On the Consistency of the Stationary Wigner Equation

Robert Kosik[1], Mischa Thesberg[1], Josef Weinbub[2], and Hans Kosina[1]
[1]*Institute for Microelectronics, TU Wien, Austria*
[2]*Christian Doppler Laboratory for High Performance TCAD at the Institute for Microelectronics, TU Wien, Austria*
kosina@iue.tuwien.ac.at

The Wigner equation describing stationary quantum transport has a singularity at zero momentum (k=0). Numerically the singularity is usually dealt with by just avoiding that point in the grid, a method used, e.g, by Frensley [1]. However, results obtained by this method are known to depend strongly on the discretization and meshing parameters. The method can even yield unphysical results.

We believe that the shortcomings of Frensley's method and related numerical methods are due to the improper treatment of the equation at k=0. We propose a revised approach. We explicitly include the point k=0 in the grid and derive two equations for that point. The first one is an algebraic constraint which ensures that the solution of the Wigner equation has no singularity at k=0. The second is a transport equation for k=0. The resulting system, which we refer to as the constrained Wigner equation, is overdetermined. These results are in line with the recent analysis in [2].

An important technical tool is the sigma equation which is the von Neumann equation in a rotated coordinate system. The constrained Wigner equation can be related to a sigma equation with inflow boundary conditions in the spatial coordinate and fully homogeneous boundary conditions in the other coordinate. With these boundary conditions the sigma equation is overdetermined as well. The numerical solution from Frensley's method is related to a sigma equation with anti-periodic boundary conditions in the non-spatial coordinate.

In a single spatial dimension the constrained Wigner and sigma equation have been prototyped. Results fit well with results from the quantum transmitting boundary method.

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[1] W. R. Frensley, Rev. Mod. Phys. **62**, 745 (1990)
[2] R. Li *et al.*, Front. Math. China **12**, 907 (2017)

$$\frac{\partial f(r,k)}{\partial r} = \frac{1}{k}\frac{m}{\hbar}\int f(r,k-k')V_w(r,k')dk' \qquad (k \neq 0)$$

$$\frac{\partial f(r,0)}{\partial r} = -\frac{m}{\hbar}\int f_k(r,k')V_w(r,k')dk' \qquad (k = 0)$$

$$\int f(r,k')V_w(r,k')dk' = 0 \qquad \text{(regularity constraint)}$$

Fig. 1: Set of equations referred to as the constrained Wigner equation.

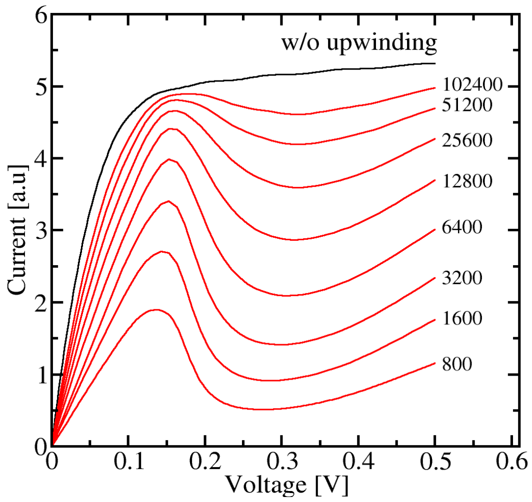

Fig. 2: Breakdown of Frensley's Method. *The upper black line is the numerical solution of the unconstrained sigma equation (anti-periodic BCs) without upwinding. The red lines are I–V curves obtained with Frensley's discretization using upwinding. The grid is refined from Nx=800 up to Nx=102400.*

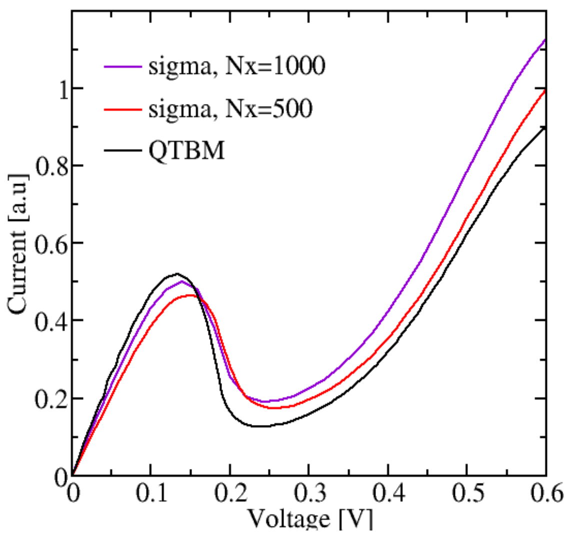

Fig. 3: The numerical solutions of the constrained sigma equation change with grid refinement, but they are quite stable. The resonance from the quantum transmitting boundary method (QTBM) is reproduced.