Quantum Correction to the Semiclassical Electron-Phonon Scattering Operator

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Abstract. A quantum kinetic equation approach is adopted in order to incorporate quantum effects such as collisional broadening due to finite lifetime of single particle states, and collisional retardation due to finite collision time. A quantum correction to the semiclassical electron distribution function is obtained using an asymptotic expansion for the quantum electron-phonon collision operator in its weak formulation. Based on this expansion, the evolution of a highly peaked, nonequilibrium distribution function in Si and Ge is analyzed. It is shown that in Ge and Si, where the electron-phonon interaction is weak, the quantum correction due to the finite collision time leads to an extra broadening of new replicas of the initial distribution function. As the observation time exceeds the collision duration, the quantum correction starts to diminish and the semiclassical solution for a particular replica is recovered.

1 Introduction

The semiclassical Boltzmann transport equation is successfully used for transport description and modeling in conventional semiconductor devices since the early development of semiconductor technology. A particular advantage of the Boltzmann equation is that it can be solved by a Markov-chain Monte Carlo algorithm which opens an immediate opportunity for direct transport process simulation. In the standard Monte-Carlo algorithm the carriers are moving on classical trajectories between the two consecutive collisions. Classical trajectories are characterized by the well defined values of coordinates $\mathbf{r}$ and momenta $\mathbf{p}$ which are related through the classical equations of motion. The scattering events are considered to be isolated from each other and instantaneous in both time and space. Locality of scattering events in time and space is one of the main assumptions underlying the semiclassical transport description based on the Boltzmann equation and should be re-evaluated in case of emerging quantum effects. Indeed, due to the quantum uncertainty principle a carrier may not have the well defined coordinate and momentum simultaneously. Therefore, the particle motion on the trajectory between collisions may not be described classically if the device dimension is comparable to the carrier de-Broglie wavelength. Similar, the scattering events may not be considered as local events in phase

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space. Locality of scattering in time may also be questioned. Due to the energy-time uncertainty, the energy conservation during scattering is justified only when the collision duration is large. This limit is usually referred to as the limit of a completed collision leading to the famous Fermi golden rule. When the duration of scattering is finite and the scattering may not be considered completed at an observation time moment t, the particle state at this moment t depends on the history of states the particle has assumed at all times $t' < t$, leading to the memory effect. This effect is in clear contradiction to the Markovian nature of the semiclassical Boltzmann equation and may not be described by the classical transport picture.

Going beyond the semiclassical approach in transport description becomes increasingly relevant. Indeed, with the 90 nm technology node being commercially implemented, the physical transistor gate length is already in the range of 45 nm. According to the International Technology Roadmap for Semiconductors, for the 32 nm technology node the physical gate length will be in the range of 10 nm, where quantum effects are expected to play a dominant role in determining the transport through the device.

Several advanced computational techniques for including the quantum effects were proposed recently. The method based on the Nonequilibrium Green's function formalism treats the quantum effects in the most complete and consistent way. However, due to its completeness, this method is rather complex and computationally costly [1]. Another approach is based on the solution of the Schrödinger equation using the modal analysis for an arbitrary 2D geometry (QDAME) [4]. Scattering can be included in this method by a Pauli master equation, and testing was successful for the resonant tunneling diode. Nevertheless, the QDAME applications to double-gate MOSFETs were so far limited to ballistic coherent regime [4].

An alternative method to address the quantum effects is the Wigner function approach [11]. Similar to the classical distribution function, the Wigner function depends on position and momentum simultaneously. Another attractive feature of the Wigner function approach is that it allows to include all scattering processes in the device via the Boltzmann scattering integral. It brings a unique opportunity to treat classical collisions on equal footing with the quantum scattering described by the quantum collision operator [3]. The question however rises as to whether the use of the classical Boltzmann scattering operator in the Wigner equation is justified. It is well known that the semiclassical transport theory based on the Boltzmann equation neglects several quantum mechanical effects such as collisional broadening due to the finite lifetime of single particle states, collisional retardation due to the finite collision duration, and intra-collisional field effects [10]. To answer this question, we shall begin from a complete quantum description of carrier scattering. The Levinson equation [5] which describes an interaction of a single electron with an equilibrium phonon bath represents a convenient starting point.

