Numerical solution of the Schrödinger equation on unbounded domains

Maike Schulte

Institute for Numerical and Applied Mathematics

Westfälische Wilhelms-Universität Münster

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➜ Transparent boundary conditions (TBC)

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- ➜ Simulation of quantum wave guides

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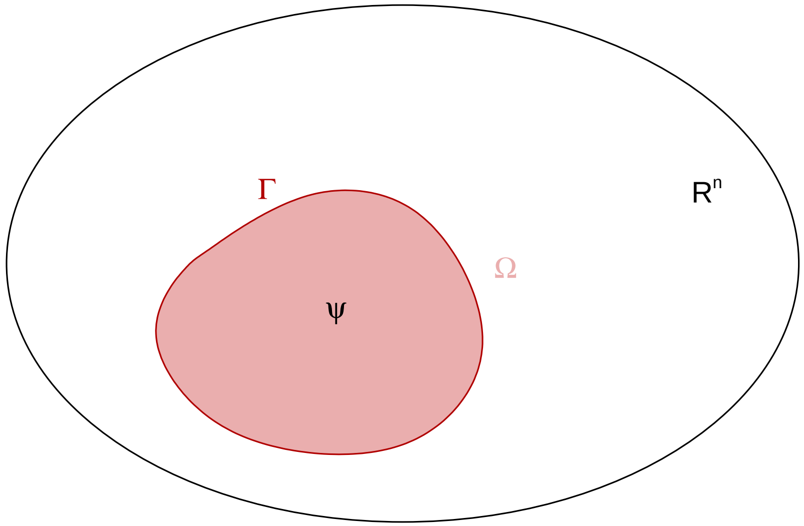
- ➜ more realistic simulations
- ➜ solving the Schrödinger equation on circular domains

TRANSPARENT BOUNDARY CONDITIONS (IN GENERAL)



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 Ω. Therefore we need new artificial boundary conditions on Γ. We call these artificial BC transparent, if the solution of the IVBP on Ω corresponds to the whole-space solution of the IVP restricted on Ω.

ANALYTICAL TBC FOR THE SCHRÖDINGER EQUATION

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

$$\begin{aligned} \mathrm{i}\hbar\frac{\partial}{\partial t}\psi(x,t) &= \left(-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial x^2} + V(x,t)\right)\psi(x,t), \qquad x \in \mathbb{R},\ t > 0 \\ \psi(x,0) &= \psi^I(x) \in L^2(\mathbb{R}) \end{aligned}$$

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

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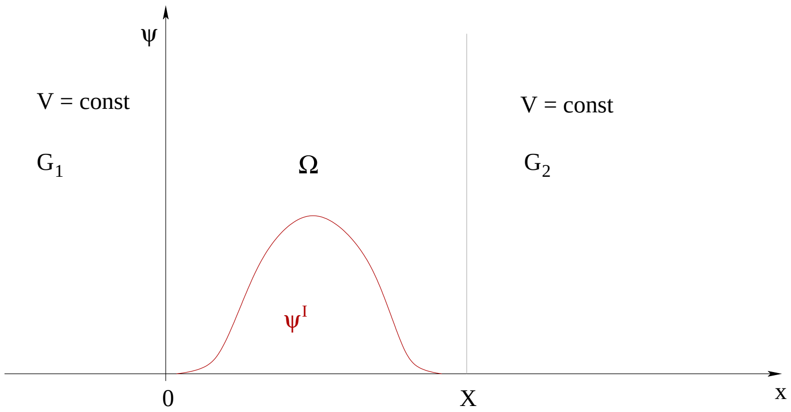
Assumptions:

- supp $\psi^I \subseteq \Omega$
- potential $V(.,t) \in L^\infty(\mathbb{R})$, $V(x,.)$ is piecewise continuous
- V constant on $\mathbb{R}\backslash\Omega$ (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 Ω with TBC at $x = 0$ and $x = X$.

Derivation of TBC



$x \in G:$

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

$$\psi(x,0) = \psi^I(x)$$

$$\psi_x(0,t) = (T_0\psi)(0,t)$$

$$\psi_x(X,t) = (T_X\psi)(X,t)$$

$x \in G_2:$

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

$$v(x,0) = 0$$

$$v(X,t) = \Phi(t) \qquad t > 0,\ \Phi(0) = 0$$

$$\lim_{x\to\infty} v(x,t) = 0$$

$$v_x(0,t) = (T_X\Phi)(t)$$

Laplace-transformation on the exterior domains:

$$\begin{aligned}
\hat{v}_{xx}(x,s) + \frac{2\mathrm{i}m^*}{\hbar}\Big(s + \frac{\mathrm{i}V_X}{\hbar}\Big)\hat{v}(x,s) &= 0 \qquad x > X \\
\hat{v}(X,s) &= \hat{\Phi}(s) \\
\lim_{x\to\infty} \hat{v}(x,s) &= 0 \\
\hat{v}_x(X,s) &= \widehat{(T_X\Phi)}(s)
\end{aligned}$$

solution:

$$\begin{aligned}
\hat{v}(x,s) &= e^{-\mathrm{i}\sqrt[+]{\frac{2\mathrm{i}m^*}{\hbar}\left(s+\frac{\mathrm{i}V_X}{\hbar}\right)}(x-X)}\,\hat{\Phi}(s) \\
\Rightarrow \qquad \widehat{(T_X\Phi)}(s) &= -\sqrt{\frac{2m^*}{\hbar}}\,e^{-\frac{\mathrm{i}\pi}{4}}\sqrt[+]{s + \frac{\mathrm{i}V_X}{\hbar}}\,\hat{\Phi}(s)
\end{aligned}$$

