Inclusion of the Pauli Principle in a Deterministic Boltzmann Equation Solver for Semiconductor Devices

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Abstract—The Pauli principle is included in a deterministic Boltzmann solver for multi-dimensional semiconductor devices. The Newton-Raphson scheme is applied to solve the nonlinear Boltzmann equation, and it is found that the inclusion of the Pauli principle introduces no numerical problems, even for semiconductor devices. The impact of the Pauli principle is numerically investigated for a scaled SiGe HBT.

I. INTRODUCTION

The Pauli principle limits the occupancy of a state to a single electron per spin direction. Its impact on simulation might be significant at low temperatures or in heavily-doped regions.

Inclusion of the Pauli principle into a Boltzmann equation solver is not a trivial task, especially for the device case. Its impact in Monte Carlo simulations is rather CPU intensive, because the distribution function is inherently known at all times [6]. However, even in this scheme, the inclusion of the Pauli principle has been reported only for bulk systems [4]. In this work, the Pauli principle is included in a deterministic Boltzmann solver for devices, and its impact on simulation is numerically investigated.

II. IMPLEMENTATION

Several modifications of the physical models – the scattering operator, the boundary conditions, and the bandgap narrowing model – must be made in order to consider Fermi-Dirac statistics.

The Pauli principle introduces an additional factor in the scattering operator. For notational simplicity, only one scattering with the energy transfer of \( \hbar \omega \) is explicitly shown in the following, however, its extension to the general case is straightforward. The scattering operator is decomposed into the in-scattering and out-scattering terms:

\[
S_{l,m}^{in}(\epsilon) = S_{l,m}^{out}(\epsilon) = S_{l,m}^{in}(\epsilon) - S_{l,m}^{out}(\epsilon). \tag{1}
\]

When the transition rate depends only on the relative angle between the initial and final wave vectors, the projection of the in-scattering term (a transition from \( \epsilon - \hbar \omega \) to \( \epsilon \)) yields [7]

\[
S_{l,m}^{in}(\epsilon) = \sum_{l',m',l''} \left[ Z_{l',m'}(\epsilon - \hbar \omega) g_{l',m'}(\epsilon) a_{l',m',l''} \right]
\times g_{l',m'}(\epsilon + \hbar \omega) c_{l',m'}(\epsilon) \epsilon_{l',m',l''}, \tag{2}
\]

where \( Z \) is the (angle dependent) density-of-states, \( g \) the generalized energy distribution function which is a product of the density-of-states and the distribution function, \( \epsilon \) the coefficient for the transition rate, and \( [Z - g] \) the so-called Pauli factor projected onto energy. Similarly, the projection of the out-scattering term (a transition from \( \epsilon \) to \( \epsilon + \hbar \omega \)) yields [7]

\[
S_{l,m}^{out}(\epsilon) = \sum_{l',m',l''} \left[ Z_{l',m'}(\epsilon + \hbar \omega) - g_{l',m'}(\epsilon + \hbar \omega) \right]
\times g_{l',m'}(\epsilon) c_{l',m'}(\epsilon + \hbar \omega) a_{l',m',l''}, \tag{3}
\]

The integral of the triple product, \( a_{l,m,l',m',m''} \), is given by

\[
a_{l,m,l',m',m''} = \int Y_{l,m} Y_{l',m'} Y_{l'',m''} d\Omega, \tag{4}
\]

where \( Y_{l,m} \) is a spherical harmonic. Therefore, a term like \( g_{l',m'}^{l''} g_{l''}^{l'} \) is newly introduced because of the Pauli principle, and the Boltzmann equation becomes nonlinear. In order to have quadratic convergence of the Newton-Raphson scheme like in [8], the dependence of \( g_{l',m'}^{l''} g_{l''}^{l'} \) on the electrostatic potential is considered in the Jacobian matrix.

