Quantum theory of transient transport in a high electric field

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A quantum theory of transient transport is developed, based on two previously derived generalized Langevin equations, one for the center-of-mass momentum and the other for the center-of-mass kinetic energy, for an interacting system of electrons, impurities, and phonons. The high-field transient transport equations obtained are found to be self-contained differential-integral equations. We show that the nonlinearity due to the high field, in the case of transient transport, not only alters the transport time but also renormalizes the electron mass. The main conclusion is that the usual low-field transient transport equation is not valid in the high-electric-field situation.

The theoretical study of transient transport has been stimulated greatly in recent years by the remarkable advance in research on submicrometer devices.[1,2] Previously, we have obtained the momentum and energy high-field transport equations for the steady state, originating from the rigorously derived generalized Langevin equations (GLE's).[3,4] Here, we extend the preliminary discussion of transient transport given in Ref. 4. In our approach, the GLE's are obtained directly by solving the Heisenberg equation for the momentum and energy of the center-of-mass electrons. This affords a convenient way to obtain the high-field transient transport equations, which will be shown to have a self-contained differential-integral equation form. One of our main interests in the present paper is the comparison between the steady-state and the transient transport equations. Our main conclusion is that the nonlinearity due to the high field in the transient transport not only alters the transport time, but also renormalizes the electron mass, which is complementary to the result of a recent publication.[5]

The GLE of the center-of-mass momentum for a many-electron system with electron-impurity, electron-phonon, and electron-electron interactions in the presence of a uniform electric field $\mathbf{E}$, had been previously derived by us.[3] For brevity, the e-e interaction will be neglected. Then the momentum GLE is

$$M\ddot{R}_\alpha(t)+\int_{-\infty}^{t}\mu_{\alpha\beta}(\dot{\mathbf{R}};t,t')M\dot{R}_\beta(t')dt'=F_\alpha(t)+NeE_\alpha\ , \tag{1}$$

where the dot denotes differentiation with respect to t, N is the total number of electrons, M, $\mathbf{R}$, and $M\dot{\mathbf{R}}$ are the mass, coordinate, and momentum of the center of mass of the electrons, respectively, $F_\alpha(t)$ represents the fluctuation force in the α direction (the detailed forms can be found in Ref. 3) and, as usual, repeated indices denotes summation. The second term on the left-hand side (LHS) is the frictional force, which contains a memory matrix in a non-Markov form

$$\mu_{\alpha\beta}(\dot{\mathbf{R}};t,t')\equiv\sum_{\mathbf{k},\mathbf{q},s}\mu^s_{\mathbf{kq},\alpha\beta}(\dot{\mathbf{R}};t,t')\equiv\sum_{\mathbf{k},\mathbf{q},s}d^s_{\mathbf{kq};\alpha\beta}\exp\left[-i\omega^s_{\mathbf{kq}}(t-t')+i\mathbf{q}\cdot\int_{t'}^{t}\dot{\mathbf{R}}(t_1)dt_1\right]\ , \tag{2}$$

where we have used the fact that $\mathbf{R}(t)-\mathbf{R}(t')=\int_{t'}^{t}\dot{\mathbf{R}}(s)ds$; also s stands for different interacting mechanisms, i.e., $s=i,A,E$ for impurity, phonon absorption, phonon emission, respectively, and

$$d^i_{\mathbf{kq},\alpha\beta}=\frac{q_\alpha q_\beta\,|U^i_q|^2}{M\omega_{\mathbf{kq}}}\phi_{\mathbf{kq}},\quad \omega^i_{\mathbf{kq}}=\omega_{\mathbf{kq}}\ , \tag{3a}$$

$$d^A_{\mathbf{kq},\alpha\beta}=\frac{q_\alpha q_\beta\,|M_q|^2}{M\omega^A_{\mathbf{kq}}}\phi_{\mathbf{kq}}b_{\mathbf{q}}b^\dagger_{\mathbf{q}},\quad \omega^A_{\mathbf{kq}}=\omega_{\mathbf{kq}}+\Omega_{\mathbf{q}}\ , \tag{3b}$$

$$d^E_{\mathbf{kq},\alpha\beta}=\frac{q_\alpha q_\beta\,|M_q|^2}{M\omega^E_{\mathbf{kq}}}\phi_{\mathbf{kq}}b^\dagger_{-\mathbf{q}}b_{-\mathbf{q}},\quad \omega^E_{\mathbf{kq}}=\omega_{\mathbf{kq}}-\Omega_{\mathbf{q}}\ . \tag{3c}$$