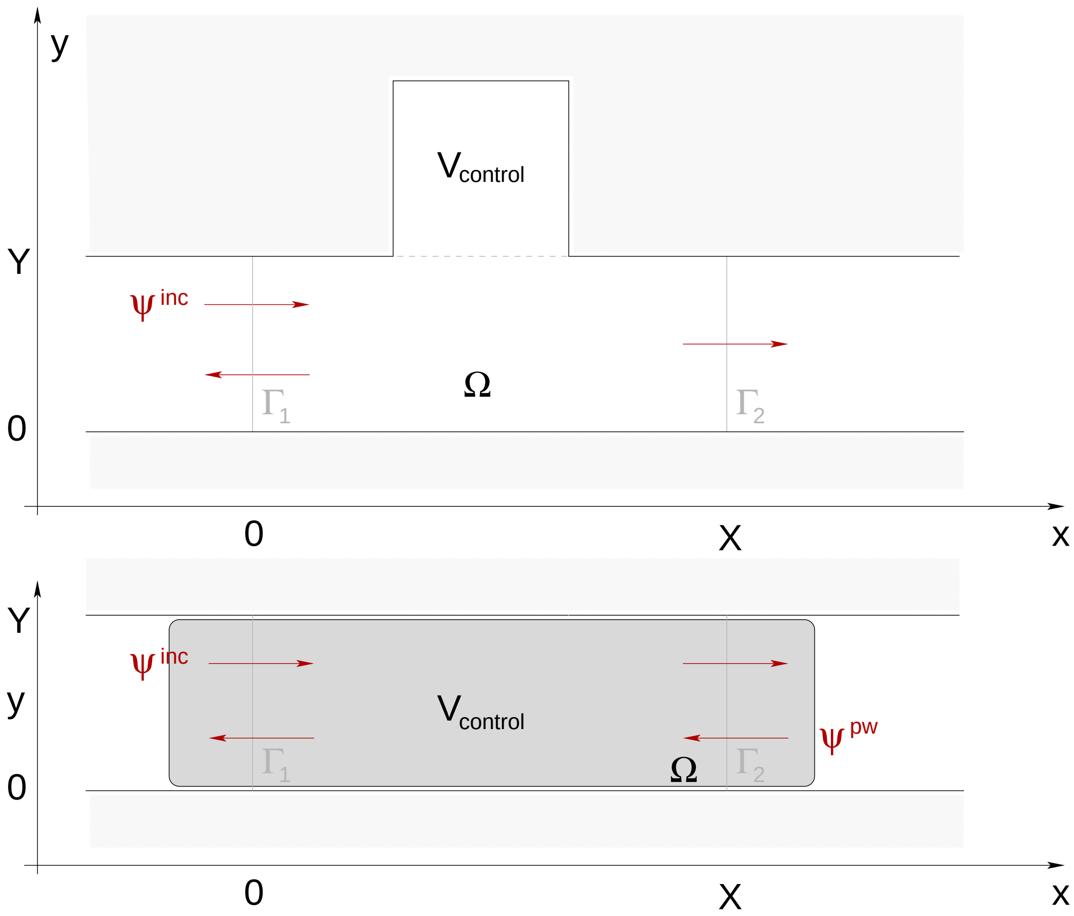
With the inverse Laplace-Transformation follows the analytical TBC

$$\psi_x(X,t) = -\sqrt{\frac{\hbar}{2\pi m^*}}\,e^{-\mathrm{i}\frac{\pi}{4}}\,e^{-\mathrm{i}\frac{V_X}{\hbar}t}\,\frac{d}{dt}\int_0^t \frac{\psi(X,\tau)e^{\mathrm{i}\frac{V_X\tau}{\hbar}}}{\sqrt{\tau-t}}\,d\tau.$$

[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)]

  $\Rightarrow$ only conditionally stable, not transparent!

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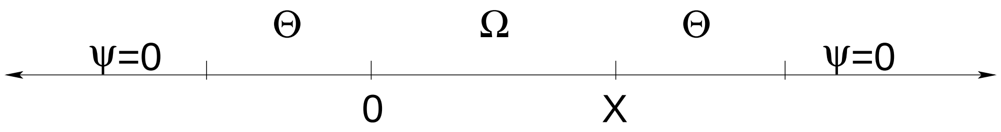
- Create a buffer zone Θ of the length d with a complex potential $V(X) = W - \mathrm{i}A$ around the computational domain Ω with Dirichlet 0-BC at $\partial\Theta$ and *absorbing boundary conditions* on $\partial\Omega$ [e.g. L. Burgnies (1997)]



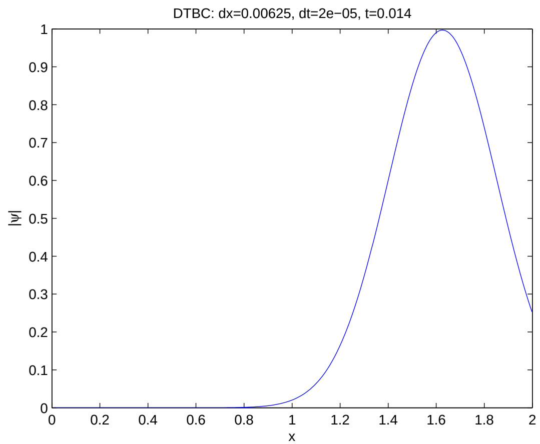
  $\Rightarrow$ unconditionally stable, unphysical reflections at the boundary, huge numerical costs

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:

