Discrete Transparent Boundary Conditions for Time-Dependent Systems of Schrödinger Equations

Andrea Zisowsky (Berlin)

The time evolution of the multi-band electronic states in nano-scale semiconductor heterostructures can be described by a system of time-dependent *kp*-SCHRÖDINGER equations. Since this coupled system is usually posed on an unbounded domain, we derive *transparent boundary conditions* (TBC) to confine the domain to a finite computational region. In order to maintain stability and to avoid numerical reflections we construct *discrete transparent boundary conditions* (DTBC) using the $\mathcal{Z}$-transformation method on a completely discrete level. Since these exact DTBCs are non-local in time and thus rather costly, we present a sum-of-exponentials ansatz to approximate the DTBCs, that allows a very fast calculation of the boundary terms. These results have been obtained in collaboration with ANTON ARNOLD, MATTHIAS EHRHARDT and THOMAS KOPRUCKI.