A Quasi-Particle Model of the Electron - Wigner Potential Interaction

M. Nedjalkov, H. Kosina, and S. Selberherr

Institute for Microelectronics, TU - Vienna,
Gusshausstrasse 27-29 / E360, A-1040 Vienna, Austria
e-mail: Nedjalkov@iue.tuwien.ac.at

The Wigner-function (f_w) formalism has been recognized as a convenient approach to describe electron transport in mesoscopic systems. The approach combines a rigorous quantum-kinetic level of treatment with the classical concepts for phase space and open boundary conditions. Moreover the classical Boltzmann collision operator B is used to account for the phonon interaction in picosecond transport regimes. In this case the Wigner equation reads: $(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r)f_w = V_w[f_w] + B[f_w]$ where V_w is the Wigner potential. Particularly useful is the conjugate integral form of the equation with a kernel denoted by K. Physical averages are expressed as series obtained by consecutive iterations of the kernel K. The series can be interpreted in terms of particle trajectories. A particle picture is associated to the transport process [1], where the Wigner potential acts as a scattering source. A general property of this approach is that particles accumulate weight with each scattering event. As used for the evaluation of physical averages, the weight can cause severe problems for the numerical aspects of the task [2]. The weight accumulation originates from the Wigner potential whose modulus $|V_w|$, does not ensure mass conservation. We use this property for a model where the action of the Wigner potential gives rise to generation of particle pairs.

The kernel K is modified by a decomposition of the antisymmetric function V_w into two positive functions $V_w = V_w^+ - V_w^-$. Furthermore a function $\nu(\mathbf{r}) = \int V_w^{\pm}(\mathbf{r},\mathbf{k})d\mathbf{k}$ is introduced. For better clarity the coherent one-dimensional case is presented:

$$K = \left\{\nu(t')e^{-\int_0^{t'}\nu(y)dy}\right\}_1 \left(\{\delta(k_x - k_x')\}_2 + \left\{\frac{V_w^+(x(t'), k_x - k_x')|}{\nu(t')}\right\}_2 - \left\{\frac{V_w^-(x(t'), k_x - k_x')|}{\nu(t')}\right\}_2\right) \quad (1)$$

Here $x(t) = x + v_x t$ and $\nu(t) = \nu(x(t))$. The kernel links phase space points in a way which can be viewed as particle propagation. The terms in the curly brackets are conditional probability densities with a subscript denoting the order of their application. $\{.\}_1$ selects the time t' of a transition between the initial state $(k_x, x, 0)$ and $(k_x, x(t'), t')$, The process is associated with a particle undergoing free flight. The terms $\{.\}_2$ simultaneously select three values of k_x' corresponding to three states $(k_x', x(t'), t')$. They are initial states for the free flights in the subsequent iteration of K and, thus, are associated with tree particles. The δ function shows that one of them, the initial particle, which survives at the end of the free flight and is further continued. The other two are newborn particles. As generated by $\pm V_w^{\pm}/\nu$ they carry opposite signs. The signs are used in the evaluation of the averages, and do not affect the evolution process. For convenience particles are marked as positive and negative.

In the general case, the events of phonon scattering are complementary to events of interaction with the Wigner potential. It follows that quasi-particles are Boltzmann-like particles, subject to processes of free flights and scattering by phonons which proceed in a classical way. The interaction with the Wigner potential occurs during the free flights and results in generation of pairs of positive and negative particles. The generation rate and the distribution of the newborn particles in the phase space depends on V_w according to (1). Positive and negative particles located close together have the same evolution but opposite contribution to the averages and therefore cancel each other. Generation and cancellation of particles are characteristic features of this quantum transport model. The model significantly improves the numerical properties of the simulation task. Monte Carlo simulations of resonant-tunneling diode have been carried out. The obtained I-V characteristics and the distribution of generic physical quantities have been compared with results obtained by other methods.

Acknowledgment: This work has been supported by the European Commission project NANOTCAD, IST-1999-10828.

References

1 C. Jacoboni, A. Bertoni, P. Bordone, R. Brunetti, Wigner-function Formulation for Quantum Transport in Semiconductors: Theory and Monte Carlo Approach, *Mathematics and Computers in Simulations*, 55, 1-3, 67-78, 2001

2 M. Nedjalkov, R. Kosik, H. Kosina, S. Selberherr, Wigner Transport through Tunneling Structures - Scattering Interpretation of the Potential Operator, *Proc. Simulation of Semiconductor Processes and Devices*, (Kobe,Japan) 187-190, 2002