Bergische Universität Wuppertal

Fachbereich Mathematik und Naturwissenschaften

Lehrstuhl für Angewandte Mathematik
und Numerische Mathematik

Lehrstuhl für Optimierung und Approximation

Preprint BUW-AMNA-OPAP 10/12

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September 2010

http://www.math.uni-wuppertal.de

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Abstract Using pseudodifferential calculus and factorization theorems we construct a hierarchy of novel absorbing boundary conditions (ABCs) for the stationary Schrödinger equation with general (linear and nonlinear) exterior potential $V(x)$. Doing so, we 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.

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 chemistry, optics, underwater acoustics, ...). The considered problem can appear in different forms: time-dependent or stationary equation, linear or nonlinear equation, inclusion of a variable potential among others.

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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 modelling 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 [2] and the references therein for further details.

In this work, we focus on the solution to the *stationary Schrödinger equation*. For a given potential V, eventually nonlinear ($V := V(x,\psi)$), we want to solve the following equation

$$\left(-\alpha \frac{d^2}{dx^2} + V\right)\psi = E\psi, \qquad x \in \mathbb{R}, \tag{1}$$

or rewritten as

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

with some parameter α that allows for some flexibility. More precisely, we study the extension of the recently derived *time-domain boundary conditions* [3] to the following two situations:

- **linear and nonlinear scattering:** E is a given value and the potential V being linear (independent of ψ) or nonlinear, we want to compute ψ as the solution of (1).
- **stationary states:** we determine here the pair (ψ, 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 ψ. In particular, we seek the fundamental stationary state which is linked to the *smallest eigenvalue*. In practice, higher order states are also of interest.

For the stationary Schrödinger equation (2), boundary conditions for solving linear scattering problems with a constant potential outside a finite domain have been proposed e.g. by Ben Abdallah, Degond and Markowich [6], by Arnold [5] for a fully discrete Schrödinger equation and in a two-dimensional quantum waveguide by Lent and Kirkner [7]. The case of bound states can be found for the one-dimensional linear Schrödinger equation with constant potential in [8].

The goal of this work is to propose and validate some new boundary conditions for modeling variable potentials stationary one-dimensional Schrödinger equations with application to scattering computation. We provide the whole theory which is related to previous developments [3] as well as numerical schemes for their validation. Finally, let us point out that these absorbing boundary conditions can be extended to higher dimensional problems and other situations like variable mass problems.

2 Absorbing boundary conditions: from the time-domain to the stationary case

In order to derive some *absorbing boundary conditions (ABCs)* for the stationary Schrödinger equation (2), let us first start with the time-domain situation. In case of the time-dependent Schrödinger equation with a linear or nonlinear potential $\widetilde{V}$

$$\begin{cases} i\partial_t u + \partial_x^2 u + \widetilde{V} u = 0, & \forall (x,t) \in \mathbb{R} \times \mathbb{R}^+, \\ u(x,0) = u_0(x), & x \in \mathbb{R}, \end{cases} \tag{3}$$

the following *second- and fourth-order ABCs*

$$\text{ABC}_2^2 \qquad \partial_{\mathbf{n}} u - i\text{Op}\left(\sqrt{-\tau + \widetilde{V}}\right) u = 0, \tag{4}$$

$$\text{ABC}_2^4 \qquad \partial_{\mathbf{n}} u - i\text{Op}\left(\sqrt{-\tau + \widetilde{V}}\right) u + \frac{1}{4}\text{Op}\left(\frac{\partial_{\mathbf{n}}\widetilde{V}}{-\tau + \widetilde{V}}\right) u = 0, \tag{5}$$

on $\Sigma \times \mathbb{R}^+$ were derived recently in [3]. Here, Op denotes a pseudodifferential operator and the fictitious boundary Σ is located at the two interval endpoints x_ℓ and x_r. The outwardly directed unit normal vector to the bounded computational domain $\Omega =]x_\ell; x_r[$ is denoted by $\mathbf{n}$.

To obtain some ABCs for the stationary equations (1) or (2), we consider these equations supplied with a new potential: $\widetilde{V} := -V/\alpha$. Moreover, we are seeking some *time-harmonic solutions* $u(x,t) := \psi(x) e^{-i\frac{E}{\alpha}t}$ and since

$$i\partial_t u = \frac{E}{\alpha} \psi(x)\, e^{-i\frac{E}{\alpha}t},$$

the variable $-\tau$ can be identified with E/α. This yield some *stationary ABCs* on Σ that we designate by SABC^M ('S' stands for stationary and M denote the order) :

$$\text{SABC}^2 \quad \partial_{\mathbf{n}}\varphi = i\frac{1}{\sqrt{\alpha}}\sqrt{E - V}\,\varphi, \quad \text{on } \Sigma, \tag{6}$$

$$\text{SABC}^4 \quad \partial_{\mathbf{n}}\varphi = i\frac{1}{\sqrt{\alpha}}\sqrt{E - V}\,\varphi + \frac{1}{4}\frac{\partial_{\mathbf{n}} V}{E - V}\,\varphi. \tag{7}$$