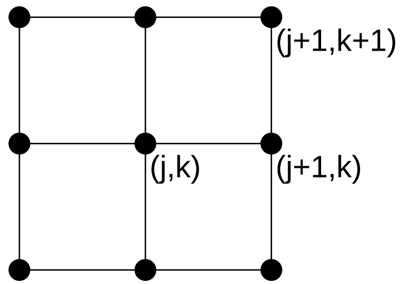
- Crank-Nicolson scheme in time, $t_n = n\Delta t$, $n \in \mathbb{N}$, $H := -\frac{1}{2}\Delta + V$ Hamilton-Operator, $\Omega = [0, X] \times [0, Y]$

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

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

- 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:



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

with

$$\psi_{j,k}^{n+\frac{1}{2}} = \frac{1}{2}\left(\psi_{j,k}^{n+1} + \psi_{j,k}^n\right)$$
$$D_t^+ \psi_{j,k}^n = \frac{\psi_{j,k}^{n+1} - \psi_{j,k}^n}{\Delta t}, \qquad n \geq 0$$
$$D_x^2 \, \psi_{j,k}^n = \frac{\psi_{j-1,k}^n - 2\psi_{j,k}^n + \psi_{j+1,k}^n}{\Delta x^2}, \qquad j \in \mathbb{Z}$$
$$D_y^2 \, \psi_{j,k}^n = \frac{\psi_{j,k-1}^n - 2\psi_{j,k}^n + \psi_{j,k+1}^n}{\Delta y^2}, \qquad k \in \mathbb{N}$$

Discrete Sine-Transformation in y-direction:

$$\hat{\psi}^n_{j,m} \quad := \quad \frac{1}{K}\sum_{k=1}^{K-1} \psi^n_{j,k} \sin\left(\frac{\pi k m}{K}\right) \qquad m = 0, \ldots, K$$

Motivation:

Solve discrete stationary Schrödinger equation in 1D:

$$\begin{aligned} -\frac{1}{2}\Delta_y^2\, \chi^m_{j,k} &= E^m\, \chi^m_{j,k}, \qquad k = 0, \ldots, K \\ \chi^m_{j,0} &= \chi^m_{j,K} = 0. \end{aligned}$$

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

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

Hence follows for $m = 0, \ldots, K$

$$\Rightarrow -\frac{1}{2\Delta y^2}\widehat{\left(\psi^n_{j,k-1} - 2\psi^n_{j,k} + \psi^n_{j,k+1}\right)}_m \quad = \quad \frac{1}{\Delta y^2}\left(1 - \cos\left(\frac{\pi m}{K}\right)\right)\hat{\psi}^n_{j,m}.$$

Sine-Transformation of the discrete Schrödinger equation on the exterior domains $j \leq 0,\ j \geq J$ yields for the modes $m = 0, \dots, K$:

$$C^m_{j+1} \hat{\psi}^{n+1}_{j+1,m} + C^m_{j-1} \hat{\psi}^{n+1}_{j-1,m} + R^m_j \hat{\psi}^{n+1}_{j,m}$$

$$= (D - C^m_{j+1}) \hat{\psi}^n_{j+1,m} + (D - C^m_{j-1}) \hat{\psi}^n_{j-1,m} + (B^m_j - R^m_j) \hat{\psi}^n_{j,m}.$$

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Definition [$\mathcal{Z}$ **- Transformation**]:
The $\mathcal{Z}$*-Transformation of a sequence* $(\psi^n)_{n\in\mathbb{N}}$ *is given by*

$$\mathcal{Z}\left\{\psi^n\right\} = \Psi(z) := \sum_{n=0}^{\infty} \psi^n z^{-n} \qquad z \in \mathbb{C},\ |z| > 1.$$

One can show:

- $\mathcal{Z}\left(\hat{\psi}^{n+1}_{j,m}\right) = -z\hat{\psi}^0_{j,m} + z\Psi^m_j(z)$
- $\psi^0_{J+1,k} = \psi^0_{J-1,k} = \psi^0_{J,k} = 0$ for $k = 0, \ldots, K$
- V_j constant for $j \leq 1,\ j \geq J-1 \Rightarrow C^m_j = C^m,\ R^m_j = R^m,\ B^m_j = B^m$

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

One can show:

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

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

This difference equation with constant coefficients is solved by $\Psi_j(z) = \nu^j(z)$:

$$\nu^2(z) + \left[\frac{R\,z + R - B}{C\,z + C - D}\right]\nu(z) + 1 = 0,$$

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

$\Rightarrow |\nu(z)| > 1$ und $\nu(z)\Psi_J(z) = \Psi_{J-1}(z)$ $\quad\to \mathcal{Z}$-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

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

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: $\mathcal{O}(\Delta x^4 + \Delta y^4 + \Delta t^2)$
- same numerical effort like discretized analytical TRB
- $s_{j,m}^{(n)} = \mathcal{O}(n^{-3/2})$
- 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:

$$D_t^+ ||\psi||_A^2 = 0 \quad \text{with} \quad ||\psi||_A^2 := \langle \psi, A\psi \rangle. \tag{1}$$

some drawbacks:

- DTBC are non-local in time
  - $\rightarrow$ high memory costs: the solution $\psi_{j,m}^{n}$ has to be saved in x_0 and x_J for all time steps $n = 1, 2, \ldots$
  - $\rightarrow$ in each time step $n = 1, 2, \ldots$ you have to calculate K convolutions of the length n (FFT not useable, $\Rightarrow \mathcal{O}(Kn^2)$)

