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IN HOT-ELECTRON TRANSPORT THEORY**

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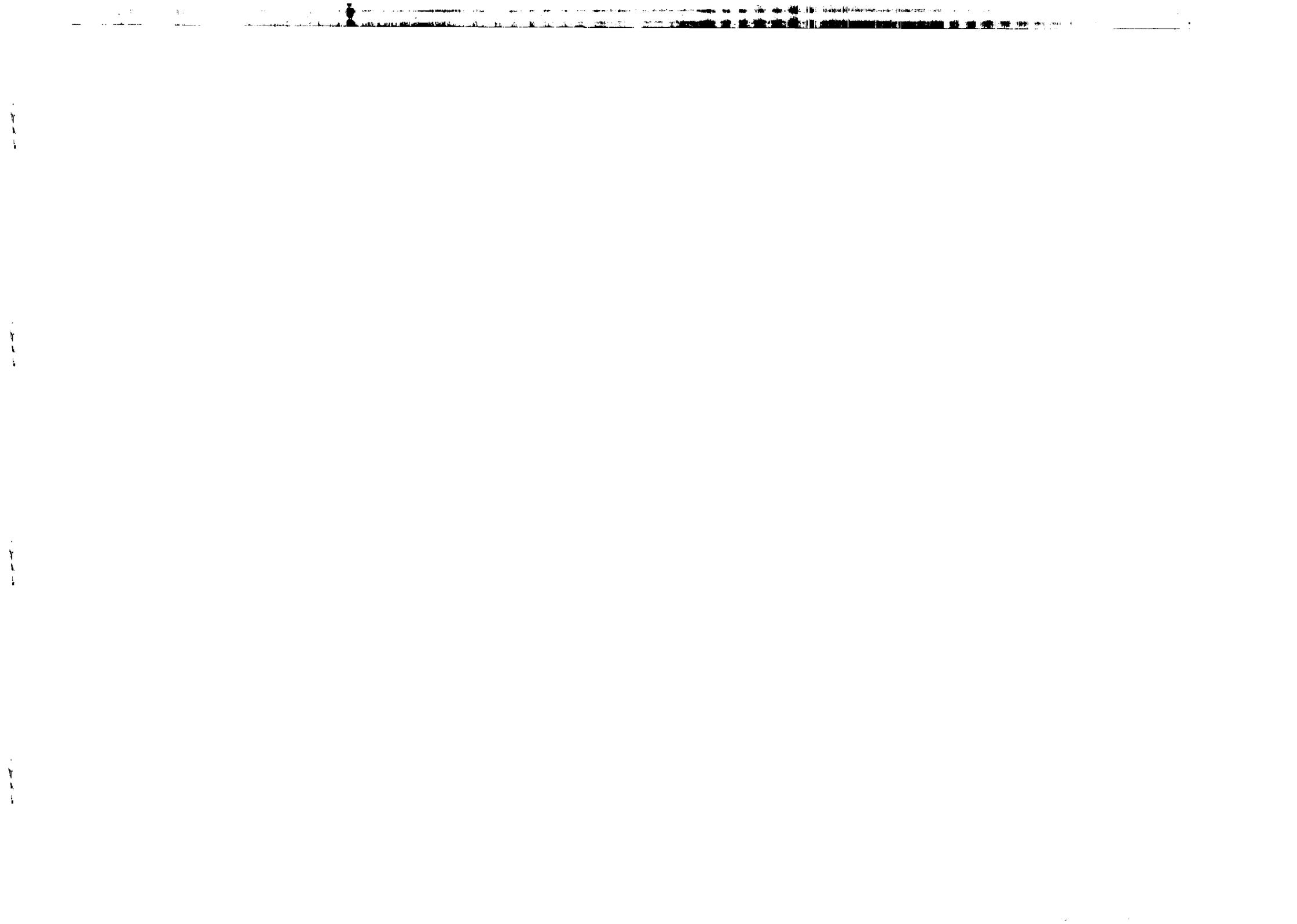


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**NONEQUILIBRIUM STATISTICAL OPERATOR  
IN HOT-ELECTRON TRANSPORT THEORY †**

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**ABSTRACT**

The Nonequilibrium Statistical Operator method developed by Zubarev is generalized and applied to the study of hot-electron transport in semiconductors. The steady-state balance equations for momentum and energy are derived to the lowest order in the electron-lattice coupling. We show that the derived balance equations are exactly the same as those obtained by Lei and Ting. This equivalence stems from the fact that to the linear order in the electron-lattice coupling, two statistical density matrices have identical effect when they are used to calculate the average value of a dynamical operator. The application to the steady-state and transient hot-electron transport in multivalley semiconductors is also discussed.

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**1. Introduction**

Since the early pioneering measurement<sup>1</sup> of nonlinear transport behavior in Ge and the later discovery of the Gunn effect<sup>2</sup> in GaAs, hot-electron transport in semiconductors has received a great deal of attention<sup>3</sup>. Rapid development of submicrometer semiconductor devices, which may be employed in high-speed computers and telecommunication systems, further enhances the importance of hot-electron transport, since miniaturization of devices has led to high-field strengths well outside the linear-response region, where Ohm's law holds, for any reasonable voltage signal. For example, applying a potential difference of 1 V across a field effect transistor of length  $0.25 \mu\text{m}$  gives a field of 40 KV/cm which far exceeds the typical fields at room temperature required to produce hot electrons.

Physical understanding of most of the microscopic processes which underlie the performances of semiconductor devices at high electric fields is provided by research into hot-electron phenomena<sup>4</sup>. Although there exists a number of theoretical approaches to this problem, most of the realistic calculations concern themselves with the solution of the Boltzmann transport equation<sup>3-5</sup> and numerical methods based on the iterative procedure<sup>6</sup> or the Monte Carlo simulation<sup>7,8</sup>. In particular, with the aid of modern large and fast computers, it would become possible to obtain exact numerical solutions of the Boltzmann equation for microscopic physical models.

It is well known that hot-electron transport is a typical irreversible process of dissipative dynamic systems. It is very important to construct a statistical density matrix adequate to describe irreversible processes of the nonequilibrium systems. The balance-equation approach<sup>9</sup> is based on the use of a equilibrium distribution for a decoupled electron-lattice system as an initial condition for Liouville's equation. This way of constructing a statistical density matrix seems to be different from the Nonequilibrium Statistical Operator (NSO) method<sup>13</sup>, but similar to the early Mori approach based on the solution of the Liouville equation with the initial condition of local equilibrium<sup>14</sup>. Then it is necessary to make a careful comparison between the balance-equation approach and the NSO method. An agreement between them will provide a powerful backing for the theoretical basis of the balance-equation approach.

The NSO method is an advanced generalization of statistical methods based on Boltzmann and Gibbs fundamental ideas, and it is considered as a powerful formalism that offers an elegant and concise way for an analytical treatment in the theory of irreversible processes. Among various types of NSO the elegant treatment of Zubarev<sup>15,16</sup> deserves particular attention. So we resort in this work to the use of the Zubarev method to study steady-state and transient hot-electron transport properties. The NSO method was applied to the study of transport properties in solid-state systems first by Kalashnikov<sup>17</sup>. Since he made a weak-field assumption that the electron drift velocity  $v_e$  is much smaller than the mean velocity of an electron, the balance equations obtained by Kalashnikov is valid only to the linear order in  $v_e$ . They may be suitable to so-called warm-electron transport, but cannot correctly describe nonlinear transport behavior in the hot-electron region. Recently, new applications of the NSO method to the hot-electron transport has been made by authors and their co-workers<sup>18-21</sup>, the derived balance equations being identical to those obtained by Lei and Ting<sup>9</sup>. Although their equivalence was shown<sup>18</sup> in the case of neglecting the electron-electron interaction, here we shall show that the inclusion of the Coulombic many-body effect does not change this conclusion. It then follows that these two approaches must have something in common. For the steady-state case, the statistical density matrices, used in these two approaches, will be pointed out to have identical effect on the calculation of averages to the lowest order in the electron-lattice coupling.

