PHYSICAL REVIEW B VOLUME 28, NUMBER 4 15 AUGUST 1983

Correlation functions for high-field transport in semiconductors

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(Received 21 March 1983)

The relevant correlation functions for the differential mobility and the diffusion coefficient are developed here for the far-from-equilibrium steady state appropriate to high-field transport in semiconductors. We present a unified analysis for the evolution of several generic correlation functions related to this steady state. We emphasize the initial values and the temporal evolution of these functions.

I. INTRODUCTION

High-electric-field transport has been studied for some three decades.[1,2] In recent years it has become of much more interest due to the advent of semiconductor devices on the micrometer and submicrometer dimensional scale.[3] Theoretically, such hot-carrier transport has been discussed primarily in terms of the Boltzmann equation.[1,4] However, semiconductor transport in high electric fields is a classical example of a far-from-equilibrium system.[5] On the short-time scales appropriate to the submicrometer dimensions, the Boltzmann equation ceases to have general validity,[6,7] and more exact approaches have been sought.

In general, we are concerned with the evolution of the average velocity and energy of the carrier ensemble in the presence of the high electric field. Approaches tend to be centered on either solving the Liouville equation[8-11] or on developing appropriate generalized Langevin equations for the macrovariables of interest.[12] In either case retarded relaxation integrals are encountered,[11,13] and these in turn involve kernels which lead to the evaluation of a set of correlation functions. While these correlation functions do not normally appear in classical mechanics, it has been recognized for some time that parameters such as the differential mobility and diffusion constant are related to these functions.[14] However, treatment of these correlation functions for high-field transport has been treated only by Green's functions based upon the Boltzmann equation. Since these same parameters are of considerable importance in evaluating transport and noise properties of submicrometer devices, we set out here to provide a more general derivation of these correlation functions from first principles.

As is known for other far-from-equilibrium systems, we show that the transport parameters of interest, differential mobility and diffusion constant, can be readily obtained through a unique set of Green's functions to which we add proper knowledge of all relevant moments of the nonequilibrium statistical distribution (NESD) that are required. In Secs. II and III we analyze the differential mobility and the diffusion constant for an ensemble of electrons in the presence of a steady, high electric field. These terms are evaluated in the high-temperature (classical) limit, although the derivations are more general. In these sections we introduce the appropriate Green's functions and the relevant initial values of the correlation functions, where the latter are intimately related to the distribution function n_k.

In Sec. IV we introduce a method to calculate the nonequilibrium density matrix. This treatment parallels that previously given by Zubarev,[15] but differs somewhat in approach. The results are used in Sec. V to evaluate the distribution function n_k. Finally, Sec. VI is devoted to the evolution equations for the Green's functions developed here. These evolution equations clearly show the role of memory effects[16] and the intracollisional field effect.[10,17]

Throughout the developments reported here, a second-quantization formalism is used, even though we often take the high-temperature classical limit in order to isolate the thermodynamical character of the results. However, we find this formalism provides an advantageous basis for the future incorporation of a full electron-electron interaction into these results. Furthermore, we restrict our treatment to the steady-state (stationary) situation.[18] The extension of these results to the case of nonstationary transport is in principle straightforward.

II. DIFFERENTIAL MOBILITY

We consider a low-density electron gas that remains in contact with the lattice and is subjected to a high electric field. The Hamiltonian of the entire system is given by

$$H = H_e + H_F + H_{eL} + H_L \ , \tag{1}$$

where the terms on the right-hand side are, respectively, the complete electronic Hamiltonian, including the electron-electron interactions, the field term (equal to $-e\vec{F}\cdot\vec{x}$), the electron-lattice interaction, and the Hamiltonian of the lattice variables. Unless otherwise noted, we limit these latter variables to the phonon field. The Liouville equation for the density matrix now becomes (we take $\hbar=1$ throughout for simplicity)

$$i\frac{\partial\rho}{\partial t} = [H,\rho] \ , \tag{2}$$

where the square brackets are the usual commutator. If the strong electric field $\vec{F}$ applied to the electronic system is static, we assume that a quasiequilibrium density matrix ρ_z (our NESD) exists and satisfies

$$[H,\rho_z] = 0 \ . \tag{3}$$

In calculating the differential mobility, we assume that

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a small ac field $\delta\vec{E}(t)$ is added to the static field $\vec{F}$. This in turn perturbs the density matrix, which can then be written as $\rho=\rho_z+\Delta\rho$. Up to first order in δE, the deviation $\Delta\rho$ is given by the solution to

$$i\frac{\partial\Delta\rho}{\partial t}+[\Delta\rho,H]=-e\left[\sum_i x_i,\rho_z\right]\delta E(t)\ , \tag{4}$$

where the index i runs over the electrons. The solution of this equation is given by the usual formulation of linear-response theory as[19]

$$i\,\Delta\rho=\int_{-\infty}^{t} e\,\delta E(u)\left[\rho_z,\sum_i x_i(u-t)\right]du\ , \tag{5}$$

where $x_i(t)$ is written in the Heisenberg representation using the Hamiltonian (1). It is then straightforward to show that

$$\langle\delta J\rangle=-i\int_{-\infty}^{t} e\,\delta E(u)\mathrm{Tr}\left\{\rho_z\left[\sum_i x_i,J(t-u)\right]\right\}du\ , \tag{6}$$

where

$$\langle\delta A\rangle=\mathrm{Tr}(\Delta\rho A)\ . \tag{7}$$

The Fourier transform of the differential mobility $\mu(\omega)$ is found by

$$\mu(\omega)=\int_0^{\infty} e^{-i\omega\tau}\hat{\mu}(\tau)d\tau\ , \tag{8}$$

where, from (6),

$$\hat{\mu}(\tau)=-i\frac{e}{Nm}\Theta(\tau)\mathrm{Tr}\left\{\rho_z\left[\sum_i x_i,P_e(\tau)\right]\right\}\ , \tag{9}$$

and $\Theta(\tau)$ is the Heaviside step function.