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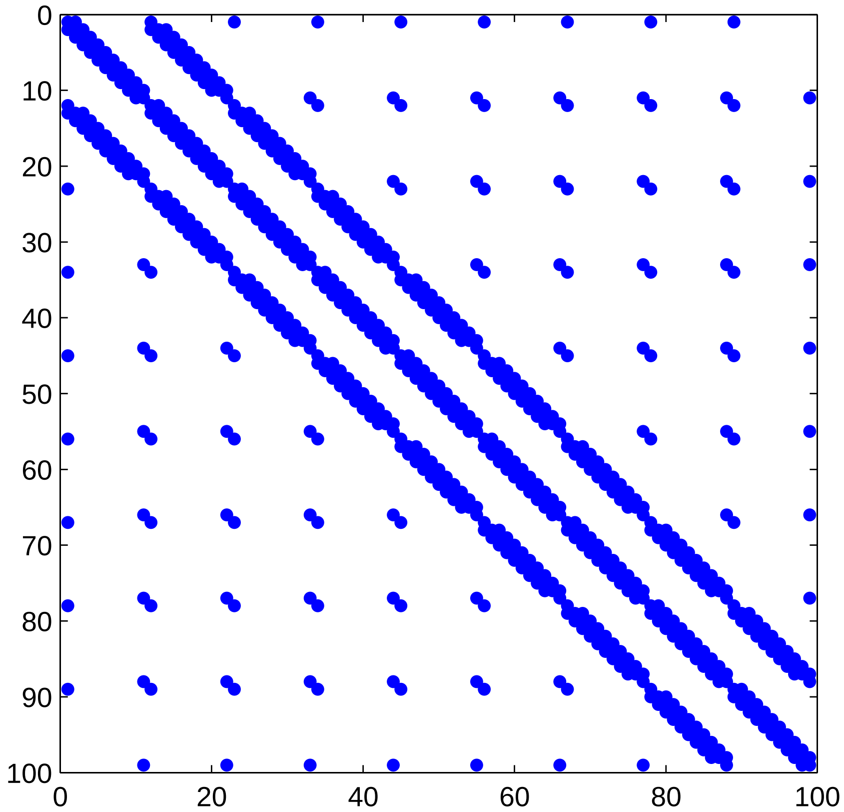
    (FFT not useable, $\Rightarrow \mathcal{O}(Kn^2)$)
- These DTBC are given in the Sine-transformed form: BC of one mode is a linear combination of all other boundary points
  - $\rightarrow$ diagonal structure of the system matrix is destroyed

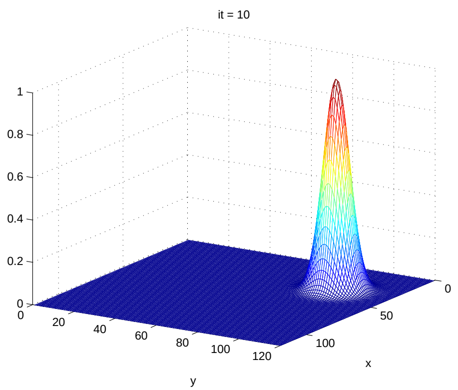


Sparsity pattern of the system matrix for $J = K = 10$

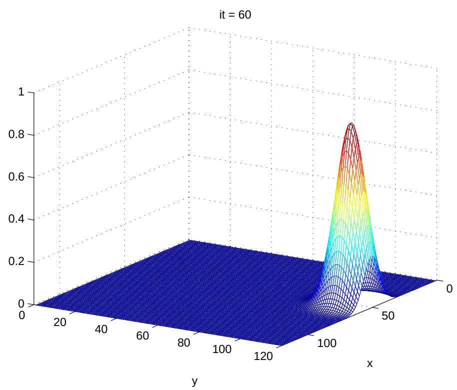
Example 1:

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

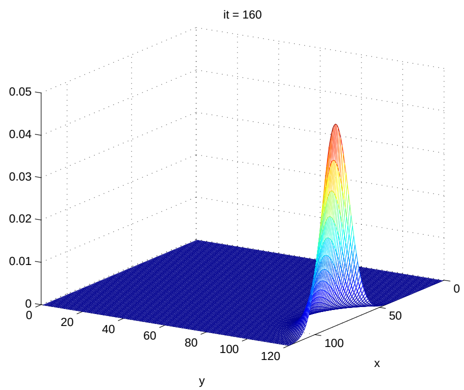
$$\psi^I(x, y) = e^{\mathrm{i}k_x x + \mathrm{i}k_y y - 60\left(\left(x - \frac{1}{2}\right)^2 + \left(y - \frac{1}{2}\right)^2\right)}, \qquad (x, y) \in \Omega$$



$T = 10$



$T = 60\Delta t$



$T = 80\Delta t$

Approximation of DTBC

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

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

*

APPROXIMATION OF DTBC

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

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

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

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

[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

$$\begin{aligned} c_l^{(n)} &= q_l^{-1} c_l^{(n-1)} + b_l q_l^{-1} \psi^{n-1}, \qquad n = 1, \dots, N \\ c_l^{(0)} &= 0 \end{aligned}$$

*

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with

$$\begin{aligned} c_l^{(n)} &= q_l^{-1}c_l^{(n-1)} + b_l q_l^{-1}\psi^{n-1}, \qquad n = 1,\ldots,N \\ c_l^{(0)} &= 0 \end{aligned}$$

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

$$\begin{aligned} q_l^* &= \frac{q_l\bar{a} - \bar{b}}{a - q_l b} \\ b_l^* &= b_l q_l \frac{a\bar{a} - b\bar{b}}{(a - q_l b)(q_l\bar{a} - \bar{b})} \frac{1 + q_l^*}{1 + q_l} \end{aligned}$$

