SIMULATION OF SEMICONDUCTOR PROCESSES AND DEVICES Vol. 12
Edited by T. Grasser and S. Selberherr - September 2007

Inclusion of the Pauli Principle in the Langevin-Boltzmann Equation for Bulk Systems

C. Jungemann

Institute for Electronics, Bundeswehr University, 85577 Neubiberg
Jungemann@ieee.org

Abstract

The Pauli principle, which limits the occupancy of a single state to one electron, is included in a deterministic solver for the Langevin-Boltzmann equation (LBE) based on a spherical harmonics expansion. The Newton-Raphson scheme for solving the nonlinear BE converges within a few steps and the increase in CPU time is less than a factor of ten. Even in the case of an extremely degenerate electron gas no numerical problems occur. The approach works well for transport and noise, and the Nyquist theorem is satisfied with high numerical precision at equilibrium. For electrons in bulk silicon a non-negligible impact of the Pauli principle is found only at very high electron densities.

1 Introduction

The Pauli Principle limits the occupancy of a state to a single electron per spin direction [1]. It has a strong impact on transport at high electron densities, when the value of the distribution function $f_\nu(\boldsymbol{k},t)$ at low energies approaches its maximum of one. This reduces scattering, because electrons can be scattered only into empty states. This effect is accounted for in the scattering integral of the BE by multiplying the transition rate with the probability that the final state is empty: $1-f_\nu(\boldsymbol{k},t)$. Evaluation of this factor requires the knowledge of the distribution function at all times during a simulation. In the case of the Monte Carlo method this entails an ensemble simulation [2], which can be very CPU intensive. This problem does not occur in the case of a solver based on a spherical harmonics expansion (SHE) of the distribution function [3], because the distribution function is inherently known at all times [4]. In addition, the SHE approach has many advantages in the case of noise calculations [5]. Here, a solver for the Langevin-Boltzmann equation (LBE) including the Pauli principle is presented.

2 Model

The electron model is based on the analytical six valley band structure and phonon scattering mechanisms developed by the Modena group [6]. Impurity scattering is modeled according to the Brooks-Herring approach [7], where the scattering rate is modified in a heuristic way such that the experimental mobility is reproduced correctly at high doping concentrations [8]. The SH expansion is truncated at an order, for which the truncation error is negligible under bulk conditions (usually the third order). Energy is

discretized with an equi-distant grid and the spacing is 1meV. Details of the expansion can be found in Ref. [9]. Due to the Pauli principle the scattering integral of the BE becomes nonlinear

$$\frac{\partial f_\nu(\boldsymbol{k},t)}{\partial t} - \frac{e}{\hbar}\boldsymbol{E}^{\mathrm{T}}\boldsymbol{\nabla}_{\boldsymbol{k}} f_\nu(\boldsymbol{k},t) = \frac{\Omega_{\mathrm{s}}}{(2\pi)^3}\sum_{\nu'=1}^{6}\int \left\{\left[1-f_\nu(\boldsymbol{k},t)\right] W_{\nu,\nu'}(\boldsymbol{k}|\boldsymbol{k}')\, f_{\nu'}(\boldsymbol{k}',t) - \left[1-f_{\nu'}(\boldsymbol{k}',t)\right] W_{\nu',\nu}(\boldsymbol{k}'|\boldsymbol{k})\, f_\nu(\boldsymbol{k},t)\right\} \mathrm{d}^3k' \,. \quad (1)$$

and the LBE is solved by the Newton-Raphson method. The initial condition is the equilibrium Fermi-Dirac distribution, which ensures that the Pauli factor $1-f_\nu(\boldsymbol{k},t)$ is positive. Noise is calculated based on the Langevin approach [10, 11, 5] and fluctuations of the distribution function in the Pauli factor are automatically included. This is in contrast to Ref. [4], where those fluctuations were ignored leading to a large error [12].

3 Bulk Results

In order to exemplify the impact of the Pauli principle and to test the robustness of the numerical approach a rather high electron density of $10^{21}/\mathrm{cm}^3$ is investigated, which leads to a strongly degenerate electron gas even at room temperature. The Newton-Raphson scheme nevertheless converges within a few iterations and convergence becomes quadratic close to the solution (Fig. 1). Even at an electric field of $100\mathrm{kV}/\mathrm{cm}$ the distribution function is close to a value of one at low energies (Fig. 2) and the Pauli principle has a strong impact. This is shown for the drift velocity in Fig. 3. At low electric fields simulations with and without the Pauli principle yield the same velocity, because the impurity scattering model was calibrated in both cases to reproduce the experimental low-field mobility. At high electric fields a large difference occurs and for an electric field of $100\mathrm{kV}/\mathrm{cm}$ the drift velocity evaluated including the Pauli principle is about twice as large as without. An analogous result is obtain for noise. The power spectral density of the velocity fluctuations is shown for zero frequency in Fig. 4 and at low electric fields both methods yield the same result. This is due to the Nyquist theorem, which takes the same form in both cases and since the low-field mobility is the same, the noise must be the same. The Nyquist theorem is satisfied with a numerical accuracy of more than four digits. Similar to the case of the drift velocity, at high electric fields large differences occur between simulations with and without the Pauli principle and the result including the Pauli principle is about three times as large as the other one at $100\mathrm{kV}/\mathrm{cm}$.
A case, which is not discussed in this paper and where the Pauli principle has a strong impact, is the one of deep traps. Even in the case of a dilute electron gas in the conduction bands, deep traps are often located below the Fermi level. In this case the Pauli principle has a strong impact on the occupancy of the traps and the corresponding noise [12].