We can write the appropriate variables of (9) in a second quantized form as

$$P_e=\sum_k k c_k^\dagger c_k\ , \tag{10}$$

$$\sum_i x_i=\sum_{k_1,k_2}\langle k_1|x|k_2\rangle c_{k_1}^\dagger c_{k_2}\ . \tag{11}$$

Now, with the identity

$$\langle k_1|x|k_2\rangle=i\frac{\partial}{\partial k_1}\delta(k_1-k_2)\ , \tag{12}$$

and the usual calculational rules for generalized distributions, we can rewrite (9) as

$$\hat{\mu}(\tau)=-\frac{e}{Nm}\sum_{k,k_1}\Theta(\tau)k\,\mathrm{Tr}\left\{\rho_z\left[\frac{\partial c_{k_1}^\dagger}{\partial k_1}c_{k_1},c_k^\dagger(\tau)c_k(\tau)\right]\right\}\ . \tag{13}$$

Expression (13) is quite general and does not rest upon any approximations other than the linear response used for (5). The generalized differential mobility $\hat{\mu}(\tau)$ is now seen to depend upon a generic operator function

$$\psi_{k_1}(k,\tau)=\Theta(\tau)\left\langle\left[\frac{\partial c_{k_1}^\dagger}{\partial k_1}c_{k_1},c_k^\dagger(\tau)c_k(\tau)\right]\right\rangle_z\ , \tag{14}$$

where the angular brackets denote an average over ρ_z.

Let us now focus on the specific effects of the high electric field, neglecting the possible electron-electron interaction. Then we find (in Sec. VI) that the evolution of $\psi_{k_1}(k,\tau)$ for $\tau>0$ is dependent primarily upon the initial condition $\psi_{k_1}(k,0)$, a result valid for the high-temperature or classical limit. Furthermore, it is easy to obtain this initial condition as

$$\psi_{k_1}(k,0)=\delta(k-k_1)\frac{\partial n_{k_1}}{\partial k_1}\ , \tag{15}$$

where

$$n_{k_1}=\langle c_{k_1}^\dagger c_{k_1}\rangle_z \tag{16}$$

is the ensemble-averaged number operator or distribution function. Now consider the following propagator or Green's function:

$$G(k_1,k;\tau)=\Theta(\tau)\left\langle 0\left|\mathrm{Tr}_L\left(\frac{e^{-\beta_L H_L}}{Z_L}c_{k_1}c_k^\dagger(\tau)c_k(\tau)c_{k_1}^\dagger\right)\right|0\right\rangle\ , \tag{17}$$

where β_L $(=1/k_BT_L)$ is the inverse lattice temperature and $Z_L=\mathrm{Tr}(e^{-\beta_L H_L})$ is a pseudopartition function. In both Z_L and the trace in (17), the trace is actually carried out only over the lattice variables since the problem involves a mixed representation.[20,21] The state $|0\rangle$ in (17) is the vacuum state of the electronic Fock space.

We recognize that $G(k_1,k;\tau)$ is related to the generic function $\psi_{k_1}(k,\tau)$. In fact, these two functions obey the same evolution equation (see Sec. VI). Furthermore, the value of $G(k_1,k;\tau)$ is uniquely defined by its initial condition $G(k_1,k;0)$, which is

$$G(k_1,k;0)=\delta(k-k_1)\ . \tag{18}$$

Then from (15)–(18) we have

$$\psi_{k_1}(k,\tau)=G(k_1,k;\tau)\frac{\partial n_{k_1}}{\partial k_1}\ . \tag{19}$$

The Green's function $G(k_1,k;\tau)$ approaches a value independent of k_1 in the limit

$$\lim_{\tau\to\infty}G(k_1,k;\tau)=f_k \tag{20}$$

with

$$\sum_k f_k=1\ . \tag{21}$$

Clearly f_k is related to n_k, and the normalization condition (21) arises from the fact that the Hamiltonian commutes with the particle number.

We can now use (19) to help with the calculation of $\hat{\mu}(\tau)$. Using (19) in (13), we obtain after a trivial integration by parts,

$$\hat{\mu}(\tau)=\frac{e}{Nm}\int\int dk_1 dk\, k n_{k_1}\frac{G(k_1,k;\tau)}{\partial k_1}$$
$$=\frac{e}{Nm}\left\langle\frac{\partial}{\partial k}\int dk_1 G(k,k_1;\tau)k_1\right\rangle , \qquad (22)$$

where we have interchanged variables in the last line, and

$$\langle\mathscr{F}\rangle=\int dk\, n_k\mathscr{F} \qquad (23)$$

represents a distribution-function average.