When the NSO method and balance-equation approach are applied to the transient hot-electron transport problem, superficially, there is a small difference between them, the former including seemingly more memory or intra-collisional field effect. In reality, their difference can be shown to be of the high order of magnitude in the electron-lattice coupling. Consequently, in second-order approximation in the electron-lattice coupling, the same evolution equations for the transient hot-electron transport can be obtained by the NSO method and by the extension of the balance-equation approach. It has been shown that for electric fields with moderate strengths, the memory effect included in the evolution equations has little influence upon the solutions of evolution equations<sup>22</sup>, and the calculated results for the evolution equations without memory effect coincide well with those obtained from the Monte Carlo simulation<sup>20,21</sup>.

In Section 2 we give the Hamiltonian of an electron-lattice system including Coulombic many-body effect, in terms of a separation of the center-of-mass motion from the relative motion of electrons. In Sections 3 we proceed to construct a NSO in the relative electron-lattice system along the line proposed by Zubarev. Section 4 is devoted to the derivation of the steady-state balance equations for momentum and energy based on the NSO method. There we show the equivalence of the derived balance equations to the Lei-Ting equations<sup>9</sup> and trace this equivalence to its source. Sections 5 and 6 are devoted to the application of the NSO method to the steady-state and transient hot-electron transport in multivalley semiconductors. Finally concluding remarks are included in Section 7.

## 2. Hamiltonian

Let us consider an electron-lattice system, which consists of  $N$  conduction electrons interacting with each other, in an applied uniform electric field  $\mathbf{E}$ . The electrons are accelerated by the applied field and scattered by phonons and  $n_i$  randomly distributed impurities, forming an electric current with drift velocity  $v_e$ . The total Hamiltonian of this system can be written in terms of the center-of-mass variables and electron variables in the relative coordinates<sup>9</sup>:

$$H = H_c + H_e + H_{ph} + H_{el}, \quad (1)$$

where  $H_c$  and  $H_e$  stand for the center-of-mass and relative parts of the electron Hamiltonian, respectively.  $H_{ph}$  is the free-phonon Hamiltonian, and  $H_{el}$  is the interaction of carriers with the lattice.

For hot-electron transport problems, it is necessary to separate the motion of the center of mass from the relative motion of the electrons. The former can be regarded as a mechanical movement of a single body with mass  $Nm$ , which obeys the classical equation of motion. Its drift velocity  $v_e$  depends on the external drifting force and internal resistance due to the electron-lattice coupling. The Hamiltonian  $H_c$  includes the kinetic energy of the center of mass and its potential energy in the external field:

$$H_c = \frac{\mathbf{P}^2}{2Nm} - Ne\mathbf{E} \cdot \mathbf{R}, \quad (2)$$

with  $\mathbf{P}$  and  $\mathbf{R}$  as the momentum and coordinate for the center of mass, respectively.

The relative electron system, which consists a large number of interacting particles, should satisfy the quantum statistics. It was in the statistical ensemble of the relative electron systems that the effective temperature  $T_e$  of hot electrons can be defined. In the representation of second quantization,

$$H_e = \sum_{\mathbf{p}} \epsilon_{\mathbf{p}} c_{\mathbf{p}}^\dagger c_{\mathbf{p}} + (1/2) \sum_{\mathbf{q}} v_c(\mathbf{q}) \rho_{\mathbf{q}} \rho_{-\mathbf{q}}. \quad (3)$$

Here  $c_p^\dagger$  and  $c_p$  are the Fermi operators in the state with energy  $\epsilon_p$  and momentum  $p$ ,  $\epsilon_p = p^2/2m$  for a parabolic energy band.  $\rho_q = \sum_q c_{p+q}^\dagger c_q$  is the electron density operator, and  $v_c(q)$  being the Coulomb potential between electrons.

$$H_{ph} = \sum_{q,\lambda} \Omega_{q\lambda} b_{q\lambda}^\dagger b_{q\lambda}. \quad (4)$$

$b_{q\lambda}^\dagger$  and  $b_{q\lambda}$  in the above equation are the phonon field operators in the state with momentum  $q$ , energy  $\Omega_{q\lambda}$ , and polarization index  $\lambda$ . Two types of electron-lattice coupling will be taken into account, one is the electron-phonon interaction, the other is the interaction with randomly distributed impurities:

$$H_{el} = \sum_{q,n} u(q) e^{iq(R-R_0)} \rho_q + \sum_{q,\lambda} M(q,\lambda) e^{iqR} (b_{q\lambda} + b_{-q,\lambda}^\dagger) \rho_q, \quad (5)$$

where  $u(q)$  is the impurity potential in momentum space, and  $M(q,\lambda)$  is the electron-phonon matrix element, which satisfies  $M(q,\lambda) = M^*(-q,\lambda)$ .

We wish to point out that the electron-lattice coupling plays an important role in the hot-electron transport theory. On the one hand, it is considered a small perturbation so that the frequency of electron-lattice collisions  $\tau_{el}^{-1}$  is much smaller than that of mutual collisions of electrons  $\tau_{ee}^{-1}$ . Then it is possible to assume the nonequilibrium distribution of electrons to be dependent on a set of macroparameters such as effective temperature and chemical potential of hot electrons. Further, the effective temperature of hot electrons may be much higher than the lattice temperature. On the other hand, the electron-lattice interaction is also indispensable to irreversible transport processes since all dissipative mechanisms are included in it. Therefore, the transport equations are usually set up to the lowest order in  $H_{el}$ .

### 3. Nonequilibrium Statistical Operator

We shall consider the nonequilibrium ensemble of the systems with the Hamiltonian in (1). Let us assume that the nonequilibrium state of the ensemble may be described by a basic set of average values  $\langle P_m \rangle^t = Tr\{P_m \rho(t)\}$  of some operators  $P_m$ . Here  $\rho(t)$  is the NSO which will be defined later. As the first step of constructing the NSO, which satisfies Liouville's equation and can describe irreversible transport processes, a quasi-equilibrium statistical operator is introduced as

$$\rho_t = \exp\{-\phi - \sum_m P_m F_m(t)\} \equiv \exp[-S(t,0)], \quad (6)$$

with

$$\phi = \ln Tr\{\exp[-\sum_m P_m F_m(t)]\},$$

where  $S(t,0)$  is the entropy operator of the system.  $F_m(t)$  are the thermodynamic parameters conjugate to the average values of  $P_m$ , and they are determined from the conditions<sup>16</sup>:

$$\langle P_m \rangle^t \equiv Tr\{P_m \rho_t\} = Tr\{P_m \rho(t)\} \equiv \langle P_m \rangle^t. \quad (7)$$

In the application of the NSO method to a specific problem of the statistical mechanics of irreversible processes, one of key steps is to choose operators  $P_m$  and their thermodynamically conjugated parameters  $F_m(t)$ . For the hot-electron transport with strong electric field and weak electron-lattice coupling, the energy which relative electrons obtain from the external field is redistributed among them in such a way that the relative electron system becomes almost in equilibrium within itself, but not in equilibrium with respect to the lattice. So  $\rho_t$  should be defined in both the relative electron and free phonon systems. A most forthright choice of  $P_m$  and  $F_m(t)$  is<sup>19,22</sup>

$$P_m = \{H_e; H_{ph}\},$$

and

$$F_m(t) = \{\beta_e(t); \beta\}, \quad (8)$$

so that

$$\rho_t = \exp\{-\phi - \beta_e(t)H_e - \beta H_{ph}\}, \quad (9)$$

where  $\beta_e(t)$  is the inverse effective temperature of hot electrons, and  $\beta$  the inverse equilibrium temperature of the lattice. This statistical operator is close in form to the equilibrium Gibbsian distribution but with different parameters  $\beta$  and  $\beta_e$  which depends on time. Its physical meaning is easily understood. Imagine that the electron-lattice interaction, together with the electric field, is mathematically cut off at the time  $t$ , so that the center of mass, the relative electrons, and the phonon system are decoupled from each other. Then the center of mass moves with a constant velocity  $v_c(t)$ , and the relative electrons and free phonons, as two isolated systems, attain their thermal equilibrium states very quickly, respectively, with hot-electron temperature  $T_e(t)$  and lattice temperature  $T$ . The above picture requires that there exist strong collisions among electrons ( $\tau_{ee} \ll t$ ,  $t$  being the characteristic time of variation of the external field) so that they can be thermalized immediately after the field is applied. The  $\rho_t(t)$  given by (9) is a generalized Gibbsian distribution of the decoupled systems in their frozen equilibrium states, and it can be used to determine instantaneous values of the macrovariables from the conditions (7).

