Energy broadening associated with finite collision duration in hot carrier transport in semiconductors

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1. Introduction

Recent fascinating progress in fabrication techniques has made it possible to construct very small device structures. Investigations of hot carrier transport in such small devices are usually based on the semi-classical Boltzmann transport equation (BTE). As the electron energy increases, however, the mean free time between two successive scatterings with phonons becomes comparable to the collision duration time, defined here as the characteristic time required to build up the energy conserving delta-function in the collision term ($\approx$ hundreds fs), so that the energy broadening associated with such small time scale is no longer negligible [collisional broadening (CB)]. In addition, since the wavevector (momentum) of an electron is not a good eigenstate of the total Hamiltonian, the electron state continuously changes during collision duration [intra-collisional field effects (ICFE)].[1] Therefore, these quantum effects could be important in deep submicron devices in which the mean free time of hot electrons could be less than 100 fs and a quantum kinetic transport equation (QTE) should be used to analyze hot carrier problems.

In the present work, a QTE which takes the aforementioned quantum effects into account is derived from the quantum Liouville equation. A new simple strategy for incorporating the energy broadening associated with finite collision duration (CB) is suggested to generalize the conventional Monte Carlo simulations.

2. Quantum kinetic equation under strong electric field

The microscopic behavior of the entire system of electrons and phonons under an electric field is *completely* described by the quantum Liouville equation. Here, we give just an outline showing how to derive the QTE. The details will be reported somewhere.

By employing the projection technique,[2] by which the variables of the reservoir (phonon bath) can be eliminated, we obtain the *exact* QTE for the electron subsystem. The collision term of this QTE contains the complete history of electron dynamics. To simplify the collision term, we make the Born approximation. The Born approximation physically corresponds to the lowest order correction and ignores the higher order contributions such as the multiple scatterings. We then obtain the following QTE:

$$\frac{\partial f_{\mathbf{k}}(t)}{\partial t} + e\mathbf{F}\cdot\frac{\partial f_{\mathbf{k}}(t)}{\partial \mathbf{k}} = -2\sum_{\mathbf{q},\eta=\pm}|M_{\mathbf{q}}|^2\left(N_{\mathbf{q}}+\frac{1}{2}+\eta\frac{1}{2}\right)$$
$$\int_0^t d\tau\left\{\cos\left[\Delta_\eta\tau-\alpha\tau^2\right]f_{\mathbf{k}-e\mathbf{F}\tau}(t-\tau)-\cos\left[\Delta_\eta\tau+\alpha\tau^2\right]f_{\mathbf{k}-\mathbf{q}-e\mathbf{F}\tau}(t-\tau)\right\}, \quad (1)$$

where $f_{\mathbf{k}}(t)$ is the electron distribution function with momentum $\mathbf{k}$ at time t, $M_{\mathbf{q}}$ the

coupling constant with phonons, $\mathbf{F}$ the uniform electric field, $N_{\mathbf{q}}$ the phonon occupation number, $\Delta_\eta = \epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}} - \eta\omega_{\mathbf{q}}$ ($\epsilon_{\mathbf{k}}$: the electron energy; $\omega_{\mathbf{q}}$: the phonon energy) and $\alpha = \frac{e\mathbf{q}\cdot\mathbf{F}}{2m}$ ($\mathbf{q}$: the phonon wave-vector; m: the electron effective mass). $\hbar$ is taken to be unity throughout this work. To be consistent with the Born approximation, the upper bound of the time integration in Eq.(1) is replaced by the free-flight time τ_{sc}. Since the electron distribution would not change significantly during the time interval τ_{sc}, we may approximate $f_{\mathbf{k}-e\mathbf{F}\tau}(t-\tau)$ to $f_{\mathbf{k}}(t)$. These are the essential steps taken in this work and are what differentiates it from previous treatments given in [3]. It is not consistent with the Born approximation to integrate over the whole time range without taking the time dependence of the electron distribution into account.