The result (22) is quite general, even with a Poisson-bracket formalism. It has been previously obtained in the classical case of a Boltzmann-equation approach,[22] and emphasizes the role of G in determining $\hat{\mu}(\tau)$ in any practical case. Furthermore, since G is independent of k_1 for $\tau\rightarrow\infty$, we clearly see from (22) that $\mu(\tau)\rightarrow 0$ in this limit. A further point worth noting is that if n_k does not correspond to the equilibrium case, (22) introduces the failure of the normal fluctuation-dissipation theorem.[23]

III. DIFFUSION COEFFICIENT

Now that some understanding of the general Green's function has been achieved, we want to turn to a consideration of the diffusion coefficient. By classical considerations we examine the basis of introducing a velocity-velocity correlation function in the absence of the electron-electron interaction. In this we introduce a generalized correlation function which once again emphasizes the role of the generic Green's function that appeared in the preceding section. We return briefly to this task in Sec. IV, where the effect of interacting electrons is discussed with regard to the diffusion coefficient.

In the classical framework, the diffusion coefficient of an ensemble of electrons is defined by the spreading of the packet in space. This leads to one definition as[24]

$$D=\frac{1}{2N}\frac{d}{dt}\left\langle\sum_i[\Delta R_i(t)]^2\right\rangle \qquad (24)$$

and

$$D=\frac{1}{N}\int_0^\infty dt\left\langle\sum_i\Delta v_i\Delta v_i(t)\right\rangle , \qquad (25)$$

where $\Delta v_i=v_i-\langle v_i\rangle$ and (25) is valid in the stationary case. Within this classical framework these definitions are accurate even with the electron-electron interaction included. On the other hand, the quantum case is more difficult as it is not easy to introduce the velocity terms inside the kernel of (25) when the electron-electron interaction is present due to the indistinguishability of the electrons. For this reason we limit the present treatment to independent particles, for which

$$\frac{1}{N^2}\left\langle\sum_i\Delta v_i\Delta v_i(t)\right\rangle=\langle\Delta v_e\Delta v_e(t)\rangle , \qquad (26)$$

where

$$v_e(t)=\frac{1}{N}\sum_i v_i(t) . \qquad (27)$$

In this case we can define the diffusion coefficient in the quantum case as

$$D=\frac{1}{Nm^2}\int_0^\infty dt\langle P_e[P_e(t)-\langle P_e\rangle_z]\rangle_z , \qquad (28)$$

where

$$\langle\mathscr{F}\rangle_z=\mathrm{Tr}(\rho_z\mathscr{F}) \qquad (29)$$

involves an average over the NESD ρ_z.[15] Here P_e is the average momentum of the ensemble of N electrons. This definition remains valid even in the classical case as well. In Sec. IV we extend the definition to include the role of the chemical potential in a manner which confirms (28).

At this point, however, it is convenient to generalize the average (29) that appears twice in (28). For this we introduce the general set of correlation functions

$$S(\Delta A,\Delta B(t))=\Theta(t)\mathrm{Tr}[\rho_z A\,\Delta B(t)] , \qquad (30)$$

where A and B are two arbitrary "one-particle" operators, expressible as

$$A=\sum_k a(k)c_k^\dagger c_k ,$$
$$B=\sum_k b(k)c_k^\dagger c_k . \qquad (31)$$

In particular, functions of this form are an excellent test of the Zubarev approach[15,25] to nonequilibrium thermodynamics. Indeed, from (30) it is clear that at $t=0$ the classical noninteracting limit results in the correlation functions (30) simply reducing to the moments of the distribution function. Note in particular that definition (30) is not symmetrical in its arguments for the quantum case.

We remark in passing that the classical limit is one readily calculated by, e.g., using an ensemble Monte Carlo (EMC) approach with an electron system.[26,27] This is particularly true as the EMC treatment of transport satisfies a more general retarded kinetic equation rather than the Boltzmann equation and so fits our need for improved treatments (over the Boltzmann equation).[28] Thus the EMC approach provides an easy and direct method for simulating the various correlation functions.

Using the set of definitions (31) for the operators, we can now expand the generalized correlation function as

$$S(\Delta A,\Delta B(t))=\Theta(t)\sum_{k_1,k_2}a(k_1)b(k_2)\langle\delta F_{k_1}\delta F_{k_2}(t)\rangle_z , \qquad (32)$$

where $F_k=c_k^\dagger c_k$, so that

$$\langle\delta F_{k_1}\delta F_{k_2}(t)\rangle_z=\Theta(t)\langle(c_{k_1}^\dagger c_{k_1}-\langle c_{k_1}^\dagger c_{k_1}\rangle_z)$$
$$\times c_{k_2}^\dagger(t)c_{k_2}(t)\rangle_z . \qquad (33)$$

The evaluation of S can now be readily carried out through the use of the generic correlation functions that now appear in (32). When $t=0$, (32) reduces to[20]

$$\langle\delta F_{k_1}\delta F_{k_2}(0)\rangle_z=\delta(k_1-k_2)n_{k_1} \qquad (34)$$

in the high-temperature limit of independent electrons. Furthermore, in this latter limit, the general case of $t>0$ leads to the correlation function (32) satisfying the same differential equation as $G(k_1,k_2;t)$ with a similar set of initial conditions (this is shown in Sec. VI). Thus we may write

$$\langle \delta F_{k_1} \delta F_{k_2}(t) \rangle = n_{k_1} G(k_1,k_2;t) \; . \tag{35}$$