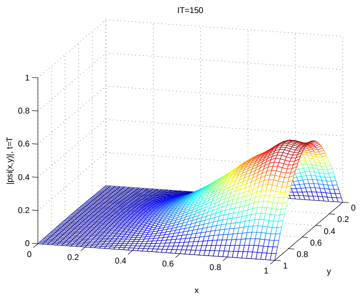
- ➜ Numerical effort: $\mathcal{O}(Kn^2) \rightarrow \mathcal{O}(KLn)$
- ➜ Memory: $\mathcal{O}(Kn) \rightarrow \mathcal{O}(KL)$

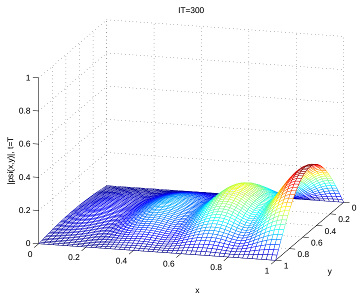
Example 2:

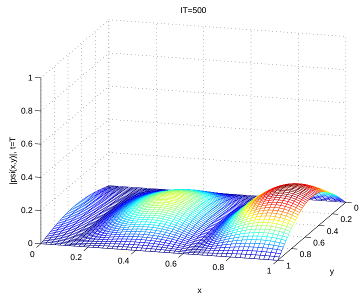
free 2D Schrödinger-Equation in $\Omega = [0,1] \times [0,1]$

Initial function:

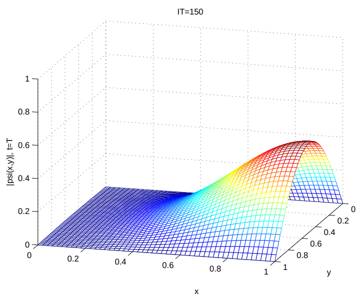
$$\psi^I(x,y) = \sin(\pi y) e^{\mathrm{i}k_x x - 60\left(x-\frac{1}{2}\right)^2}, \qquad (x,y) \in \Omega$$