In the application of the NSO method to hot-electron transport theory, Kalashnikov<sup>17</sup> chose a more complicate form for  $P_m$  and  $F_m(t)$ . They are

$$P_m = \{H_e'; P; N; P_1; H_{ph} + H_{el}\},$$

and

$$F_m(t) = \{\beta_e(t); -v_c(t)\beta_e(t); -\beta_e(t)[\mu(t) - mv_c^2(t)/2]; 0; \beta\}. \quad (10)$$

Here  $H_e'$  is the electron Hamiltonian in the laboratory system,  $N$  is the number-of-electron operator, and  $P_1$  is the momentum operator of the lattice.  $\mu(t)$  is the nonequilibrium chemical potential of hot electrons.

$\rho_l(t)$ , which is obtained by substituting (10) into (6), differs superficially from that defined by (9). In reality, it can be shown that they are almost identical. First, the complex structure of (10) stems mainly from the fact that the  $\rho_l(t)$  is defined in the laboratory system. By means of a canonical transformation from the relative electron system into the laboratory one<sup>16</sup>, the expression (9) for  $\rho_l$  becomes

$$\rho_l(t) = \exp\{-\phi - \beta_c(t)[H'_e - v_c(t)P - Nm v_c^2(t)/2] - \beta H_{ph}\}, \quad (11)$$

from which one can understand the origin of the operators  $H'_e$ ,  $P$  and  $N$  which appear in (10). Second, the introduction of operators  $N$  and  $P_1$  into the set of  $P_m$  in (10) doesn't seem to be necessary. This is because a statistical ensemble of the relative electron systems with constant electron number can be described by a cononical distribution, and the average momentum of the lattice is usually assumed to be zero. Finally, we wish to point out that if introducing the electron-lattice interaction  $H_{el}$  into the set of  $P_m$ , as used in (10), one has some trouble in choosing its thermodynamically conjugated parameter  $F_m$ . The trouble is that it is difficult to determine whether the  $F_m$  corresponding to  $H_{el}$  is chosen to be  $\beta$  of the lattice, or  $\beta_c(t)$  of the hot electrons, or an unknown function of both. Fortunately it has been shown<sup>18</sup> that in the approximation to the lowest order of  $H_{el}$ , which is usually used in hot-electron transport theory, the choice of this  $F_m$  is irrelevant to the final expression of the balance equations in steady-state hot-electron transport. So it is quite convenient to exclude  $H_{el}$  from the set of  $P_m$  from the outset. Therefore, the two choices of  $P_m$  and  $F_m(t)$  are approximately equivalent to each other. Since  $P_m$  and  $F_m(t)$  given by (8) have a much simpler form, in this work, we shall apply them to construct the NSO, and then to derive the balance equations for hot-electron transport. If Kalashnikov's choice in the form (10) is used, the same result for the balance equations can also be obtained as long as all the correlation functions which appear in the balance equations are correctly calculated<sup>18</sup>.

The density matrix of the real system, of course, deviates from the quasi-equilibrium distribution because the  $\rho_l$  can neither satisfy Liouville's equation nor describe irreversible processes. However, it can be used to formulate boundary conditions to the Liouville equation<sup>16</sup>, in the same way as the free-particle wave function is used to formulate boundary conditions to the Schrödinger equation in the quantum theory of scattering.

It is well known that the Liouville equation is symmetric under the time-reversal transformation (in the quantum case, this means the replacement  $(t, iL) \Rightarrow (-t, -iL^+)$ , where  $L$  is the Liouville's operator of the system). However, the macroscopic evolution of the system with dissipative structures must be irreversible. This poses the question of how to obtain irreversible behavior in the macroscopic description of the state of the system generated by a statistical operator satisfying Liouville's equation. Zubarev's approach to this question is to introduce into Liouville's equation an infinitesimally small source that breaks time-reversal symmetry<sup>16</sup>. Then the NSO for the relative electron-lattice system has the form

$$\rho(t) = \exp\{-\varepsilon \int_{-\infty}^0 dt' e^{\varepsilon t'} S(t+t', t')\}, \quad (12)$$

with

$$S(t, t') = e^{iHt'} S(t, 0) e^{-iHt'},$$

$$S(t, 0) = \phi(t) + \beta_c(t)H_e + \beta H_{ph}. \quad (13)$$

where  $\varepsilon$  is a positive number and will tend to zero after the thermodynamic limiting process in the calculation of averages. As shown in (13), the first argument of  $S(t, t')$  denotes the time dependence though the parameters  $F_m(t)$ , and the second denotes the Heisenberg picture time dependence of operators  $P_m(t)$ . Integrating by part, the operator  $\rho(t)$  can be written as

$$\rho(t) = \exp\{-S(t, 0) + \int_{-\infty}^0 dt' e^{\varepsilon t'} \dot{S}(t+t', t')\}, \quad (14)$$

where

$$\dot{S}(t, t') = e^{iHt'} \dot{S}(t, 0) e^{-iHt'},$$

with

$$\dot{S}(t, 0) = \beta_c(t)\dot{H}_e + \beta\dot{H}_{ph} + \dot{\beta}_c(t)(H_e - \langle H_e \rangle^t), \quad (15)$$

as the entropy production operator. In the limit of  $E=0$  and  $\beta_c(t) = \beta$ , the second term in the exponent of (14) can be shown to be  $-\beta H_{el}$  when the entropy production operator is evaluated to the lowest order in the  $H_{el}$ . Then the density matrix reduces to the well-known form  $\rho(t) = \exp(-\phi - \beta H)$  for the equilibrium state. It has been shown<sup>22</sup> that the first two terms on the right hand side of (15) are of the first order in  $H_{el}$  whereas the last term is at least second order of magnitude in  $H_{el}$ . In the hot-electron transport theory, as already mentioned, the  $H_{el}$  is usually regarded as a small perturbation since the energy exchange between the electron and lattice systems is generally assumed to be small. If we confine  $\rho(t)$  to terms of the first order in  $H_{el}$ , the last term in (15) may be neglected. Further, using the following operator equation in the approximation linear in  $B$ :

$$\exp(A+B) \simeq \{1 + \int_0^1 d\tau e^{A\tau} B e^{-A\tau}\} e^A, \quad (16)$$

where  $A$  and  $B$  stand for arbitrary operators, and replacing  $A$  and  $B$  by  $-S(t, 0)$  and  $\int_{-\infty}^0 dt' e^{\varepsilon t'} \dot{S}(t+t', t')$ , respectively, we obtain the expansion of  $\rho(t)$  to the first-order approximation in  $H_{el}$ :

$$\rho(t) = \{1 + \int_{-\infty}^0 dt' e^{\varepsilon t'} \int_0^1 d\tau [\beta_c(t+t')\dot{H}_e(t', i\tau) + \beta\dot{H}_{ph}(t', i\tau)]\} \rho_l. \quad (17)$$

where

$$\dot{H}_e(t', i\tau) = e^{-\tau S(t, 0)} e^{iHt'} \dot{H}_e e^{-iHt'} e^{\tau S(t, 0)}, \quad (18)$$

and

$$\dot{H}_e = -i[H_e, H] = -\sum_{\mathbf{q}, \alpha} u(\mathbf{q}) c^{i\mathbf{q}(\mathbf{R}-\mathbf{R}_\alpha)} \dot{\rho}_{\mathbf{q}} - \sum_{\mathbf{q}, \lambda} M(\mathbf{q}, \lambda) c^{i\mathbf{q}\mathbf{R}} (b_{\mathbf{q}\lambda} + b_{-\mathbf{q}\lambda}^\dagger) \dot{\rho}_{\mathbf{q}}, \quad (19)$$

with

$$\dot{\rho}_{\mathbf{q}} = -i[\rho_{\mathbf{q}}, H] = -i[\rho_{\mathbf{q}}, H_e]. \quad (20)$$

The  $\dot{H}_{ph}(t', i\tau)$  has the same dependences of  $t'$  and  $\tau$  as  $\dot{H}_e(t', \tau)$  given by (18), but

$$\dot{H}_{ph} = i \sum_{\mathbf{q}, \lambda} M(\mathbf{q}, \lambda) \Omega_{\mathbf{q}\lambda} e^{i\mathbf{q}\mathbf{R}} (b_{\mathbf{q}\lambda} - b_{-\mathbf{q}\lambda}^\dagger) \rho_{\mathbf{q}}. \quad (21)$$

By means of the approximate expression (17) for  $\rho(t)$ , one can obtain the balance equations in second-order approximation in the electron-lattice interaction.