In this paper we analyze a quantum correction to the semiclassical scattering operator which is based on a recently obtained asymptotic expansion of

Levinson's scattering operator [9]. This method allows calculating a correction to the distribution function simultaneously with solving of the Boltzmann equation, which is the advantage as compared to the previously used techniques. An application of the algorithm to describe the transient processes in Si and Ge is investigated in details for the case of electron-phonon interaction. Taking a highly nonequilibrium initial distribution function which is sharply peaked around a certain energy as example, it is shown that for Si and especially for Ge the method adequately describes the quantum correction to the distribution function due to the finite collision time.

2 Basic Equations

A suitable quantum kinetic equation for the Wigner function describing the interaction of a single electron with an equilibrium phonon bath has been proposed by Levinson [5]. In case of vanishing electric field and spatially uniform semiconductor the Levinson equation has the following form:

$$\frac{\partial f}{\partial t} = \int_0^t dt' \int d\mathbf{p}' [S(p,p',t-t')f(p',t') - S(p',p,t-t')f(p,t')]. \qquad (1)$$

Here, $\mathbf{p}$ denotes the momentum and $p = |\mathbf{p}|$ is its absolute value. The kernel $S(p,p',t)$ corresponding to an electron-optical phonon scattering is taken in the form

$$S(p,p',t) = \frac{2VF^2n}{(2\pi\hbar)^3} \left\{ \cos\left[\frac{t}{\hbar}(E(p) - E(p') - \hbar\omega)\right] + \frac{n+1}{n} \cos\left[\frac{t}{\hbar}(E(p) - E(p') + \hbar\omega)\right] \right\}, \qquad (2)$$

where $\hbar F$ denotes the electron-phonon interaction matrix element, $\hbar\omega$ the phonon energy, V the normalization volume, $n = (\exp(\beta\hbar\omega) - 1)^{-1}$ is the phonon occupation number corresponding to the temperature $k_BT = 1/\beta$, and $E(p)$ is the single particle energy. Due to an explicit time dependence of the kernel (2), the Levinson equation can fully describe the effects caused by the finiteness of the collision time. Numerical integration of the equation by Monte Carlo methods is, however, quite involved and can be performed for short evolution times only, due to fast growth of variances with time [2]. Our goal is to develop an approximate scheme which is computationally sound and less expensive. The path we would like to explore is based on the assumption of weak electron-phonon interaction. This assumption allows one to obtain an asymptotic expansion of the scattering operator (2) in powers of the dimensionless interaction constant. The principal term of this expansion reproduces the semiclassical Boltzmann scattering integral. The second term in the series describes the correction to the Boltzmann scattering integral due to the finite collision time. To derive it, we rewrite (1) in scaled variables, introduced in [9]. Measuring electron energies E in units of optical phonon energy $\epsilon = E/(\hbar\omega)$ and introducing the new variable $\widetilde{t} = t/t_0$, where $t_0 = (\lambda\omega)^{-1}$, the resulting equation takes the form [9]:

$$\frac{\partial f}{\partial \widetilde{t}} = \int_0^{\widetilde{t}/\lambda} d\tau \int d\varepsilon \rho(\epsilon')[s(\varepsilon,\varepsilon',\tau) f(\varepsilon', \widetilde{t} - \lambda\tau) - s(\varepsilon,\varepsilon',\tau) f(\epsilon, \widetilde{t} - \lambda\tau)], \quad (3)$$

$$s(\epsilon,\epsilon',\tau) = \sum_{\nu=\pm 1} a_\nu \cos(\tau(\epsilon - \epsilon' + \nu)), \quad a_{-1} = \frac{n}{n+1}, \quad a_1 = 1,$$

where $\rho(\epsilon) = 4\pi\sqrt{2\epsilon}$ is the density of states, corresponding to the parabolic dispersion $E = p^2/(2m)$. The dimensionless electron-phonon interaction constant λ is given by

$$\lambda = \frac{2VF^2 n}{(2\pi)^3}\sqrt{\frac{m^3}{\hbar^3\omega}}. \quad (4)$$

