},\lambda_3)|^2=\frac{\hbar D_{LL}^2}{2Vd\Omega_{LL}} \tag{45}$$

with $D_{LL}=1.0\times10^9$ eV/cm and $\hbar\Omega_{LL}=29.0$ meV.

For intervalley electron-phonon scattering between Γ valley and any one of the four L valleys, the matrix element is taken as

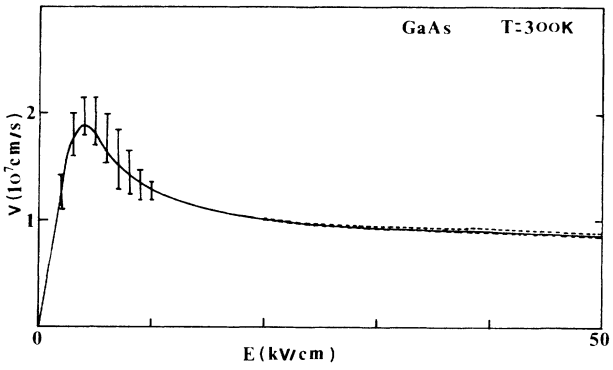

FIG. 1. Steady-state drift velocity v vs electric field E for GaAs at $T=300$ K. The solid curve is the calculated result, the error bars are experimental data compiled by Ref. 13, and the upper and lower dashed curves are experimental data from Refs. 14 and 15, respectively.

$$|M_{12}(\mathbf{q},\lambda)|^2=\frac{\hbar D_{L\Gamma}^2}{2Vd\Omega_{L\Gamma}}\ , \tag{46}$$

with $D_{L\Gamma}=1.1\times10^9$ eV/cm and $\hbar\Omega_{L\Gamma}=20.8$ meV.

The calculated results of the steady-state drift velocity v, defined by Eq. (32), as a function of electric field less than 50 kV/cm are shown in Figs. 1 and 2, together with compiled experimental data,[13–15] showing reasonably good agreement between theory and experiments. The present results are also in concordance with Monte Carlo simulations[13] and a Boltzmann equation calculation using relaxation time approximation.[7]

In Fig. 3 we plot the calculated values of the fraction of carriers in Γ valley N_1/N and the electron temperatures normalized to the lattice temperature T_e/T for Γ and L valleys as functions of the electric field E at $T=300$ K.

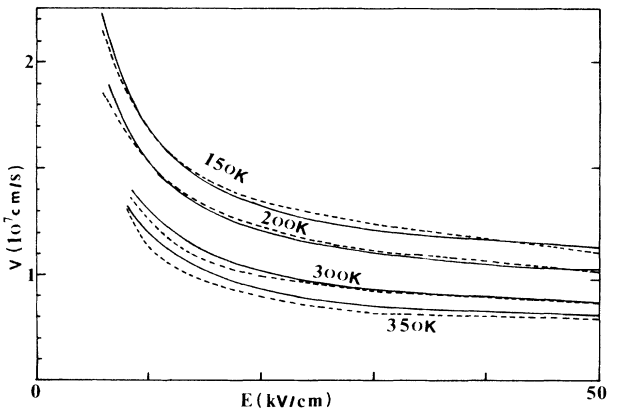

FIG. 2. Steady-state drift velocity v vs electric field E for GaAs at $T=150$, 200, 300, and 350 K. The solid curves are calculated results and the dashed lines are the experimental data from Ref. 15.

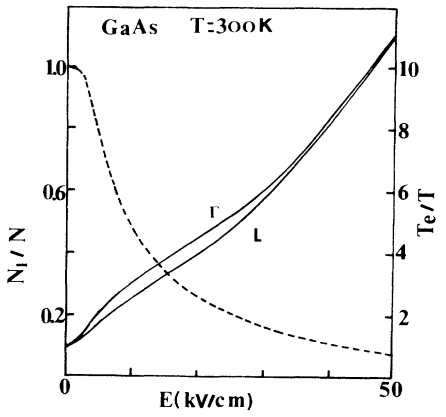

FIG. 3. The calculated results for the fraction of carriers in Γ valley, N_1/N (dashed curve), and the electron temperatures normalized to the lattice temperature for Γ and L valleys, are shown as functions of the electric field E at $T=300$ K (solid curves).