This last result is somewhat peculiar, as the normal fixed point[29] $\langle \delta F_{k_1} \delta F_{k_2}(t \to \infty) \rangle \to 0$ is not achieved with (34). The reason for this lies in (34) which is used in the low-density limit. This expression breaks the normal property (which arises from conservation of the particle number)

$$\sum_{k_2} \langle \delta F_{k_1} \delta F_{k_2}(0) \rangle = 0 \; , \tag{36}$$

which is required to give the aforementioned fixed-point limit. However, this effect is small. It only appears in the very long-time limit of the correlation function and is density dependent. In the long-time limit, other complicated behavior is also at work to create long-time tails on the correlation functions (see the discussion of Ref. 24). They have a deep thermodynamical character and should not be mixed with our density-dependent artifact.

It appears now that the calculations of the differential mobility and the correlation functions of interest involve a requirement of n_k in order to establish the initial conditions at $t=0$. From this, we need only a knowledge of the evolution of the Green's function $G(k_1,k_2;t)$. We begin by determining n_k in Secs. IV and V. To achieve this, we use a method that parallels that of McLennan[30] and Zubarev[15] in treating nonequilibrium thermodynamics. In this approach we find that $n_k = \langle F_k \rangle_z$. First, in Sec. IV the central features of the density matrix ρ_z are discussed. In this treatment, the chemical potential of the electron ensemble is introduced. Then in Sec. V, the distribution function n_k is developed.

IV. DENSITY MATRIX ρ_z

We now turn our attention to the calculation of the density matrix ρ_z. This function is found by solving the Liouville equation (2), which in turn is achieved in two steps. First, we introduce a trial quasiequilibrium density matrix. Second, we solve the Liouville equation in terms of deviations from this trial function. Here we take ρ_L as the trial operator so that we can write $\rho_z = \rho_L + \Delta\rho$. Then ($\hbar = 1$)

$$i\frac{\partial \Delta\rho}{\partial t} - [H,\Delta\rho] = [H,\rho_L] - i\frac{\partial \rho_L}{\partial t} \; . \tag{37}$$

The source term on the right-hand side contains all the irreversibility that is involved in the evolution of ρ_z.[12] Now ρ_L is defined to be an operator functional of a selected set of macrovariables, much in the sense of a "displaced Maxwellian." More specifically, we write ρ_L as

$$\rho_L = \exp[-\sigma(t)] \; , \tag{38}$$

with[11,15]

$$\sigma(t) = \psi(t) + \sum_m F_m(t) P_m \; . \tag{39}$$

Here $\psi(t)$ provides the normalization and has the properties that are entailed in a partition function. The P_m are the set of macrovariables

$$\{P_m\} = \{\vec{P}_e, H_e, N_e, H_L, H_{e-L}, \dots\} \; , \tag{40}$$

where $\vec{P}_e$ is the electronic momentum, etc. The parameters $F_m(t)$ are the corresponding conjugate forces, thus ensuring the requirement

$$\mathrm{Tr}(\rho P_m) = \mathrm{Tr}(\rho_L P_m) \; . \tag{41}$$

These are given by the set, respectively, for the set (40)

$$\{F_m\} = \{-\beta_e \vec{v}_D, \beta_e, -\beta_e(\mu - \tfrac{1}{2} m v_D^2), \beta_L, \beta_L, \dots\} \; , \tag{42}$$

where β_e and β_L are the inverse electron and lattice temperatures, $\vec{v}_D$ is the drift velocity of the electron ensemble, and μ is the chemical potential of the ensemble.

We now solve the Liouville equation. While at first appearance it may seem that a direct attack on (37) is called for, we shall proceed otherwise. We note that if $\rho(t)$ satisfies the Liouville equation, then any quantity $S(t)$ defined through $\rho(t) = \exp[-S(t)]$ also satisfies the Liouville equation. If we define $S(t) = \Delta S(t) + \sigma(t)$, then the evolution equation for ΔS is just

$$i\frac{\partial \Delta S}{\partial t} - [H,\Delta S] = [H,\sigma] - i\frac{\partial \sigma}{\partial t} \; . \tag{43}$$

Thus if we choose $\rho(t=-\infty) = \rho_0$ for the initial condition on $\rho(t)$, where ρ_0 is the density matrix in equilibrium, we find that $\Delta S(t=-\infty) = 0$ is the appropriate initial condition for (43). By introducing the causal Green's function in (43), it is then straightforward to obtain

$$\Delta S(t) = -i \int_{-\infty}^{t} dt' \exp[\eta(t'-t) + i\hat{H}(t'-t)] \times \left[[H,\sigma(t')] - i\frac{\partial \sigma(t')}{\partial t'} \right] , \tag{44}$$

where $\hat{H}$ is the commutator-generating super operator of the system Hamiltonian H and η is the usual convergence factor.