In the limit of small λ corresponding to weak interaction the time scale t_0 becomes much larger than the period of lattice vibrations. Considering an asymptotic behavior of the collision operator in the left-hand side of (3) for small λ when $\widetilde{t}/\lambda \gg 1$, the Levinson equation becomes [9]:

$$\partial_{\widetilde{t}} f = \Theta_0[f] + \lambda\Theta_1[\partial_{\widetilde{t}} f] + o(\lambda), \quad (5)$$

where $\Theta_0[f]$ represents the Boltzmann scattering integral,

$$\Theta_0[f](p,t) = \sum_{\nu=\pm 1} \pi a_\nu \int d\varepsilon' \rho(\varepsilon')[\delta(\varepsilon - \varepsilon' + \nu) f(\varepsilon', t) - \delta(\varepsilon' - \varepsilon + \nu) f(\varepsilon, t)] \quad (6)$$

For the sake of brevity we omit the tilde and use the notation t for the scaled variable $\widetilde{t}$ here and below, unless it is specified otherwise.

The correction scattering operator $\Theta_1[\partial_{\widetilde{t}} f]$ formulated in a weak sense can be written as [9]

$$\int d\varepsilon \rho(\varepsilon)\Theta_1[\partial_t f](\phi(\varepsilon) = \sum_{\nu=\pm 1} a_\nu \int d\varepsilon \int d\varepsilon' \ln|\varepsilon' - \varepsilon + \nu| \times \frac{\partial}{\partial\varepsilon'}\frac{\partial}{\partial\varepsilon}\left\{\rho(\varepsilon')\rho(\varepsilon)\frac{\partial f(\varepsilon', t)}{\partial t}(\phi(\varepsilon) - \phi(\varepsilon'))\right\}, \quad (7)$$

where $\phi(\varepsilon)$ is a smooth test function. The weak formulation of the collision operator Θ_1 conserves mass locally since (7) is explicitely equal to zero for constant test functions.

In contrast to the the Boltzmann scattering integral being a functional of the distribution function, the correction scattering operator (7) depends on its time derivative $\partial_t f(\varepsilon', t)$. The time derivative is a consequence of memory effects present in the original Levinson equation. Expression (7) shows that the correction term $\Theta_1[\partial_t f]$ also depends on the values of the distribution function outside of the constant energy shell defined by the Fermi golden rule (6). These off-shell contributions are caused to the finiteness of the collision time and therefore provide the quantum mechanical correction to the Fermi golden rule.

3 Multiple Trajectories Monte Carlo Method

Equation (5) with scattering operators $\Theta_0[f]$ and $\Theta_1[\partial_t f]$, defined by (6) and (7), respectively, represents our starting point. We formally solve the equation (5) for $f(\varepsilon, t)$ using an iteration technique. We are looking for a solution of the form $f(\varepsilon,t) = f_0(\varepsilon,t)+\lambda f_1(\varepsilon,t)$, where $f_1(\varepsilon,t)$ is a correction term to the semiclassical solution $f_0(\varepsilon,t)$. The substitution into (5) allows to reduce the problem of finding an inverse of the operator $(I - \lambda\Theta_1)[\partial_t f]$, which is hardly treatable with Monte Carlo technique, to a simpler problem of computing the effect of the scattering operator Θ_1 acting on the first time derivative $\partial_t f_0(\varepsilon,t)$. Thus we arrive to the system of two coupled Boltzmann equations for f_0 and for the correction f_1:

$$\partial_t f_0 = Q_0[f_0], \qquad \partial_t f_1 = Q_0[f_1] + Q_1[\partial_t f_0],$$

with the initial conditions $f_0(\varepsilon, 0) = \phi_0(\varepsilon)$ and $f_1(\varepsilon, 0) = 0$.