Significant simplification can be obtained when the transition rate does not depend on the scattering angle:

\[
\epsilon_{l} = \epsilon_{0} \delta_{l,0}. \tag{5}
\]

The in-scattering term is given by

\[
S_{l,m}^{in}(\epsilon) = [Z_{l,m}(\epsilon) - \epsilon_{l,m}(\epsilon)]
\times \epsilon_{0,0}(\epsilon - \hbar \omega)c_{l,0}(\epsilon) Y_{0,0}. \tag{6}
\]

The out-scattering term is given by

\[
S_{l,m}^{out}(\epsilon) = [Z_{0,0}(\epsilon + \hbar \omega) - \epsilon_{0,0}(\epsilon + \hbar \omega)]
\times \epsilon_{l,m}(\epsilon)c_{0}(\epsilon + \hbar \omega) Y_{0,0}. \tag{7}
\]

Note that the velocity-randomizing scattering mechanism – for example, phonon scattering with constant matrix elements – is corresponding to this case.
Dirac statistics, step function, and \( v_n \) where \( \Delta n \) principle.

In the maximum H-transformation and the maximum entropy dissipation principle is stable even in the case of the extremely scaled SiGe HBTs shown in [14].

A two-dimensional SiGe HBT whose cutoff frequency is about 260GHz at room temperature has been simulated. The maximum doping level in the emitter region is as high as \( 2 \times 10^{20}/\text{cm}^3 \). The analytical band model and the parameters of the related phonon scattering mechanisms proposed by the Modena group [15] have been utilized for electrons. In the case of impurity scattering an approximation by an isotropic-elastic process [9], [16] is employed. A third-order spherical harmonics expansion for the electron distribution function is used.

In Fig. 1 typical convergence behavior of the simulation is shown for different bias points. The initial solution is obtained by solving the nonlinear Boltzmann equation for a fixed electrostatic potential. Once an initial solution of the Boltzmann equation is obtained, a fully-coupled scheme is used for the Boltzmann and Poisson equations. Only when the maximum value of the potential correction at a certain Newton-Raphson iteration exceeds the energy spacing (typically 5meV in this work), additional fixed potential simulations are performed. Usually two or three iterations are sufficient to achieve a converged solution of the nonlinear Boltzmann equation, as shown in Fig. 3. When the temporal solution of the Newton-Raphson iteration is close enough to the converged solution, such fixed potential iterations naturally disappears. In every simulation the last Newton-Raphson step shows a huge decrease of the norm of the update vector.

In Fig. 4 the electron distribution function in the emitter region is shown for different Newton-Raphson iterations. In the first step its maximum value is larger than unity. However, the result of the second iteration already is very close to the Fermi-Dirac distribution.

In Fig. 5 the electron distribution function with or without the Pauli principle is shown. In the emitter region the degeneracy effect in the electron distribution function is clearly visible. However, for other regions (base and collector), the difference due to the statistics is negligible because the bandgap narrowing is modified in order to compensate it. The electron distribution function in the collector region demonstrates that our injection boundary condition [8] can handle such highly non-equilibrium distributions without any difficulties.

In Fig. 6 the electron density of the SiGe HBT is shown along the vertical position. For comparison, its counterpart for Maxwell-Boltzmann statistics is also displayed and the differences are rather small. Note that the electron density shows considerable differences without the bandgap correction, as shown in Fig. 7.
In Fig. 8 the cutoff frequency of the SiGe HBT in the quasi-stationary limit [17] is shown. Since macroscopic quantities such as the electron density agree well between the two statistics, again the impact of the Pauli principle is small, although the internal distribution function is quite different in the heavily-doped region.

IV. CONCLUSION

We have implemented a deterministic Boltzmann solver including the Pauli principle. Several modifications of the physical models – the scattering operator, the boundary condition, and the bandgap narrowing model – were made in order to consider Fermi-Dirac statistics. The resultant Boltzmann equation is stable and convergence degradation is not observed.

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REFERENCES

Fig. 6. Electron density along the vertical position for different $V_{BE}$ values, 0.74V, 0.79V, 0.84V, and 0.89V. The lateral position is fixed to the center of the emitter window. $V_{CE} = 1.2$V.

Fig. 7. Electron density obtained from simulations with or without the bandgap narrowing correction. The Pauli principle is included. Simulation condition is the same with Fig. 6.