V. SUMMARY

We have demonstrated that the balance-equation approach[8] based on the separation of the center of mass from the relative motion of electrons can be extended to multivalley semiconductor systems, i.e., systems composed of two or more groups of carriers: each has different effective mass and the particle numbers of the different groups can exchange with each other. The equation of motion of the center of mass, and the energy and particle number balance equations for each subsystem are derived, including full dynamic Coulomb interactions between carriers in different valleys. The equations obtained are good for numerical calculation for steady-state and transient transport in a uniform high electric field. We have carried out numerical computation for GaAs steady-state transport at field $E<50$ kV/cm with the simplest Γ-L model without including intervalley Coulomb interaction. Reasonably good agreement with experiments is obtained. For better results for GaAs at higher field a more realistic model including X valleys and the nonparabolicity of the Γ valley is desirable. To adapt the present approach to this case is a subject for future study.

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APPENDIX A

The time derivatives of center-of-mass momentum and relative electron energy of the carrier system 1 are as follows:

$$\dot{P}_{1x}=-i[P_{1x},H]$$
$$=N_1eE_x-i\sum_{\mathbf{q},a}u_1(\mathbf{q})\mathbf{q}_x e^{i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_a)}\rho_{1\mathbf{q}}-i\sum_{\mathbf{q},\lambda}M_1(\mathbf{q},\lambda)\mathbf{q}_x e^{i\mathbf{q}\cdot\mathbf{R}_1}(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})\rho_{1\mathbf{q}}$$
$$+i\sum_{\mathbf{q},\lambda}M_{21}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_2}\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_2-\mathbf{R}_1)}\mathbf{k}_x c^{\dagger}_{2\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}$$
$$-i\sum_{\mathbf{q},\lambda}M_{12}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_1}\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_2)}(\mathbf{k}_x+\mathbf{q}_x)c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{2\mathbf{k}\sigma}$$
$$-i\sum_{\mathbf{q}}v_c(\mathbf{q})\mathbf{q}_x e^{i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_2)}\rho_{1\mathbf{q}}\rho_{2,-\mathbf{q}}\ , \tag{A1}$$

$$\dot{H}_{1e}=-i[H_{1e},H]$$
$$=-i\sum_{\mathbf{q},a}u_1(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_a)}\sum_{\mathbf{k},\sigma}(\varepsilon_{1\mathbf{k}+\mathbf{q}}-\varepsilon_{1\mathbf{k}})c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}$$
$$-i\sum_{\mathbf{q},\lambda}M_1(\mathbf{q},\lambda)e^{i\mathbf{q}\cdot\mathbf{R}_1}(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})\sum_{\mathbf{k},\sigma}(\varepsilon_{1\mathbf{k}+\mathbf{q}}-\varepsilon_{1\mathbf{k}})c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}$$
$$+i\sum_{\mathbf{q},\lambda}M_{21}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_2}\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_2-\mathbf{R}_1)}\varepsilon_{1\mathbf{k}}c^{\dagger}_{2\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}$$
$$-i\sum_{\mathbf{q},\lambda}M_{12}(\mathbf{q},\lambda)(b_{\mathbf{q}\lambda}+b^{\dagger}_{-\mathbf{q}\lambda})e^{i\mathbf{q}\cdot\mathbf{R}_1}\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_2)}\varepsilon_{1\mathbf{k}+\mathbf{q}}c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{2\mathbf{k}\sigma}$$
$$-i\sum_{\mathbf{q}}v_c(\mathbf{q})e^{i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_2)}\sum_{\mathbf{k},\sigma}(\varepsilon_{1\mathbf{k}+\mathbf{q}}-\varepsilon_{1\mathbf{k}})c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}\rho_{2,-\mathbf{q}}\ . \tag{A2}$$

The expressions for $\dot{P}_{2x}$ and $\dot{H}_{2e}$ can be obtained from (A1) and (A2) by exchanging the indices $1\leftrightarrow 2$. The time derivative of the energy of the phonon system is

$$\dot{H}_{\rm ph}=-i[H_{\rm ph},H]$$
$$=i\sum_{\mathbf{q},\lambda}M_1(\mathbf{q},\lambda)\Omega_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}_1}(b_{\mathbf{q}\lambda}-b^{\dagger}_{-\mathbf{q}\lambda})\rho_{1\mathbf{q}}+i\sum_{\mathbf{q},\lambda}M_2(\mathbf{q},\lambda)\Omega_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}_2}(b_{\mathbf{q}\lambda}-b^{\dagger}_{-\mathbf{q}\lambda})\rho_{2\mathbf{q}}$$
$$+i\sum_{\mathbf{q},\lambda}M_{12}(\mathbf{q},\lambda)\Omega_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}_1}(b_{\mathbf{q}\lambda}-b^{\dagger}_{-\mathbf{q}\lambda})\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_2)}c^{\dagger}_{1\mathbf{k}+\mathbf{q}\sigma}c_{2\mathbf{k}\sigma}$$
$$+i\sum_{\mathbf{q},\lambda}M_{21}(\mathbf{q},\lambda)\Omega_{\mathbf{q}\lambda}e^{i\mathbf{q}\cdot\mathbf{R}_2}(b_{\mathbf{q}\lambda}-b^{\dagger}_{-\mathbf{q}\lambda})\sum_{\mathbf{k},\sigma}e^{i\mathbf{k}\cdot(\mathbf{R}_2-\mathbf{R}_1)}c^{\dagger}_{2\mathbf{k}+\mathbf{q}\sigma}c_{1\mathbf{k}\sigma}\ . \tag{A3}$$