To obtain a forward Monte Carlo algorithm, we are following the standard procedure [7] writing the equations in integral form for an adjoint function $g_j(\varepsilon,t)$ defined in such a way that the average $(A, f_j) \equiv \int_0^\infty dt \int d\varepsilon\ \rho(\varepsilon)A(\varepsilon,t)f_j(\varepsilon,t)$ of an observable $A(\varepsilon,t)$ can be expressed as

$$(A, f_j) \equiv \int_0^\infty dt' \int d\varepsilon'\ \rho(\varepsilon') f_j^{(0)}(\varepsilon', t') g_j(\varepsilon', t'), \qquad j = 0, 1, \tag{8}$$

where the source-terms are defined as $f_1^{(0)}(\varepsilon,t) = \int_0^t dt' e^{-\kappa_0(\varepsilon)(t-t')} Q_1[\partial_t f_0](\varepsilon, t')$, $f_0^{(0)}(\varepsilon,t) = e^{-\kappa_0(\varepsilon)t}\phi_0(\varepsilon)$.

It can be shown [7] that the function $g_j(\varepsilon', t)$ must satisfy the adjoint equation

$$g_j(\varepsilon', t') = \int_0^\infty dt \int d\varepsilon\rho(\varepsilon)\ K(\varepsilon, t, \varepsilon', t') g_j(\varepsilon, t) + A(\varepsilon', t'), \qquad j = 0, 1, \tag{9}$$

with the free term given by the observable $A(\varepsilon', t)$. The kernel K in (9) is defined as $K(\varepsilon, t, \varepsilon', t') = H(t')H(t-t')e^{-\kappa_0(\varepsilon)(t-t')} S_0(\varepsilon, \varepsilon')$, where $\kappa_0(\varepsilon)$ is the total out-scattering rate: $\kappa_0(\varepsilon) = 4\pi^2 \sum_{\nu=\pm1} a_\nu \sqrt{2(\varepsilon - \nu)} H(\varepsilon - \nu)$.

It is important that neither the kernel nor the source term in (9) depend on j, so the index j can be omitted. Therefore, the sets of trajectories necessary to calculate f_0 and f_1 are similar. Different statistical averages are obtained by different terms $f_j^{(0)}$ in the inner product (8).

The solution of (9) is found through corresponding Neumann series. The forward Monte Carlo method is used to evaluate the series numerically. The algorithm is designed to compute f_0 together with its time derivative $\partial f_0/\partial t$. It allows to solve both equations for f_0 and f_1 simultaneously providing better computational scaling at large time compared to previously used techniques.

4 Results

We now apply the method developed to practically relevant semiconductors. In Si and Ge the constant of electron interaction with nonpolar optical phonons is expressed as [8]:

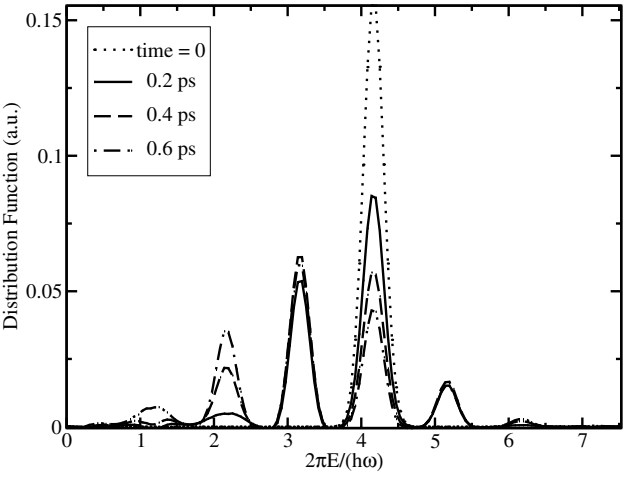

Fig. 1. Distribution $f_0(\varepsilon, t)$ with the quantum correction term $\lambda f_1(\varepsilon, t)$ added in Ge at the time instances $t_1 = 2 \times 10^{-13}$ s, $t_2 = 4 \times 10^{-13}$ s, $t_3 = 6 \times 10^{-13}$ s

$$F^2 = \frac{\hbar^2 (D_t K)^2}{2V\rho_0 \hbar\omega}, \tag{10}$$

leading to the dimensionless constant of electron-phonon interaction $\mu = \lambda\pi\rho(\varepsilon)$, which for $\varepsilon = 1$ is equal to $\mu \approx 0.055$. An even smaller value of the constant $\mu \approx 0.02$ is found in Ge. Because the values of the electron-phonon interaction constant in Si and Ge are comparable, results of simulations in Si and Ge are similar. Below we consider in details the case of Ge.