Here $\omega_{\mathbf{kq}}=(\mathbf{k}\cdot\mathbf{q})/m$ and $\Omega_{\mathbf{q}}$ is the energy of the $\mathbf{q}$-mode phonon, $M_{\mathbf{q}}$ is the electron-phonon matrix element, $U_{\mathbf{q}}$ denotes the Fourier transform of the impurity potential, and $U^i_{\mathbf{q}}=U_{\mathbf{q}}\sum_a e^{i\mathbf{q}\cdot\mathbf{R}_a}$, with $\mathbf{R}_a$ the position of the ath impurity. In addition, $b^\dagger_k,b_k$ are phonon creation and annihilation operators, and

$$\phi_{\mathbf{kq}}=C^\dagger_{\mathbf{k}-\mathbf{q}/2}C_{\mathbf{k}-\mathbf{q}/2}-C^\dagger_{\mathbf{k}+\mathbf{q}/2}C_{\mathbf{k}+\mathbf{q}/2} \tag{3d}$$

are electron operators. We stress that the GLE (1) for the center-of-mass momentum is derived exactly and rigorously from the Heisenberg equations of motion, and it is still in its operator form. Once the ensemble average of (1) is taken, one can study a variety of transport properties, such as conductivity, through the use of the memory function. Also, we note the dependence of the memory function on the external field through the velocity of the center of mass, $\dot{\mathbf{R}}$. In the low-field case, which we studied in Ref. 3, this factor can be neglected and the memory function is independent of the field strength. In this paper we study the high-field transport, and use $\dot{\mathbf{R}}$ in the argument of μ to stress the field-dependent nonlinear effects.

To this point we have obtained the generalized Langevin equation (GLE) (1) for the center-of-mass momentum. From this equation we can derive the GLE of the center-of-mass energy operator $\varepsilon_{\dot{\mathbf{R}}}(t)=\frac{1}{2}M\dot{R}^{2}(t)$. Multiplying both sides of (1) by $\dot{R}(t)$, and noticing that

$$\frac{d}{dt}\varepsilon_{\dot{R}}(t)=\dot{\mathbf{R}}\cdot(M\ddot{\mathbf{R}}) ,$$

we obtain the GLE energy equation

$$\frac{d}{dt}\varepsilon_{\dot{R}}(t)+\int_{-\infty}^{t}\mu_{\varepsilon,\alpha}(\dot{\mathbf{R}};t,t')\varepsilon_{\dot{R}_\alpha}(t')dt'+Q(t) = W(t)+Ne\mathbf{E}\cdot\dot{\mathbf{R}}(t) , \quad (4)$$

where

$$W(t)=\dot{\mathbf{R}}(t)\cdot\mathbf{F}(t) \quad (5)$$

is the instantaneous power supplied by the fluctuation force $F(t)$. The second and third terms on the LHS of (4) act as a frictional power, where the α component of the energy memory function μ_ε (note that ε is a label signifying "energy") is

$$\mu_{\varepsilon,\alpha}(\dot{\mathbf{R}};t,t')=2\sum_{\mathbf{k},\mathbf{q},s}\left[\frac{1}{i\omega_{\mathbf{kq}}^{s}}d_{\mathbf{kq},\alpha\alpha}^{s}\delta(t-t') + \frac{\mathbf{q}\cdot\dot{\mathbf{R}}(t)}{\omega_{\mathbf{kq}}^{s}}\mu_{\mathbf{kq},\alpha\alpha}^{s}(\dot{\mathbf{R}};t,t')\right] , \quad (6)$$

$d_{\mathbf{kq}}^{s}$ and $\mu_{\mathbf{kq}}^{s}(\dot{\mathbf{R}};t,t')$ are the same as in (2), and $Q(t)$ represents the contribution to the frictional power due to the acceleration, which has the form

$$Q(t)=\sum_{\mathbf{k},\mathbf{q},s}\frac{i}{\omega_{\mathbf{kq}}^{s}}M\dot{R}_\alpha(t)\int_{-\infty}^{t}\mu_{\mathbf{kq},\alpha\beta}^{s}(\dot{\mathbf{R}};t,t')\ddot{R}_\beta(t')dt' . \quad (7)$$

We note that in Ref. 4, the $Q(t)$ in (4) has been neglected since we concentrated in that paper on the case of steady-state transport (for which $\ddot{R}=0$). The presence of $Q(t)$ in (4) is a clear indication of the differences between the transient and steady-state transport equations, which we will discuss later.

We have now two GLE operator equations (1) and (4), illustrating the microscopic evolution of the momentum and energy of the electronic center of mass, respectively. We stress that, as distinct from the low-field case, the memory functions depend on $\dot{\mathbf{R}}$. Also, this nonlinear dependence of $\dot{\mathbf{R}}$ makes the GLE's (1) and (4) different from their linear correspondences. In particular, the acceleration enters the frictional term in the nonlinear GLE's (1) and (4). In the energy GLE (4) this is represented explicitly by the term $Q(t)$, whereas it is implicitly contained in the memory term of the momentum GLE (1) which we will discuss more later. On averaging equations (1) and (4) over the ensemble, we will obtain the macroscopic momentum and energy transport equations. In general, at any time t we can denote the velocity $\dot{\mathbf{R}}(t)$ as the sum of the time-dependent drift velocity $\mathbf{V}(t)=\overline{\dot{\mathbf{R}}(t)}$ and its fluctuation $\delta\dot{\mathbf{R}}(t)=\dot{\mathbf{R}}(t)-\overline{\dot{\mathbf{R}}(t)}$, i.e.,

