Modeling boundary conditions for solving stationary Schrödinger equations

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Abstract

In this talk we present some novel absorbing boundary conditions (ABCs) for modeling the solution of linear and nonlinear variable potentials one-dimensional stationary Schrödinger equations. Using pseudodifferential calculus and factorization theorems we construct a hierarchy of novel ABCs and generalize the well-known quantum transmitting boundary condition of Kirk and Lentner to the case of space-dependent potential. Moreover, we propose a rapidly converging iterative method based on finite elements suitable for computing scattering solutions and bound states.

The accuracy of our new absorbing boundary conditions is investigated numerically for two different situations. The first problem is related to the computation of linear scattering problems. The second application concerns the computation of energies and ground-states for linear and nonlinear Schrödinger equations. It turns out that these absorbing boundary conditions and their variants lead to a higher accuracy than the usual Dirichlet boundary condition. Finally, our approach also offers the possibility to construct ABCs for higher dimensional problems.

References

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