Discrete transparent boundary conditions for the Schrödinger equation on circular domains

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Abstract

In this talk we present some novel transparent boundary conditions (TBCs) for the time–dependent Schrödinger equation on a circular computational domain. First we derive the two–dimensional discrete TBCs in conjunction with a conservative Crank–Nicolson finite difference scheme. The presented discrete initial boundary–value problem is unconditionally stable and completely reflection–free at the boundary. Then, since the discrete TBCs for the Schrödinger equation with a spatially dependent potential include a convolution w.r.t. time with a weakly decaying kernel, we construct *approximate* discrete TBCs with a kernel having the form of a finite sum of exponentials, which can be efficiently evaluated by recursion. In numerical tests we finally illustrate the accuracy, stability, and efficiency of the proposed method.

As a by-product we also present a new formulation of discrete TBCs for the 1D Schrödinger equation, with convolution coefficients that have better decay properties than those from the literature.

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