Let us remark that we constructed for the time-dependent case two families of ABCs, denoted by ABC_1^M and ABC_2^M [3]. These ABCs all coincide if the potential is time-independent. In the stationary case, all the potentials fall into this category and thus the ABCs are equivalent. Hence, we get the unique class of stationary ABCs, SABC^M (without subscript index). For convenience, the form of the boundary conditions (6)–(7) is based on ABC_2^M (we refer to [3] for more technical details).

In the next section we investigate numerically these absorbing boundary conditions in the case of linear scattering problems.

3 Application to linear scattering problems

Let us consider an incident right-traveling plane wave

$$\varphi^{\text{inc}}(x) = e^{ikx}, \quad k > 9, \qquad x \in]-\infty; x_\ell], \tag{8}$$

coming from $-\infty$. The parameter k is the real valued positive wave number and the variable potential V models an inhomogeneous medium. We consider a bounded computational domain $\Omega =]x_\ell; x_r[$ and assume that the wave $\varphi - \varphi^{\text{inc}}$ is perfectly reflected back at the left endpoint x_ℓ. Furthermore, we assume that the wave is totally transmitted in $[x_r; \infty[$, propagating then towards $+\infty$. As a consequence, we have to solve the following *boundary value problem*

$$\begin{aligned} &\left(-\alpha \frac{d^2}{dx^2} + V\right)\psi = E\psi, && \text{for } x \in \Omega, \\ &\partial_{\mathbf{n}}\varphi = g_{M,\ell}\varphi + f_{M,\ell}, && \text{at } x = x_\ell, \\ &\partial_{\mathbf{n}}\varphi = g_{M,r}\varphi, && \text{at } x = x_r, \end{aligned} \tag{9}$$

with $f_{M,\ell} = \partial_{\mathbf{n}}\varphi^{\text{inc}}(x_\ell) - g_{M,\ell}\varphi^{\text{inc}}(x_\ell)$. Here, the order M is equal to 2 or 4 according to the choice of SABC^M (6) or (7) and thus we have

$$g_{2,(\ell,r)} := i\frac{1}{\sqrt{\alpha}}\sqrt{E - V_{\ell,r}}, \tag{10}$$

$$g_{4,(\ell,r)} := g_{2,(\ell,r)} + \frac{1}{4}\frac{\partial_{\mathbf{n}} V_{|x=x_{\ell,r}}}{E - V_{|x=x_{\ell,r}}}. \tag{11}$$

In the sequel of this paper, we will also use the following other concise writing

$$\partial_{\mathbf{n}}\varphi = g_M\varphi + f_M, \quad \text{on } \Sigma, \tag{12}$$

for each function being adapted with respect to the endpoint. Finally, for a plane wave, we have the *dispersion relation*: $E = \alpha k^2 + V_\ell$, where $V_\ell = V(x_\ell)$.

We use a *finite element method (FEM)* to solve numerically this problem. One benefit of using FEM in this application is that the ABCs can be incorporated directly into the variational formulation. The interval $[x_\ell; x_r]$ is decomposed into n_h elementary uniform segments of size h. Classically, the ABCs are considered as *(impedance) Fourier-Robin boundary conditions*. Let $\varphi \in \mathbb{C}^{n_h+1}$ denote the vector of nodal values of the $\mathbb{P}_1$ interpolation of φ and let $\mathbb{S} \in \mathscr{M}_{n_h+1}(\mathbb{R})$ the $\mathbb{P}_1$ stiffness matrix associated with the bilinear form $\int_\Omega \partial_x\varphi\,\partial_x\psi\,dx$. Next we introduce $\mathbb{M}_{V-E} \in \mathscr{M}_{n_h+1}(\mathbb{R})$ as the generalized mass matrix arising from the linear approximation of $\int_\Omega (V-E)\varphi\psi\,dx$, for any test-function $\psi \in H^1(\Omega)$. Let $\mathbb{B}_M \in \mathscr{M}_{n_h+1}(\mathbb{C})$ be the matrix of the boundary terms related to the ABC SABC^M. The right-hand side $\mathbf{b}_M \in \mathbb{C}^{n_h+1}$ is given by $\mathbf{b} = \left(\alpha f_{M,\ell}, 0, \ldots, 0\right)^\top$ and the linear system reads

$$(\alpha\mathbb{S} + \mathbb{M}_{V-E} + \mathbb{B}_M)\varphi = \mathbf{b}_M, \tag{13}$$

For an example we study the stationary Schrödinger equation (1) with $\alpha = 1/2$:

$$-\frac{1}{2}\frac{d^2}{dx^2}\varphi + V\varphi = E\varphi, \quad x \in \mathbb{R}, \tag{14}$$

and consider an incident right-traveling plane wave with wave number $k = 10$. We analyze the results for a *Gaussian potential* $V(x) = A\exp\{-(x-x_c)^2/w^2\}$, centered at $x_c = 20$ with the amplitude $A = -5$ and the parameter $w = 3$.