$$\dot{\mathbf{R}}(t)=\mathbf{V}(t)+\delta\dot{\mathbf{R}}(t), \quad \overline{\delta\dot{\mathbf{R}}(t)}=0 , \quad (8)$$

where we use a bar to denote the ensemble average over the center-of-mass coordinates. Then after averaging over the whole system, the GLE's (1) and (4) are replaced by

$$M\dot{V}(t)+\int_{-\infty}^{t}\overline{\langle\mu(\dot{\mathbf{R}};t,t')\rangle M\ddot{R}(t')}dt'=NeE , \quad (9)$$

$$\frac{d}{dt}(\varepsilon_{V(t)}+\overline{\varepsilon_{\delta\dot{R}}})+\int_{-\infty}^{t}\overline{\langle\mu_{\varepsilon,\alpha}(\dot{\mathbf{R}};t,t')\rangle\varepsilon_{\dot{R}_\alpha}(t')dt'} +\overline{Q(t)}=NeEV(t) , \quad (10)$$

where we have taken the external field $\mathbf{E}$ along x direction and the subscript x is suppressed. In particular, we note that we are dealing with the xx component of μ in (9) (since μ is a diagonal matrix). The symbol $\langle\ \rangle$ denotes the ensemble average over relative electrons, phonons, and impurities, $\varepsilon_{\delta\dot{R}_\alpha}=\frac{1}{2}M\delta\dot{R}_\alpha(t)^2$ and $\varepsilon_{\delta\dot{R}}=\sum_\alpha\varepsilon_{\delta\dot{R}_\alpha}$. We note that the operation $\langle\ \rangle$ has been discussed elsewhere,[3] so the remaining complication of the present Eqs. (9) and (10) lies in the average over the center-of-mass as the memory functions defined in (2) and (6) are all functions of $\dot{\mathbf{R}}$. It is convenient to write the time-dependent factor in the memory function (2) as

$$-i\omega_{\mathbf{kq}}^{s}(t-t')+i\mathbf{q}\cdot\int_{t'}^{t}\{[\mathbf{V}(t_1)+\delta\dot{\mathbf{R}}(t_1)-\mathbf{V}(t)]+\mathbf{V}(t)\}dt_1=i\omega_s(V)(t-t')+i\mathbf{q}\cdot\int_{t'}^{t}\left[-\int_{t_1}^{t}\dot{\mathbf{V}}(t_2)dt_2+\delta\dot{\mathbf{R}}(t_1)\right]dt_1 , \quad (11)$$

where

$$\omega_s(V)=\mathbf{q}\cdot\mathbf{V}(t)-\omega_{\mathbf{kq}}^{s}=q_xV(t)-\omega_{\mathbf{kq}}^{s}\equiv\omega_0(V)-\omega_{\mathbf{kq}}^{s} , \quad (12)$$

and $\omega_{\mathbf{kq}}^{s}$ is defined in (3). We emphasize that $\mathbf{V}(t)$ is along the x direction since $\mathbf{E}$ is taken to be along the x direction (but, of course, velocity fluctuations can be along any direction). Substituting (11) back into (2) makes apparent the explicit dependence on $\dot{\mathbf{V}}(t)$ of the memory functions appearing in (9) and (10). In other words Eqs. (9) and (10) are a set of complicated self-contained differential-integral equations. Therefore, one must seek approximations with respect to the $\dot{\mathbf{V}}(t)$ contained in (11). Here we make two approximations to evaluate the integral of $\dot{\mathbf{V}}(t)$ in (11), viz.,

$$\frac{d}{dt}\dot{V}(t)\approx 0 \quad \text{and} \quad \int_{t_1}^{t}\dot{\mathbf{V}}(t_2)dt_2\approx\int_{t-t_c}^{t}\dot{\mathbf{V}}(t_2)dt_2 . \tag{13}$$

The first condition in (13) is to assume that the rate of change of the acceleration of the center of mass is very small, which is consistent with the experimental results for the transient velocity.[6] The second approximation in (13) is to assume that the acceleration contribution to the memory function in (9) and (10) has an effective range of time t_c, which is introduced in the present calculation phenomenologically. By using (11) and (13), the memory function (2) can be written as

$$\begin{aligned}\mu_{\alpha\beta}(\dot{\mathbf{R}};t,t')&=\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\mu^{s}_{\mathbf{kq},\alpha\beta}(\dot{\mathbf{R}};t,t')\\ &=\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}d^{s}_{\mathbf{kq},\alpha\beta}\exp\left[i\omega^{c}_{s}(V)(t-t')+i\mathbf{q}\cdot\int_{t'}^{t}\delta\dot{\mathbf{R}}(t_1)dt_1\right] ,\end{aligned}\tag{14}$$

where

$$\omega^{c}_{s}(V)=\omega_{s}(V)-q_x\dot{V}(t)t_c=\omega_0(V)-q_x\dot{V}(t)t_c-\omega^{s}_{\mathbf{kq}} , \tag{15}$$

