Particle modeling of semiconductor quantum devices

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Abstract

With the scaling down of semiconductor device deeply into the sub-0.1μm region, it is increasingly important to take quantum mechanical effects of carrier transport into account in device simulation. However, it is difficult to simulate practical devices where clear semi-classical and quantum features coexist, as is the case for nanoscale devices at normal temperatures. In this paper, we present a particle description of quantum phenomena based upon a quantum force derived from the Wigner's transport formalism. The quantum force can be incorporated into the driving force term of the Boltzmann transport equation, which enables us to utilize the well-developed particle Monte Carlo computational techniques. We demonstrate that the quantum transport effects such as quantum tunneling and energy quantization are incorporated in the standard Monte Carlo technique.

1 Introduction

With the progress of LSI technology, the electronic device size is scaling down to the sub-0.1μm region. In such an ultrasmall device, it is more important to take quantum mechanical effects of carrier transport into account in device simulation. In the classical and semi-classical transport regimes, the electron transport has been well described by the classical Boltzmann transport equation with the scattering processes represented in terms of Fermi's golden rule. However, when the device size reaches below 0.1μm and approaches the deBroglie wavelength of electrons, the semi-classical descrip-
tion of device operation is no longer available. In such a quantum transport regime, not only the device geometric shape, but also the electron's wave or particle natures directly appear on the device operating properties. So far, the transmission coefficient model [1], the Wigner function model [2]-[4] and the Green's function model [5]-[9] have been widely used for various nanostucture devices. These quantum mechanical models have provided the powerful tool, but in practical applications it is limited to one-dimensional problems for its computational expenses. In this paper, we will propose a novel quantum device model based upon a direct solution of the Boltzmann equation for multi-dimensional practical use. In this model, the quantum effects are represented in terms of quantum mechanically corrected force in the classical Boltzmann equation.

2 Nonequilibrium Green's function model

Non-equilibrium quantum-field theory has been in existence for almost 40 years and only recently has become a variable technique for the simulation of semiconductor devices. This formalism is based upon the double-time correlation functions of the field operator of a single fermion, where the following different Green's functions are defined. They are the advanced $G^A$, retarded $G^R$, time-ordered $G^t$, anti-time ordered $G^\tau$, and $G^<, G^>$, which have no name [10]. These six Green's functions are not independent, but mutually related through

$$G^A = [G^R]^\dagger, \quad G^> - G^< = G^R - G^A, \quad G^< + G^> = G^t + G^\tau.$$  \hspace{1cm} (1)

For equal times, $G^<$ and $G^>$ reduce to the one-particle densities of electrons and holes, respectively, and therefore have the character of a distribution function. In addition, the full double-time $G^<$ and $G^>$ also contain the dynamical information on the evolution of the one-particle excitations of both types. $G^{R,A}$ describe the propagation of an extra particle added to the system. Following the generalized Keldysh arguments along the contour, we use a useful notation which expresses four of these Green's functions as the elements of a two-by-two matrix [10]. For interacting systems whether in equilibrium or not, the Green's functions satisfy the Dyson equation given in terms of the matrix notation [10].

$$\bar{G}(x_1, x_2) = \bar{g}(x_1, x_2) + \int dx_3 \int dx_4 \bar{g}(x_1, x_3) \bar{\Sigma}(x_3, x_4) \bar{G}(x_4, x_2).$$  \hspace{1cm} (2)

Here, the notation is simplified by letting as $x_1 = (r_1, t_1)$, and

$$\bar{G} = \begin{pmatrix} G^t & -G^< \\ G^> & -G^\tau \end{pmatrix}, \quad \bar{g} = \begin{pmatrix} g^t & -g^< \\ g^> & -g^\tau \end{pmatrix}, \quad \bar{\Sigma} = \begin{pmatrix} \Sigma^t & -\Sigma^< \\ \Sigma^> & -\Sigma^\tau \end{pmatrix}.$$  \hspace{1cm} (3)
As found in (2), the Green's functions are expressed as the noninteracting terms $\tilde{g}$ plus the contribution from the interactions provided by the self-energy functions. The self-energy represents all the interacting effects, which consists of the boundary coupling effects at the device-electrode interfaces, the various scattering effects, and the electron-electron interaction effects. We should note that only the two Green's functions $G^<\!$ and $G^R$ are used for the quantum transport, and generally the two Dyson equations in terms of $G^<$ and $G^R$ are solved self-consistently.

