A Monte Carlo Method Seamlessly Linking Quantum and Classical Transport Calculations

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A quantum Monte Carlo method taking into account both interference and dissipation effects is presented. The method solves the space-dependent Wigner equation

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla_r + q\mathbf{E}\cdot\nabla_k\right) f_w = Q[f_w] + \Theta_w[f_w]\,. \tag{1}$$

Scattering processes are treated semi-classically by the Boltzmann collision operator $Q[f_w]$. The classical force term $q\mathbf{E}$ is separated from the Wigner potential and included in the Liouville operator on the left hand side [1]. For sufficiently small potential gradients the Wigner potential vanishes and only the classical force term remains. Consequently, the presented MC method simplifies gradually to the classical MC method when the classical limit is approached. Introducing the truncated Wigner potential, $V_w^+(\mathbf{k}) = \mathrm{Max}(0, V_w(\mathbf{k}))$, the potential operator is reformulated as [2]

$$\Theta_w[f_w](\mathbf{k},\mathbf{r}) = \int V_w^+(\mathbf{q},\mathbf{r})\,[f_w(\mathbf{k}-\mathbf{q},\mathbf{r}) - f_w(\mathbf{k}+\mathbf{q},\mathbf{r})]\,d\mathbf{q}\,. \tag{2}$$

A particle model is presented which interprets (2) as a generation term. Pairs of numerical particles carrying the statistical weights $+1$ and -1 are generated at a rate $\gamma(\mathbf{r}) = \int V_w^+(\mathbf{q},\mathbf{r})\,d\mathbf{q}$. In this picture, (1) has the form of a Boltzmann equation augmented by a generation term Θ_w, such that in principle any MC method for solving the Boltzmann equation can be employed, extended by a mechanism for generating particle pairs. The challenge of employing such algorithm is to handle the avalanche of numerical particles properly. This problem has been solved for stationary conditions. Particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation.

Resonant tunneling diodes (RTD) have been simulated using the new MC algorithm. The Wigner generation rate $\gamma(\mathbf{r})$ reaches fairly high values in this structure (Fig. 1) and is used to distinguish between classical ($\gamma = 0$) and quantum regions ($\gamma > 0$). To apply well-posed boundary conditions, significant parts of the highly doped contact regions are included in the simulation domain. Fig. 2 demonstrates that the electron concentration and the mean energy are nearly constant in the contact regions and not affected by the strong onset of the Wigner generation rate. The influence of phonon scattering on the electron concentration is shown in Fig. 3 and Fig. 4. Phonon scattering leads to an increase in the valley current and a resonance voltage shift as shown in Fig. 5. The mean energy, which is strongly affected by the variance of the MC method, is given in Fig. 6.

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[1] P.Bordone, A.Bertoni, R.Brunetti, C.Jacoboni: "Monte Carlo Simulation of Quantum Electron Transport Based on Wigner Paths," in "Abstracts Seminar on Monte Carlo Methods," Salzburg, Sep.2001, p.53.

[2] H.Kosina, M.Nedjalkov, and S.Selberherr: "Quantum Monte Carlo Simulation of a Resonant Tunneling Diode Including Phonon Scattering", in "Proc. Nanotech 2003", San Francisco, Feb.2003 (in print).

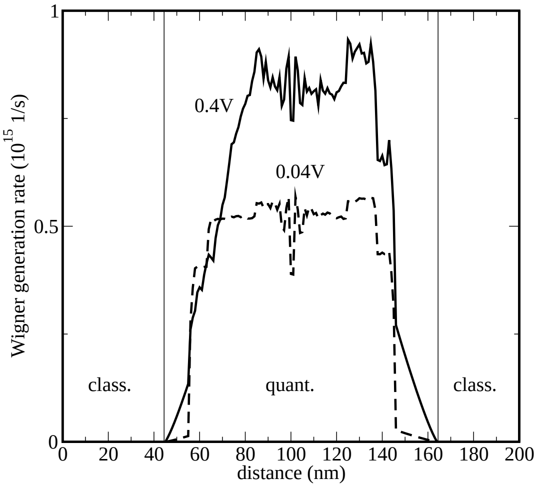

Figure 1: Pair generation rate $\gamma(x)$ caused by the Wigner potential.

