Stochastic Interpretation of Wigner Transport in Nanostructures

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A stochastic interpretation of the quantum transport in nanoscale electronic devices is proposed. Considered is the Wigner equation which accounts for the coherent part of the transport via the Wigner potential V_w and for dissipation processes due to the lattice imperfections such as phonons via the Boltzmann collision operator B.

$$\left(\frac{\partial}{\partial t} + \frac{\hbar \mathbf{k}}{m}\frac{\partial}{\partial \mathbf{r}}\right) f_w(\mathbf{r},\mathbf{k},t) = (V_w f_w)(\mathbf{r},\mathbf{k},t) + (B f_w)(\mathbf{r},\mathbf{k},t) \tag{1}$$

At present, deterministic methods can only solve the coherent Wigner equation or include dissipation in the relaxation time approximation [1].

The stochastic approach is motivated by the Monte Carlo (MC) method for device simulation, where the collision operator is treated exactly, but the coherent part is presented by its classical limit. This limit leads to a classical force term transforming (1) into the Boltzmann equation. How to account for the complete potential term is the main concern of the approach. It is shown that the action of the Wigner potential operator can be interpreted in terms of scattering events in a strict analogy with the Boltzmann operator B. In this way the entire right hand side of equation (1) is treated as a scattering term where the interaction with the quantum potential appears as an additional scattering mechanism. An out-scattering rate from the Wigner potential can be introduced which has a meaning similar to the phonon and impurity out-scattering rates. A particle picture can be associated to the transport process. Particles which are injected from the device boundaries are scattered by phonons and the potential. Two peculiarities are due to the quantum character of the transport process. The potential interaction is non-local, i.e. particles are subject to potential scattering away from the physical location of the tunneling barrier. Second, a sign is associated to the particles. This sign can become negative which is in accordance with the fact that the Wigner function allows negative values.

A Monte Carlo method based on the particle picture has been developed. It retains the basic features of the weighted Single Particle MC method [2]. The method has been applied for simulation of stationary coherent transport in a resonant-tunneling diode. The obtained I-V characteristics and the distribution of the generic physical quantities in the device demonstrate the correctness of the approach.

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[1] J. Sun, G. Haddad, P. Mazumder, and J. Schulman, Proceedings of IEEE **86**, 641 (1998).

[2] H. Kosina, M. Nedjalkov, and S. Selberherr, in *Proc. Modeling and Simulation of Microsystems, MSM 2001,* edited by M. Laudon and B. Romanowicz (Computational Publications, 2001), pp. 11–14.