In the steady-state transport, (2) is Fourier transformed with respect to the relative time $(t_1 - t_2)$. Following the tight-binding approximation of the Dyson equation by Caroli [11], the equation of motion for $G^<$ and $G^R$ in the device is given as

$$G^< = g^< + g^< \Sigma^A G^A + g^R \Sigma^< G^A + g^R \Sigma^R G^<, \quad (4)$$

$$G^R = g^R + g^R \Sigma^R G^R, \quad (5)$$

where Green's functions and the self-energies are matrices in site space and functions of energy. $g^<$ and $g^R$ are determined in advance when the electro-static potential is given. In the single-band tight-binding model, the steady state current density $J_l$ and the electron density $n_l$ at a layer $l$ are represented by using the Fourier transformed correlation function $G^<\!$ [5][6]

$$J_l = \frac{2e}{\hbar A} \sum_{k_\parallel} \int \frac{dE}{2\pi} 2Re \left\{ t_{l,l+1} G^<_{l+1,l}(k_\parallel, E) \right\}, \quad (6)$$

$$n_l = -\frac{2i}{A\Delta} \sum_{k_\parallel} \int \frac{dE}{2\pi} \left\{ G^<_{l,l}(k_\parallel, E) \right\}, \quad (7)$$

where $k_\parallel$ is a transverse wave vector, and $t_{l,m}$ denotes the hopping energy between the $l$th and $m$th layers. $A$ and $\Delta$ are the cross section of the device and the layer spacing, respectively.

We have developed a multi-band, non-equilibrium Green's function and Poisson simulator for GaAs/AlAs resonant tunneling diodes [8][9], where realistic complex multi-band structures based on the tight-binding $sp^3s^*$ model are used to include the $\Gamma$-X valley-mixing, nonparabolicity effects and evanescent modes at the heterointerfaces. Further, space charge effect is incorporated by solving the Poisson equation simultaneously.

In the study of quantum dots, the intradot interaction has been well incorporated in terms of self-energy within the Hartree-Fock approximation [7]. Further, the current fluctuations as well as the time-averaged transport characteristics are discussed to investigate the temporal correlation of the tunneling electrons. To evaluate the current fluctuations, the noise power spectrum has been calculated, which is related to the Fourier transform of the current correlation function as

$$S_l(E) = \int_{-\infty}^{\infty} d\tau e^{iE\tau/\hbar} \left\langle \Delta \hat{I}_l(\tau) \Delta \hat{I}_l(0) + \Delta \hat{I}_l(0) \Delta \hat{I}_l(\tau) \right\rangle \quad (8)$$
where \( \Delta \hat{I}_1(\tau) = \hat{I}_1(\tau) - \langle \hat{I}_1(\tau) \rangle \) denotes the current fluctuation operator. Therefore, the noise power spectrum is expressed in the form of the two-electron Green's function, that will give us another information on the electron transport in nanostructure devices. In connection with this discussion, it is noteworthy that in the formal linear response theory pioneered by Kubo [17] the frequency dependent conductivity (dissipation) is also represented by using the current-current correlation function (fluctuation).

### 3 Wigner function model

Starting from the Dyson equation (2), the quantum Boltzmann equation (QBE) has been derived by Keldysh [12], Kadanoff and Baym [13], and Mahan [10] afterwards. When the independent variables are changed to the center-of-mass coordinates \((r, t) = (r_1 + r_2, t_1 + t_2)/2\) and the relative coordinates \((w, \tau) = (r_1 - r_2, t_1 - t_2)\), a quantum mechanical distribution function \(G^<(k, \omega; r, t)\) is defined as Fourier transform of \(G^<(w, \tau; r, t)\) with respect to the relative coordinates. The QBE is a differential kinetic equation for the Green's function \(G^<\), which is formulated by using standard techniques (eqn. (31) in [4]).