and the last equality follows from (12). In general one can also assume that the fluctuation is relatively small, i.e., $\delta\dot{R}(t)\ll V(t)$. It follows from (2) and (14) that, to lowest order,

$$\begin{aligned}\overline{\langle\mu_{\alpha\beta}(\dot{\mathbf{R}};t,t')\rangle}&=\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\langle d^{s}_{\mathbf{kq},\alpha\beta}e^{i\omega^{c}_{s}(V)(t-t')}\rangle\\ &\equiv\mu_{\alpha\beta}(V;t-t') ,\end{aligned}\tag{16}$$

i.e., the dependence on time takes a relatively simple form. To lowest nonvanishing order in $\delta\dot{\mathbf{R}}(t)$, the evaluation of (9) and (10) is now quite straightforward. After some algebra we obtain from (9) and (16) the momentum transport equation

$$M\dot{V}(t)+\frac{MV(t)}{\tau(V)}+\int_{-\infty}^{t}\langle\mu^{\delta}_{\alpha}(V(t);t-t')\rangle[M\overline{\delta\dot{R}^{\,2}_{\alpha}(t')}/V(t)]dt'+A_m(t)M\dot{V}(t)+A^{\delta}_{m,\alpha}(t)\frac{M}{V(t)}\frac{d}{dt}\overline{\delta\dot{R}^{\,2}_{\alpha}(t)}=NeE , \tag{17}$$

where the inverse of the instantaneous momentum transport time

$$\frac{1}{\tau(V)}=\int_{-\infty}^{t}\langle\mu_{xx}(V;t-t')\rangle dt'=\int_{0}^{\infty}\langle\mu_{xx}(V;t')\rangle dt' \tag{18}$$

and $\mu_{xx}(V;t')$ is defined in (16). The third term on the LHS of (17) is the contribution due to velocity fluctuations, with

$$\mu^{\delta}_{\alpha}(V;t-t')\equiv\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\frac{\omega_0(V)\omega^{s}_{\mathbf{kq}}}{[\omega^{c}_{s}(V)]^2}d^{s}_{\mathbf{kq},\alpha\alpha}e^{i[\omega_0(V)-\omega^{s}_{\mathbf{kq}}](t-t')} , \tag{19}$$

and it represents a new contribution to the balance equation, previously discussed by us.[4] For clarity, we emphasize that the superscript "δ" is a label, signifying contributions due to fluctuations, in contrast to the subscript "α" which denotes spatial directions. The last two terms on the LHS of (17) are contributions due to acceleration, with

$$A_m(t)=\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\left\langle\frac{d^{s}_{\mathbf{kq},xx}}{[\omega^{c}_{s}(V)]^2}\left[1+2\left[\frac{\overline{\mathbf{q}\cdot\delta\dot{\mathbf{R}}(t)}}{\omega^{c}_{s}(V)}\right]^2\right]\right\rangle , \tag{20}$$

$$A^{\delta}_{m,\alpha}(t)=\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\left\langle\frac{d^{s}_{\mathbf{kq},\alpha\alpha}\omega_0(V)}{2[\omega^{c}_{s}(V)]^3}\left[\frac{\omega_0(V)}{\omega^{c}_{s}(V)}-\frac{3}{2}\right]\right\rangle , \tag{21}$$

and $\omega_0(V)=q_xV(t)$. Similarly, from (10) and (16) we obtain the energy transport equation

$$\dot{\varepsilon}_v(t)+\frac{d}{dt}\overline{\varepsilon_{\delta\dot{R}}(t)}+\frac{\frac{1}{2}MV^2(t)}{\tau_\varepsilon(V)}+\int_{-\infty}^{t}\langle\mu^{\delta}_{\varepsilon,\alpha}(V;t-t')\rangle\overline{\varepsilon_{\delta\dot{R}_\alpha}(t')}dt'+A_\varepsilon(t)\dot{\varepsilon}_v(t)+A^{\delta}_{\varepsilon,\alpha}(t)\frac{d}{dt}\overline{\varepsilon_{\delta\dot{R}_\alpha}(t)}=NeEV(t) , \tag{22}$$

where the inverse of the instantaneous energy transport time

$$\frac{1}{\tau_\varepsilon(V)}=\int_{-\infty}^{t}\langle\mu_\varepsilon(V;t-t')\rangle dt'=\int_{0}^{\infty}\langle\mu_\varepsilon(V;t')\rangle dt' , \tag{23}$$

where $\mu_\varepsilon(V;t-t')$ is defined as in (6) except that the argument on the RHS is $(t-t')$, analogous to (16), and $\mathbf{q}\cdot\dot{\mathbf{R}}(t)$ is replaced by $q_xV(t)$. The fourth term on the LHS of (22) is due to the velocity fluctuations and

$$\mu^{\delta}_{\varepsilon,\alpha}(V;t-t')\equiv\sum_{\substack{\mathbf{k},\mathbf{q}\\ s}}\frac{2i(\omega^{s}_{\mathbf{kq}})^2}{[\omega^{c}_{s}(V)]^3}d^{s}_{\mathbf{kq},\alpha\alpha}\delta(t-t') . \tag{24}$$

