A Fermi-Statistics-Based Model for Quantum Semiconductor Device Simulations

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Abstract: In this paper, we derive a Fermi-statistics-based self-consistent stationary model for quantum semiconductor device simulations. This new model is comprehensive in both physical and mathematical aspects. It is capable of describing hot electron transport as well as significant quantum mechanical effects for advanced devices with dimensions comparable to the de Broglie wave-length. Moreover, quantum mechanical Fermi-Dirac statistics is also introduced to estimate the electron concentration. The model is completely self-adjoint for all state variables and hence provides many appealing mathematical features such as global convergence, fast iterative solution, and highly parallelizable. Numerical simulations on diode with the length down to 30 nm using this model have been performed and compared with that using the Boltzmann-statistics-based transport model. It is shown that the maximal electron temperature is significantly reduced by the new model up to 76 % comparing with that of the previous model in literature.

Key–Words: Maxwell-Boltzmann statistics, Fermi-Dirac statistics, semiconductor device simulation

1 Introduction

In order to keep pace with the increasing speed of miniaturization of modern semiconductor technology, a great variety of device models that account for quantum effects, accuracy, robustness, and efficiency in real-life simulations have been intensively developed and tested in recent years, see e.g. [1, 2, 3] and references therein. Among them, a class of macroscopic quantum mechanical (QM) models based on the density gradient (DG) theory of Ancona and Tiersten [1] have been shown to accurately simulate multi-dimensional devices with lengths ranging from 50 nm down to 6 nm [2, 3]. This model is a quantum corrected version of the classical drift-diffusion (DD) model, with \( O(\hbar^2) \) corrections to the stress tensor, and is viewed as one of the hierarchy of the quantum hydrodynamic (QHD) models [4, 5]. In this paper, we consider in particular the quantum-corrected energy transport model (QCET) proposed in [6, 7] which is one of the most advanced DG models in the sense that it extends the commonly used quantum drift-diffusion (QDD) model by including the energy balance equations in order to take the hot electron effects into account.

Semiconductor statistics includes both classical statistics and quantum statistics. Classical or Maxwell-Boltzmann statistics is derived on the basis of purely classical physics arguments. In contrast, quantum or Fermi-Dirac statistics takes into account results of quantum mechanics, namely the Pauli exclusion principle and the finiteness of the number of states in an energy interval. The finiteness of states is a result of the Schrödinger equation [8, 9]. If the difference between the quasi-Fermi energy and the band energy is small, i.e., the lightly doping concentration is applied, then one can use Maxwell-Boltzmann statistics to achieve the simpler and better approximation for the carrier concentrations. However, the validity of Boltzmann statistics becomes a very poor assumption when heavily doped devices are considered.

The purpose of this paper is to extend the QCET model to consider the Fermi-Dirac (FD) statistics and shows this new extension is capable of describing hot electron transport as well as significant QM effects for advanced devices. Our model (FDET) is able to explain that electron temperature essentially differs from the lattice temperature. It is clear that this effect cannot be described by the DG model alone. Moreover, Fermi-Dirac statistics is also taken into account to avoid the poor approximation of Maxwell-Boltzmann statistics. Section 2 discusses the DG model and the QCET model with emphasis on Maxwell-Boltzmann statistics. A full self-adjoint formulation of the Fermi-statistics-based model is then given. In Section 3,
numerical results of simulation on various diodes to compare with the results in the literature to demonstrate the effectiveness of the proposed model. A short concluding remark is given in Section 4.

2 Semiconductor Models and Statistics

For the modelling of nanoscale semiconductor devices, the DG theory was developed by observing that the electron gas is energetically sensitive not only to its density but also to the gradient of the density. It captures the nonlocality of quantum mechanics to the lowest-order of $\hbar^2$ where $\hbar$ is the reduced Planck constant and can be rigorously derived from quantum mechanics [1, 10]. Specifically, a third order derivative term of quantum correction is added to the carrier current density as [6]

$$
J_n = \begin{array}{l}
-q\mu_n n \nabla \phi + qD_n \nabla n \\
-2q\mu_n b_n \nabla \left[ \frac{\Delta \sqrt{n}}{\sqrt{n}} \right], \\
\end{array}
\quad (1)
$$

$$
J_p = \begin{array}{l}
-q\mu_p p \nabla \phi - qD_p \nabla p \\
+ 2q\mu_p b_p \nabla \left[ \frac{\Delta \sqrt{p}}{\sqrt{p}} \right],
\end{array}
\quad (2)
$$