In the following discussions, we restrict ourselves to the CB and ignore the electric field (ICFE) in the right-hand side (rhs) of Eq.(1). This may be justified when the electric field is not extremely large, i.e., F is greater than a few tens kV/cm.[4] Equation (1) then reads

$$\frac{\partial f_{\mathbf{k}}(t)}{\partial t} + e\mathbf{F}\cdot\frac{\partial f_{\mathbf{k}}(t)}{\partial \mathbf{k}} = -2\sum_{\mathbf{q},\eta} |M_{\mathbf{q}}|^2 \left(N_{\mathbf{q}} + \frac{1}{2} + \eta\frac{1}{2}\right) \frac{\sin(\Delta_\eta \tau_{sc})}{\Delta_\eta} \left[f_{\mathbf{k}}(t) - f_{\mathbf{k}-\mathbf{q}}(t)\right], \quad (2)$$

where the first and second terms of the rhs are the *out-scattering* and *in-scattering* terms, respectively. Notice that Eq.(2) is very similar in form to the conventional BTE, the only difference being that the retardation associated with collision duration is explicitly included in Eq.(2) *as a function of free-flight time τ_{sc} between two successive scatterings.* If the retardation is ignored, which corresponds to taking the limit of $\tau_{sc} \to \infty$, the usual energy-conserving delta-function recovers. Therefore, the retardation due to collision duration broadens the electron energy which is otherwise strictly conserved.

According to our previous study, the energy broadening has negligible effects on the out-scattering term whereas the in-scattering term is greatly affected.[5] This allows us to ignore the broadening in the out-scattering terms and to sum all those terms. Consequently, a standard numerical technique such as the Monte Carlo method can be employed to numerically evaluate Eq.(2). The only modification required is that the final energy of electron after scattering has to be determined with a proper probability function whose width is roughly given by $1/\tau_{sc}$. The way that the electron lifetime is introduced *during* simulations is different from the previous treatments in which the electron lifetime is estimated from the self-energy *before* the simulations by assuming that the whole system is in thermal equilibrium.

3. Numerical calculation results

For numerical evaluations, we employ the material parameters of GaAs ($m = 0.067m_0$ and $\omega_{\mathbf{q}} = 36$ meV) and assume deformation-type scatterings for simplicity. The coupling constant ($D = 3\times10^9$ eV/cm) is chosen so that the magnitude of the total scattering rate at the energy ranges considered here is similar to that of the Fröhlich scattering ($\approx 10^{13}$ 1/s).

We first show the onset of energy broadening by considering a system where electrons are excited with 150 meV at $t = 0$ and relax to their steady state under a uniform electric field. Figure 1 shows the time evolutions of the electron energy distribution after photo-excitation under F = (a) 0 and (b) 1 kV/cm. When no electric field is

applied, the shape of the energy distribution differs greatly for the two cases of with and without energy broadening. Therefore, even for a moderate scattering rate ($\approx 10^{13}$ 1/s), transport is already in the CB regime and standard approximations leading to the Fermi golden rule break down. Nevertheless, application of moderately strong electric fields greatly suppresses the phonon emission and absorption peaks and leads to results which are almost identical to the semiclassical results obtained from the Fermi golden rule.

Figure 2 shows the energy distributions under steady state regimes for $F =$ (a) 10 and (b) 50 kV/cm. When the strength of the electric field is large, the energy distribution obtained with energy broadening deviates from the one with no broadening; the high energy tail is more enhanced. This can be understood from the fact that the density of state is proportional to $\epsilon_{\mathbf{k}}^{1/2}$ and thus a high energy state is more often selected as a final state during simulations. This result is consistent with those obtained previously from other treatments of CB.[3] Figure 3 shows the average energy and drift velocity plotted as a function of the electric field. Because of the enhancement of the high energy tail, the average energy becomes larger as the electric field increases; the deviation between the two cases, with and without energy broadening, becomes significant when electric field is very strong ($\geq$ a few tens kV/cm). On the other hand, the drift velocity shows no significant difference within the range of numerical fluctuations in both cases. This is because the coupling constant for the deformation-type scattering has no wave-vector (direction) dependence and, therefore, the final state after scattering is directed at random.

4. Conclusions

A quantum kinetic equation which incorporates the ICFE and CB has been derived from the quantum Liouville equation by the projection technique. A new simple strategy for incorporating the energy broadening associated with finite collision duration has been introduced to generalize conventional Monte Carlo simulations. It has been shown that even for a moderate scattering rate ($\approx 10^{13}$ 1/s), transport is already in the CB regime and standard approximations leading to the Fermi golden rule break down. It is expected, therefore, that the use of the QTE is crucial in analyses of the device transport characteristics in deep submicron regimes, where the scattering rate of electrons in the high energy tail easily exceeds 10^{13} 1/s.