Simulation results of initial evolution of highly nonequilibrium distribution with the quantum correction taken into account are shown in Fig. 1. The appearance of additional replicas is clearly seen at energies which are multiples of the phonon energy, at first in the proximity of the initial energy distribution. With time passing the solutions propagate away from the initial energy ε_0 gradually creating more remote replicas. This is accompanied by an amplitude decrease of the initial peak. In contrast to zero-temperature results [6], our simulations were done at room temperature T=300 K. This leads to the possibility of phonon absorption which results in the creation of additional replicas with energies higher than the initial energy ε_0. However, the amplitude of these replicas is much smaller compared to those at energies lower than ε_0, reflecting the fact that phonon absorptions by nonequilibrium electrons is less probable than phonon emission.

In order to show the differences between the behavior with and without quantum corrections, a snapshot at time step $t = 6 \times 10^{-13}$ s is shown in Fig. 2. One can clearly see the additional broadening of more remote replicas when the quantum correction is taken into account in contrast to the classical solution. This is the result of scattering outside of an energy shell determined by the Fermi golden rule energy conserved delta-function, which is allowed due to the finiteness

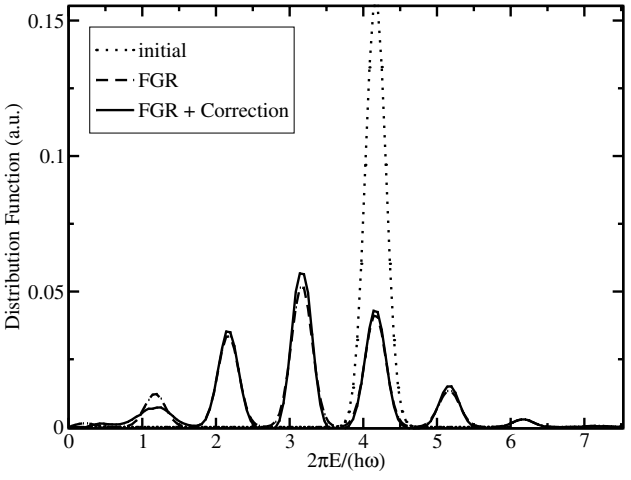

Fig. 2. Comparison of the semiclassical Boltzmann distribution $f_0(\varepsilon, t)$ and the distribution $f_0(\varepsilon, t)$ together with the quantum correction term $\lambda f_1(\varepsilon, t)$ added in Ge at the time $t = 6 \times 10^{-13}$ s. Additional broadening of remote replicas is due to the finiteness of the collision time.

of the collision time until the collision is complete. Similar collisional peak broadening was reported previously while solving the Levinson equation directly [6]. At the same time, neighboring replicas are becoming almost indistinguishable from those determined solely by the Fermi golden rule. This clearly shows that the quantum correction decreases at large time. In order to explain such a behavior, we note that the neighboring replicas correspond to emission (absorption) of only a single phonon. After some time, there will be almost no electrons left which did not emit (absorb) a phonon. For all electrons which emitted or absorbed a phonon, the collision process may be considered as completed, and the Fermi golden rule enforced energy conservation delta function is recovered. It is therefore expected that differences between the solutions with and without corrections will disappear, starting from replicas close to the initial peak.

5 Conclusion

Based on the asymptotic expansion of the Levinson equation, the quantum correction to the classical distribution function due to the finite collision time is analyzed. The Monte Carlo algorithm is developed in order to solve the Boltzmann equation simultaneously with the equation for the quantum correction. For the electron phonon interaction the method is also applied to calculate the quantum corrections in Si and Ge, where the electron phonon interaction is weaker than in GaAs. It is shown that for a highly nonequilibrium initial distribution peaked around a certain energy, the quantum correction leads to an extra broadening of replicas of the initial distribution peak appearing at frequencies

shifted by a multiple of the phonon frequency. At the same time the quantum correction disappears for longer times when the limit of completed collision is recovered.

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