where $\phi$ is the electrostatic potential, $n$ and $p$ are the electron and hole charge, $J_n$ and $J_p$ are the current densities, $\mu_n$ and $\mu_p$ are the electron and hole mobilities, $D_n$ and $D_p$ are the electron and hole diffusion coefficients expressed by the Einstein relation with the mobilities, the coefficients $b_n = \frac{n^2}{12q\mu_n}$ and $b_p = \frac{p^2}{12q\mu_p}$ are the material parameters measuring the strength of the gradient effects in the gas. In the above equations, vectors are denoted by bold letters. To alleviate the difficulty in discretization caused by this higher order term, additional variables called the quantum potentials

$$
\phi_{qn} \equiv 2b_n \left[ \frac{\Delta \sqrt{n}}{\sqrt{n}} \right],
\quad (3)
$$

$$
\phi_{qp} \equiv -2b_p \left[ \frac{\Delta \sqrt{p}}{\sqrt{p}} \right],
\quad (4)
$$

have been introduced in [10] and thus can be lumped with the classical drift term to obtain

$$
J_n = \begin{array}{l}
-q\mu_n n \nabla (\phi + \phi_{qn}) + qD_n \nabla n, \\
\end{array}
\quad (5)
$$

$$
J_p = \begin{array}{l}
-q\mu_p p \nabla (\phi + \phi_{qp}) - qD_p \nabla p.
\end{array}
\quad (6)
$$

2.1 Boltzmann Statistics

For Boltzmann statistics, we have the quantum correction expressions of the carriers [6, 10]

$$
n = n_i \exp\left(\frac{\phi - \varphi_n + \phi_{qn}}{V_T}\right)
= n_i \exp\left(\frac{\phi + \phi_{qn}}{V_T}\right) \equiv \zeta_n^2, \tag{7}
$$

$$
p = n_i \exp\left(\frac{\varphi_p - \phi - \phi_{qp}}{V_T}\right)
= n_i \exp\left(\frac{-\phi - \phi_{qp}}{V_T}\right) \equiv \zeta_p^2, \tag{8}
$$

where $V_T = (k_B T_L)/q$ is the thermal voltage, $k_B$ is Boltzmann’s constant, $T_L$ is the lattice temperature and $\varphi_n$ and $\varphi_p$ are the generalized quasi-Fermi potentials, $u = \exp(\sqrt{\zeta_n}/V_T)$, $v = \exp(\sqrt{\zeta_p}/V_T)$, $\zeta_n = \sqrt{n}$ and $\zeta_p = \sqrt{p}$ are new variables used in the QCET model [6, 7]. The current continuity equations then become

$$
\frac{1}{q} \nabla \cdot J_n = R(\phi, u, v, \zeta_n, \zeta_p), \quad (9)
$$

$$
\frac{1}{q} \nabla \cdot J_p = -R(\phi, u, v, \zeta_n, \zeta_p), \quad (10)
$$

where

$$
J_n = +qD_n n_i \exp\left(\frac{\phi + \phi_{qn}}{V_T}\right) \nabla u, \quad (11)
$$

$$
J_p = -qD_p n_i \exp\left(-\frac{\phi - \phi_{qp}}{V_T}\right) \nabla v, \quad (12)
$$

and $R$ is the generation-recombination rate.

2.2 Fermi Statistics

For Fermi statistics, the electron density $n$ is approximately by introducing the band parameters $\omega_{qn}$ as [4]

$$
n = n_i \exp\left(\frac{\phi - \varphi_n + \phi_{qn} + \omega_{qn}}{V_T}\right)
= n_i \exp\left(\frac{\phi + \phi_{qn} + \omega_{qn}}{V_T}\right) u \equiv \zeta_n^2, \tag{13}
$$

The band parameter $\omega_{qn}$ is determined as

$$
\omega_{qn} = \log\left(\frac{n}{N_c}\right) - G_{1/2} \left(\frac{n}{N_c}\right), \quad (14)
$$

where $N_c$ is the density of states in the conduction band, and $G_{1/2}$ is the inverse-Fermi function of order 1/2. A convenient fit for numerical implementation is
given in [11]. The electron current density then becomes [4]

\[ J_n = -q \mu_n n \nabla (\phi + \phi_{qn} + \omega_{qn}) + q D_n \nabla n, \]

\[ = -q \mu_n n \nabla (\phi + \phi_{qn} + \omega_{qn}) + q D_n \nabla \left[ n \exp\left(\frac{\phi + \phi_{qn} + \omega_{qn}}{V_T}\right)\right], \]

\[ = +q D_n \nabla \left[ n \exp\left(\frac{\phi + \phi_{qn} + \omega_{qn}}{V_T}\right)\right], \]

which defines the generalized quasi-Fermi potential as in

\[ \phi_{qn} = -q \mu_n n \nabla \varphi_n \]  

with the quantum correction in electron concentration. Using (13) we rewrite the quantum potential as

\[ \phi_{qn} = V_T \ln\left(\frac{e^2}{\mu n_i}\right) - \phi - \omega_{qn}. \]

