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PROPERTIES OF THE NUMEROV-CRANK-NICOLSON SCHEME ON A NON-UNIFORM MESH FOR THE 1D TIME-DEPENDENT SCHRÖDINGER EQUATION

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We deal with the initial-boundary value problem for the 1D time-dependent Schrödinger equation

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m_0}\frac{\partial^2\psi}{\partial x^2} + V\psi \quad \text{on} \quad (0,\infty), \quad \text{for} \quad t>0,$$
$$\psi|_{x=0}=0, \quad \|\psi(\cdot,t)\|_{L^2(0,\infty)}<\infty \quad \text{for} \quad t>0, \quad \psi|_{t=0}=\psi^0(x) \quad \text{on} \quad (0,\infty),$$

where i is the imaginary unit, $\hbar>0$ and $m_0>0$ are physical constants, the sought wave function $\psi=\psi(x,t)$ is complex-valued and $V=V(x)$ is the given real coefficient (potential). We assume that $V(x)=V_\infty$ and $\psi^0(x)=0$ for $x\ge X_0$ with sufficiently large $X_0>0$.

The Crank-Nicolson scheme in time with the Numerov averages on the non-uniform space mesh is studied, with approximate transparent boundary conditions (TBCs) [1]. The uniform in time and L^2 and H^1 in space stability is proved both with respect to the initial function and free terms in the equation and the approximate TBC. The stability analysis develops one given in [2] and additionally includes accurate bounds for the skew-Hermitian parts of the Numerov sesquilinear forms together with sufficient (and necessary) conditions for their positive definiteness. The results depend on properties of the mesh and the Hölder or Lipschitz smoothness of V; conditions like $h_\omega=O(\tau_\omega)$ arise for the mean mesh steps h_ω and τ_ω in space and time which probably are necessary.

We briefly present the similar stability results for the Numerov-Crank-Nicolson scheme on the *infinite* space mesh. Note that, for rigorous derivation of the *discrete* TBC, some stability bounds of such type together with the existence of the solution are obligatory.

In the case of the discrete TBC, we also derive error estimates in both L^2 and H^1 mesh space norms based on the stability bounds on the infinite space mesh. They are of higher orders $O(h^3+\tau^2)$ and $O(h^4+\tau^2)$ in dependence with the properties of the space mesh and are given in terms of *the Sobolev regularity* of ψ^0 (and V) that is implemented by the delicate error analysis; they *contain no* unpleasant terms with the mesh steps in negative powers in contrast to the cases of other approximate TBCs and are new even in the case of the uniform meshes.

Numerical results are presented for tunneling through smooth and rectangular potentials-wells, including the global Richardson extrapolation in time to ensure also higher order in time.

REFERENCES

[1] A. Zlotnik. The Numerov-Crank-Nicolson scheme on a non-uniform mesh for the time-dependent Schrödinger equation on the half-axis. *Kinetic Relat. Models*, **8** (3):587–613, 2015.

[2] A.A. Zlotnik and A.V. Lapukhina. Stability of a Numerov type finite-difference scheme with approximate transparent boundary conditions for the nonstationary Schrödinger equation on the half-axis. *J. Math. Sci.*, **169** (1):84–97, 2010.