Numerical solution of the Schrödinger equation on unbounded domains

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Transparent boundary conditions (TBC)
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Analytical transparent boundary conditions for the Schrödinger equation
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→ Derivation of discrete transparent boundary conditions (DTBC) for the Schrödinger equation for a higher order compact 9-point scheme
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→ more realistic simulations
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more realistic simulations

solving the Schrödinger equation on circular domains
Definition (TBC):
Consider a given whole-space initial value problem (IVP) on $\mathbb{R}^n$ and $\Omega \subset \mathbb{R}^n$, $\Gamma = \partial \Omega$. We are interested in the solution of the IVP on $\Omega$. Therefore we need new artificial boundary conditions on $\Gamma$. We call these artificial BC transparent, if the solution of the IVBP on $\Omega$ corresponds to the whole-space solution of the IVP restricted on $\Omega$. 
IVP: time-dependent Schrödinger equation (here: 1D)

\[ i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left( -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t), \quad x \in \mathbb{R}, \; t > 0 \]

\[ \psi(x, 0) = \psi^I(x) \in L^2(\mathbb{R}) \]

on a domain of interest \( \Omega = \{ x \in \mathbb{R} | 0 < x < X \} \).
**Analytical TBC for the Schrödinger Equation**

IVP: time-dependent Schrödinger equation (here: 1D)

\[
i\hbar \frac{\partial}{\partial t} \psi(x, t) = \left( -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x^2} + V(x, t) \right) \psi(x, t), \quad x \in \mathbb{R}, \ t > 0
\]

\[
\psi(x, 0) = \psi^I(x) \in L^2(\mathbb{R})
\]

on a domain of interest \( \Omega = \{ x \in \mathbb{R} | 0 < x < X \} \).

**Assumptions:**

- \( \text{supp} \ \psi^I \subseteq \Omega \)
- potential \( V(., t) \in L^\infty(\mathbb{R}) \), \( V(x, .) \) is piecewise continuous
- \( V \) constant on \( \mathbb{R} \setminus \Omega \) (here: \( V(x, t) = 0 \) for \( x \leq 0 \) and \( V(x, t) = V_X \) for \( x \geq X \))

**Goal:**

Calculate the solution \( \psi(x, t) \in \mathbb{C} \) on \( \Omega \) with TBC at \( x = 0 \) and \( x = X \).
**DERIVATION OF TBC**

\[ \psi(x,0) = \psi^I(x) \]
\[ \psi_x(0,t) = (T_0 \psi)(0,t) \]
\[ \psi_x(X,t) = (T_X \psi)(X,t) \]

\[ i\hbar \psi_t = -\frac{\hbar^2}{2m^*} \psi_{xx} + V(x,t)\psi \]

\[ x \in G : \]
\[ x \in G_2 : \]
\[ \psi(x,0) = \psi^I(x) \]
\[ \psi_x(0,t) = (T_0 \psi)(0,t) \]
\[ \psi_x(X,t) = (T_X \psi)(X,t) \]

\[ v(x,0) = 0 \]
\[ v(X,t) = \Phi(t) \quad t > 0, \ \Phi(0) = 0 \]

\[ \lim_{x \to \infty} v(x,t) = 0 \]
\[ v_x(0,t) = (T_X \Phi)(t) \]
Laplace-transformation on the exterior domains:

\[
\hat{v}_{xx}(x, s) + \frac{2im^*}{\hbar} \left( s + \frac{iV_x}{\hbar} \right) \hat{v}(x, s) = 0 \quad x > X
\]

\[
\hat{v}(X, s) = \hat{\Phi}(s)
\]

\[
\lim_{x \to \infty} \hat{v}(x, s) = 0
\]

\[
\hat{v}_x(X, s) = (T_X \hat{\Phi})(s)
\]

solution:

\[
\hat{v}(x, s) = e^{-i \sqrt{\frac{2im^*}{\hbar} \left( s + \frac{iV_x}{\hbar} \right)}} (x-X) \hat{\Phi}(s)
\]

\[
\Rightarrow (T_X \hat{\Phi})(s) = -\sqrt{\frac{2m^*}{\hbar}} e^{-\frac{i\pi}{4}} + \sqrt{s + \frac{iV_x}{\hbar}} \hat{\Phi}(s)
\]