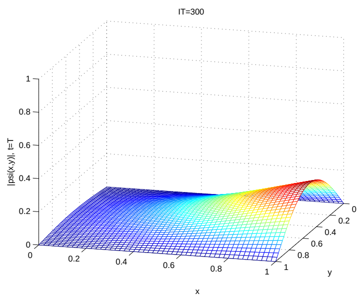


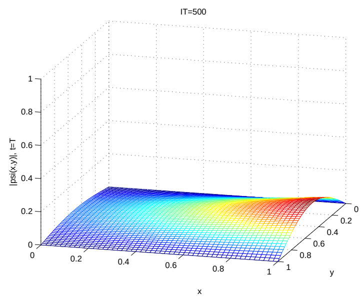




$L = 5:$ $\quad T = 150\Delta t$ $\quad T = 300\Delta t$ $\quad T = 500\Delta t$

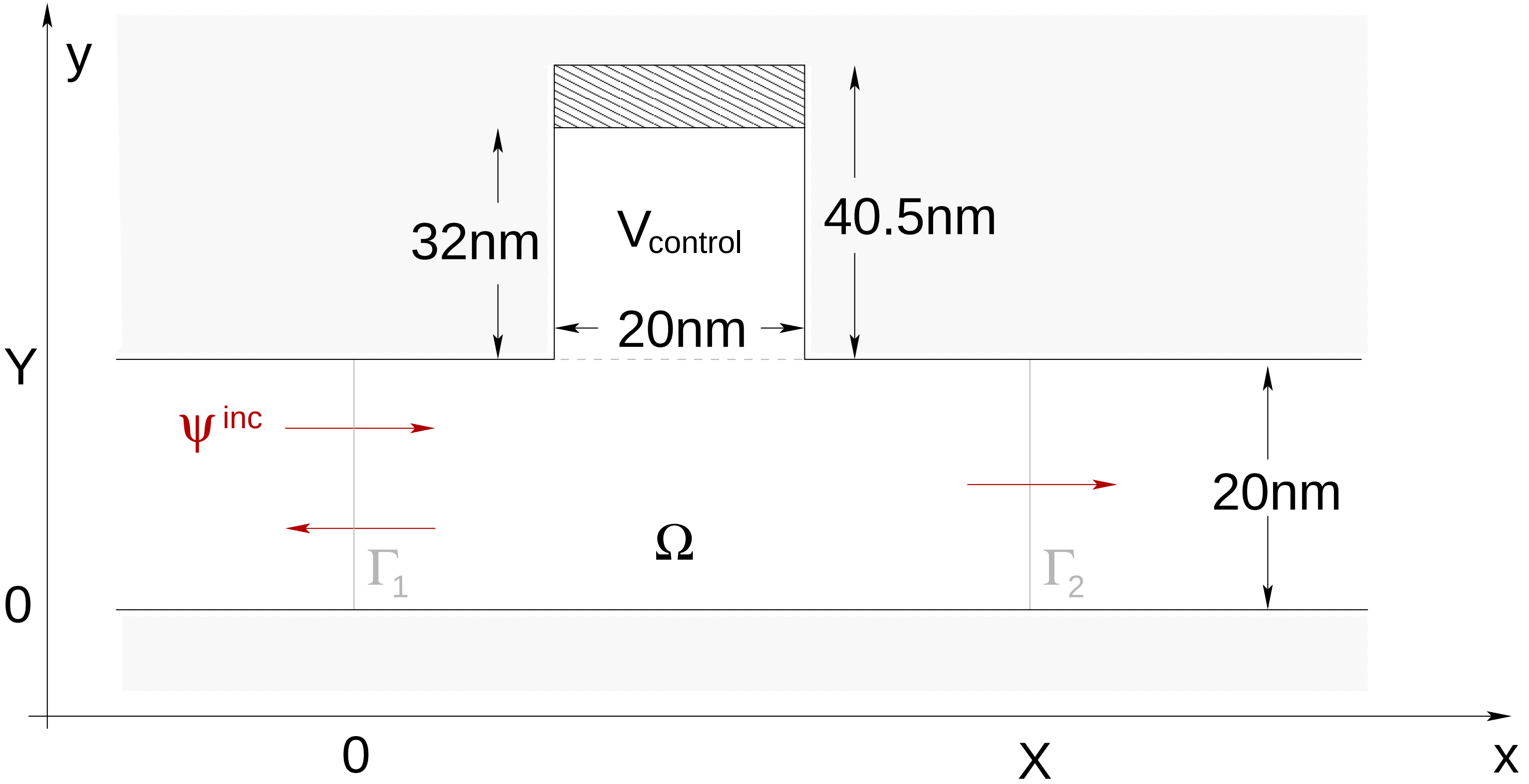






$L = 20:$ $\quad T = 150\Delta t$ $\quad T = 300\Delta t$ $\quad T = 500\Delta t$

SIMULATION OF QUANTUM WAVEGUIDES



- Incoming wave at $x = 0$:

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

- inhomogeneous DTBC at $x = 0$, DTBC at $x = X$

Little trick to suppress oscillations in time:

ψ^{inc} oscillates like $e^{\frac{-\mathrm{i}Et}{\hbar}}$ in time.

E big:

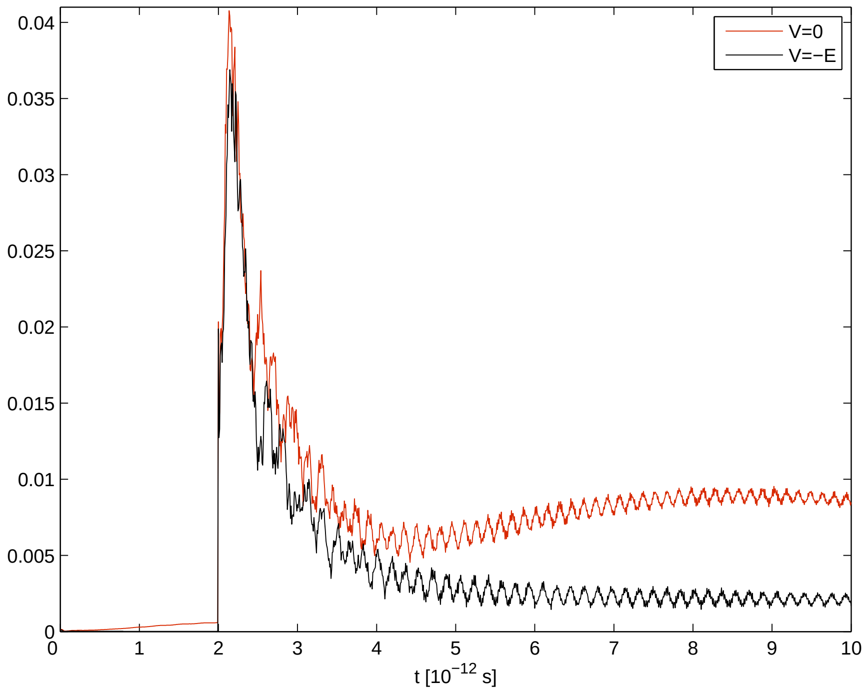
- ➜ fast oscillation of the solution in time
- ➜ small time step size is necessary
- ➜ high numerical effort for the analysis of steady state and long-time behaviour

Define

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

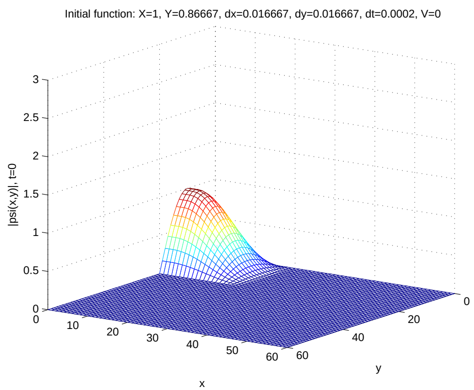
φ solve the modified Schrödinger equation

$$\mathrm{i}\hbar\varphi_t \quad = \quad -\frac{\hbar^2}{2m^*}(\varphi_{xx}+\varphi_{yy}) + \underbrace{(V-\omega\hbar)}_{=:\tilde{V}}\varphi$$

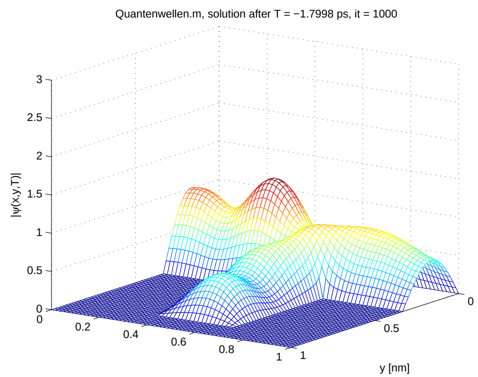


$$f_1(t) = ||\psi_1(x,y,t) - \psi_{ref}(x,y,t)||_2$$
$$f_2(t) = ||\psi_2(x,y,t) - \psi_{ref}(x,y,t)||_2$$

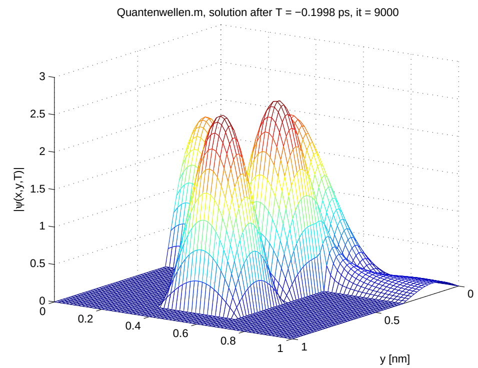
ψ_1 is calculated with $\tilde{V} = 0$, ψ_2 with $\tilde{V} = -E$ and ψ_{ref} is a numerical reference solution, which has been calculated with high accuracy.