In the original definition of $\sigma(t)$ above, the time parameter corresponds to the time at which the thermodynamic variables are evaluated. We may extend this definition to the two-time function as

$$\sigma(t,u) = \psi(t) + \sum_m F_m(t) P_m(u) \; , \tag{45}$$

where the time evolution of $P_m(u)$ is given as $\exp(i\hat{H}u)P_m$. It is then easy to write

$$\Delta S(t) = -\int_{-\infty}^{0} dt\, e^{\eta t'} \dot{\sigma}(t+t',t') \; , \tag{46}$$

where

$$\dot{\sigma}(t,u) = \frac{\partial \sigma(t,u)}{\partial t} + i[H,\sigma(t,u)] \; . \tag{47}$$

With these definitions the final expression for ρ_z is easily found as

$$\rho_z(t) = \exp\left[-\sigma(t) + \int_{-\infty}^{0} dt' e^{\eta t'} \dot{\sigma}(t+t',t') \right] , \tag{48}$$

which is the same form obtained by Zubarev.[15] Up to this point, the result (48) for ρ_z depends only upon formal considerations. Insight is only required in the choice of the macrovariable set (40) and the corresponding conjugate forces (42). A "proper" selection of these ensures that the metric "distance" (in the Hilbert space of operators) between ρ_z and ρ_L is minimized so that an expansion in terms of low powers of $S(t)$ may readily be utilized.

We must still calculate the quantity $\dot{\sigma}$. First, it is clear that if $H_{eL}=0$, ρ_L is a solution to the Liouville equation with the current choice of macrovariables. In this case, the source term $\dot{\sigma}$, which describes the irreversibility, must vanish. From the definition (47) for $\dot{\sigma}$, we may write[11,25]

$$\dot{\sigma}(t,0)=\sum_m \dot{P}_{m,L}F_m(t) + \sum_{m,l}(P_m-\langle P_m\rangle^t)\frac{\partial F_m}{\partial\langle P_l\rangle}\langle \dot{P}_{l,L}\rangle \,, \tag{49}$$

where $\dot{P}_{m,L}=i[H_{eL},P_m]$. The determination of ρ_z is then completed by using (49) and (39) in (48).

Let us look at the role of the chemical potential now by examining the diffusion processes in the reference frame traveling at v_e. In this frame of reference,

$$\rho_L=\exp[-\psi(t)-\beta_e H_e+\beta_e\mu N_e-\beta_L H_{eL}-\beta_L H_L'] \,, \tag{50}$$

where H_L' is the lattice Hamiltonian in the moving frame. The diffusion flux is then[15]

$$D=\frac{\beta_e}{m^2}\int_0^\infty dt\,(P_e;P_e(t))\frac{\partial\mu}{\partial n} \,, \tag{51}$$

where n is the density of particles and the quantum correlation functions are defined through

$$(P_e;P_e(t))=\int_0^1 du\,\mathrm{Tr}[\Delta P_e e^{-u\sigma}P_e(t)e^{u\sigma}\rho_L] \,. \tag{52}$$

If (51) and (28) are compared for the case of independent electrons, where $\partial\mu/\partial n=(n\beta_e)^{-1}$, it is clear that we can draw a correspondence between the two if the "N-electron system" of Sec. III refers to a unit volume. Nevertheless, differences between the two lie in the definitions of the correlation functions involved. However, in the classical limit, the correlation function (52) can be written

$$(P_e;P_e(t))=\mathrm{Tr}[\rho_L\Delta P_e P_e(t)] \,. \tag{53}$$

Using (41) and the fact that the two correlation functions satisfy the same evolution equations, in the classical case of noninteracting electrons, we find that the two formulations are equivalent. Thus the general formula for D is that of (51). If electron-electron interactions become important in the system, these will enter (51) through the correlation function and through μ.

Up to now we have not considered the role of the impurities which give a positive background of charge to ensure neutrality. If we wish to include electron-electron interactions, then it will also be necessary to include the electron-impurity interaction in ρ_L and H in order to cover the long-range Coulomb terms in the potentials. Furthermore, in any diffusion experiment, the presence of an electric field arising from the direct Coulomb interaction leads to an additional current which is treated by the differential mobility discussed above.

V. INITIAL VALUE OF THE CORRELATION FUNCTIONS

At this point we now turn our attention to the evaluation of n_k, the distribution function needed in order to calculate the initial values of the various correlation functions. First, it should be recalled that

$$n_k=\mathrm{Tr}(\rho_z c_k^\dagger c_k) \,, \tag{54}$$

and that we use (48) for ρ_z. In the calculations to follow, we will retain the high-temperature (noninteracting) limit. These calculations will be carried out only up to second order in H_{eL}, as this is the lowest order which leads to dissipation. After considerable algebra, (54) may be rewritten as

$$\begin{aligned} n_k={}&\langle c_k^\dagger c_k\rangle_0+\frac{\beta_L^2}{2}(\langle c_k^\dagger c_k H_{eL}^2\rangle_0-\langle c_k^\dagger c_k\rangle\langle H_{eL}^2\rangle_0)-\beta_L\int_{-\infty}^0 dt' e^{\eta t'}\langle c_k^\dagger c_k\dot{\sigma}_1(0,t')H_{eL}\rangle_0 \\ &+\tfrac{1}{2}\int_{-\infty}^0 dt' e^{\eta t'}\int_{-\infty}^0 dt'' e^{\eta t''}\langle c_k^\dagger c_k\dot{\sigma}_1(0,t')\dot{\sigma}_1(0,t'')\rangle_0+\int_{-\infty}^0 dt' e^{\eta t'}\langle c_k^\dagger c_k\dot{\sigma}_2(0,t')\rangle_0+\cdots \,, \end{aligned} \tag{55}$$