With the inverse Laplace-Transformation follows the analytical TBC

\[
\psi_x(X, t) = -\sqrt{\frac{\hbar}{2\pi m^*}} e^{-\frac{i\pi}{4}} e^{-\frac{iV_x}{\hbar} t} \int_0^t \frac{\psi(X, \tau)e^{i\frac{V_x \tau}{\hbar}}}{\sqrt{\tau - t}} d\tau.
\]

[J. S. Papadakis (1982)]
Application of DTBC for the Schrödinger equation:

- Simulation of quantum transistors in quantum waveguides (with inhomogeneous DTBC for the 2D Schrödinger equation)
- Analyse steady states and transient behaviour
FORMER STRATEGIES:

- Discretization of the analytic TBCs with an numerical approximation of the convolution integral [e.g. B. Mayfield (1989)]

⇒ only conditionally stable, not transparent!
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  ⇒ only conditionally stable, not transparent!

- Create a buffer zone $\Theta$ of the length $d$ with a complex potential $V(X) = W - iA$ around the computational domain $\Omega$ with Dirichlet $0$-BC at $\partial\Theta$ and absorbing boundary conditions on $\partial\Omega$ [e.g. L. Burgnies (1997)]

  ⇒ unconditionally stable, unphysical reflections at the boundary, huge numerical costs
SUCCESSFUL STRATEGIES

- Family of absorbing BCs (also for the non-linear Schrödinger equation, wave equation)

  [J. Szeftel (2005)]

- discretize the whole space problem with an unconditionally stable scheme (e.g. Crank-Nicolson finite difference scheme) and calculate new discrete transparent boundary conditions for the full discretized Schrödinger equation

  [A. Arnold, M. Ehrhardt (since 1995)]
Derivation of discrete TRB

Discretize 2D Schrödinger equation:

- Crank-Nicolson scheme in time, $t_n = n\Delta t$, $n \in \mathbb{N}$, $H := -\frac{1}{2} \Delta + V$
- Hamilton-Operator, $\Omega = [0, X] \times [0, Y]$

$$
\left(1 + \frac{iH\Delta t}{2}\right)\psi(x, y, t + \Delta t) = \left(1 - \frac{iH\Delta t}{2}\right)\psi(x, y, t)
$$

$$
\Rightarrow \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \left(\psi^{n+1}(x, y) + \psi^n(x, y)\right)
= g^{n+\frac{1}{2}}(x, y) \left(\psi^{n+1}(x, y) + \psi^n(x, y)\right) + W\psi^n(x, y)
$$

- compact 9-point scheme in space, $x_j = j\Delta x$, $y_k = k\Delta y$ with $j \in \mathbb{Z}$, $0 \leq k \leq K$

- DTBC at $x_0 = 0$ and $x_J = X = J\Delta x$ with $J \in \mathbb{Z}$

- 0-BC at $y = 0$ and $y = Y = K\Delta y$ with $K \in \mathbb{N}$
9-point discretization scheme:

\[
\left(D_x^2 + D_y^2 + \frac{\Delta x^2 + \Delta y^2}{12} D_x^2 D_y^2\right) \psi_{j,k}^{n+\frac{1}{2}} \\
= \left(I + \frac{\Delta x^2}{12} D_x^2 + \frac{\Delta y^2}{12} D_y^2\right) \left[2V_{j,k}^{n+\frac{1}{2}} \psi_{j,k}^{n+\frac{1}{2}} - 2i D_t^+ \psi_{j,k}^n\right]
\]

with

\[
\psi_{j,k}^{n+\frac{1}{2}} = \frac{1}{2} \left(\psi_{j,k}^{n+1} + \psi_{j,k}^n\right)
\]

\[
D_t^+ \psi_{j,k}^n = \frac{\psi_{j,k}^{n+1} - \psi_{j,k}^n}{\Delta t}, \quad n \geq 0
\]

\[
D_x^2 \psi_{j,k}^n = \frac{\psi_{j-1,k}^n - 2\psi_{j,k}^n + \psi_{j+1,k}^n}{\Delta x^2}, \quad j \in \mathbb{Z}
\]

\[
D_y^2 \psi_{j,k}^n = \frac{\psi_{j,k-1}^n - 2\psi_{j,k}^n + \psi_{j,k+1}^n}{\Delta y^2}, \quad k \in \mathbb{N}
\]
**Discrete Sine-Transformation in y-direction:**

\[ \hat{\psi}_{j,m}^n := \frac{1}{K} \sum_{k=1}^{K-1} \psi_{j,k}^n \sin \left( \frac{\pi km}{K} \right) \quad m = 0, \ldots, K \]