The density gradient equation then becomes

\[ \phi_{qn} = 2b_n \left[ \frac{\Delta \sqrt{n}}{\sqrt{n}} \right] \]

\[ = V_T \ln\left(\frac{e^2}{\mu n_i}\right) - \phi - \omega_{qn}. \]

We express it as a self-adjoint form,

\[ \Delta \zeta_n = \frac{c_n}{2b_n} \left[ V_T \ln\left(\frac{e^2}{\mu n_i}\right) - \phi - \omega_{qn} \right]. \]

### 2.3 A Fermi-Statistics-Based Model

As in [6, 7], we consider the following energy transport model

\[ \Delta \phi = \frac{q}{\varepsilon_s} (n - p + N_A^- - N_D^+), \]

\[ \nabla \cdot S_n = J_n \cdot E - \left( \frac{\omega_{n} - \omega_0}{\tau_{nw}} \right), \]

and Eqns. (1) and (3) where \( \varepsilon_s \) is the permittivity constant of semiconductor, \( N_A^- \) and \( N_D^+ \) are the densities of ionized impurities, \( S_n \) is the electron energy flux, \( E \) is the electric field, \( \tau_{nw} \) is the electron energy relaxation time, \( \omega_0 \) is the thermal energy, and \( \omega_n \) is the electron average energy. These physical variables are tightly coupled together with the following auxiliary relationships

\[ E = -\nabla \phi, \]

\[ S_n = \frac{J_n}{-q} \omega_n + \frac{J_n}{-q} k_B T_n + Q_n, \]

where \( Q_n \) is the electron heat flux, \( T_n \) is the electron temperature, \( m_n^* \) is the electron effective mass, \( v_n \) is the electron velocity, \( \kappa_n \) is the electron heat conductivity. Using the variable

\[ g_n = T_n / \exp\left(\frac{5 \varphi_n}{4 V_T}\right), \]

we can rewrite the electron energy flux as a self-adjoint form. More precisely,

\[ S_n = \frac{5 J_n}{-2 q} k_B g_n \exp\left(\frac{5 \varphi_n}{4 V_T}\right) \]

\[ - \kappa_n \left[ \exp\left(\frac{5 \varphi_n}{4 V_T}\right) \nabla g_n + \frac{5}{4 V_T} g_n \exp\left(\frac{5 \varphi_n}{4 V_T}\right) \nabla \varphi_n \right] \]

\[ + \frac{J_n}{-q} \left( m_n^* |v_n|^2 \right) \]

\[ = -\kappa_n \exp\left(\frac{5 \varphi_n}{4 V_T}\right) \nabla g_n + \frac{J_n}{-q} \left( m_n^* |v_n|^2 \right). \]

Hence, we obtain the following self-adjoint form

\[ \nabla \cdot \left( \kappa_n \exp\left(\frac{5 \varphi_n}{4 V_T}\right) \nabla g_n \right) = R_n, \]

where

\[ R_n (g_n) = n \left( \frac{\omega_{n} - \omega_0}{\tau_{nw}} \right) - \frac{J_n}{q} \nabla \left( \frac{1}{q} \frac{m_n^*}{q^2 n^2} |J_n|^2 \nabla J_n \right). \]

Our new model (FDET) for Fermi Statistics with the four state variables \( \phi, u, \zeta_n \), and \( g_n \) is re-organized as follows:

\[ \Delta \phi = F, \]

\[ \frac{1}{q} \nabla \cdot J_n = R, \]

\[ \Delta \zeta_n = Z_n, \]

\[ \nabla \cdot G_n = R_n, \]
where
\[ F = \frac{q n_i}{e_s} \left[ n \exp\left(\phi + \phi_{qn} + \omega_{qn}\right) \right] - v \exp\left(\frac{-\phi - \phi_{qn}}{V_T}\right) + q \left(N_A - N_D^+\right) \] (37)
\[ J_n = +q D_n i_n \exp\left(\frac{\phi + \phi_{qn} + \omega_{qn}}{V_T}\right) \nabla u, \] (38)
\[ Z_n = \frac{\zeta_n}{2b_n} \left[ V_T \ln\left(\zeta_n^2\right) - V_T \ln\left(n_{in}\right) \right] - \phi - \omega_{qn}, \] (39)
\[ \phi_{qn} = V_T \ln\left(\zeta_n^2\right) - V_T \ln\left(n_{in}\right) - \phi - \omega_{qn}, \] (40)
\[ G_n = \kappa_n \exp\left(\frac{\nabla \phi_{qn}}{4V_T}\right) \nabla g_n, \] (41)
and Eqn. (32). It should be noted that effective approximation of the gradient of current density in formula (32) is in general very difficult to acquire. Simplified models for the formula based on physical consideration are possible. For example, by assuming that the drift energy is only a small part of the total kinetic energy [12], (32) can be reduced to
\[ R_n(g_n) = n \left(\frac{\omega_n - \omega_0}{\tau_{nw}}\right) - J_n E, \] (42)
which will be used in our numerical simulations.