where $\dot{\sigma}_1$ is the lowest-order part of $\dot{\sigma}$,

$$\dot{\sigma}_1(0,t')=\sum_m \dot{P}_{mL}(t')F_m \,, \tag{56a}$$

$\dot{\sigma}_2(0,t')$ is the second-order part of $\dot{\sigma}$,

$$\dot{\sigma}_2(0,t')=\sum_{m,l}[P_m(t')-\langle P_m\rangle^t]\frac{\partial F_m}{\partial\langle P_l\rangle}\langle \dot{P}_{l,L}\rangle \,, \tag{56b}$$

and angular brackets with subscript zero refer to the averages being taken with respect to ρ_L in the absence of H_{eL}. If we write the interaction terms as

$$H_{eL}=\sum_{k,q,\lambda}(U_{q\lambda}b_{q\lambda}c_{k+q}^\dagger c_k+\text{c.c.}) \,, \tag{57}$$

then standard decoupling procedures[31] can be employed in order to rewrite (55) as

$$\begin{aligned}
n_k = n_k^0 & \left[1 + \beta_L^2 \sum_{q,\lambda} N_{q\lambda} | U_{q\lambda} |^2 \right] \\
& + n_k^0 \beta_L \sum_{q,\lambda} [(\beta_e - \beta_L) E_{k,k-q} - \beta_L \vec{\mathrm{V}}_D \cdot \vec{\mathrm{q}}] \, | U_{q\lambda} |^2 \\
& \qquad \times \int_{-\infty}^{0} dt' e^{\eta t'} \{ G_k^{(1)}(t') G_{k-q}^{(2)}(t') [D_{q\lambda}^{(2)}(t') + D_{-q\lambda}^{(1)}(t')] \} \\
& - \tfrac{1}{2} \sum_{q,\lambda} [(\beta_e - \beta_L) E_{k,k-q} - \beta_e \vec{\mathrm{v}}_D \cdot \vec{\mathrm{q}}]^2 \, | U_{q\lambda} |^2 \\
& \qquad \times \int_{-\infty}^{0} dt' \int_{-\infty}^{0} dt'' e^{\eta(t'+t'')} n_k(t'') G_k^{(1)}(t') \langle c_{k-q}(t') c_{k-q}^{\dagger}(t'') \rangle_0 \\
& \qquad\qquad \times [\langle b_{q\lambda}(t') b_{q\lambda}^{\dagger}(t'') \rangle_0 + \langle b_{-q\lambda}^{\dagger}(t') b_{-q\lambda}(t'') \rangle_0] \\
& + \frac{1}{N} \left[\frac{\langle \dot{H}_{eL} - \vec{\mathrm{v}}_D \cdot \dot{\vec{\mathrm{P}}}_{e,L} \rangle}{\langle \tilde{\epsilon}^2 \rangle_0 - \langle \tilde{\epsilon} \rangle_0^2} (\tilde{\epsilon}_k - \langle \tilde{\epsilon}_k \rangle_0) + \frac{\beta_e}{m} \langle \dot{P}_{e,L} \rangle (k - \langle k \rangle_0) \right] \int_{-\infty}^{0} dt' e^{\eta t'} n_k(t') G_k(t') \, . \qquad (58)
\end{aligned}$$

While (58) is quite busy, we note that several simple and usual notations are being used, including separate electron and phonon Green's functions. These latter notations are defined through

$$\begin{aligned}
& G_{kk'}^{(1)}(t) = i\Theta(-t) \langle c_k c_{k'}^{\dagger}(t) \rangle_0 \, , \\
& G_{kk'}^{(2)}(t) = i\Theta(-t) \langle c_k(t) c_{k'}^{\dagger} \rangle_0 \, , \\
& D_{q\lambda,q'\lambda'}^{(1)}(t) = i\Theta(-t) \langle b_{q\lambda}^{\dagger}(t) b_{q'\lambda'} \rangle_0 \, , \qquad (59) \\
& D_{q\lambda,q'\lambda'}^{(2)}(t) = i\Theta(-t) \langle b_{q\lambda}(t) b_{q'\lambda'}^{\dagger} \rangle_0 \, , \\
& n_{kk'}(t) = i\Theta(-t) \langle c_k^{\dagger} c_{k'}(t) \rangle_0 \, ,
\end{aligned}$$

with $I_k(t) = I_{kk}(t)$, where I stands for any of the functions in (59). Further, $E_{k,k\pm q} = E(k) - E(k \pm q)$ and $\tilde{\epsilon}_k = E(k) - \mu' - v_D k$. If $\phi(k)$ is any real function of k, we define $\langle \phi(k) \rangle_0$ by $N \langle \phi(k) \rangle_0 = \sum_k \phi(k) n_k^0$. We note that in the presence of a high electric field, these energies are evolving functions of time due to the intracollisional field effect.[10,17,32] If this latter effect is ignored in the off-diagonal terms, then the diagonal terms of the various electronic Green's functions satisfy, as an example,

