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A fast method to implement non-local discrete transparent boundary conditions for the Schrödinger equation

Discrete transparent boundary conditions (DTBCs) for the time-dependent Schrödinger equation were introduced in the numerical simulations of whole space problems in order to reduce the computational domain to a finite region. They include a convolution w.r.t. time with a weakly decaying kernel that leads to very costly numerical evaluation for large-time simulations. As a remedy we construct approximate DTBCs with a kernel having the form of a finite sum-of-exponentials, which can be evaluated in an efficient recursion.

1. Introduction

Discrete transparent boundary conditions for the discrete 1D–Schrödinger equation

$$-iR(\psi_{j,n+1}-\psi_{j,n}) = \psi_{j+1,n+1}-2\psi_{j,n+1}+\psi_{j-1,n+1}+\psi_{j+1,n}-2\psi_{j,n}+\psi_{j-1,n}-wV_{j,n+\frac{1}{2}}\left(\psi_{j,n+1}+\psi_{j,n}\right), \qquad (1)$$

where $R=4\Delta x^2/\Delta t$, $w=2\Delta x^2$, $V_{j,n+\frac{1}{2}} := V(x_j,t_{n+\frac{1}{2}})$, $x_j=j\Delta x$, $j\in\mathbb{Z}$; and $V(x,t)=V_-=const$ for $x\le 0$; $V(x,t)=V_+=const$ for $x\ge X$, $t\ge 0$, $\psi(x,0)=\psi^I(x)$, with $\operatorname{supp}\psi^I\subset[0,X]$, were introduced in [1]. The DTBC at e.g. the left boundary point $j=0$ reads, cf. Th. 3.8 in [2]:

$$\psi_{1,n}-s_0\psi_{0,n} = \textstyle\sum_{k=1}^{n-1} s_{n-k}\psi_{0,k}-\psi_{1,n-1}, \quad n\ge 1. \qquad (2)$$

The convolution kernel $\{s_n\}$ can be obtained by explicitly calculating the inverse Z–transform of the function $\hat{s}(z) := \frac{z+1}{z}\hat{\ell}(z)$, where $\hat{\ell}(z)=1-i\zeta\pm\sqrt{-\zeta(\zeta+2i)}$, $\zeta=\frac{R}{2}\frac{z-1}{z+1}+i\Delta x^2 V_-$ (choose sign such that $|\hat{\ell}(z)|>1$).

The use of (2) for calculations permits us to avoid any boundary reflections and it renders the fully discrete scheme unconditionally stable, like the Crank-Nicolson scheme (1). However, the linearly in t increasing numerical effort to evaluate the DTBCs can sharply raise the total computational costs. A strategy to overcome this drawback will be the key issue of this paper.

2. Approximation of Convolution Coefficients by Sums of Exponentials

We evaluate numerically the several first convolution coefficients s_n appearing in the DTBC (2): $s_n\approx s_n^{(N)} = \rho^n N^{-1}\sum_{k=0}^{N-1}\hat{s}(\rho e^{i\varphi_k})\,e^{in\varphi_k}$, $n=0,1,\dots,N-1$. Here $\varphi_k=2\pi k/N$, and $\rho>1$ is a regularization parameter.

Our fast method to calculate the discrete convolution in (2) is based on the approximation of the coefficients s_n by the following ansatz (sum of exponentials):

$$s_n\approx\tilde{s}_n := \begin{cases} s_n, & n=0,\dots,\nu-1,\\ \sum_{l=1}^{L} b_l q_l^{-n}, & n=\nu,\nu+1,\dots, \end{cases} \qquad (3)$$

where $L,\nu\in\mathbb{N}$ are fixed numbers. In order to find the required $\{b_l,q_l\}$, we fix L and ν in (3) (e.g. $\nu=1$), and consider the Padé approximation $\frac{P_{L-1}(x)}{Q_L(x)}$ for the formal power series: $f(x) := s_\nu+s_{\nu+1}x+s_{\nu+2}x^2+\dots$, $|x|\le 1$.