### 3 Results and Discussions

To demonstrate the effectiveness and accuracy of the FDET model, several numerical studies have been made for sample diode device structures. A benchmark device, namely, an abrupt $n^- n-n^+$ silicon diode is used to verify our methods and formulation with the results reported in literature. Numerical experiments are performed first on a 600 nm silicon diode at 300 K with $n^+ = 5.0 \times 10^{17} cm^{-3}$ and $n = 2.0 \times 10^{15} cm^{-3}$. The length of the $n$-region is approximately 400 nm. The steady state results for this problem are illustrated by the dotted and solid curves with respective to the FDET and DGET models in Figs. 1(a)-1(d) where the applied voltage $V_G$ is taken as 2.0V. The dotted curve coincides with the solid curve. This represents that the new model can be applied to devices with larger size, i.e., where the QM effects are negligible. These results agree also very well with that previously reported in the literature [13, 14, 15]. Moreover, the role, $\phi_{qn}$, in the QCET model has been changed to $\phi_{qn} + \omega_{qn}$ in the FDET model. The quantum potential has been corrected significantly because the additional band parameter is considered. See Fig. 2.

To verify QM effects with our model, we then reduce the scale down to two cases. Case (1) is a 120

![Figure 1: The numerical results of 600 nm silicon diode.](image1)

![Figure 2: The behaviors of $\phi_{qn}$, $\omega_{qn}$ and $\phi_{qn} + \omega_{qn}$ (600nm).](image2)
Electron Quantum Potential $\phi_{qn}$ models is more visible in Case (2). Fig. 5 shows increased one order comparing with those of the 600 nm silicon diode. The applied voltage $V_O$ is taken as 1.2V. Case (2) is a 30 nm silicon diode with $n^+ = 5.0 \times 10^{19} \text{cm}^{-3}$ and $n = 2.0 \times 10^{15} \text{cm}^{-3}$. The length of the $n$-region is approximately 80 nm. The applied voltage $V_O$ is taken as 0.8V. Figs. 3 shows the significant change of the electron density and temperature. The maximal temperatures of DGET and FDET models are $T_{th} = 4225K$ and $T_n = 3962K$, respectively. Fig. 3(c) and 4 show $\phi_{qn}$, $\omega_{qn}$ and $\phi_{qn} + \omega_{qn}$ increased one order comparing with those of the 600 nm diode.

The difference between the DGET and FDET models is more visible in Case (2). Fig. 5 shows the numerical results. Since the larger doping ($n^+ = 5.0 \times 10^{19} \text{cm}^{-3}$) is applied, Fermi statistics should be considered. Causing the introduction of the band parameter $\omega_{qn}$, we can see the significant dissimilarity in the $n^+$-regions and the junctions. Moreover, the maximal temperatures of DGET and FDET models are more different than the Case (1). They are $T_n = 3309K$ and $T_n = 2512K$, respectively. The corresponding thermal energies are $E_{th} = \frac{2}{3}k_B T = 0.428eV$ and $E_{th} = 0.325eV$. The maximal temperature of the new model is reduced by up to 76 % comparing with that of the QCET model. Since the behaviors of $\phi_{qn}$, $\omega_{qn}$ and $\phi_{qn} + \omega_{qn}$ are similar to previous cases except the order, we skip the presentation of the figure.
4 Conclusion

A Fermi-statistics-based self-consistent stationary model is proposed here for nanoscale semiconductor device simulations. It is capable of describing hot electron transport as well as significant quantum correction effects for advanced devices. Moreover, quantum mechanical Fermi-Dirac statistics is also introduced to calculate the electron concentration to avoid the poor approximation of Maxwell-Boltzmann statistics. The model is completely self-adjoint for all state variables and hence provides many appealing mathematical features. Numerical simulations on diode with the length down to 30 nm using this model have been performed and compared with that using the Boltzmann-statistics-based transport model. It is shown that the maximal electron temperature is significantly reduced by the new model up to 76% comparing with that of the QCET model.

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