

Semidiscrete transparent boundary conditions for the Schrödinger equation based on convolution quadrature

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The Schrödinger equation is one of the central equations of quantum mechanics. It is commonly posed on the full space \mathbb{R}^d . In order to discretize this equation, for example using finite elements, one needs to restrict the problem to a bounded domain Ω . The question arises which boundary conditions should be imposed on the artificial boundary $\partial\Omega$. In this talk I present a “semi-discrete” approach that is based on first discretizing the time variable and then deriving boundary conditions for the sequence of approximations. This talk mostly focuses on the simplest case of one spatial dimension, considering the possible time discretizations using multistep and Runge-Kutta methods, but also suggests the possible generalization to higher dimensions using boundary element methods (BEM).