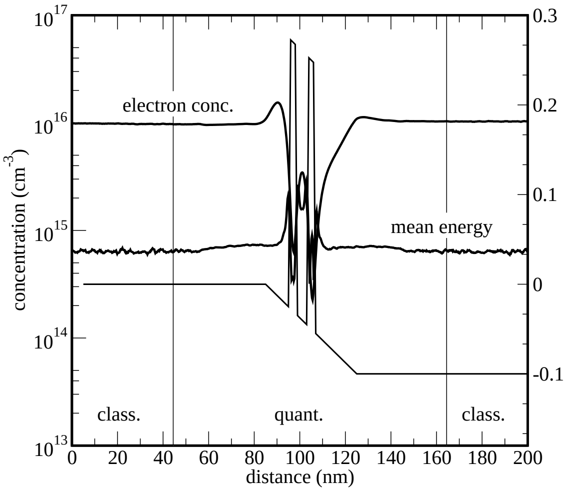

Figure 2: Electron concentration and mean electron energy in the RTD at T=300K and 0.1V bias.

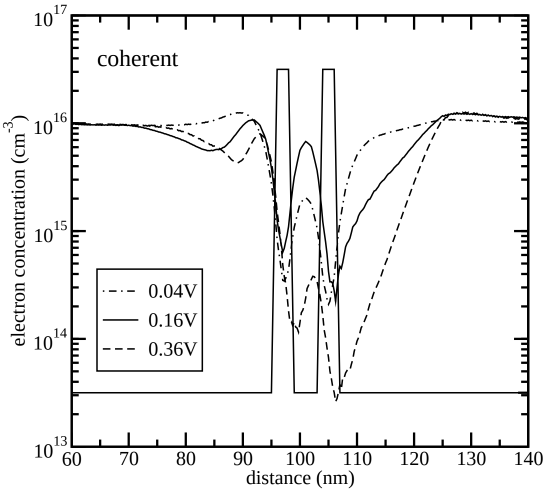

Figure 3: Electron concentration in the RTD without scattering.

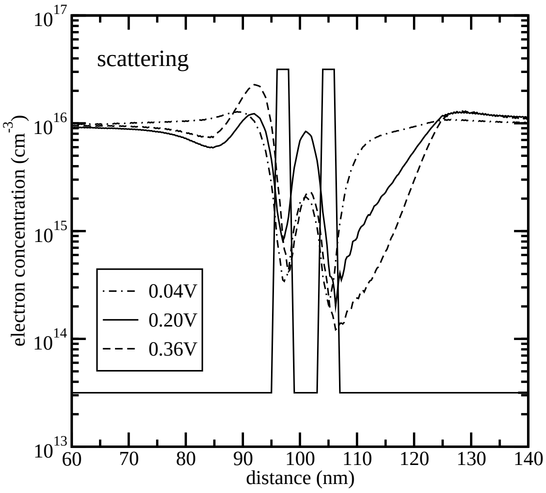

Figure 4: Electron concentration in the RTD including phonon scattering.

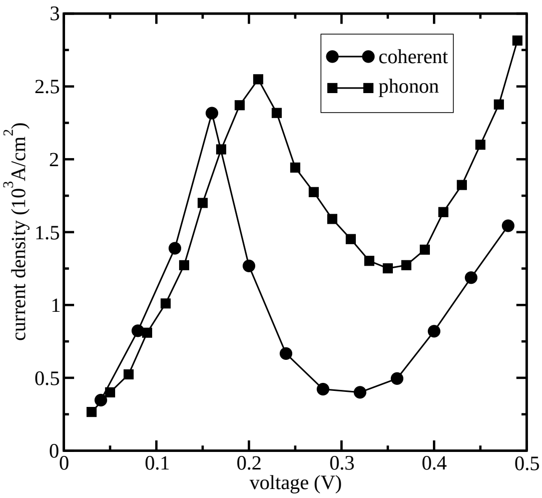

Figure 5: Influence of phonon scattering on the IV-characteristics of the RTD.

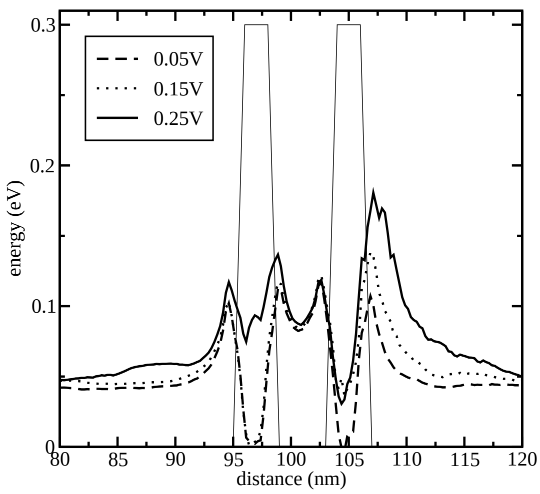

Figure 6: Mean electron energy for different applied voltages.