Numerical methods with discrete transparent boundary conditions for solving the time-dependent Schrödinger equation in unbounded domains

A.A. Zlotnik

Department of Mathematics at Faculty of Economic Sciences, National Research University Higher School of Economics, Myasnitskaya 20, 101000 Moscow, Russia

This a joint study together with B. Ducomet (France), I. Zlotnik and A. Romanova (Russia).

The linear time-dependent Schrödinger equation is among the key equations in quantum mechanics and electronics, nuclear, atomic and molecular physics, wave physics, etc. Often it should be solved in unbounded space domains. To overcome this difficulty, among a lot of existing approaches we adopt the so-called discrete transparent boundary conditions (TBCs). Their advantages are the complete (100%) absence of spurious reflections from artificial boundaries, reliable computational stability and ability to ensure small relative errors in practice, the clear mathematical background and the corresponding rigorous conservative properties and stability theory, error estimates without mesh steps in negative powers in theory, etc.

We construct and study a collection of new efficient discretization methods. Among these methods are the Crank-Nicolson-polylinear finite element method with the discrete TBC, any order Crank-Nicolson-finite element method in space with the discrete TBC, splitting in potential finite-difference schemes of the 2^{nd} and 4^{th} orders of accuracy in space with the discrete TBCs, and high order of accuracy methods in time based on the global Richardson extrapolation in time, see [1-7].

We develop a rigorous stability theory and theoretical and practical error analysis.

A number of numerical results on computing the tunnel effect for various barriers/wells are presented.

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