Similar to the momentum transport equation (17), the last two terms on the LHS of the energy transport equation (22) are contributions due to acceleration, with

$$A_\varepsilon(t)=\sum_{\mathbf{k},\mathbf{q},s}\left\langle \frac{d^s_{\mathbf{kq},xx}}{[\omega^c_s(V)]^2}\left[1+2\left[\frac{\overline{\mathbf{q}\cdot\delta\dot{\mathbf{R}}(t)}}{\omega^c_s(V)}\right]^2 \times\left[1-\frac{\omega^c_s(V)}{\omega_0(V)}\right]\right]\right\rangle , \quad (25)$$

$$A^\delta_{\varepsilon,\alpha}(t)=\sum_{\mathbf{k},\mathbf{q},s}\left\langle \frac{d^s_{\mathbf{kq},\alpha\alpha}}{[\omega^c_s(V)]}\left[1-4\frac{\omega_0(V)}{\omega^c_s(V)}+\left[\frac{\omega_0(V)}{\omega^c_s(V)}\right]^2\right]\right\rangle . \quad (26)$$

In summary, Eqs. (17) and (22) are the momentum and energy transient transport equations. For steady-state conditions, one has $\dot{V}(t)=0$ and

$$\frac{d}{dt}\overline{\varepsilon_{\delta\dot{R}}(t)}=0 ,$$

then the terms in (17) and (22) due to acceleration vanish and one recovers the steady-state transport equations[4] [with $V(t)=V_d$ and $t_c=0$]. Also, we have previously shown that the total effect of the velocity fluctuations is to broaden the energy level and to reduce the overall mobility.[4] In the following discussion we will concentrate on the effects of the acceleration on the transport properties and neglect the velocity fluctuations to write (17) and (22) as

$$[1+A(V)]M\dot{V}(t)+\frac{MV(t)}{\tau(V)}=NeE , \quad (27)$$

$$[1+A(V)]\dot{\varepsilon}_v(t)+\frac{\varepsilon_v(t)}{\tau_\varepsilon(V)}=NeEV(t) , \quad (28)$$

where $A(V)$ represents the $A_m(t)$ and $A_\varepsilon(t)$, which are defined in (20), and (25), at $\delta\dot{R}=0$, in which case the time dependence is solely determined by $V(t)$. Explicitly,

$$A(V)=\sum_{\mathbf{k},\mathbf{q},s}\left\langle \frac{d^s_{\mathbf{kq},xx}}{[\omega^c_s(V)]^2}\right\rangle . \quad (29)$$

We note that the second term on the LHS of (28) can be shown to be[4]

$$\frac{\varepsilon_v(t)}{\tau_\varepsilon(V)}=\langle \dot{H}_e\rangle+\langle \dot{H}_{\text{ph}}\rangle , \quad (30)$$

where $\langle \dot{H}_e\rangle$, $\langle \dot{H}_{\text{ph}}\rangle$ represents the energy changing rate of the relative electrons and phonons, respectively. Equation (30) is equivalent to saying that the dissipation of the center-of-mass electrons is through the relative electrons and phonons. As $\langle H_e\rangle$ is a function of the electron temperature T_e, from (28) and (30) one can calculate the rate of change of $T_e(t)$ and then obtain the rate of change of the drift velocity $V(t)$ from (27). Thus, (27) and (28) are numerically solvable to obtain the time dependent $T_e(t)$ and $V(t)$. We leave the details of the numerical work for a future study and here just make a few more comments about the physics of our transient transport equations (27) and (28).

First, the momentum transport equation (27), can be rewritten into a form similar to the classical Langevin equation

$$\dot{V}(t)+\frac{V(t)}{\tau^*(V)}=\frac{eE}{m^*(V)} , \quad (31)$$

where

$$m^*(V)=m(1+A(V)), \quad \tau^*(V)=\tau(V)[1+A(V)] . \quad (32)$$

To the lowest order of $V(t)$ (linear GLE case), it may be verified that (32) becomes velocity independent, which will be denoted by $m^*=m^*(V\to 0)$, $\tau^*=\tau^*(V\to 0)$. Then (31) has the same form as the classical Langevin equation and it is straightforward to obtain from it the well-known Drude form of the dynamical conductivity

$$\sigma(\omega)=\frac{iNe^2}{m^*(\omega+i/\tau^*)} , \quad (33)$$

which is in agreement with the result of Ting and Nee,[7] except that they have neglected the low-field contribution of

$$A=\left.\frac{\partial\mu_2}{\partial\omega}\right|_{\omega=0}$$

in (33). On the other hand, in the high-field case, the $A(V)$ of (31) is time dependent through the instantaneous velocity, and so is the $m^*(V)$ and $\tau^*(V)$ of (33). In consequence, the transient equations (27) and (28), where $A(V)$ plays an important role, are quite different from the usual low-field transport equations. This latter conclusion is at variance with the recent work of Xing and Ting,[5] who found that the nonlinear transient transport equations still have the ordinary form of the transport equation, i.e., with the $A(V)$ in (27) and (28) missing and the t_c contained in $1/\tau(V)$ and $1/\tau_\varepsilon(V)$ neglected. We feel that the absence of $A(V)$ in Ref. 5 (where the nonlinear GLE has not been derived) is the result of using an unjustified "classical approximation" (absence of memory effects) in the high-field case [see, in particular, Ref. 5, Eq. (53)]. This extra term gives strong support to the use of nonlinear GLE's in the analysis of nonlinear transient transport problems.

