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Absorbing Boundary Conditions for Solving N-Dimensional Stationary Schrödinger Equations with Unbounded Potentials and Nonlinearities

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Abstract. We propose a hierarchy of novel absorbing boundary conditions for the one-dimensional stationary Schrödinger equation with general (linear and nonlinear) potential. The accuracy of the new absorbing boundary conditions is investigated numerically for 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, we give the extension of these ABCs to N-dimensional stationary Schrödinger equations.

AMS subject classifications: 35J10, 65M60, 65N30

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1 Introduction

The solution of the Schrödinger equation occurs in many applications in physics, chemistry and engineering (e.g., quantum transport, condensed matter physics, quantum

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chemistry, optics, underwater acoustics, $\cdots$). The considered problem can appear in different forms: time-dependent or stationary equation, linear or nonlinear equation, inclusion of a variable potential among others. One of the main difficulty when solving the Schrödinger equation and most particularly from a numerical point of view, is to impose suitable and physically admissible *boundary conditions* to solve numerically a bounded domain equation modeling an equation originally posed on an unbounded domain. Concerning the time-domain problem, many efforts have been achieved these last years. We refer the interested reader e.g., to the recent review paper [1] and the references therein for further details.

In this paper, we begin to focus on the solution to the one-dimensional *stationary Schrödinger equation*. For a given potential V possibly extending to infinity, eventually nonlinear ($V:=V(x,\varphi)$), we want to solve the following equation

$$\left(-\alpha\frac{d^2}{dx^2}+V\right)\varphi=E\varphi,\quad x\in\mathbb{R}, \tag{1.1}$$

or rewritten as

$$\left(\frac{d^2}{dx^2}+\frac{1}{\alpha}\left[E-V\right]\right)\varphi=0,\quad x\in\mathbb{R}, \tag{1.2}$$

with some parameter α that allows for some flexibility. More precisely, we study the extension of the recently derived *time-domain boundary conditions* [2] to the computation of stationary states: we determine here the pair (φ,E), for a given linear or nonlinear potential V. This eigenvalue problem is also known as the *computation of ground states*. The energy of the system is then the eigenvalue E and the associated stationary state is the eigenfunction φ. In particular, we seek the fundamental stationary state which is linked to the *smallest eigenvalue*. In practice, higher order states are also of interest. After a careful numerical validation of the 1D case, we develop some ABCs for the generalized N-dimensional case

$$-\alpha\Delta u+V(\mathbf{x})u+f(u)u=Eu$$

in $\mathbb{R}^N$ for an unbounded potential V and general nonlinearities. Another related problem which is not treated here is linear and nonlinear scattering. We refer to our extended version of the present paper [3] where a thorough study of scattering problems with the ABCs is developed.

Let us note here that numerical approaches based on solving the stationary Schrödinger with ABCs is not the only practical possibility. Indeed, other solutions may be used. The most widely used approach with applications for example in Bose-Einstein condensation is to bound the infinite space with a sufficiently large computational domain and then to impose a Dirichlet boundary condition on this fictitious boundary. The fact that we may fix the field at zero at the boundary is related to the property that ground states decay exponentially fast in the far-field. Then, spectrally accurate solutions can be efficiently obtained following the works by Bao et al. [4,5]. Other solutions include whole space solutions based on spectral methods (see [6,7]). Let us also note the following other