**Motivation:**

Solve discrete stationary Schrödinger equation in 1D:

\[ -\frac{1}{2} \Delta_y^2 \chi_{j,k}^m = E^m \chi_{j,k}^m, \quad k = 0, \ldots, K \]

\[ \chi_{j,0}^m = \chi_{j,K}^m = 0. \]

The eigenfunctions \( \chi_{j,k}^m = \sin \left( \frac{\pi km}{K} \right) \) provide the energies

\[ E^m = \frac{1}{\Delta y^2} \left( 1 - \cos \left( \frac{\pi m}{K} \right) \right). \]

Hence follows for \( m = 0, \ldots, K \)

\[ \Rightarrow -\frac{1}{2\Delta y^2} \left( \psi_{j,k-1}^n - 2\psi_{j,k}^n + \psi_{j,k+1}^n \right)_m = \frac{1}{\Delta y^2} \left( 1 - \cos \left( \frac{\pi m}{K} \right) \right) \hat{\psi}_{j,m}^n. \]
Sine-Transformation of the discrete Schrödinger equation on the exterior domains \( j \leq 0, \ j \geq J \) yields for the modes \( m = 0, \ldots, K \):

\[
C_{j+1}^m \hat{\psi}_{j+1,m}^n + C_{j-1}^m \hat{\psi}_{j-1,m}^n + R_j^m \hat{\psi}_{j,m}^n \\
= (D - C_{j+1}^m) \hat{\psi}_{j+1,m}^n + (D - C_{j-1}^m) \hat{\psi}_{j-1,m}^n + (B_j^m - R_j^m) \hat{\psi}_{j,m}^n.
\]
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$$= (D - C_{j+1}^m)\hat{\psi}_{j+1,m}^n + (D - C_{j-1}^m)\hat{\psi}_{j-1,m}^n + (B_j^m - R_j^m)\hat{\psi}_{j,m}^n.$$  

**Definition [\(Z\)-Transformation]:**

The \(Z\)-Transformation of a sequence \((\psi^n)_{n \in \mathbb{N}}\) is given by

$$Z \{\psi^n\} = \Psi(z) := \sum_{n=0}^{\infty} \psi^n z^{-n} \quad z \in \mathbb{C}, \ |z| > 1.$$
One can show:

- \[ Z \left( \hat{\psi}_{j,m}^{n+1} \right) = -z \hat{\psi}_{j,m}^0 + z \Psi_j^m(z) \]
- \[ \psi_{j+1,k}^0 = \psi_{j-1,k}^0 = \psi_{j,k}^0 = 0 \text{ for } k = 0, \ldots, K \]
- \[ V_j \text{ constant for } j \leq 1, j \geq J-1 \Rightarrow C_j^m = C^m, R_j^m = R^m, B_j^m = B^m \]

\[ \Rightarrow \Psi_{J+1}(z) + \left[ \frac{R z + R - B}{C z + C - D} \right] \Psi_J(z) + \Psi_{J-1}(z) = 0. \]
One can show:

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\[ \Rightarrow \Psi_{J+1}(z) + \left[ \frac{Rz + R - B}{Cz + C - D} \right] \Psi_J(z) + \Psi_{J-1}(z) = 0. \]

This difference equation with constant coefficients is solved by \[ \Psi_j(z) = \nu^j(z) : \]
\[ \nu^2(z) + \left[ \frac{Rz + R - B}{Cz + C - D} \right] \nu(z) + 1 = 0, \]

Physical background forces decay of the solution for \[ j \to \infty \]

\[ \Rightarrow |\nu(z)| > 1 \quad \text{und} \quad \nu(z) \Psi_J(z) = \Psi_{J-1}(z) \quad \rightarrow Z\text{-transformed DTBC} \]
Theorem [DTBC for the 2D Schrödinger equation]: Discretize the 2D Schrödinger-Equation with the compact 9-point difference scheme in space and with the Crank-Nicolson scheme in time. Then the DTBC at $x_J = J \Delta x$ and $x_0 = 0$ for $n \geq 1$ read

$$\hat{\psi}^{n}_{1,m} - s^{(0)}_{0,m} \hat{\psi}^{n}_{0,m} = \sum_{\nu=1}^{n-1} s^{(n-\nu)}_{0,m} \hat{\psi}^{\nu}_{0,m} - a^{m}_{1} \hat{\psi}^{n-1}_{1,m},$$

$$\hat{\psi}^{n}_{J-1,m} - s^{(0)}_{J,m} \hat{\psi}^{n}_{J,m} = \sum_{\nu=1}^{n-1} s^{(n-\nu)}_{J,m} \hat{\psi}^{\nu}_{J,m} - a^{m}_{J-1} \hat{\psi}^{n-1}_{J-1,m}.$$