The numerical reference solution is computed on the large domain $]0;58[$ using the fourth-order ABC. At the fictitious boundary points x_ℓ and x_r of the computational domain, the values of the potential are $V(58) \approx 10^{-69}$ and $V(0) \approx 10^{-19}$, i.e. from a numerical point of view, the potential can be considered as compactly supported in this reference domain. Then, the ABCs are highly accurate [2] yielding a suitable *reference solution* φ_{ref} with spatial step size $h = 5 \cdot 10^{-3}$.

We next compute the solution obtained by applying the ABCs on a smaller computational domain by shifting the right endpoint to $x_r = 18$, now the potential being far from vanishing at this endpoint. In the negative half-space $x < x_\ell = 0$, the potential is almost equal to zero and hence the second-order ABC is very accurate.

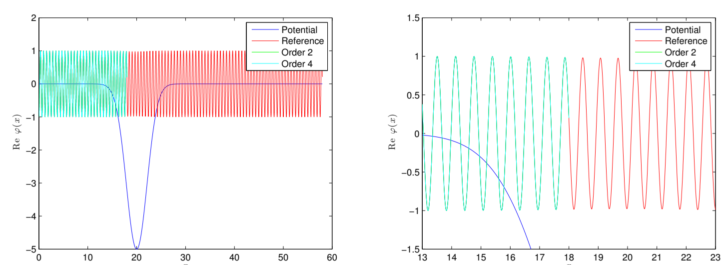

Fig. 1 Real parts of the numerical solutions.

Figure 1 shows the computed solutions (denoted by φ_{num}), superposed on the potential and reference solution, with the second-order (green) and fourth-order (cyan) ABCs placed at the right endpoint x_r. Since the solutions are complex valued, we only plot here their real parts. Note that we would obtain roughly the same curves for their complex parts. The ABCs give quite good results as it can be clearly observed in Figure 1 (right) where we zoom around the boundary $x_r = 18$ to distinguish the different curves. At first sight, the curves coincide. Next we plot in Figure 2 (left) the error curves on the real part $x \mapsto |\text{Re}(\Delta\varphi(x))|$ and in Figure 2 (right) we show the modulus $x \mapsto |\Delta\varphi(x)|$, with the error $\Delta\varphi = \varphi_{\text{num}} - \varphi_{\text{ref}}$.

We can see that the approximation error by using the SABC^2 is roughly $5 \cdot 10^{-4}$ while the error associated with ABC^4 is almost 10^{-6}, which is also the linear finite element approximation error $h^2 \approx 10^{-6}$. Hence, not only the results are precise but they are also of increasing accuracy as the order of the SABC increases.

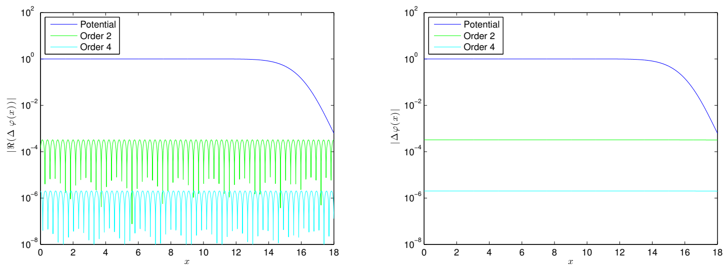

Fig. 2 Errors $|\varphi_{\text{num}} - \varphi_{\text{ref}}|$ for the potential $V(x) = -5e^{-(x-20)^2/9}$, real part (left), modulus (right).

Conclusion

We have proposed some accurate and physically admissible absorbing boundary conditions for modeling linear (and nonlinear) stationary Schrödinger equations with variable potentials. Based on numerical schemes, these boundary conditions have been validated for linear scattering computations.

A more detailed discussion and examples including the consideration of linear and nonlinear eigenstate computation with applications to many possible given variable potentials and nonlinearities can be found in [4].

Acknowledgements This work was supported partially by the French ANR fundings under the project MicroWave NT09_460489 (http://microwave.math.cnrs.fr/)

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