Secondly, we remark that the $A(V)$ in (27) and (28) is related to the imaginary part of the memory function (16). Actually, if one performs the Fourier transform of (16) defined by

$$\mu(V;\omega)\equiv\mu_1(V;\omega)+i\mu_2(V;\omega)=\int_0^\infty \mu(V;t')e^{i\omega t'}dt' , \quad (34)$$

then it follows that

$$A(V)=-\sum_{\mathbf{q}}\frac{\partial}{\partial\omega}\mu_2(V;q,\omega)\bigg|_{\omega=0}\equiv-\frac{\mu_2(V;\omega)}{\omega}\bigg|_{\omega=0}, \tag{35}$$

where we used $\mu(V;\omega)=\sum_{\mathbf{q}}\mu(V;q,\omega)$, and where we have dropped the subscript xx since, from henceforth, we will be considering μ_{xx} only. In general, the $\mu_2(V;\omega)$ of (34) has a rather complicated form, and large-scale numerical work is needed to evaluate the $A(V)$ of (35). Nevertheless, in the highly degenerate case, when the influence of the electron temperature on the Fermi distribution function of relative electrons can be neglected ($\varepsilon_F \gg T_e$), then the evaluation of $\mu_2(V;\omega)$ simplifies dramatically in the case of impurity scattering. Also for definiteness, we take the impurity interaction as extremely short ranged (i.e., $U_q=U$) in the following discussion.

Substituting (3a) into (16) and taking the Fourier transform according to (34) we obtain

$$\mu_2(V;\omega)=\frac{n_i U^2}{M}\sum_{\mathbf{q}} q_x^2\frac{1}{\omega+\omega_0}[\chi_1(q,\omega+\omega_0)-\chi_1(q,0)], \tag{36}$$

where n_i is the impurity density, $\omega_0=q_x V(t)$, and $\chi_1(q,\omega)$ represents the real part of the density response function, the general form of which is

$$\chi_1(q,\omega)=-N_d(\varepsilon_F)L_d(q,\omega). \tag{37}$$

Here d denotes dimension, $N_2(\varepsilon_F)=m/2\pi$, $N_3(\varepsilon_F)=mk_F/\pi^2$, and $L_d(q,\omega)$ is the Lindhard function corresponding to dimension d. The explicit expressions for $L_2(q,\omega)$ and $L_3(q,\omega)$ are listed in (A1) and (A2), respectively. Combining (35)–(37), we get the $A(V)$ of noninteracting electrons in the case of short-range impurity scattering as

$$A_d(V)=\frac{1}{\varepsilon_F\tau_d}\frac{d}{2\pi^2(2k_F)^{d+2}}\int d^dq\, q_x^2\frac{\partial\phi_d}{\partial\omega}\bigg|_{\omega=0}, \tag{38}$$

where the relaxation time $\tau_d=[2\pi N_i U^2 N_d(\varepsilon_F)]^{-1}$, and

$$\frac{\partial\phi_d}{\partial\omega}\bigg|_{\omega=0}=(4\varepsilon_F)^2\left[\frac{L_d(q,0)-L_d(q,\omega_0)}{\omega_0^2}+\frac{1}{\omega_0}\frac{\partial L_d(q,\omega+\omega_0)}{\partial\omega}\bigg|_{\omega=0}\right]. \tag{39}$$

We will now investigate separately the three- and two-dimensional cases, in that order. When $d=3$, an analytical expression for (38) can be derived (see Appendix A), which is

$$A_3(V)=\frac{1}{\varepsilon_F\tau}\left[\frac{3}{10}x_u+\frac{3(x_u^2-1)^2}{8v^2}\ln\frac{1-v^2/(1+x_u)^2}{1-v^2/(1-x_u)^2}+\left[-\frac{1+x_u^2}{4}+\frac{3v^2}{40}\right]\ln\frac{(x_u+1)^2-v^2}{(x_u-1)^2-v^2}\right.$$
$$\left.+\frac{4x_u}{5v^2}\left[1+\frac{1-5x_u^2}{4vx_u}\ln\frac{(x_u+v)^2-1}{(x_u-v)^2-1}\right]+\frac{4x_u^3}{5v^2}\left[1+\frac{x^2-5}{4v}\ln\frac{x_u^2-(v+1)^2}{x_u^2-(v-1)^2}\right]\right], \tag{40}$$

where $v=V(t)/V_F$, $x=q/2k_F$, x_u is the upper cutoff for the wave number occurring in the integral of (38). Equation (40) is an exact result for the short-range impurity situation, from which one can deduce the low-field result

$$A_3(0)=\frac{1}{\varepsilon_F\tau}\left[x_u+\frac{x_u^2+1}{2}\ln\frac{x_u-1}{x_u+1}\right], \tag{41}$$

and to find the $v\to 0$ behavior of $A(V)$

$$\lim_{\substack{v\to 0\\ x_u\gg 1}}\left[\frac{A_3(V)-A_3(0)}{v^2}\right]\sim\frac{1}{\varepsilon_F\tau x_u}. \tag{42}$$