The convolution coefficients $s^{(n)}_{j,m}$ can be calculated by

$$s^{(n)}_{j,m} = \alpha^{m}_{j} \frac{(\lambda^{m}_{j})^{-n}}{2n-1} \left[ P_{n}(\mu^{m}_{j}) - P_{n-2}(\mu^{m}_{j}) \right]$$

with the Legendre-Polynomials $P_{n}$ ($P_{-1} \equiv P_{-2} \equiv 0$).
Advantages of the new DTBC:

- no numerical reflections
- 3-point recursion for $s^{(n)}$
- these DTBC have exactly the same structure like the DTBC calculated with the 5-point scheme [A. Arnold, M. Ehrhardt]
- convergence: $O(\Delta x^4 + \Delta y^4 + \Delta t^2)$
- same numerical effort like discretized analytical TRB
- $s_{j,m}^{(n)} = O(n^{-3/2})$
- CN-FD scheme with DTBC is unconditionally stable, with $A := I + \frac{\Delta x^2}{12} D_x^2 + \frac{\Delta y^2}{12} D_y^2$ follows:

$$D_t^+ ||\psi||_A^2 = 0 \quad \text{with} \quad ||\psi||_A^2 := \langle \psi, A\psi \rangle.$$  \hspace{1cm} (1)
some drawbacks:

- DTBC are non-local in time
  → high memory costs: the solution $\psi_{j,m}^n$ has to be saved in $x_0$ and $x_J$ for all time steps $n = 1, 2, \ldots$

  → in each time step $n = 1, 2, \ldots$ you have to calculate $K$ convolutions of the length $n$
  (FFT not useable, $O(Kn^2)$)
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  - in each time step $n = 1, 2, \ldots$ you have to calculate $K$ convolutions of the length $n$
    (FFT not useable, $\Rightarrow O(Kn^2)$)

- These DTBC are given in the Sine-transformed form: BC of one mode is a linear combination of all other boundary points
  - diagonal structure of the system matrix is destroyed
Sparsity pattern of the system matrix for $J = K = 10$
Example 1:

free 2D Schrödinger equation on $\Omega = [0, 2] \times [0, 2]$ with the initial data:

$$\psi^I(x, y) = e^{ik_xx + ik_yy - 60 \left( \left( x - \frac{1}{2} \right)^2 + \left( y - \frac{1}{2} \right)^2 \right)}, \quad (x, y) \in \Omega$$
APPROXIMATION OF DTBC

- Idea: Approximate the convolution coefficients $s_{j,m}^{(n)}$ by a sum of exponentials:

$$s^{(n)} \approx \tilde{s}^{(n)} = \sum_{l=1}^{L} b_l q_l^{-n}, \quad n \in \mathbb{N}, \ |q_l| > 1, \ L \leq 40$$
**APPROXIMATION OF DTBC**

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s^{(n)} \approx \tilde{s}^{(n)} = \sum_{l=1}^{L} b_l q_l^{-n}, \quad n \in \mathbb{N}, \ |q_l| > 1, \ L \leq 40
\]

- \( b_l, q_l \) are calculated by the Padé - Approximation of

\[
f(x) = \sum_{n=0}^{2L-1} s^{(n)} x^n, \quad |x| \leq 1
\]

[A.Arnold, M. Ehrhardt, I. Sofronov (2003)]
Recursion formula for the convolution coefficients:

\[
\sum_{t=0}^{n-1} \tilde{s}^{(n-t)} \psi^t = \sum_{l=1}^{L} c_l^{(n)}
\]

with

\[
c_l^{(n)} = q_l^{-1} c_l^{(n-1)} + b_l q_l^{-1} \psi^{n-1}, \quad n = 1, \ldots, N
\]

\[
c_l^{(0)} = 0
\]
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\]

