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Quantum Corrections to Semiclassical Transport in Nanoscale Devices using Entropy Principles

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I. Background

The simulation of nanoscale devices requires, at least rudimentarily, the inclusion of quantum effects. Quite a lot of attention has been paid to the quantum mechanical modelling of free (collisionless) transport. Efforts here include the direct solution of the Schrödinger equation [2], [11], macroscopic moment equations (quantum hydrodynamic models) [9], [10], and extensions of semiclassical Monte Carlo methods, either directly [13], [8] or via effective potential approaches [6], [1], [12]. Comparably little work has been done on the inclusion of quantum effects into collision operators. Collisions can be treated quite rigorously using Green's functions or by Wigner function methods for the phonon system [7]. Using classical collision operators in collusion with quantum corrected transport models has the disadvantage that equilibrium solutions of the resulting system do not correspond to admissible quantum mechanical states, since the semiclassical phonon collision operator increases the classical entropy and not the correct quantum mechanical entropy, given by $S = Tr[\rho(\ln \rho - 1)]$, where ρ denotes the density matrix of the mixed state.

II. Quantum entropy principles

In recent work [3], [4], [5] we have developed the framework to extend semiclassical transport equations, like the Boltzmann equation, to a quantum mechanical setting via the local maximization of the quantum entropy. This results in a modification of the semiclassical phonon collision operator. The resulting operator dissipates the quantum entropy, while maintaining the local conservation properties of the semiclassical collision operator. In the Wigner picture, i.e. in terms of the Wigner function $f_w(\mathbf{r}, \mathbf{k})$, for a given potential $V(\mathbf{r})$ it is of the form

$$Q[f_w](\mathbf{r}, \mathbf{k}) = \tag{1}$$

$$\int K(\mathbf{r}, V, \mathbf{k}, \mathbf{k}')\phi(\mathbf{r}, \mathbf{k}')\ d\mathbf{k}' - \kappa(\mathbf{r}, \mathbf{k}, V)\phi(\mathbf{r}, \mathbf{k})\ ,$$

where $\phi(\mathbf{r}, \mathbf{k})$ is the quantum mechanical entropy variable, i.e. a generalization of the quasi- Fermi function. The relation between the Wigner function f_w and the entropy variable ϕ is given by a nonlocal, potential dependent, integral relation of the form

$$f_w(\mathbf{r}, \mathbf{k}) = \int A(V, \mathbf{r}, \mathbf{k}, \mathbf{r}', \mathbf{k}')\phi(\mathbf{r}', \mathbf{k}')\ d\mathbf{r}'d\mathbf{k}'\ . \tag{2}$$

The quantum corrected collision operator acts like a classical collision operator on the entropy variable ϕ, but is nonlocal in space because of the nonlocal relation (2) between f_w and ϕ. The resulting collision operator dissipates the quantum entropy and drives the system to a quantum mechanically correct equilibrium. It maintains the local conservation properties, i.e. a collision event results in the exchange of an amount $\hbar\omega$ of energy with the lattice. The operator Q in (1) is amenable to Monte Carlo discretizations as well as series expansion methods. We will present preliminary results for a tunneling diode using a spherical harmonics expansion method of the resulting Wigner - Boltzmann equation. Figures 1-4 show the relation between the Wigner function f_w and the entropy variable ϕ, which would classically be given by $f_w = e^{-H}\phi$, for a potential barrier. Figure 1 shows the potential and Figure 2 shows the Wigner function f_w for a constant entropy variable ϕ. Figures 3 and 4 show

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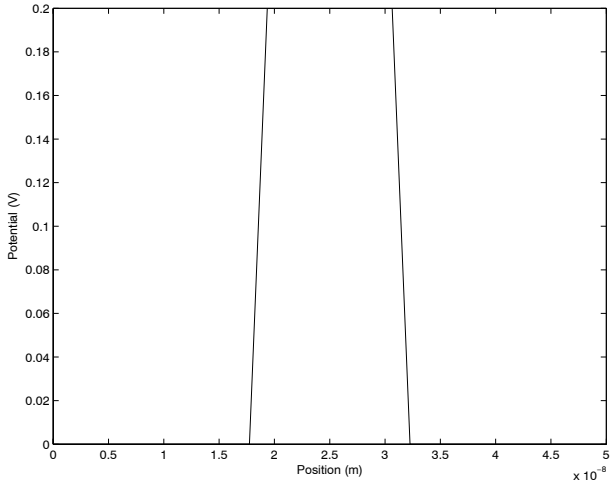

Fig. 1. Potential

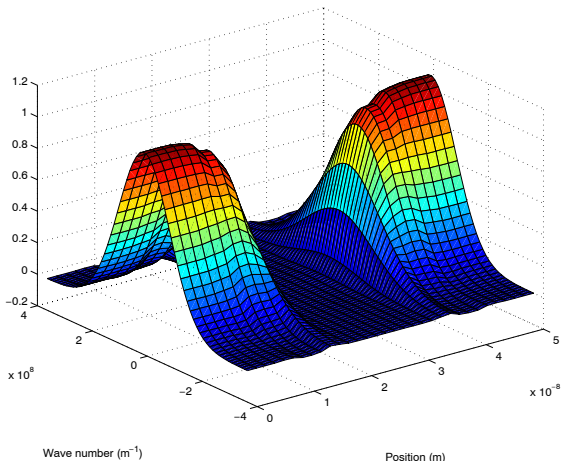

Fig. 2. Wigner function f_w for a constant entropy variable ϕ

the corresponding relations for an entropy variable ϕ which is concentrated inside the potential barrier.

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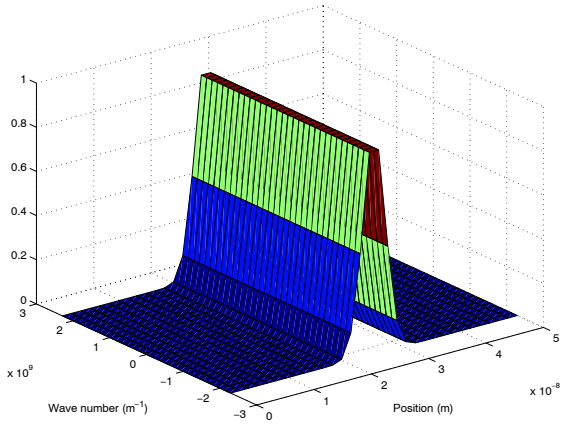

Fig. 3. ϕ concentrated inside the barrier

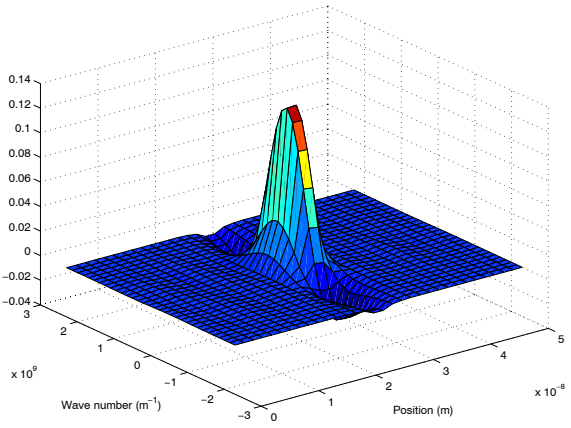

Fig. 4. Wigner function f_w corresponding to ϕ in Figure 3