Finally, the rates of change of the particle number operators are given by

$$d\hat{N}_1/dt=-d\hat{N}_2/dt=-i(H^{12}_{e\text{-ph}}-H^{21}_{e\text{-ph}})\ . \tag{A4}$$

APPENDIX B

The frictional forces and energy-loss rates for carrier systems 1 and 2 due to intravalley interaction are

$$F_1(v_1)=n_i\sum_{\mathbf{q}}|u_1(\mathbf{q})|^2\mathbf{q}_x\Pi_2^{(1)}(\mathbf{q},\omega_1)+2\sum_{\mathbf{q},\lambda}|M_1(\mathbf{q},\lambda)|^2\mathbf{q}_x\Pi_2^{(1)}(\mathbf{q},\omega_1+\Omega_{\mathbf{q}\lambda})\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\omega_1+\Omega_{\mathbf{q}\lambda}}{T_{1e}}\right]\right]\ , \tag{B1}$$

$$F_2(v_2)=n_i\sum_{\mathbf{q}}|u_2(\mathbf{q})|^2\mathbf{q}_x\Pi_2^{(2)}(\mathbf{q},\omega_2)+2\sum_{\mathbf{q},\lambda}|M_2(\mathbf{q},\lambda)|^2\mathbf{q}_x\Pi_2^{(2)}(\mathbf{q},\omega_2+\Omega_{q\lambda})\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\omega_2+\Omega_{\mathbf{q}\lambda}}{T_{2e}}\right]\right]\ , \tag{B2}$$

$$W_1(v_1)=2\sum_{\mathbf{q},\lambda}|M_1(\mathbf{q},\lambda)|^2\Omega_{\mathbf{q}\lambda}\Pi_2^{(1)}(\mathbf{q},\omega_1+\Omega_{\mathbf{q}\lambda})\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\omega_1+\Omega_{\mathbf{q}\lambda}}{T_{1e}}\right]\right]\ , \tag{B3}$$

$$W_2(v_2)=2\sum_{\mathbf{q},\lambda}|M_2(\mathbf{q},\lambda)|^2\Omega_{\mathbf{q}\lambda}\Pi_2^{(2)}(\mathbf{q},\omega_2+\Omega_{\mathbf{q}\lambda})\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\omega_2+\Omega_{\mathbf{q}\lambda}}{T_{2e}}\right]\right]\ , \tag{B4}$$

with $\omega_1\equiv\mathbf{q}_x v_1$, and $\omega_2\equiv\mathbf{q}_x v_2$.

The force experienced by the center of mass, and the energy-loss rate of carrier system 1 due to intervalley Coulomb interaction are

$$F_{12}(v_1-v_2)=\sum_{\mathbf{q}} |\nu_c(\mathbf{q})|^2 q_x \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\left[n\left[\frac{\omega}{T_{1e}}\right]-n\left[\frac{\omega-\omega_{12}}{T_{2e}}\right]\right]\Pi_2^{(1)}(\mathbf{q},\omega)\Pi_2^{(2)}(\mathbf{q},\omega-\omega_{12}) , \tag{B5}$$

$$W_{12}(v_1-v_2)=\sum_{\mathbf{q}} |\nu_c(\mathbf{q})|^2 \int_{-\infty}^{\infty} \frac{d\omega}{\pi}\omega\left[n\left[\frac{\omega}{T_{1e}}\right]-n\left[\frac{\omega-\omega_{12}}{T_{2e}}\right]\right]\Pi_2^{(1)}(\mathbf{q},\omega)\Pi_2^{(2)}(\mathbf{q},\omega-\omega_{12}) , \tag{B6}$$

with

$$\omega_{12}\equiv\omega_1-\omega_2=\mathbf{q}_x(v_1-v_2) . \tag{B7}$$

In Eqs. (B1)–(B6) $\Pi_2^{(1)}(\mathbf{q},\omega)$ and $\Pi_2^{(2)}(\mathbf{q},\omega)$ are the imaginary parts of the electron density-density correlation functions for carrier systems 1 and 2 at temperatures T_{1e} and T_{2e}, respectively. Under random-phase approximation the density-density correlation functions can be written as ($j=1,2$)