$$(\omega + E_k - i\eta) G_k^{(1)}(\omega) = 1 - ieF \frac{\partial}{\partial k'} G_{kk'}^{(1)}(\omega) \Big|_{k' \to k} + G_k^{(1)}(\omega) \sum_{q,\lambda} \frac{2N_{q\lambda} | U_{q\lambda} |^2 (\omega + E_{k+q} - i\eta)}{(\omega + E_{k+q} - i\eta)^2 - \omega_{q\lambda}^2} \, , \qquad (60)$$

where $\omega_{q\lambda}$ and $N_{q\lambda}$ are the frequency and density of the q,λ mode. It is in general still a difficult task to solve (60) for $G_k^{(1)}(\omega)$. On the other hand, crude approximations simplify this task. One approximation is to replace the last term by the relaxation time approximation, in which this term becomes $iG_k^{(1)}(\omega)/\tau_k$. Then one can solve (60) in the real plane by utilizing the method of characteristics. Following this procedure yields

$$G_{kk'}^{(1)}(t) = i\Theta(-t) \delta_{k',k+eFt} \exp \left[i \int_0^t \omega_k(t') dt' \right] , \qquad (61)$$

with

$$\omega_k(t') = E_{k+eFt'} + i/\tau_{k+eFt'} \, . \qquad (62)$$

Equivalent forms can be obtained for the phonon Green's functions. Thus, for example,

$$(\omega + \omega_q - i\eta) D_q^{(1)}(\omega) = N_{q\lambda} + D_q^{(1)}(\omega) \sum_k | U_q |^2 \frac{n_k - n_{k+q}}{\omega + E_{k+q} - E_k - i\eta} \, . \qquad (63)$$

Finally, it should be mentioned that the first term on the right-hand side of (58) does not lead to irreversibility since n_k^0

is just the classical displaced Maxwellian. This latter result arises from the quasiequilibrium nature of ρ_L.[12,15] The second and third terms actually lead to the dissipation effects in n_k, as they build the third- and higher-order moments of the function.

VI. EVOLUTION OF $G(k_1,k;t)$

In the preceding section we obtained the values of n_k, which give the initial values of the various correlation functions. We now turn to evaluation of the equations which provide the temporal evolution of these various functions. It is apparent that the evolution equations for the Green's function $G(k_1,k;t)$, defined in (17), and for the generic functions, defined in (14) and (32), involve a knowledge of the evolution of the operator product $c_k^\dagger(t)c_k(t)$. With the definition (57), we may immediately determine that

$$i\frac{\partial c_k^\dagger(t)c_k(t)}{\partial t}=-ieF\frac{\partial}{\partial k}[c_k^\dagger(t)c_k(t)]+\sum_{q,\lambda}U_{q\lambda}^*b_{q\lambda}^\dagger(t)[c_k^\dagger(t)c_{k+q}(t)-c_{k-q}^\dagger(t)c_k(t)]$$
$$+\sum_{q,\lambda}U_{q\lambda}b_{q\lambda}(t)[c_k^\dagger(t)c_{k-q}(t)-c_{k+q}^\dagger(t)c_k(t)]\ . \tag{64}$$

It is clear from this that the evolution of the operator product $c_k^\dagger(t)c_k(t)$ involves the knowledge of the evolution of higher-order products such as $b_{q\lambda}^\dagger(t)c_k^\dagger(t)c_{k+q}(t)$. When these terms appear in correlation functions such as (14) or (33), their evolution gives rise to higher-order terms which may be reflected back into the diagonal terms by standard decoupling procedures.[8] The only direct influence of these off-diagonal operator products lies in their initial values, which in the high-temperature or random-phase limits may be taken as zero. Indeed, this result establishes the validity of expressions (19) and (35).

Let us now turn to the evolution of G itself. The diagonal terms may be obtained from (64) and

$$i\frac{\partial G(k_1,k;t)}{\partial t}=i\delta(t)\delta_{k_1,k}-ieF\frac{\partial G(k_1,k;t)}{\partial k}+\sum_{q,\lambda}U_{q\lambda}^*[H_\lambda^{(1)}(k_1,k,k+q;t)-H_\lambda^{(1)}(k_1,k-q,k;t)]$$
$$+\sum_{q,\lambda}U_{q\lambda}[H_\lambda^{(2)}(k_1,k,k-q;t)-H_\lambda^{(2)}(k_1,k+q,k;t)]\ , \tag{65}$$

where $H_\lambda^{(1)}$ and $H_\lambda^{(2)}$ are defined through

$$H_\lambda^{(i)}(k_1,k,k\pm q;t)=\Theta(t)\left\langle 0\left|\mathrm{Tr}_L\left[\frac{e^{-\beta_L H_L}}{Z_L}c_{k_1}b_{q\lambda}^*(t)c_k^\dagger(t)c_{k\pm q}(t)c_{k_1}^\dagger\right]\right|0\right\rangle\ , \tag{66}$$

where the upper sign is taken for $i=1$ (and $b_{q\lambda}^*=b_{q\lambda}^\dagger$) and the lower sign is taken for $i=2$ (and $b_{q\lambda}^*=b_{q\lambda}$). In writing the evolution equations for these latter terms, we shall ignore the electronic coupling via the phonon field as this just leads to higher-order terms. Thus by decoupling the electron and phonon fields,

$$i\frac{\partial H_\lambda^{(i)}(k_1,k,k\pm q;t)}{\partial t}=(E_{k\pm q}-E_k\mp\omega_q)H_\lambda^{(i)}(k_1,k,k\pm q;t)-ieF\frac{\partial H_\lambda^{(i)}(k_1,k,k\pm q;t)}{\partial k}$$
$$+(U_{q\lambda}^*)^\dagger N_{q\lambda}[G(k_1,k;t)-G(k_1,k\pm q;t)]\ . \tag{67}$$