#### 4. Balance Equations For Momentum and Energy

We now focus our attention on steady-state hot-electron transport. In steady state, the center of mass moves with a constant  $v_e$  along the electric field direction. At the same time, the total energy of the relative electron system must be constant, the energy supplied per unit time by the electric field to the electron system being equal to the energy transfer rate from the electron system to the lattice. Therefore, the steady-state hot-electron transport is determined by the following balance equations for momentum and energy<sup>17</sup>

$$Nm\dot{v}_e = \langle \dot{\mathbf{P}} \rangle^t = 0, \quad (22)$$

$$c_e \dot{T}_e = \langle \dot{H}_e \rangle^t = 0, \quad (23)$$

where  $c_e$  is the heat capacity of the relative electron system, and the averages with the NSO will be approximately calculated by means of (17).

If the external electric field  $\mathbf{E}$  is assumed to be along the x-direction, the center-of-mass momentum operator  $\mathbf{P}$  has only x-component  $P_x$  and its derivative is equal to

$$\dot{P}_x = NeE + \dot{P}_{el}, \quad (24)$$

with

$$\dot{P}_{el} = -i \sum_{\mathbf{q}, \alpha} q_x u(\mathbf{q}) e^{i\mathbf{q}(\mathbf{R}-\mathbf{R}_0)} \rho_{\mathbf{q}} - i \sum_{\mathbf{q}, \lambda} q_x M(\mathbf{q}, \lambda) e^{i\mathbf{q}\mathbf{R}} (b_{\mathbf{q}\lambda} + b_{-\mathbf{q}\lambda}^\dagger) \rho_{\mathbf{q}}, \quad (25)$$

Substituting (17) into (22) and (23), we obtain

$$NeE + \int_{-\infty}^0 dt' e^{\epsilon t'} \int_0^1 d\tau \{ \beta_e \langle \dot{P}_{el} \dot{H}_e(t', i\tau) \rangle_I + \beta \langle \dot{P}_{el} \dot{H}_{ph}(t', i\tau) \rangle_I \} = 0, \quad (26)$$

$$\int_{-\infty}^0 dt' e^{\epsilon t'} \int_0^1 d\tau \{ \beta_e \langle \dot{H}_e \dot{H}_e(t', i\tau) \rangle_I + \beta \langle \dot{H}_e \dot{H}_{ph}(t', i\tau) \rangle_I \} = 0. \quad (27)$$

Here all the correlation functions should be calculated in the relative electron-lattice system by means of the quasi-equilibrium density matrix  $\rho_I$  given by (9). Since in the steady state the  $\rho_I$  is independent of time  $t$ , for simplicity, we have omitted the superscripts of all the correlation functions. The solutions of the balance equations (26) and (27) determine the steady-state values  $v_e$  and  $\beta_e$  as functions of the external field.

The next step is to calculate the correlation functions which appear in the balance equations (26) and (27). In Ref. 17, a weak-field approximation was made under the

consideration of warm-electron transport. On the basis of this approximation, only the diagonal-correlation functions like  $\langle \dot{P}_{el} \dot{P}_{el}(t', i\tau) \rangle_I$  and  $\langle \dot{H}_e \dot{H}_e(t', i\tau) \rangle_I$  were retained, while all the off-diagonal-correlation functions in the balance equations were neglected<sup>17</sup>. In the region of hot-electron transport, however, this kind of approximation will not work. It has been shown<sup>18</sup> that both the diagonal- and off-diagonal-correlation functions play important roles in hot-electron transport theory, and the latter can vanish only when  $\beta_e = \beta$ .

Up to this point, we have considered the general case of including the Coulomb interaction between carries. In the following we shall calculate the correlation functions in (26) and (27) in two separate cases. First we assume that the  $H_e$  has a simple form of a free-electron Hamiltonian. This corresponds to the case in which the influence of mutual scattering of electrons may be taken into account by a normalization of an electron-lattice coupling. Then the effect due to the electron-electron interaction, which is explicitly included in (3), will also be considered.

For free-electron and phonon operators, there are the following relationships<sup>17,18</sup>:

$$c_k(t, i\tau) = c_k \exp(\tau \beta \epsilon_k - i t \epsilon_k), \quad (28)$$

$$b_{\mathbf{q}\lambda}(t, i\tau) = b_{\mathbf{q}\lambda} \exp(\tau \beta \Omega_{\mathbf{q}\lambda} - i t \Omega_{\mathbf{q}\lambda}), \quad (29)$$

from which the  $t$  and  $\tau$  dependences of the correlation functions can be taken from the calculation of averages and the integrations over  $\tau$  and  $t'$  in (26) and (27) are easily done<sup>18</sup>. Taking the energy balance equation (27) as an example, we have

$$\begin{aligned} & \int_0^1 d\tau \{ \beta_e \langle \dot{H}_e \dot{H}_e(t', i\tau) \rangle_I + \beta \langle \dot{H}_e \dot{H}_{ph}(t', i\tau) \rangle_I \} \\ &= n_e \sum_{\mathbf{q}, \mathbf{k}} |u(\mathbf{q})|^2 \omega_{\mathbf{k}\mathbf{q}} [\exp(\beta_e \omega_{\mathbf{k}\mathbf{q}}) - 1] \exp[-it'(\omega_{\mathbf{k}\mathbf{q}} + \mathbf{q}_x v_e)] \\ & \times \langle c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}} \rangle_I + \sum_{\mathbf{K}, \mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 \omega_{\mathbf{k}\mathbf{q}} \langle c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}} \rangle_I \\ & \times \{ \langle b_{\mathbf{q}\lambda} b_{\mathbf{q}\lambda}^\dagger \rangle_I [\exp(\beta_e \omega_{\mathbf{k}\mathbf{q}} - \beta \Omega_{\mathbf{q}\lambda}) - 1] \exp[-it'(\omega_{\mathbf{k}\mathbf{q}} + q_x v_e - \Omega_{\mathbf{q}\lambda})] \\ & + \langle b_{-\mathbf{q}\lambda}^\dagger b_{-\mathbf{q}\lambda} \rangle_I [\exp(\beta_e \omega_{\mathbf{k}\mathbf{q}} + \beta \Omega_{\mathbf{q}\lambda}) - 1] \exp[-it'(\omega_{\mathbf{k}\mathbf{q}} + q_x v_e + \Omega_{\mathbf{q}\lambda})] \}, \end{aligned} \quad (30)$$

where  $\omega_{\mathbf{k}\mathbf{q}} = \epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}$ . In deriving of (30) we have used the relation  $\mathbf{q} \cdot [\mathbf{R}(t') - \mathbf{R}(0)] = q_x v_e t'$  for the steady-state transport under a constant field along the x-direction. Further, taking into account the following relations

$$\langle c_{\mathbf{k}+\mathbf{q}}^\dagger c_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}+\mathbf{q}} \rangle_I = f(\beta_e \epsilon_{\mathbf{k}+\mathbf{q}}) [1 - f(\beta_e \epsilon_{\mathbf{k}})], \quad (31)$$

$$\langle b_{\mathbf{q}\lambda} b_{\mathbf{q}\lambda}^\dagger \rangle_I = 1 + \langle b_{\mathbf{q}\lambda}^\dagger b_{\mathbf{q}\lambda} \rangle_I = 1 + n(\beta \Omega_{\mathbf{q}\lambda}), \quad (32)$$