For systems nearly homogeneous and steady-state, it is given as

\[
\left[ \frac{\partial}{\partial t} + \frac{\hbar k}{m^*} \cdot \nabla r \right] G^<(k, \omega; r, t) + \frac{1}{\hbar} \int \frac{d^3 k'}{(2\pi)^3} V(r, k - k') G^<(k', \omega; r, t)
\]

\(\simeq i \left[ \Sigma^<(k, \omega; r, t) G^>(k, \omega; r, t) - \Sigma^>(k, \omega; r, t) G^<(k, \omega; r, t) \right] , \tag{9}\)

where

\[ V(r, k - k') = i \int d^3 w e^{-i(k - k') \cdot w} \left[ U \left( r + \frac{w}{2} \right) - U \left( r - \frac{w}{2} \right) \right] . \tag{10}\]

Here, \(U(r)\) denotes the spatially varying potential energy. In the QBE (9) the retarded Green's function \(G^R\) is not included explicitly, but it will be introduced through the spectral function \(A(k, \omega; r, t) = -2\text{Im}G^R(k, \omega; r, t)\) by using the so-called Kadanoff-Baym approximation represented as

\[ G^<(k, \omega; r, t) = iA(k, \omega; r, t)f(k, r, t), \tag{11}\]

where \(f(k, r, t)\) is the Wigner distribution function defined as the energy-integral of \(G^<(k, \omega; r, t)\)

\[ f(k, r, t) = \int \frac{d\omega}{2\pi} [-iG^<(k, \omega; r, t)] . \tag{12}\]

The electron density \(n(r, t)\) and the current density \(J(r, t)\) are represented by using the Wigner distribution function as follows.

\[ n(r, t) = \int \frac{d^3 k}{(2\pi)^3} f(k, r, t), \tag{13}\]

\[ J(r, t) = e \int \frac{d^3 k}{(2\pi)^3} \frac{\hbar k}{m^*} f(k, r, t) . \tag{14}\]
A transport equation for the Wigner distribution function including scattering effects is finally derived by integrating Eq. (9) over $\omega$ as

$$\frac{\partial f}{\partial t} + \frac{\hbar k}{m^*} \cdot \nabla_r f + \frac{1}{\hbar} \int \frac{d^3 k'}{(2\pi)^3} V(r, k - k') f = \left( \frac{\partial f}{\partial t} \right)_c. \tag{15}$$

Generally, the collisional term $(\partial f/\partial t)_c$ becomes a complicated form [4]. In addition, the third term on the left-hand side of the equation (15), that is driving term, is represented by the nonlocal potential function defined by the equation (10). In the classical limit ($\hbar \to 0$), this term reduces to $-(\nabla_r U/\hbar) \cdot \nabla_k f$, which is coincident with the classical Boltzmann equation. In short, this term describes the quantum mechanical effects. The Wigner distribution function model have been widely applied to a variety of quantum devices, such as resonant-tunneling diodes [3], quantum wires [4], and quantum-structure lasers [14].

4 Quantum Monte Carlo method

The transport equation of the Wigner distribution function (15) is rewritten in the form of a modified Boltzmann equation as [15]

$$\frac{\partial f}{\partial t} + \frac{\hbar k}{m^*} \cdot \nabla_r f - \frac{1}{\hbar} \nabla_r U \cdot \nabla_k f \tag{16}$$

$$- \sum_{\alpha=1}^{\infty} \frac{(-1)^{\alpha+1}}{\hbar 4^\alpha (2\alpha + 1)!} \nabla_r^{2\alpha+1} U \cdot \nabla_k^{2\alpha+1} f = \left( \frac{\partial f}{\partial t} \right) \cdot,$$

where the fourth term on the left-hand side denotes the quantum correction due to the spatially varying potential energy $U(r)$, which accounts for various quantum effects. Although the quantum transport equation (16) provides the general and powerful tool to simulate quantum devices, it is limited to one-dimensional problems in practical application for its computational expenses. So, we propose to take only the lowest-order quantum correction by taking only the $\alpha = 1$ term in (16), because the lowest-order term induces a major contribution in the quantum correction ingredients. Further, when the system is close to equilibrium, by using a drifted Maxwell-Boltzmann distribution, the following Boltzmann-like equation is obtained from (16) [16].

$$\frac{\partial f}{\partial t} + \frac{\hbar k}{m^*} \cdot \nabla_r f - \frac{1}{\hbar} \nabla_r U \cdot \nabla_k f$$

$$\quad + \frac{1}{\hbar} F \cdot \nabla_k f = \left( \frac{\partial f}{\partial t} \right). \tag{17}$$

