Transparent Boundary Conditions for Quantum-Waveguide Simulations

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The electron transport through a quantum waveguide can be modeled in good approximation by a two-dimensional SCHRÖDINGER equation on an unbounded domain. For numerical simulations, however, it is necessary to restrict this problem to a finite domain. This is possible without changing the solution by introducing *transparent boundary conditions* (TBC), which are non-local in time (convolution type).

The numerical discretizations of these artificial boundary conditions is a main challenge, as it may easily render the initial-boundary value problem unstable. Based on a CRANK–NICHOLSON finite difference discretization of the SCHRÖDINGER equation, we shall discuss a dicrete TBC, which makes the overall scheme unconditionally stable. Further, we derive approximations of the involved discrete convolutions by exponential sums, and analyze the stability of theresulting numerical scheme.

The derived boundary conditions are illustrated by simulations of a wavequide with a resonating stab.