with  $f(x)$  and  $n(x)$  being the usual Fermi and Bose functions, respectively, and

$$\int_{-\infty}^0 dt' \exp[-it'(\omega_{\mathbf{k}\mathbf{q}} + q_x v_e \pm \Omega_{\mathbf{q}\lambda}) + \epsilon t'] = i[\omega_{\mathbf{k}\mathbf{q}} + q_x v_e \pm \Omega_{\mathbf{q}\lambda} + i\epsilon]^{-1}, \quad (33)$$

with real part being  $\pi\delta(\omega_{\mathbf{k}\mathbf{q}} + q_x v_e \pm \Omega_{\mathbf{q}\lambda})$ , we finally obtain for the energy balance equation

$$2 \sum_{\mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 (q_x v_e + \Omega_{\mathbf{q}\lambda}) \Pi_2^0(\mathbf{q}, q_x v_e + \Omega_{\mathbf{q}\lambda}) [n(\beta \Omega_{\mathbf{q}\lambda}) - n(\beta_e (q_x v_e + \Omega_{\mathbf{q}\lambda}))] \\ + n_i \sum_{\mathbf{q}} |u(\mathbf{q})|^2 q_x v_e \Pi_2^0(\mathbf{q}, q_x v_e) = 0, \quad (34)$$

where

$$\Pi_2^0(\mathbf{q}, \omega) \equiv \text{Im} \Pi^0(\mathbf{q}, \omega) = 2\pi \sum_{\mathbf{k}} [f(\beta_e \varepsilon_{\mathbf{k}}) - f(\beta_e \varepsilon_{\mathbf{k}+\mathbf{q}})] \delta(\omega - \omega_{\mathbf{k}+\mathbf{q}}), \quad (35)$$

is the imaginary part of the density-density correlation function in the absence of the Coulomb interaction between electrons.

Using a same procedure to that outlined above, we can obtain for the momentum balance equation

$$N e E + 2 \sum_{\mathbf{q}, \lambda} |M(\mathbf{q}, \lambda)|^2 q_x \Pi_2^0(\mathbf{q}, q_x v_e + \Omega_{\mathbf{q}\lambda}) [n(\beta \Omega_{\mathbf{q}\lambda}) - n(\beta_e (q_x v_e + \Omega_{\mathbf{q}\lambda}))] \\ + n_i \sum_{\mathbf{q}} |u(\mathbf{q})|^2 q_x \Pi_2^0(\mathbf{q}, q_x v_e) = 0. \quad (36)$$

Equations (35) and (36) are the main results derived from the NSO method. Comparing them with the results in Ref. 17, we find that two sets of balance equations are quite different in the region of hot-electron transport. The momentum balance equations agree with each other only when  $\beta_e = \beta$ , while the energy balance equations are the same in the approximation linear in  $v_e$ .

To see clear the difference between two sets of balance equations, we make a comparison between them by means of studying numerically their solutions for  $v_e$  and  $T_e$  for p-type Ge. We assume that the transport is due to heavy holes with a parabolic band. The scattering mechanisms include both acoustic and nonpolar optical phonons<sup>9</sup>. The parameters<sup>23,24</sup> we employ are given as follows. The heavy-hole mass is chosen as  $m = 0.31m_e$ , with  $m_e$  as the free-electron mass. The reason for such a choice is that the contribution to the current by the light holes is compensated by adjusting the mass of heavy-hole band. The density of the lattice is  $d = 5.32\text{g/cm}^3$ . The effective acoustic deformation potential  $E = 4.34\text{eV}$  and the longitudinal acoustic phonon velocity is  $v_s = 5.4 \times 10^5\text{cm/sec}$ . The optical phonon deformation field  $D = 8.86 \times 10^8\text{eV/cm}$  and the optical phonon frequency is  $\Omega_0 = 430\text{K}$ . In Fig.1,  $v_e$  and  $T_e$  are depicted as functions of electric field strength  $E$  at a given lattice temperature  $T = 77\text{K}$ . The solid curves are calculated according to (34) and (36), while the dashed curves according to the balance equations obtained by Kalashnikov<sup>17</sup>. The results have been also compared with the experimental data of Reggiani *et al.*<sup>23</sup>. In the linear region ( $E < 100\text{V/cm}$ ) the drift velocities  $v_e$  for both theories agree with each other and also with experimental data. But for  $E > 200\text{V/cm}$  the discrepancy in  $v_e$  between the solid and dashed curves begins to show up. It clearly indicates that the present result (solid curve) is consistent

with experimental data in high-field region. We also would like to emphasize here that the present result for  $v_e$  as a function of electric field agrees with that of Monte Carlo simulation<sup>23</sup> for a single isotropic hole band.

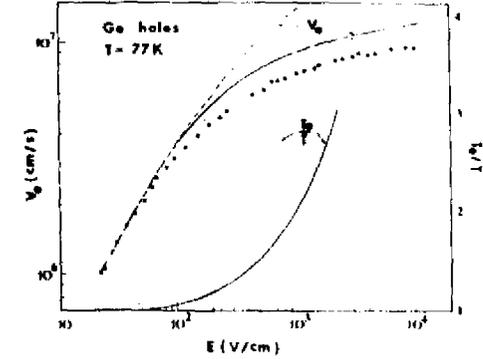


Fig.1. Hole drift velocity  $v_e$  and carrier temperature  $T_e$  as functions of electric field  $E$  at lattice temperature 77K. The solid curves present the results of Eqs. (34) and (36) and the dashed curves present the results of Kalashnikov<sup>17</sup>. The circles, squares, and dots refer to the experimental data from Ref. 23 for the direction of  $E$  along different orientations of the crystal; the circles indicate  $E \parallel \langle 100 \rangle$ , the squares are for  $E \parallel \langle 110 \rangle$ , and the dots for  $E \parallel \langle 111 \rangle$ .

It is easy to see that the balance equations (34) and (36) obtained above are identical to the Lei-Ting equations in the absence of the Coulomb interaction between carriers. We now study the effect of the electron-electron interaction on the balance equations. Let us consider the relative electron Hamiltonian in the form (3). Since the Coulomb interaction has been explicitly included in  $H_e$ , the simple relations (28) and (31), which are used in deriving balance equations in the preceding section, no longer hold. So the derivation for the balance equations cannot be straightforward as done above.

In what follows we shall generally show that in the steady state, statistical average of a dynamical operator, calculated with the approximate expression (17) for the NSO, coincides with its average over the statistical density matrix used by Lei and Ting<sup>9</sup>. So the balance equations for momentum and energy, derived from (22) and (23), must be identical with theirs.

For the steady-state hot-electron transport under consideration, both  $\beta_e$  and  $\beta$

are independent of time so that the entropy operator  $S(t,0)$  does not depend explicitly on time. In this section, for the sake of simplicity, we omit to write the arguments of the entropy operator  $S$  and rewrite the entropy production operator as

$$\begin{aligned}\dot{S}(t, i\tau) &= \beta_e \dot{H}_e(t, i\tau) + \beta \dot{H}_{ph}(t, i\tau) \\ &= (-i)e^{-\tau S} e^{iHt} [S, H_{ei}] e^{-iHt} e^{\tau S},\end{aligned}\quad (37)$$

where we have utilized the property that both  $H_e$  and  $H_{ph}$  commutes with the operator  $S$ . Then the NSO in the form (17) can be rewritten as

$$\rho(t) = \{1 + \int_{-\infty}^0 dt' e^{t't} \int_0^1 d\tau \dot{S}(t', i\tau)\} e^{-S}. \quad (38)$$

The average of a dynamical operator  $A$  over the statistical density matrix (38) is

$$\langle A \rangle^t = \langle A \rangle_t + \int_{-\infty}^0 dt' e^{t't} \int_0^1 d\tau \langle A \dot{S}(t', i\tau) \rangle_t, \quad (39)$$

where the second term, including the time correlation function, will be calculated in terms of the spectral representation for the correlation function.