Theorem 1. *Let the polynomial $Q_L(x)$ have L simple roots q_l with $|q_l|>1$, $l=1,\dots,L$. Then*

$$\tilde{s}_n=\sum_{l=1}^{L} b_l q_l^{-n}, \qquad n=\nu,\nu+1,\dots, \quad \textit{where}\ \ b_l := -\frac{P_{L-1}(q_l)}{Q_L'(q_l)}q_l^{\nu-1}\neq 0, \qquad l=1,\dots,L.$$

Remark 1. According to the definition of the Padé algorithm, we have $\tilde{s}_n=s_n$ for $n=\nu,\nu+1,\dots,2L+\nu-1$. For the remaining $\tilde{s}_n$ with $n>2L+\nu-1$, the following estimate is proved: $|\tilde{s}_n-s_n|=\mathcal{O}(n^{-\frac{3}{2}})$.

Remark 2. All our practical calculations confirm that the *condition* of Theorem 1 holds for any desired L, although we cannot prove this.

3. Fast Evaluation of the Discrete Convolution with an "Exponential" Kernel

Given the approximation (3) of the discrete convolution kernel appearing in the DTBC (2), the convolution

$$C^{(n)}(u) := \sum_{k=1}^{n-\nu} u_k \tilde{s}_{n-k} \tag{4}$$

of a discrete function u_k, $k = 1, 2, \ldots$, can be calculated efficiently by *recurrence* formulas, cf. [3]:

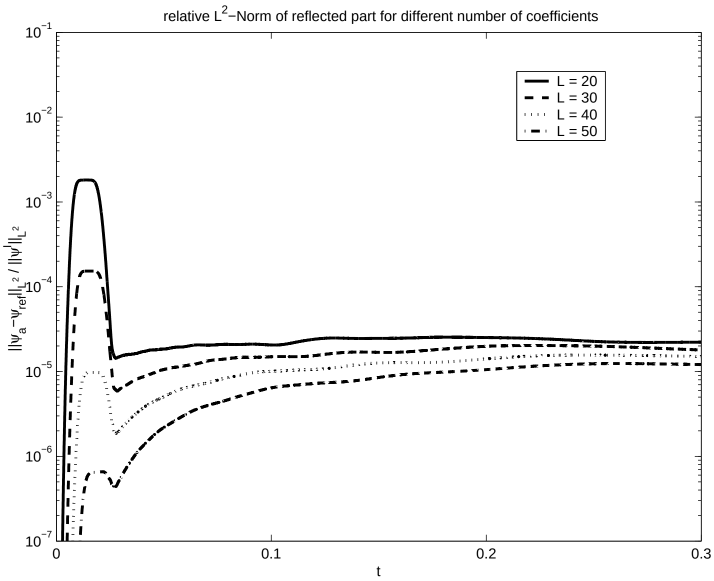
Theorem 2. *The function $C^{(n)}(u)$ from (4) for $n \geq \nu + 1$ is represented by*

$$C^{(n)}(u) = \sum_{l=1}^{L} C_l^{(n)}(u), \quad \textit{where} \quad C_l^{(n)}(u) = q_l^{-1} C_l^{(n-1)}(u) + b_l q_l^{-\nu} u_{n-\nu} \quad \textit{for} \quad n \geq \nu + 1, \quad C_l^{(\nu)}(u) \equiv 0.$$

The recursion permits us to drastically reduce the computational effort of evaluating DTBCs for long–time computations ($n \gg 1$): $\mathcal{O}(L * n)$ instead of $\mathcal{O}(n^2)$ arithmetic operations.

4. Numerical Example

As an example, we consider (1) on $0 \leq x \leq 1$ with $V_- = V_+ = 0$, and non–zero initial data ψ^I. The reference solution ψ_{ref} with $\Delta x = 1/160$, $\Delta t = 2 \cdot 10^{-5}$ is obtained by using exact DTBCs (2) at the ends $x = 0$ and $x = 1$. We vary the parameter $L = 20, 30, 40, 50$ in (3), find the corresponding approximate DTBCs, and show the error of the approximate solution ψ_a measured in $\frac{||\psi_a - \psi_{ref}||_{L_2}(t)}{||\psi^I||_{L_2}}$. The result up to $n = 15000$ is shown in the figure.



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5. References

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