4 Conclusions

A SHE solver for the LBE including the Pauli principle has been presented. The approach is numerically robust and converges within a few iterations. This approach might

also work in the case of devices in contrast to the Monte Carlo approach, which in that case requires an ensemble device simulation with a prohibitive number of particles due to the high number of dimensions of the phase space. It has been shown that at least for very high electron densities the Pauli principle has a non-negligible impact.

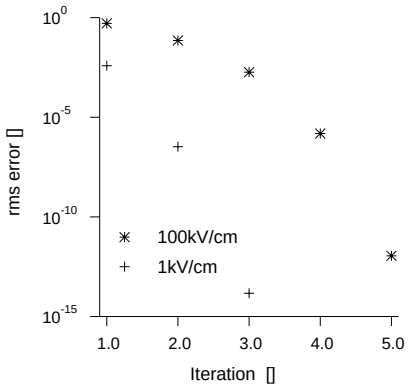

Figure 1: Root mean square error of the distribution function for an electron concentration of $10^{21}/\mathrm{cm}^3$ in silicon at 300K.

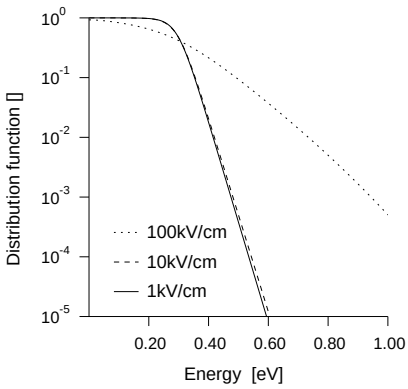

Figure 2: Electron distribution function in the valley with the principle axis along the electric field, which is in $\langle 100 \rangle$ direction, for silicon at 300K.

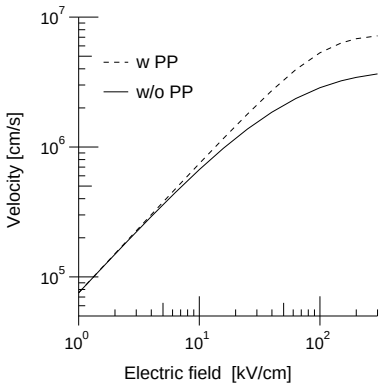

Figure 3: Drift velocity calculated with the Pauli principle (w PP) and without (w/o PP) for an electron concentration of $10^{21}/\mathrm{cm}^3$ in silicon at 300K.

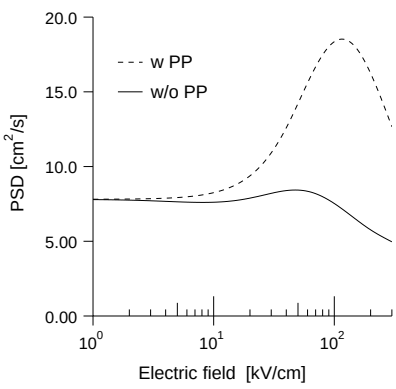

Figure 4: Power spectral density of the velocity fluctuations calculated with the Pauli principle (w PP) and without (w/o PP) for an electron concentration of $10^{21}/\mathrm{cm}^3$ in silicon at 300K.

References

[1] O. Madelung, *Introduction to Solid State Theory*, Springer, Berlin, 1978.

[2] P. Lugli and D.K. Ferry, "Degeneracy in the Ensemble Monte Carlo Method for High-Field Transport in Semiconductors," *IEEE Trans. Electron Devices*, vol. 32, no. 11, pp. 2431–2334, 1985.

[3] N. Goldsman, L. Henrickson, and J. Frey, "A physics-based analytical/numerical solution to the Boltzmann transport equation for use in device simulation," *Solid–State Electron.*, vol. 34, pp. 389–396, 1991.

[4] A. J. Piazza, C. E. Korman, and A. M. Jaradeh, "A physics-based semiconductor noise model suitable for efficient numerical implementation," *IEEE Trans. Computer–Aided Des.*, vol. 18, no. 12, pp. 1730–1740, 1999.

[5] C. Jungemann, "A deterministic approach to RF noise in silicon devices based on the Langevin Boltzmann equation," *IEEE Trans. Electron Devices*, vol. 54, no. 5, pp. 1185–1192, 2007.

[6] R. Brunetti, C. Jacoboni, F. Nava, L. Reggiani, G. Bosman, and R. J. J. Zijlstra, "Diffusion coefficient of electrons in silicon," *J. Appl. Phys.*, vol. 52, pp. 6713–6722, 1981.

[7] H. Brooks, "Scattering by ionized impurities in semiconductors," *Phys. Rev.*, vol. 83, pp. 879, 1951.

[8] C. Jungemann and B. Meinerzhagen, *Hierarchical Device Simulation: The Monte-Carlo Perspective*, Computational Microelectronics. Springer, Wien, New York, 2003.

[9] C. Jungemann, A.-T. Pham, B. Meinerzhagen, C. Ringhofer, and M. Bollhöfer, "Stable discretization of the Boltzmann equation based on spherical harmonics, box integration, and a maximum entropy dissipation principle," *J. Appl. Phys.*, vol. 100, pp. 024502–1–13, 2006.

[10] Sh. Kogan, *Electronic Noise and Fluctuations in Solids*, Cambridge University Press, Cambridge, New York, Melbourne, 1996.

[11] S. V. Gantsevich, V. L. Gurevich, and R. Katilius, "Theory of fluctuations in nonequilibrium electron gas," *Nuovo Cimento*, vol. 2, pp. 5, 1979.

[12] C. Jungemann, "A deterministic solver for the Langevin Boltzmann equation including the Pauli principle," in *Proceedings of SPIE Fluctuations and Noise Conference*, Florence, 2007.