Let  $|m\rangle$  and  $S_m$  be the eigenfunctions and eigenvalues of the operator  $S$ . Substituting (37) into (39), we write explicitly the statistical averaging for the time correlation function:

$$\begin{aligned}\langle A \dot{S}(t', i\tau) \rangle_t &= (-i) \sum_m \langle m | A e^{-\tau S} e^{iHt'} (S H_{ei} - H_{ei} S) e^{-iHt'} e^{(\tau-1)S} | m \rangle.\end{aligned}\quad (40)$$

Between the operators  $S$  and  $H_{ei}$ , we insert another complete set of states, which is unity

$$1 = \sum_m |m\rangle \langle m|,$$

which gives

$$\begin{aligned}\langle A \dot{S}(t', i\tau) \rangle_t &= (-i) \sum_{m,n} \langle m | A | n \rangle \langle n | H_{ei}(t') | m \rangle \\ &\quad (S_n - S_m) \exp\{\tau(S_m - S_n) - S_m\}.\end{aligned}\quad (41)$$

Therefore,

$$\begin{aligned}&\int_0^1 d\tau \langle A \dot{S}(t', i\tau) \rangle_t \\ &= (-i) \sum_{m,n} \langle m | A | n \rangle \langle n | H_{ei}(t') | m \rangle \{\exp(-S_m) - \exp(-S_n)\}, \\ &= (-i) \sum_m \langle m | \{A H_{ei}(t') - H_{ei}(t') A\} e^{-S} | m \rangle \\ &= (-i) \langle [A, H_{ei}(t')] \rangle_t.\end{aligned}\quad (42)$$

Substituting (42) into (39), we obtain

$$\langle A \rangle^t = \langle A \rangle_t + \int_{-\infty}^0 dt' \langle\langle A | H_{ei}(t') \rangle\rangle, \quad (43)$$

where

$$\langle\langle A(t) | H_{ei}(t') \rangle\rangle \equiv (-i) \theta(t-t') \langle [A(t), H_{ei}(t')] \rangle_t. \quad (44)$$

It is easily seen that the present result for the average value of any operator  $A$  is just the same as that in Ref. 9. This means that in the calculation of steady-state averages, the approximate NSO (17) is equivalent to the statistical density matrix used in Ref. 9, even though they differ greatly from each other in the form. It then follows from this equivalence that starting from (17), we can obtain exactly the same balance equations for momentum and energy as those given by Lei and Ting<sup>9</sup>, the Coulombic many-body effect being included. It has been shown<sup>9</sup> that the main effect of the Coulomb interaction between carries on the balance equations is that all the retarded density-density correlation functions in (34) and (36) need to be renormalized by their form in the random-phase approximation. Another important effect of electron-electron interaction is to make the charge carriers to reach fast thermalization<sup>25</sup> after an electric field is applied. Therefore, we have shown that in the presence of the electron-electron interaction, the steady-state balance equations, derived from the NSO method, is still identical with the Lei-Ting equations.

## 5. Application to Multivalley Semiconductors

Up to now the NSO approach to the steady-state hot electron transport is based on a single valley model with spherical equienergetic surfaces. However, realistic semiconductors usually have more complicated band structures, especially many-valley structures. As a typical example, n-type GaAs has a conduction band with a  $\Gamma$ -L-X valley ordering, i.e., there are one  $\Gamma$  valley, four equivalent L valleys and three equivalent X valleys in order of energy minimum. For n-type Si, the electrons which contribute to transport are those in the six equivalent valleys which are around the six minima of the conduction band along the  $\langle 100 \rangle$  directions. Since the equienergetic surfaces of each valley are near ellipsoids whose major axis is along the crystallographic directions, the effective mass of hot electrons for each valley is anisotropic. Therefore, for an external electric field along any direction, except the  $\langle 111 \rangle$  crystallographic directions, the six valleys may be not equivalent to each other due to different effective masses along the field direction. In multivalley semiconductors the electron transfer between nonequivalent valleys plays a very important role in determining their hot-electron transport properties. Both the wellknown Gunn effect<sup>2</sup> in n-type GaAs and the anisotropic effect<sup>3</sup> for the drift velocity in n-type Si originate from the redistribution of hot electrons between nonequivalent valleys via intervalley transfer.

In the single valley case, as already shown, a pair of balance equations, which determine  $v_e$  and  $T_e$  as functions of the external field strengths, are quite enough for describing the steady-state hot-electron transport. In the case of multivalley semiconductors, the balance equations for momentum and energy must be written for each valley

together with an additional balance equation for population since the hot-electron population for each valley is no longer a constant in the presence of intervalley coupling.

We now proceed to extend the NSO method to the study in the multivalley case and put stress on discussing how to construct a NSO adequate to a multivalley system. First, take each valley as an electron subsystem and separate its center-of-mass motion from the relative motion of electrons for this subsystem. The whole electron system can be regarded as consisting of various subsystems which are coupled with each other due to intervalley electron-lattice and electron-electron interactions. Then the total Hamiltonian of an electron-lattice system with  $n$  valleys can be written as

$$H = \sum_{\alpha=1}^n [H_{c\alpha} + H_{e\alpha} + H_{l\alpha}] + H_{ph} + H_{inter}, \quad (45)$$

where  $H_{c\alpha}$  and  $H_{e\alpha}$  are the center-of-mass and relative parts of the electron Hamiltonian for the  $\alpha$ th valley, respectively, and  $H_{l\alpha}$  is the intravalley electron-lattice interaction. They have the same expressions as those given by (2), (3) and (5), but it is necessary to mark all the operators and physical quantities for each valley by a valley index, since they may be different for nonequivalent valleys. For example, the single-electron energy for the  $\alpha$ th valley is  $\epsilon_{\alpha p} = p^2/(2m_{\alpha}) + \epsilon_{\alpha 0}$  where the energy minimum  $\epsilon_{\alpha 0}$  and the effective mass  $m_{\alpha}$  may generally have different values for different  $\alpha$ . The phonon Hamiltonian  $H_{ph}$  retains its original expression (4). All the intervalley couplings are included in  $H_{inter}$ :

$$\begin{aligned} H_{inter} = & \sum_{\alpha \neq \gamma} \left\{ \sum_{\mathbf{k}, \mathbf{q}} u_{\alpha\gamma}(\mathbf{q}) \exp[i(\mathbf{k} + \mathbf{q})\mathbf{R}_{\alpha} - \mathbf{k}\mathbf{R}_{\gamma}] c_{\alpha, \mathbf{k} + \mathbf{q}}^{\dagger} c_{\gamma, \mathbf{k}} \right. \\ & + \sum_{\mathbf{k}, \mathbf{q}, \lambda} M_{\alpha\gamma}(\mathbf{q}, \lambda) \exp[i(\mathbf{k} + \mathbf{q})\mathbf{R}_{\alpha} - \mathbf{k}\mathbf{R}_{\gamma}] (b_{\mathbf{q}\lambda} + b_{-\mathbf{q}\lambda}^{\dagger}) c_{\alpha, \mathbf{k} + \mathbf{q}}^{\dagger} c_{\gamma, \mathbf{k}} \\ & \left. + \sum_{\mathbf{q}} v_{\alpha}(\mathbf{q}) \rho_{\alpha, \mathbf{q}} \rho_{\gamma, -\mathbf{q}} \right\}, \quad (46) \end{aligned}$$

with

$$\rho_{\alpha, \mathbf{q}} = \sum_{\mathbf{k}} c_{\alpha, \mathbf{k} + \mathbf{q}}^{\dagger} c_{\gamma, \mathbf{k}}.$$

Here the first two terms in the summation over  $\alpha$  and  $\gamma$  are the intervalley electron-impurity and electron-phonon interactions, and the third term is the Coulomb interaction between electrons for different valleys.