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Advantages:

→ If you have calculated \( b_l, q_l \) once for a set \( \Delta x, \Delta y, \Delta t, V \), you’ll easily derive \( b_l^*, q_l^* \) for any \( \Delta x^*, \Delta y^*, \Delta t^*, V^* \) by

\[
q_l^* = \frac{q_l \bar{a} - \bar{b}}{a - q_l b}
\]

\[
b_l^* = b_l q_l \frac{a \bar{a} - \bar{b} b}{(a - q_l b)(q_l \bar{a} - \bar{b})} \frac{1 + q_l^*}{1 + q_l}
\]

→ Numerical effort: \( \mathcal{O}(K n^2) \rightarrow \mathcal{O}(K L n) \)

→ Memory: \( \mathcal{O}(K n) \rightarrow \mathcal{O}(K L) \)
Example 2:
free 2D Schrödinger-Equation in $\Omega = [0, 1] \times [0, 1]$
Initial function:

$$\psi^I(x, y) = \sin(\pi y) e^{ikx} e^{-60(x - \frac{1}{2})^2}, \quad (x, y) \in \Omega$$

$L = 5 : \quad T = 150\Delta t \quad T = 300\Delta t \quad T = 500\Delta t$

$L = 20 : \quad T = 150\Delta t \quad T = 300\Delta t \quad T = 500\Delta t$
Incoming wave at $x = 0$:

$$\psi^{inc}(0, y, t) = \sin(\pi y)e^{-\frac{iEt}{\hbar}}, \quad E = 29.9 \text{ meV}$$

inhomogeneous DTBC at $x = 0$, DTBC at $x = X$
Little trick to suppress oscillations in time:

\[ \psi^{inc} \] oscillates like \( e^{\frac{-iEt}{\hbar}} \) in time.

\( E \) big:
- fast oscillation of the solution in time
- small time step size is necessary
- high numerical effort for the analysis of steady state and long-time behaviour

Define

\[ \varphi(x, y, t) := e^{-i\omega t} \psi(x, y, t) \quad \text{mit} \quad \omega = \frac{-E}{\hbar}. \]

\( \varphi \) solve the modified Schrödinger equation

\[
i\hbar \varphi_t = -\frac{\hbar^2}{2m^*}(\varphi_{xx} + \varphi_{yy}) + (V - \omega \hbar) \varphi
\]

\[ =: \tilde{V} \]
\begin{align*}
  f_1(t) &= \| \psi_1(x, y, t) - \psi_{ref}(x, y, t) \|_2 \\
  f_2(t) &= \| \psi_2(x, y, t) - \psi_{ref}(x, y, t) \|_2
\end{align*}

\( \psi_1 \) is calculated with \( \tilde{V} = 0 \), \( \psi_2 \) with \( \tilde{V} = -E \) and \( \psi_{ref} \) is a numerical reference solution, which has been calculated with high accuracy.
Initial function: $X=1$, $Y=0.86667$, $dx=0.016667$, $dy=0.016667$, $dt=0.0002$, $V=0$

$|\psi(x,y)|$, $t=0$

Quantenwellen.m, solution after $T = -1.7998$ ps, $it = 1000$

Quantenwellen.m, solution after $T = 0.0202$ ps, $it = 10100$

Quantenwellen.m, solution after $T = 0.0802$ ps, $it = 10400$

Quantenwellen.m, solution after $T = 1.9002$ ps, $it = 19500$

$T = 0\Delta t$

$T = 1000\Delta t$

$T = 9000\Delta t$

$T = 10100\Delta t$

$T = 10400\Delta t$

$T = 19500\Delta t$
EXTENSION OF THE DTBC TO MORE ARBITRARY POTENTIALS

Drawbacks of the simulations:

• Hard walls (zero Dirichlet BCs) and edges are not practicable in industry!
  → Geometry of computational domain shall be realized by potentials also in the simulations.
  → How to choose the incoming wave and the initial function then?