The set of equations composed of (65) and (67) is now a closed set from which the evolution of the off-diagonal as well as diagonal terms can be achieved. It is easy to further obtain a Boltzmann-type equation for this evolution if we ignore the field terms and the terms involving the left-hand side of (67). The first of these is equivalent to ignoring the intracollisional field effect, which has been shown to be important in high-field transport.[32] Ignoring the latter set of terms is equivalent to ignoring memory effects in the temporal evolution of the Green's functions. In dealing with (58) in the preceding section, we made approximations equivalent to these, but these are thought to be justifiable in that n_k invokes the Green's functions only in the integrands. For such cases, preliminary indications appear to suggest that these two effects tend to partially offset each other.

Our present purpose is to look at the evolution of the Green's function itself, so that we will retain all of the above effects. We wish to concentrate primarily on the relaxation of $G(k_1,k;t)$ and shall make the explicit statement that $G\rightarrow 0$ when $t\rightarrow\infty$. As discussed previously, this introduces an error only in the long-time limit, but this error is small in the low-density limit considered here. Since we are seeking the evolution of G, we shall retain only the diagonal terms in the collision operators of (67). In order to solve (67), we introduce the Green's function associated with the complete set of streaming terms as

$$-i\Theta(t-t_0)\delta(L)\exp\left[-i\int_{t_0}^{t}dt'[\Omega_{k_0}(F,t'-t_0)-i\eta]\right]\ , \tag{68}$$

where

$$L=k-k_0-eF(t-t_0)\ , \tag{69}$$

$$\Omega_{k_0}(F,t'-t_0)=E_{k'\pm q}-E_{k'}\mp\omega_q \; , \qquad (70)$$

and

$$k'=k_0+eF(t'-t_0) \; . \qquad (71)$$

We note that $\Omega_k(F,t)=0$ is the normal long-time requirement of energy conservation, modified here by the field terms. Using (68), we can now solve (67) to yield

$$H_\lambda^{(i)}(k_1,k,k\pm q;t)=-i(U_{q\lambda}^*)^\dagger N_{q\lambda}\int_0^t dt' G(k_1,k-eF(t-t');t')\exp\left[-i\int_{t'}^t dt''[\Omega_k(F,t''-t)-i\eta]\right] . \qquad (72)$$

Expression (72) clearly includes both the memory effects and the intracollisional field effect. The two terms of (72) can now be used in (65) to yield a relaxation equation for G, which may be expressed as

$$\frac{\partial G(k_1,k_1+eFt;t)}{\partial t}=\delta(t)-R*G \; , \qquad (73)$$

where the convolution $R*G$ includes the four standard collision terms of the form

$$\sum_{q,\lambda} |U_{q\lambda}|^2 N_{q\lambda}\int_0^t dt' G(k_1,k_1+eFt';t')\exp\left[-i\int_{t'}^t dt''[\Omega_{k_1}(F,t'')-i\eta]\right] . \qquad (74)$$

It is worth repeating at this point that while (73) is a relaxation equation in which both memory and field streaming are taken into account, this is not the same equation previously given by Barker and Ferry.[33] The latter equation expressed the evolution of $n_k(t)$ which does not vanish in the long-time limit. Rather, (73) is an approximation in which the fluctuations in the diagonal terms have been ignored as having a zero initial condition. Thus the use of (73) is better suited to describing the major part of the initial relaxation rather than the long-time limit. If we had not invoked these approximations, (73) would be exactly of the type in Barker and Ferry. We add that we could have also derived a master equation for G following the procedure of Pottier,[34] in which the electric field is written in a vector potential gauge and the projection-operator technique of Zwanzig.[16,35] Applying these results to $\langle \delta F_{k_1}\delta F_{k_2}(t)\rangle$ obviously comes from an extension of the Onsager hypothesis[29] to the low-density far-from-equilibrium situation.

VII. CONCLUSIONS

In this paper we have discussed several aspects of high-field transport in semiconductors which are related to the correlation functions appropriate to the far-from-equilibrium steady state. This discussion has detailed several of the problems which arise when calculating the differential mobility and the diffusion coefficient. In this, generic correlation functions have been introduced in order to calculate the above two quantities. We have given a unified treatment of these generic functions by focusing on the evolution of a single Green's-function set. Initial values are obtained from the nonequilibrium statistical density matrix and by performing the calculations up to second order in the electron-phonon interaction. All of the calculations have been carried out in the high-temperature low-density limit.

ACKNOWLEDGMENTS

The authors wish to express their appreciation to P. Lugli, W. Porod, and R. O. Grondin for helpful discussions. This work was supported in part by the U.S. Office of Naval Research.

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