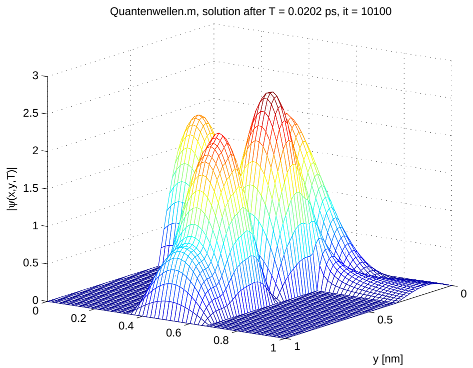
$T = 0\Delta t$



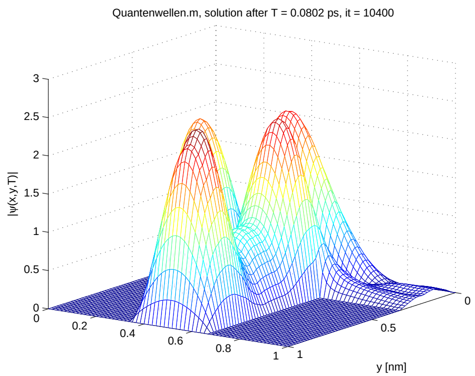
$T = 1000\Delta t$



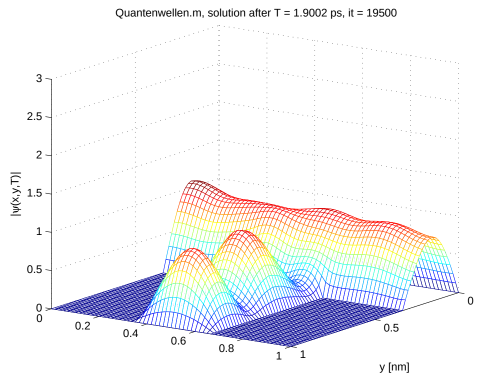
$T = 9000\Delta t$



$T = 10100\Delta t$



$T = 10400\Delta t$



$T = 19500\Delta t$

Drawbacks of the simulations:

- Hard walls (zero Dirichlet BCs) and edges are not practicable in industry!
  - $\rightarrow$ Geometry of computational domain shall be realized by potentials also in the simulations.
  - $\rightarrow$ How to choose the incoming wave and the initial function then?
- Potentials are NOT constant in the exterior domains!
  - $\rightarrow$ Decoupling of the modes for $V(x,y) \neq const.$ after Sine-Transformation is not possible

EXTENSION OF THE DTBC TO MORE ARBITRARY POTENTIALS

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Discrete Schrödinger equation:

5-point scheme in space, Crank-Nicolson in time:

$$\mathrm{i}\hbar D_t^+ \psi_{j,k}^n = -\frac{\hbar^2}{2m^*}\left(D_x^2 + D_y^2\right)\psi_{j,k}^{n+\frac{1}{2}} + V_{j,k}^{n+\frac{1}{2}}\psi_{j,k}^{n+\frac{1}{2}}$$

➜ Calculate new Eigenfunctions, which take the potential into account!

Solve the eigenvalue equation on the exterior domains ($j \le 0,\ j \ge J$):

$$-\frac{1}{2\Delta y^2}\left(\chi^n_{j,k-1,m} - 2\chi^n_{j,k,m} + \chi^n_{j,k+1,m}\right) + V_k^{n+\frac{1}{2}}\chi^n_{j,k,m} = E^n_{j,m}\chi^n_{j,k,m}$$

with

$$\Delta y \sum_{k=0}^{K} \left|\chi^n_{j,k,m}\right|^2 = 1 \qquad \text{and} \qquad \chi^n_{j,0,m} = \chi^n_{j,K,m} = 0$$

for $0 \le k,\ m \le K,\ n > 0$.

Transformation w.r.t. the eigenfunctions

$$\hat{\psi}^n_{j,m} = \Delta y \sum_{k=1}^{K-1} \chi^n_{j,k,m}\psi^n_{j,k}, \qquad 0 \le m \le K.$$

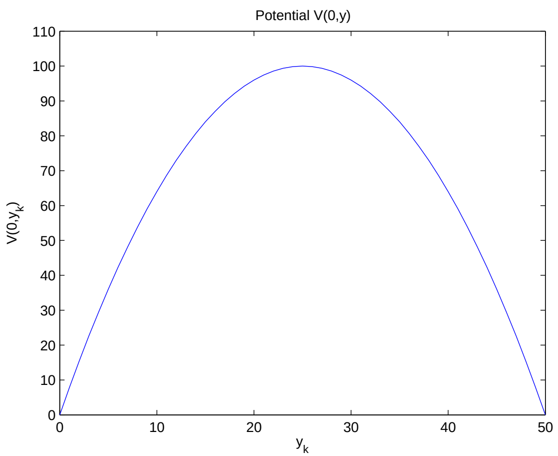
yields

$$\mathrm{i}\hbar D_t^+\,\hat{\psi}^n_{j,m} = -\frac{\hbar^2}{2m^*}D_x^2\,\hat{\psi}^{n+\frac{1}{2}}_{j,m} + E^n_{j,m}\hat{\psi}^{n+\frac{1}{2}}_{j,m}$$