The quantum effects are incorporated in terms of the quantum force $F$ in the driving term whose components are given, for example, in two-
dimensional problem, by

\[
F_x = \frac{\partial}{\partial x} \left[ \frac{1}{24} \left\{ \left( \gamma_x^2 (k_x - k_x^0)^2 - 3\gamma_x \right) \frac{\partial^2 U}{\partial x^2} \right. \right.
+ 3(\gamma_y^2 (k_y - k_y^0)^2 - \gamma_y) \frac{\partial^2 U}{\partial y^2} \left. \right\} \right],
\]

(18)

\[
F_y = \frac{\partial}{\partial y} \left[ \frac{1}{24} \left\{ \left( \gamma_x^2 (k_x - k_x^0)^2 - 3\gamma_x \right) \frac{\partial^2 U}{\partial x^2} \right. \right.
+ 3(\gamma_y^2 (k_y - k_y^0)^2 - \gamma_y) \frac{\partial^2 U}{\partial y^2} \left. \right\} \right],
\]

(19)

where \( k_x^0 \) and \( k_y^0 \) denote mean wavenumbers of \( k_x \) and \( k_y \) defined in each spatial grid, respectively, and \( \gamma_x \) and \( \gamma_y \) are given by

\[
\gamma_x = \frac{\beta \hbar^2}{m_x^*}, \quad \gamma_y = \frac{\beta \hbar^2}{m_y^*},
\]

(20)

where \( \beta = 1/k_B T \).

In this paper, we will apply the ensemble Monte Carlo method to solve the quantum transport equation. Based upon (17), the velocity and the force for particles during the free flight are respectively given by

\[
\frac{dr}{dt} = \frac{\hbar \mathbf{k}}{m^*},
\]

(21)

\[
\frac{d\mathbf{k}}{dt} = \frac{1}{\hbar} \left( -\nabla r U + \mathbf{F} \right).
\]

(22)

The velocity equation (21) is the same as used in the standard Monte Carlo technique, but the force equation (22) is modified in the quantum transport so that the particles evolve under the enforcement not only by the classical built-in potential, but also by the quantum force. In the equations of motion (21) and (22), we have described the carriers as though they have well-defined positions and momenta simultaneously. Although this seems to be inconsistent with the quantum mechanical uncertainty principle, we can interpret that the \( \mathbf{r} \) and \( \mathbf{k} \) obtained from (21) and (22) represent the centers of positions and momenta of traveling wave packets, respectively. This situation could be the same as the quantum mechanical treatment of scattering events in the semi-classical Monte Carlo approaches.

5 Simple example

To verify the validity of our proposal, we have first studied the quantum transport of a simple GaAs/AlGaAs single tunneling barrier at 300K. The barrier width and its energy height are 2.5nm and 0.22eV, respectively. The doping density in the GaAs electrodes is given as \( 10^{18} \text{cm}^{-3} \). As a collisional
Figure 1: Simulated electron distributions in space and energy of a single tunneling barrier at 300K by means of the classical (top) and the quantum corrected (bottom) Monte Carlo method.
process, the LO phonon scattering, the acoustic phonon scattering and the ionized impurity scattering are considered. Fig. 1 shows the computed electron distributions in space and energy at the bias voltage of 0.3V. The upper figure and the lower one correspond to the classical Monte Carlo simulation and the quantum corrected one, respectively. For reference, the conduction band profiles are also plotted in the solid line. Comparing these two figures, we can observe the two major quantum effects. The first one is the quantum confinement effects in the triangular potential well formed in the left electrode. The electrons are distributed away from the left barrier interface, and more surprisingly, no electrons exist under a certain energy due to the quantized subband formed in the triangular well. The second one is the quantum tunneling effects through the central barrier. In the classical particle model, only the thermally excited electrons with energy larger than the barrier height are found in the barrier region. On the other hand, in the quantum transport simulation, a few tunneling electrons are detected apart from the thermally excited ones and they are found accelerated after tunneling due to the electric field. Consequently, the quantum transport effects have been incorporated in the standard Monte Carlo techniques successfully by considering the quantum corrected driving force.

6 Conclusion

In this paper, we propose a quantum Monte Carlo device simulation applicable for ultrasmall semiconductor devices, where the quantum effects are represented in terms of quantum mechanically corrected force in the Boltzmann equation. We have demonstrated that the quantum tunneling and energy quantization effects of carriers can be incorporated in the standard Monte Carlo techniques successfully by using our model. We believe that the proposed quantum Monte Carlo technique will provide a powerful tool in the device simulation of ultrasmall MOSFET’s in ULSI circuits.

References