• Potentials are NOT constant in the exterior domains!
  → Decoupling of the modes for \( V(x, y) \neq \text{const.} \) after Sine-Transformation is not possible
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Discrete Schrödinger equation:
5-point scheme in space, Crank-Nicolson in time:

\[
i\hbar D^+_t \psi_{j,k}^n = -\frac{\hbar^2}{2m^*} \left( D_x^2 + D_y^2 \right) \psi_{j,k}^{n+\frac{1}{2}} + V_{j,k}^{n+\frac{1}{2}} \psi_{j,k}^{n+\frac{1}{2}}
\]

→ Calculate new Eigenfunctions, which take the potential into account!
Solve the eigenvalue equation on the exterior domains \((j \leq 0, j \geq J)\):

\[-\frac{1}{2\Delta y^2} (\chi_{j,k-1,m} - 2\chi_{j,k,m} + \chi_{j,k+1,m}) + V_k^{n+\frac{1}{2}} \chi_{j,k,m} = E_{j,m}^n \chi_{j,k,m}\]

with

\[\Delta y \sum_{k=0}^{K} |\chi_{j,k,m}^n|^2 = 1 \quad \text{and} \quad \chi_{j,0,m}^n = \chi_{j,K,m}^n = 0\]

for \(0 \leq k, m \leq K, n > 0\).

Transformation w.r.t. the eigenfunctions

\[\hat{\psi}_{j,m}^n = \Delta y \sum_{k=1}^{K-1} \chi_{j,k,m}^n \psi_{j,k}^n, \quad 0 \leq m \leq K.\]

yields

\[i\hbar D_t^+ \hat{\psi}_{j,m}^n = -\frac{\hbar^2}{2m^*} D_x^2 \hat{\psi}_{j,m}^{n+\frac{1}{2}} + E_{j,m}^n \hat{\psi}_{j,m}^{n+\frac{1}{2}}\]

\[\rightarrow \text{same structure as the sine-transformed Schrödinger equation!}\]

[N. Ben Abdallah, M.S. (2005)]
Example 3: 2D channel

potential $V(y) = 400y(1 - y)$

eigenfunction $\chi$ of $m = 1$

$\Rightarrow$ initial function:

$$\psi^I_{j,k} = e^{ikx_j\Delta x} \chi^0_{j,k,m}$$

$\Rightarrow$ incoming wave:

$$\psi^{inc}_{j,k,n} = e^{ikx_j\Delta x} \chi^0_{j,k,m} e^{-iE_x n \Delta t} \quad \text{with} \quad E_x = \frac{1 - \cos(k_x \Delta x)}{\Delta x^2}$$
Extension of the DTBC to more arbitrary potentials
SCHRÖDINGER EQUATION ON CIRCULAR DOMAINS

Solve the Schrödinger equation (in polar coordinates)

\[ i \psi_t = -\frac{1}{2} \left( \frac{1}{r} (r \psi_r)_r + \frac{1}{r^2} \psi_{\theta\theta} \right) + V(r, \theta, t) \psi, \quad r > 0, \ 0 \leq \theta \leq 2\pi, \ t > 0 \]

on a circular domain \( \Omega = [0, R] \times [0, 2\pi] \) with TBC at \( x = R \).

Problems:

- solve a second order difference equation with varying coefficients:
  \[
a_j \Psi_{J+1}(z) + b_j(z) \Psi_J(z) + c_j \Psi_{J-1}(z) = 0
  \]

- calculation of the convolution coefficients for the DTBC
  \( \rightarrow \) "recursion from infinity"

- singularity at \( r = 0 \) \( \rightarrow \) not equidistant offset-grid \( \tilde{r}_j = r_{j+\frac{1}{2}} \)

- approximation of the convolution coefficients and the -sum

  [A. Arnold, M. Ehrhardt, M. S., I. Sofronov (2006)]
Example 4:
free Schrödinger equation on unit disc $\Omega_1 = [0, 1] \times [0, 2\pi]$

$$\psi^I(r, \theta) = \frac{1}{\sqrt{\alpha_x \alpha_y}} e^{2ik_x r \cos \theta + 2ik_y r \sin \theta - \frac{(r \cos \theta)^2}{2\alpha_x} - \frac{(r \sin \theta)^2}{2\alpha_y}}$$
Error due to the scheme/TBC:

\[ L(\psi, \varphi, t_n, \Omega) := \left| \left| \psi(r_j, \theta_k, t_n) - \varphi(r_j, \theta_k, t_n) \right| \right|_{\Omega,2} / \left| \left| \varphi(r_j, \theta_k, t_n) \right| \right|_{\Omega,2} \]

\( \psi \): numerical solution
\( \varphi \): exact solution or numerical reference solution

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SCHRÖDINGER EQUATION ON CIRCULAR DOMAINS