Open Boundary Conditions for the Wigner and the Characteristic von Neumann Equation

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Open boundary conditions for the Wigner equation have been introduced by Frensley [1] who used inflow boundary conditions at spatial boundaries. On a coarse mesh Frensley's model produces superficially reasonable solutions, which however are an artifact of numerical diffusion. The model breaks down in the limit of a fine mesh [2].

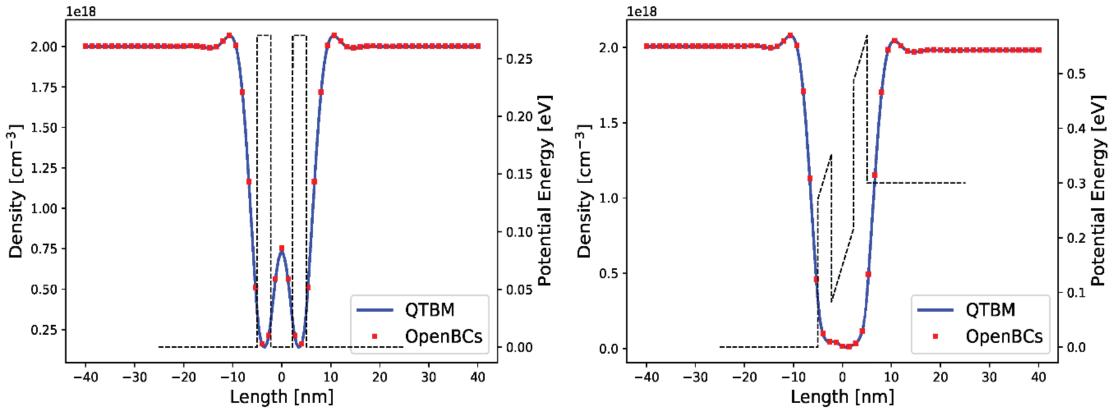
Frensley's discretization corresponds to anti-periodic boundary conditions in the non-spatial coordinate of the characteristic von Neumann equation. To remedy the breakdown an absorbing imaginary potential can be employed as suggested in [3]. The absorbing potential avoids spurious reflections at non-spatial boundaries in the characteristic equation.

Here we introduce a formulation of open boundary conditions based on a symmetric treatment of spatial and non-spatial coordinates in the characteristic equation. We apply inflow type boundary conditions also at the non-spatial boundaries. For this we use the Fourier transform of the characteristic function in the spatial coordinate which is denoted ambiguity function. We impose the condition that the flow into the domain at non-spatial boundaries is zero.

As shown in Figures 1 and 2 results based on "no inflow" boundary conditions (open BCs) closely reproduce results from the quantum transmitting boundary method (QTBM). In Figure 3 we compare results from open BCs with results when using an absorbing potential and find excellent agreement. This work clarifies the notion of open boundary conditions for the Wigner and the characteristic Neumann equation and demonstrates its numerical robustness.

Acknowledgements. This work was partly funded by FWF Austrian Science Fund, project number P33151 "Numerical Constraints for the Wigner and the Sigma Equation".

[1] W. R. Frensley, Rev. Mod. Phys. 62(3), 745–791 (1990)
[2] R. Kosik *et al.,* In: Large-Scale Scientific Computing, p. 403-410 (Springer, 2020)
[3] L. Schulz, D. Schulz, IEEE Trans. Nanotechnol. 18, 830-838 (2019)



(a) Bias = 0.0 V (b) Bias = 0.3 V

Figure 1: Comparison of the particle density in the active region of a resonant tunneling diode structure for different biases using QTBM and open BCs. The dashed black lines indicate potential energy. The coherence length used is 120 nm. Mesh size $N_r = 1000$, $N_s = 907$.

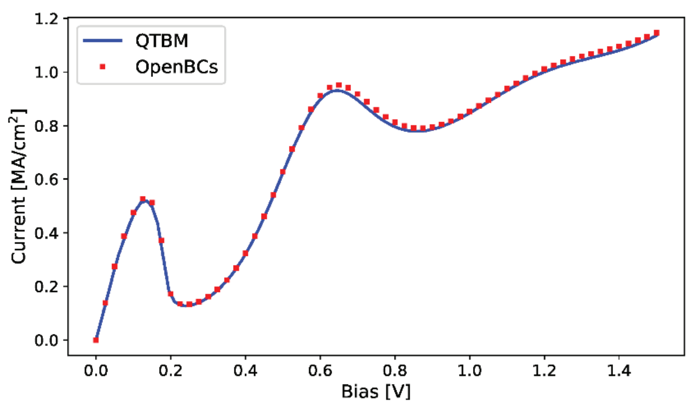


Figure 2: Simulation of the current-voltage curve for the same resonant tunneling structure as used in Fig. 1. Again, good agreement between the solution based on open BCs and the QTBM solution.

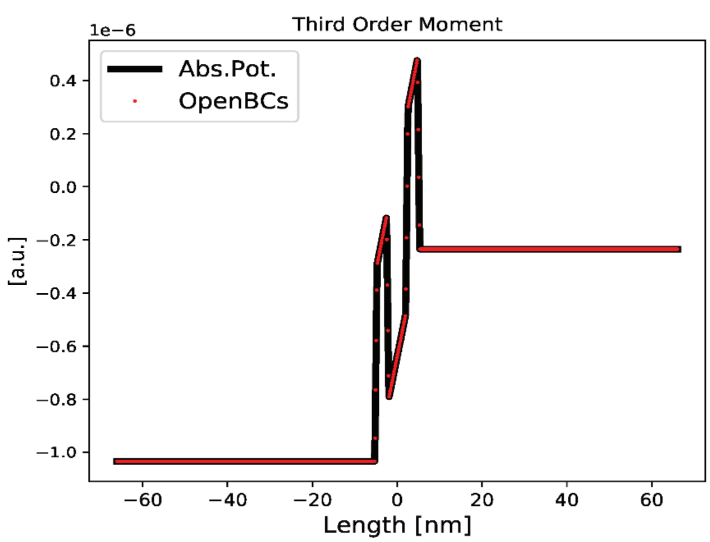


Figure 3: Quality test. The third order moment of the Wigner function (third order derivative of the characteristic function) follows the potential energy. Results from using an absorbing potential (black line) are in excellent agreement with results using open BCs (dotted red). The exact same mesh and the same discrete spatial inflow boundary conditions are used for both simulations (bias 0.3 V, barrier height 0.27 eV).