Equations (41) and (42) show in the case of short-range impurity scattering (i) $A(V)$ is inversely proportional to the relaxation time τ and the electron density (through ε_F), and (ii) as both (40) and (41) are of the order of $1/\varepsilon_F\tau x_u$ in the $v\to 0$ limit, it is clear that, since x_u is very large, the high-field correction to $A_3(0)$ of (41) will not be important.

When $d=2$ the situation is very different, as we will now show. In this case we can solve (38) by expanding (39) in powers of $v=V(t)/V_F$ (see Appendix A) to get

$$\frac{\partial\phi_2}{\partial\omega}\bigg|_{\omega=0}=\bar{\omega}_0^{-2}\sum_{n=1}^{\infty}\frac{2n-1}{2n!}B_{2n}\bar{\omega}_0^{(2n)}, \tag{43}$$

where $\bar{\omega}_0=vq_x/2k_F$ and

$$B_{2n}=\frac{\partial^{(2n)}L_2(q,\bar{\omega}_0)}{\partial\bar{\omega}_0^{(2n)}}\bigg|_{v=0}$$

is the Taylor expansion coefficient of the Lindhard function, and B_2, B_4 for $d=2$ can be found in (A9). Combining (38), (43), and (A9) we get the $v\to 0$ expression of $A(V)$ for a system of two-dimensional electrons in the case of short-range impurity scattering

$$A_2(V)=\frac{1}{\varepsilon_F\tau}\frac{1}{\pi}\left[-1+\frac{x_c}{(x_c^2-1)^{1/2}}\times\left[1+\frac{9v^2}{16(x_c^2-1)^2}\right]\right], \quad (44)$$

where to avoid the divergent problem,[8] we have introduced in the integral of (38) a lower cutoff $x_c=1+b/2$, with $b=2mD/\hbar$, and D is the diffusion constant of the center of mass (see Appendix A). The two-dimensional correspondence of (42) is

$$\lim_{\substack{v\to 0\\ b\ll 1}}\frac{A_2(V)-A_2(0)}{v^2}\sim\frac{1}{\varepsilon_F\tau b^2}. \quad (45)$$

The above formula shows that due to the low dimensionality, the high-field contribution to the $A(V)$ of (38) for the $d=2$ case is much more significant than that for the $d=3$ case seen in (42). Also, one can estimate that the high-field correction term in (44) should be included when $V(t)/V_F\gtrsim 0.1b(b\ll 1)$, i.e., significant corrections occur even for values of $V(t)$ much less than V_F, in contrast to what occurs in the three-dimensional case. We note that the above discussion serves for the qualitative understanding of the basic feature of $A(V)$. For a comprehensive study of the high-field transient equation, the electron-phonon interaction, the electron heating effects, and the fluctuation effects should be included, and one goes back to the momentum GLE (17) and energy GLE (22).

In summary, we have used the operator GLE's (1) and (4) of the momentum and the energy of the center of mass for a many-electron system, to obtain the macroscopic GLE's (9) and (10), which are suitable for the study of the quantum transient transport. To study the acceleration effect on the transient transport, we have used the lowest-order nonvanishing approximation (13) to obtain the high-field transient transport equations (17) and (22), which includes the acceleration and velocity fluctuation effects. The direct consequence of including acceleration in the analysis of nonlinear transport is the appearance of time-dependent renormalizations of the electron mass and of the transport time. When the velocity fluctuation is neglected, the renormalization factor $A(V)$ depends simply on the imaginary part of the Fourier transform of the static memory function, as seen in (35). The detailed study of the $A(V)$ for noninteracting electrons in the case of impurity scattering shows that $A(V)$ is inversely proportion to $\varepsilon_F\tau$, and the high-field contribution to $A(V)$ in the two-dimensional case is much more significant than that of the three-dimensional case. Our formalism shows that the use of the nonlinear GLE's to study the transient transport is rigorous, and we have found that the conventional transport equations cannot be used directly in this respect.