References

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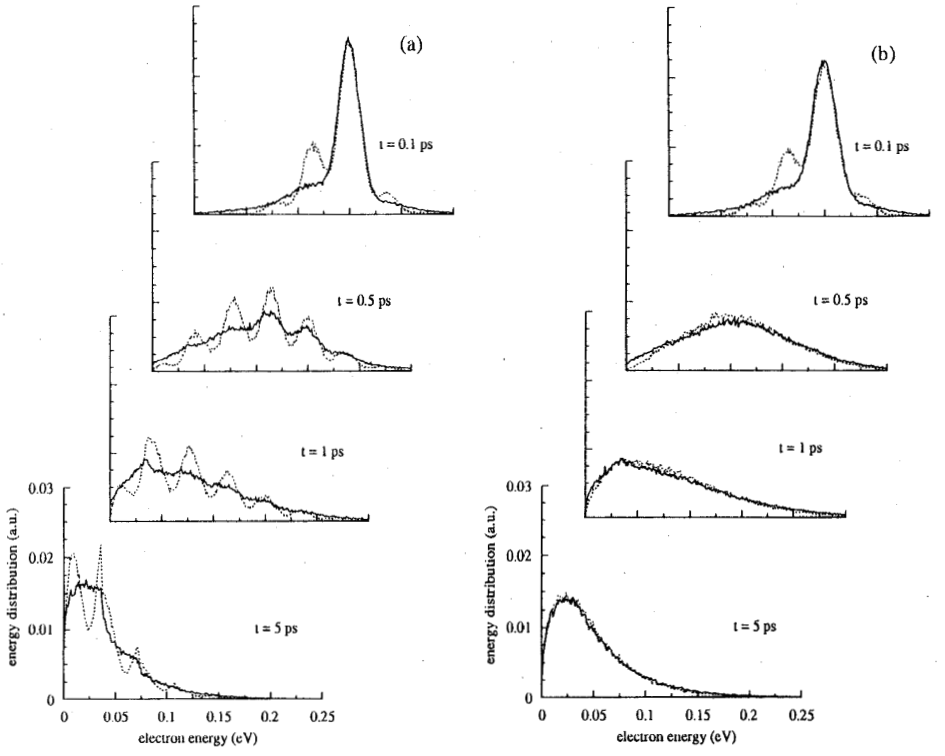

Fig.1. Time evolutions of the electron energy distribution; t = 0.1, 0.5, 1, and 5 ps . The excitation energy is 150 meV and the electric fields of F = (a) 0 and (b) 1 kV/cm are applied. The solid (dotted) curves represent results with (without) energy broadening.

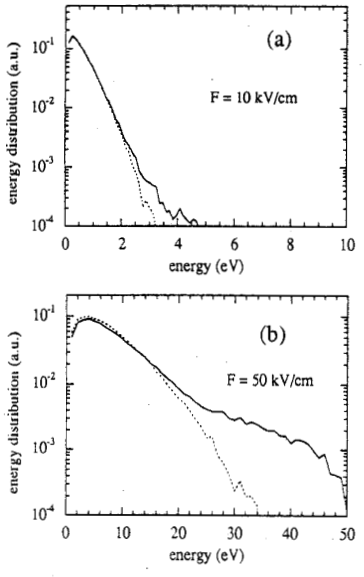

Fig.2. Electron energy distributions in a steady state at T = 300 K for F = (a) 10 and (b) 50 kV/cm. The solid (dotted) curves represent results with (without) energy broadening. Note that the energy scale is different for (a) and (b).

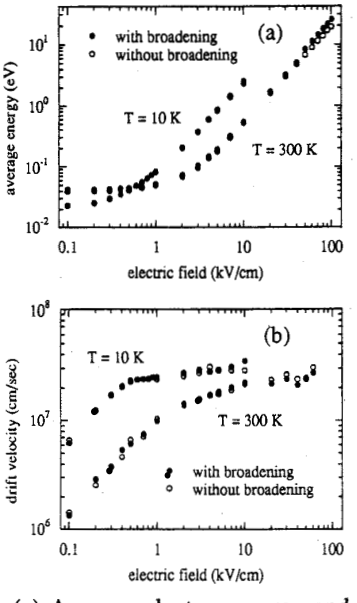

Fig.3. (a) Average electron energy and (b) drift velocity as a function of electric field for T = 10 and 300 K. The solid (open) circles represent results with (without) energy broadening.