$$\Pi^{(j)}(\mathbf{q},\omega)=\frac{\pi^{(j)}(\mathbf{q},\omega)}{1-\nu_c(q)\pi^{(j)}(\mathbf{q},\omega)} , \tag{B8}$$

in which

$$\pi^{(j)}(\mathbf{q},\omega)=2\sum_{\mathbf{k}}\frac{f((\varepsilon_{j\mathbf{k}+\mathbf{q}}-\mu_j)/T_{je})-f((\varepsilon_{j\mathbf{k}}-\mu_j)/T_{je})}{\omega+\varepsilon_{j\mathbf{k}+\mathbf{q}}-\varepsilon_{j\mathbf{k}}+i\delta} \tag{B9}$$

are the density-density correlation functions of the carrier systems in the absence of intraband Coulomb interaction.

The frictional force experienced by the center of mass of the carrier system 1 due to intervalley electron-phonon interaction is

$$\begin{aligned}F_p^{12}(v_1,v_2)=4\pi\sum_{\mathbf{k},\mathbf{q},\lambda}|M_{12}(\mathbf{q},\lambda)|^2(-k_{1x})[f(\xi_{1\mathbf{k}}/T_{1e})-f(\xi_{2\mathbf{k}+\mathbf{q}}/T_{2e})]\\ \times\left\{\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{1\mathbf{k}}}{T_{1e}}-\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}+\Omega_{\mathbf{q}\lambda})\right.\\ \left.+\left[\ln\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}-\frac{\xi_{1\mathbf{k}}}{T_{1e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}-\Omega_{\mathbf{q}\lambda})\right\} ,\end{aligned} \tag{B10}$$

in which $\xi_{1k}=\varepsilon_{1k}-\mu_1$, $\xi_{2k}=\varepsilon_{2k}-\mu_2$,

$$E_{1\mathbf{k}}=\varepsilon_{1\mathbf{k}}+\tfrac{1}{2}m_1v_1^2+k_xv_1 , \tag{B11}$$

$$E_{2\mathbf{k}}=\varepsilon_{2\mathbf{k}}+\tfrac{1}{2}m_2v_2^2+k_xv_2 . \tag{B12}$$

The expression for $F_p^{21}(v_2,v_1)$ can be obtained from Eq. (B10) by exchanging all the indices $1\leftrightarrow2$.

The energy-loss rate of the carrier system 1 due to intervalley electron-phonon interaction is

$$\begin{aligned}W_p^{12}(v_1,v_2)=4\pi\sum_{\mathbf{k},\mathbf{q},\lambda}|M_{12}(\mathbf{q},\lambda)|^2\varepsilon_{1\mathbf{k}}[f(\xi_{1\mathbf{k}}/T_{1e})-f(\xi_{2\mathbf{k}+\mathbf{q}}/T_{2e})]\\ \times\left\{\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{1\mathbf{k}}}{T_{1e}}-\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}+\Omega_{\mathbf{q}\lambda})\right.\\ \left.+\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}-\frac{\xi_{1\mathbf{k}}}{T_{1e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}-\Omega_{\mathbf{q}\lambda})\right\} .\end{aligned} \tag{B13}$$

The expression for $W_p^{12}(v_2,v_1)$ can be obtained from Eq. (B13) by exchanging all the indices $1\leftrightarrow2$.

Finally, the rate of change of the particle number of the carrier system 1 is due to intervalley electron-phonon coupling:

$$\begin{aligned}N(v_1,v_2)=-4\pi\sum_{\mathbf{k},\mathbf{q},\lambda}|M_{12}(\mathbf{q},\lambda)|^2[f(\xi_{1\mathbf{k}}/T_{1e})-f(\xi_{2\mathbf{k}+\mathbf{q}}/T_{2e})]\\ \times\left\{\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{1\mathbf{k}}}{T_{1e}}-\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}+\Omega_{\mathbf{q}\lambda})\right.\\ \left.+\left[n\left[\frac{\Omega_{\mathbf{q}\lambda}}{T}\right]-n\left[\frac{\xi_{2\mathbf{k}+\mathbf{q}}}{T_{2e}}-\frac{\xi_{1\mathbf{k}}}{T_{1e}}\right]\right]\delta(E_{2\mathbf{k}+\mathbf{q}}-E_{1\mathbf{k}}-\Omega_{\mathbf{q}\lambda})\right\} .\end{aligned} \tag{B14}$$

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