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APPENDIX A: THE DERIVATION OF (40) AND (44)

For the reader's convenience, we first list the $d=2$ and $d=3$ Lindhard functions.[9,10] They are

$$L_2(x,y)=1-\frac{1}{2x}[(\nu_-^2-1)^{1/2}\mathrm{sgn}(\nu_-)\Theta(\nu_-^2-1)-(\nu_+^2-1)^{1/2}\mathrm{sgn}(\nu_+)\Theta(\nu_+^2-1)], \quad (A1)$$

$$L_3(x,y)=1-\frac{\nu_-^2-1}{4x}\ln\frac{\nu_-+1}{\nu_--1}-\frac{\nu_+^2-1}{4x}\ln\frac{\nu_++1}{\nu_+-1}, \quad (A2)$$

where

$$x=\frac{q}{2k_F},\quad y=\frac{\omega}{4\varepsilon_F},\quad \nu_\pm=x\pm\frac{y}{x}, \quad (A3)$$

and Θ is the step fraction. Also, we have recently shown that the nonanalyticity of the above Lindhard functions can be eliminated by including the fluctuation effects due to the motion of the center of mass. In the $d=2$ case, the analytical expression we obtained is[8]

$$L_2(x,y;b)=1-\frac{1}{2\sqrt{2}x}\{\mathrm{sgn}(\nu_-)[(\gamma_-^2+4b^2x^2\nu_-^2)^{1/2}-\gamma_-]^{1/2}-\mathrm{sgn}(\nu_+)[(\gamma_+^2+4b^2x^2\nu_+^2)^{1/2}-\gamma_+]^{1/2}\}, \quad (A4)$$

where $\gamma_\pm=1+b^2x^2-\nu_\pm^2$, $b=2mD/\hbar$, D is the diffusion constant of the center of mass and, in general b is much less than 1. When $b=0$, (A3) is reduced to (A1).

When $d=3$, the angle integral contained in (38) can be carried through analytically. Using (39) and (A2), we obtain from (38)

$$A_3(V)=\frac{1}{\varepsilon_F\tau}\frac{3}{v^2}\int_0^\infty dx\,x^2I(v,x), \quad (A5)$$

where $v=V(t)/V_F$, and

$$I(v,x)=\frac{x^2-1}{2x}\ln\frac{(x-1)^2}{(x+1)^2}+\frac{4}{3}+\frac{x^2-3}{3v}\ln\frac{(v+1)^2-x^2}{(v-1)^2-x^2}-\frac{2}{3xv}\ln\frac{(x+v)^2-1}{(x-v)^2-1}+\frac{3(x^2-1)-v^2}{6x}\ln\frac{(x+1)^2-v^2}{(x-1)^2-v^2}. \quad (A6)$$

The integral of (A6) can also be done analytically, after introducing an upper cutoff x_u to replace the upper limit of ∞, and the end result is (40).

When $d=2$, if we use (39) and (A1) directly, the angle integral contained in (38) cannot be carried out analytically. Nevertheless, as we are interested in the case of $V(t) \ll V_F$, ($T_e \ll \varepsilon_F$), we can do the problem by expanding $L_2(x,\bar{\omega}_0)$ of (A1) with $\bar{\omega}_0=\omega_0/4\varepsilon_F=vq_x/2k_F$, in terms of v. For this purpose we write (A1) as

$$L_2(x,\bar{\omega}_0)=\sum_{n=0}^{\infty}\frac{B_{2n}}{2n!}\bar{\omega}_0^{2n}\ , \qquad \text{(A7)}$$

where

$$B_{2n}=\left.\frac{\partial^{(2n)}L_2}{\partial\bar{\omega}_0^{(2n)}}\right|_{v=0}$$

and the first three coefficients of B_{2n} can easily be worked out by use of (A1) to give

$$B_0=1,\quad B_2=\frac{\Theta(x^2-1)}{x^3(x^2-1)^{2/3}}\ ,$$
$$B_4=\frac{6(4x^2+1)}{x^5(x^2-1)^{7/2}}\Theta(x^2-1)\ . \qquad \text{(A8)}$$

Strictly speaking, the expansion formulas (A7) and (A8) do not hold at $x=1$, where B_{2n} is divergent as can be seen from (A8). Nevertheless, as we stated earlier this nonanalyticity does not exist in the more rigorous version of the $d=2$ Lindhard function (A4). On the other hand, the expansion formula for $L_2(x,\bar{\omega}_0;b)$ of (A4) is much more complicated and will not eventually help us for the analytical analysis of (38) and (39). Therefore, we introduce a lower cutoff $x_c=1+\alpha b/2$ [α is a number between 1 and 2, determined by demanding consistency with the result (A4)], to replace the one in the step function of (A8), to rewrite (A8) as

$$B_0=1,\quad B_2=\frac{\Theta(x^2-x_c)}{x^3(x^2-1)^{3/2}}\ ,$$
$$B_4=\frac{6(4x^2+1)}{x^5(x^2-1)^{7/2}}\Theta(x^2-x_c)\ . \qquad \text{(A9)}$$

Now the expansion formulas (A7) and (A9) are analytic, and have the same asymptotic behavior at $x=x_c$ ($x_c\approx 1+b/2$) as that of (A4) in the $b\to 0$ limit. Using (A7) and (A9), we obtain the expansion formula (43) for (39). Combining (38), (43), and (A9), after some algebra we obtain (44).

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