In the Hamiltonian (45) we consider  $H' = \sum_{\alpha} H_{e\alpha} + H_{inter}$  as a small perturbation. If  $H'$  is neglected in the zeroth approximation, as in the construction of the quasi-equilibrium statistical operator, all the electron subsystems, together with the lattice system, are decoupled from each other. So the effective temperatures of hot electrons for various valleys may be different from each other, and also from the lattice temperature. In view of the above-mentioned consideration, we choose the following basic sets of  $P_m$  and  $F_m(t)$ :

$$\{P_m\} = \{H_{e1}; \dots; H_{en}; N_1; \dots; N_n; H_{ph}\}, \quad (47)$$

and

$$\{F_m(t)\} = \{\beta_1(t); \dots; \beta_n(t); -\beta_1(t)\mu_1(t); \dots; -\beta_n(t)\mu_n(t); \beta\}, \quad (48)$$

where  $\beta_{\alpha}(t)$  and  $\mu_{\alpha}(t)$  are the inverse effective temperature and chemical potential of hot electrons for the  $\alpha$ th valley, respectively. Since the population of electrons for each valley is not constant due to intervalley transfer, the population operators  $N_{\alpha}$  should be included in the set of  $P_m$ .

Starting from (47) and (48), it is straightforward to construct the NSO and obtain its approximate expression to the first order in  $H'$ . Using a similar procedure to that in the single valley case, as already outlined in Section 4, we can obtain the analytic results for statistical averages of the time derivatives of the center-of-mass momentum  $\mathbf{p}_{\alpha}$ , relative electron energy  $H_{e\alpha}$  and population  $N_{\alpha}$  for various valleys. Their explicit expressions have been given by Ref. 20 and will not be presented here. Letting them be equal to zero for the steady state, we have  $3n$  balance equations:

$$\langle \dot{\mathbf{p}}_{\alpha} \rangle^t = 0, \quad (49)$$

$$\langle \dot{H}_{e\alpha} \rangle^t = 0, \quad (50)$$

and

$$\langle \dot{N}_{\alpha} \rangle^t = 0, \quad (51)$$

with  $\alpha = 1, 2, \dots, n$ . They form a complete set of equations to determine the  $3n$  steady-state values of  $v_{\alpha}$ ,  $T_{\alpha}$  and  $N_{\alpha}$  as functions of the electric field strengths at a given lattice temperature. The chemical potential  $\mu_{\alpha}$  ( $\alpha = 1, 2, \dots, n$ ) of  $n$  valleys, which appear in the balance equations (49)-(51), are self-consistently determined by the following relations:

$$\langle N_{\alpha} \rangle^t = \sum_{\mathbf{k}} 1 / \{ \exp[\beta_{\alpha}(\epsilon_{\mathbf{k}\alpha} - \mu_{\alpha})] + 1 \}. \quad (52)$$

Finally, the drift velocity of the whole electron system is given by

$$\mathbf{v}_e = \sum_{\alpha=1}^n (\langle N_{\alpha} \rangle^t / N) \mathbf{v}_{\alpha}, \quad (53)$$

with  $N$  the total carrier number.

For the same reason as that discussed in the single valley case, the set of balance equations derived from the NSO method should be identical with that obtained by the Lei-Ting approach. This equivalence in the multivalley case has been presented by authors and their co-workers<sup>20,26</sup>. At the same time, we have compared the numerical solutions for the set of balance equations (49)-(51) with those of Monte Carlo calculations and experimental data of n-type Si and GaAs. For n-type Si, without any adjustable parameters, our calculated results<sup>20</sup> are in good agreement with those of Monte Carlo simulation<sup>27</sup> in wide ranges of temperature and field strength. Further, the results calculated from the balance equations also agree with the experimental data for hot-electron transport in n-type GaAs<sup>28</sup>.

## 6. Extension to Transient Hot-Electron Transport

It is straightforward to extend the NSO method to the study of transient hot-electron transport. The problem is to study the motion of an ensemble of electrons in a uniform bulk sample subject to various time configurations of a uniform electric field. Thus an ensemble average will enable us to obtain the time dependence of all the dynamic parameters such as the mean carrier energy and the mean carrier velocity. Here for simplicity, we will confine our discussion to the single valley case. The application to the case of multivalley semiconductors has been made by Ref.21.

For the transient transport, a pair of evolution equations

$$Nm\dot{v}_e = \langle \dot{p} \rangle^t, \quad (54)$$

$$c_e \dot{T}_e = \langle \dot{H}_e \rangle^t, \quad (55)$$

are needed to determine the transient drift velocity  $v_e(t)$  and the effective temperature  $T_e(t)$  as functions of time resulting from a time-dependent configuration of the electric field. Further, it should be checked whether or not the statistical averages in (54) and (55) are same as those in (22) and (23) since the NSO used for the transient transport seems to be a bit different from that in the steady-state case. To make this point clear let us extend the derivation in Section 6 to the case for transient transport. We again start from the approximate NSO in the form (17), over which the average of a dynamical operator A is

$$\langle A \rangle^t = \langle A \rangle_i + \int_{-\infty}^0 dt' e^{t't'} \int_0^1 d\tau \langle A e^{-\tau S(t,0)} \dot{S}(t+t',t') e^{\tau S(t,0)} \rangle_i. \quad (56)$$

Here

$$\dot{S}(t+t',t') = (-i)e^{iHt'} \{ \beta_e(t+t') [H_e, H_{el}] + \beta [H_{ph}, H_{el}] \} e^{-iHt'}, \quad (57)$$

and

$$\langle A \rangle_i = \text{Tr}(A e^{-S(t,0)}), \quad (58)$$

is calculated with the quasi-equilibrium statistical operator  $\rho_i$  at time  $t$ . Since the entropy operator  $S(t,0)$  depends explicitly on time, the average over  $\rho_i$  must be time dependent. To calculate the time correlation function in (56) let  $|m\rangle$  be the exact eigenstates of  $H_e$  and  $H_{ph}$ ,  $E_m$  and  $\Omega_m$  be the corresponding eigenvalues of  $H_e$  and  $H_{ph}$ . We can repeat the same calculation of the spectral representation for the time correlation function as done in Section 6, yielding

$$\int_0^1 d\tau \langle A e^{-\tau S(t,0)} \dot{S}(t+t',t') e^{\tau S(t,0)} \rangle_i = (-i) \sum_{m,n} \langle m | A | n \rangle \langle n | H_{el}(t') | m \rangle \times \{ \exp[-S_m(t)] - \exp[-S_n(t)] \} \gamma_{mn}(t+t',t), \quad (59)$$

where

$$S_m(t) = \beta_e(t) E_m + \beta \Omega_m,$$

and

$$\gamma_{mn}(t+t',t) = [S_m(t+t') - S_n(t+t')]/[S_m(t) - S_n(t)],$$

is a factor including some memory effect. Substituting (59) into (56) and integrating by parts, we obtain

$$\begin{aligned} \langle A \rangle^t = & \langle A \rangle_i - i \int_{-\infty}^0 dt' e^{t't'} \sum_{m,n} \langle m | A | n \rangle \langle n | H_{el}(t') | m \rangle \\ & \times \{ \exp[-S_m(t)] - \exp[-S_n(t)] \} + i \int_{-\infty}^0 dt' \dot{\gamma}_{mn}(t+t',t) \int_{-\infty}^{t'} ds e^{s't} \\ & \times \sum_{m,n} \langle m | A | n \rangle \langle n | H_{el}(s) | m \rangle \{ \exp[-S_m(t)] - \exp[-S_n(t)] \}, \end{aligned} \quad (60)$$

where

$$\dot{\gamma}_{mn}(t+t',t) = \dot{\beta}_e(t+t')(E_m - E_n)/[S_m(t) - S_n(t)].$$

It is obvious that the second term on the right-hand side of (60) is of the first order in  $H_{el}$  while the third term is of the third order of magnitude in  $H_{el}$  because  $\dot{\beta}_e$  is directly proportional to the square of  $H_{el}$ , as will be shown later. Therefore, when we construct the evolution equations in second order approximation in  $H_{el}$ , the third term in (60) should be neglected. Further, making the variable transformation  $t' \rightarrow t' - t$  for the integral over  $t'$  in (60) and using the relation, valid in the first approximation in  $H_{el}$

$$\langle m | A | n \rangle \langle n | H_{el}(t' - t) | m \rangle = \langle m | A(t) | n \rangle \langle n | H_{el}(t') | m \rangle,$$

we have

$$\begin{aligned} \langle A \rangle^t = & \langle A \rangle_i - i \int_{-\infty}^t dt' e^{t'(t-t')} \sum_{m,n} \langle m | A(t) | n \rangle \langle n | H_{el}(t') | m \rangle \\ & \times \{ \exp[-S_m(t)] - \exp[-S_n(t)] \}. \end{aligned} \quad (61)$$

On the analogy of (42), we can write (61) as

$$\langle A \rangle^t = \langle A \rangle_i + \int_{-\infty}^t dt' \langle\langle A(t) | H_{el}(t') \rangle\rangle^t, \quad (62)$$

where

$$\langle\langle A(t) | H_{el}(t') \rangle\rangle^t = -i\theta(t-t') \langle [A(t), H_{el}(t')] \rangle_i, \quad (63)$$

is a retarded double-time Green function. Equation (62) seems to have the same form as (43) for the steady-state case, but they have two major differences. One is the time-dependent statistical density matrix, as already mentioned, the other is that the center-of-mass coordinate,  $R(t) = R(t') + \int_{t'}^t v_e(s) ds$  with  $v_e(t)$  as the drift velocity, can not simply be expressed by  $R(t') + v_e(t-t')$ , as in the steady state, since  $v_e$  is time dependent in the transient transport case.

To obtain the evolution equations for  $v_e(t)$  and  $T_e(t)$  we substitute (19) and (21) into (62) and calculate the retarded Green function. Omitting the tedious calculations we write down the final result only:

$$Nm\dot{v}_e = NcE(t) - i \sum_q q_x \int_{-\infty}^{\infty} dt' \exp[q_x \int_{t'}^t v(s) ds] \{n_i | u(q) |^2 \langle \langle \rho_q(t) | \rho_{-q}(t') \rangle \rangle^t + \sum_{\lambda} |M(q, \lambda)|^2 [\langle \langle \rho_q(t) b_{q\lambda}(t) | \rho_{-q}(t') b_{-q\lambda}^\dagger(t') \rangle \rangle^t + \langle \langle \rho_q(t) b_{-q\lambda}^\dagger(t) | \rho_{-q}(t') b_{-q\lambda}(t') \rangle \rangle^t] \}, \quad (64)$$

$$c_e \dot{T}_e = - \sum_q \int_{-\infty}^{\infty} dt' \exp[q_x \int_{t'}^t v(s) ds] \{n_i | u(q) |^2 \langle \langle \dot{\rho}_q(t) | \rho_{-q}(t') \rangle \rangle^t + \sum_{\lambda} |M(q, \lambda)|^2 [\langle \langle \dot{\rho}_q(t) b_{q\lambda}(t) | \rho_{-q}(t') b_{-q\lambda}^\dagger(t') \rangle \rangle^t + \langle \langle \dot{\rho}_q(t) b_{-q\lambda}^\dagger(t) | \rho_{-q}(t') b_{-q\lambda}(t') \rangle \rangle^t] \}. \quad (65)$$

Here we wish to point out that the evolution equations (63) and (64), derived from the NSO method, are exactly the same as those obtained by extending the Lei-Ting approach to the transient hot-electron transport<sup>22</sup>. This shows that the conclusion that two statistical density matrices in the linear approximation in  $H_{el}$  has identical effect on the calculation of averages is applicable not only to the steady-state transport, but also to the transient hot-electron transport. It is worth to mention that the evolution equations (63) and (64) contain the memory effect of the drift velocity, which is included in their exponent factors. When the evolution equation (63) is linearized, we can obtain a Langevin-like equation for the drift velocity. It has been shown that the memory effect or the intra-collisional field effect has little influence upon the solutions of evolution equations, at least for applied electric fields with moderate strengths<sup>22</sup>. Further, the evolution equations without memory effect have been applied to the calculations of transient hot-electron transport in p-type Ge and n-type GaAs under electric fields with several time-dependent configurations<sup>21,22</sup>. The calculated results coincide well with those obtained by interactive procedure and Monte Carlo simulation.

## 7. Concluding Remarks

We have applied the NSO method to the study of steady-state and transient hot-electron transport, including Coulombic many-body effect. After making a careful comparison between the NSO method and the balance-equation approach<sup>9</sup>, we conclude that they yield the identical balance or evolution equations in the second-order approximation in  $H_{el}$ , which is usually used in hot-electron transport theory. This identity stems from the fact that though they belong to two different statistical methods, their statistical density matrices to lowest order in  $H_{el}$  have the same effect on the calculation of averages. It is conjecturable that such identity can not extend beyond this approximation; if so the balance or evolution equations obtained by the NSO method and the balance-equation approach may differ from each other only by high-order terms in  $H_{el}$ .

The essential feature of the balance-equation approach is the separation of the center-of-mass motion from the relative motion of electrons in the Hamiltonian and in the density matrix. After the separation the external electric field acts only on the center of mass, and the electrons which move relative to the center of mass do not directly experience the external field. They couple with the center of mass and with the lattice only through the electron-lattice interaction  $H_{el}$ . Taking into account the inequality  $\tau_{el} \gg \tau_{ee}$  for the electron-lattice system under consideration, we can regard  $H_{el}$  as a small perturbation. In the zeroth approximation the relative electrons decouple themselves from the center of mass and from the lattice. So for time intervals larger than  $\tau_{ee}$  but smaller than  $\tau_{el}$  the hot-electron system in a nonequilibrium state may be described by an effective temperature  $T_e$  which indicates the mean energy of the relative motion of hot electrons, and the center-of-mass motion described by the average value of the momentum operator of the center of mass. On the other hand, the perturbation operator  $H_{el}$  provides dissipative mechanisms for the irreversible transport processes, so both steady-state balance equations and transient evolution equations are set up in terms of the perturbation expansion of  $H_{el}$ , usually in the second-order approximation in  $H_{el}$ . Therefore, the "separation" idea provides a very clear physical picture, as well as a simple mathematical treatment, for the hot-electron transport. In this work, since the beginning of applying the NSO method to the study of hot-electron transport we have absorbed this advanced idea, with the result that the present derivation for balance equations is greatly simplified in contrast to earlier ones<sup>17,18</sup>.

A difficult problem in the nonequilibrium dissipative theory is how to obtain irreversible behavior in the macroscopic description of the state of the system generated by a statistical operator  $\rho(t)$ , if it satisfies Liouville equation with time-reversal invariance. This can be obtained in terms of Prigogine's dynamic condition for dissipativity<sup>27</sup>:

$$\frac{\partial \rho(t)}{\partial t} + i\Lambda(t)\rho(t) = 0. \quad (66)$$

Here  $\Lambda$  is a modified Liouville operator composed of an odd and an even part under time-reversal, and  $\rho(t)$  is a transformed NSO now having irreversibility built in it. All available approaches to the nonequilibrium statistical problems introduce at some point in their derivations condition analogous to Prigogine's principle. As already mentioned, the Zubarev approach is to introduce into Liouville's equation an infinitesimally small source that break time-reversal symmetry. The modified Liouville equation is<sup>16</sup>

$$\frac{\partial \ln \rho(t)}{\partial t} - i[\ln \rho(t), H] = -\epsilon(\ln \rho(t) - \ln \rho_l), \quad (67)$$

where  $\epsilon \rightarrow +0$  after the thermodynamic limiting process. In construting the above equation which is linear in  $\ln \rho(t)$ , it has been considered that the logarithm of a statistical operator satisfying Liouville's equation also satisfies Liouville's equation. It is easily shown that the NSO (12) is just the solution of (67). Although this point is not explicitly put forward in the balance-equation approach by Lei and Ting<sup>9</sup>, when they select the retard solution of Liouville's equation and use the retarded Green functions, an infinitesimally small source which violates the time-reversal symmetry has been implicitly introduced into Liouville's equation.

In this work we restrict ourselves to consider the spatially homogeneous distribution of hot electrons interacting with thermal-equilibrium scatterers in semiconductors.

This approach may be easily extended to take into account the spatial inhomogeneities of the system and the deviation of the scatterers from thermal equilibrium such as phonon drag effect. Besides hot-electron transport problems, the NSO method has been also applied to different problems in the theory of irreversible processes<sup>13</sup>. The successes on various applications show that the NSO method may constitute a very powerful theoretical tool in the study of dissipative dynamic systems.

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