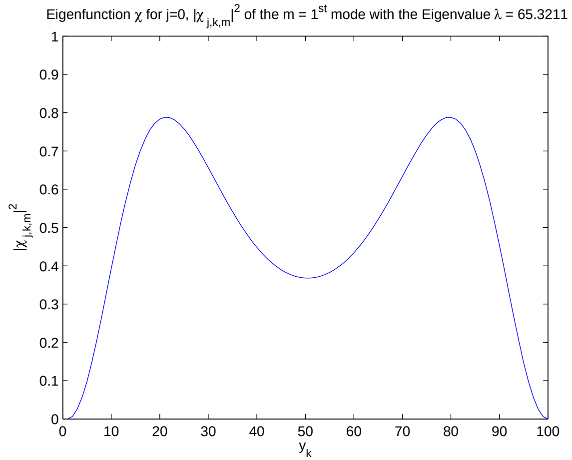
➜ same structure as the sine-transformed Schrödinger equation!

[N. Ben Abdallah, M.S. (2005)]

Example 3: 2D channel



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



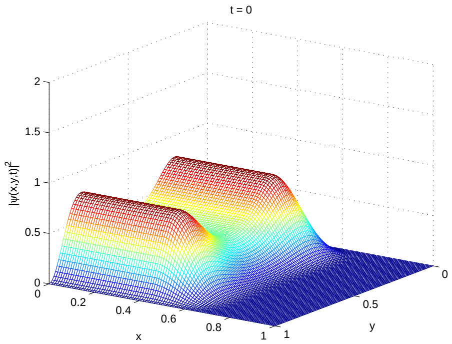
eigenfunction χ of $m = 1$

➜ initial function:

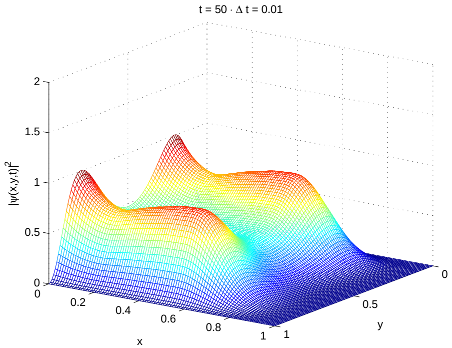
$$\psi^{I}_{j,k} = e^{\mathrm{i}k_x j\Delta x}\chi^{0}_{j,k,m}$$

➜ incoming wave:

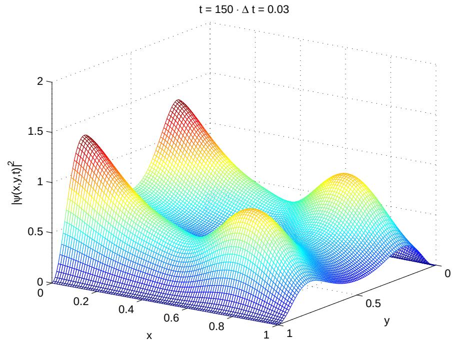
$$\psi^{inc}_{j,k,n} = e^{\mathrm{i}k_x j\Delta x}\chi^{0}_{j,k,m}e^{-\mathrm{i}E_x n\Delta t} \qquad \text{with} \qquad E_x = \frac{1-\cos(k_x\Delta x)}{\Delta x^2}$$



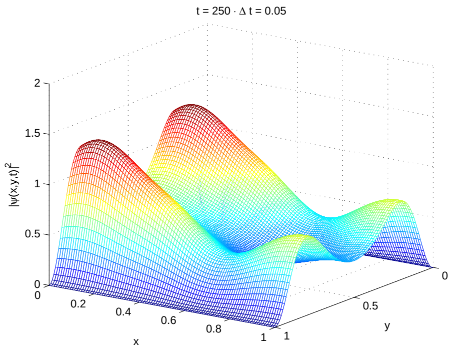
$T = 0\Delta t$



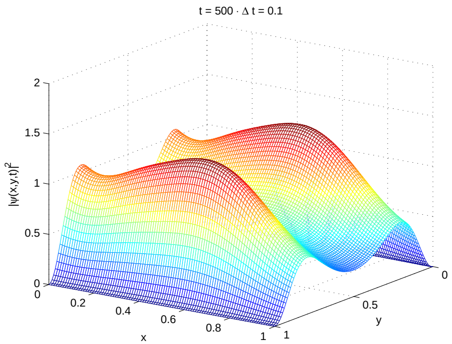
$T = 50\Delta t$



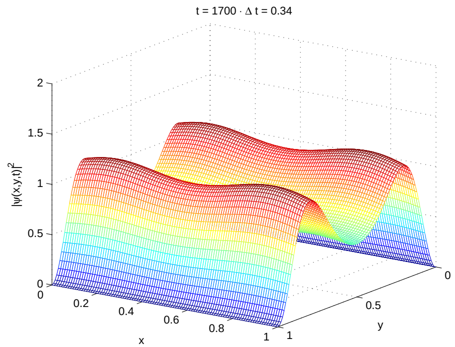
$T = 150\Delta t$



$T = 250\Delta t$



$T = 500\Delta t$



$T = 1700\Delta t$

SCHRÖDINGER EQUATION ON CIRCULAR DOMAINS

Solve the Schrödinger equation (in polar coordinates)

$$\mathrm{i}\psi_t = -\frac{1}{2}\left(\frac{1}{r}(r\psi_r)_r + \frac{1}{r^2}\psi_{\theta\theta}\right) + V(r,\theta,t)\psi, \qquad r > 0, 0 \le \theta \le 2\pi,\ t > 0$$

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:

$$a_j \Psi_{J+1}(z) + b_j(z)\Psi_J(z) + c_j \Psi_{J-1}(z) = 0$$

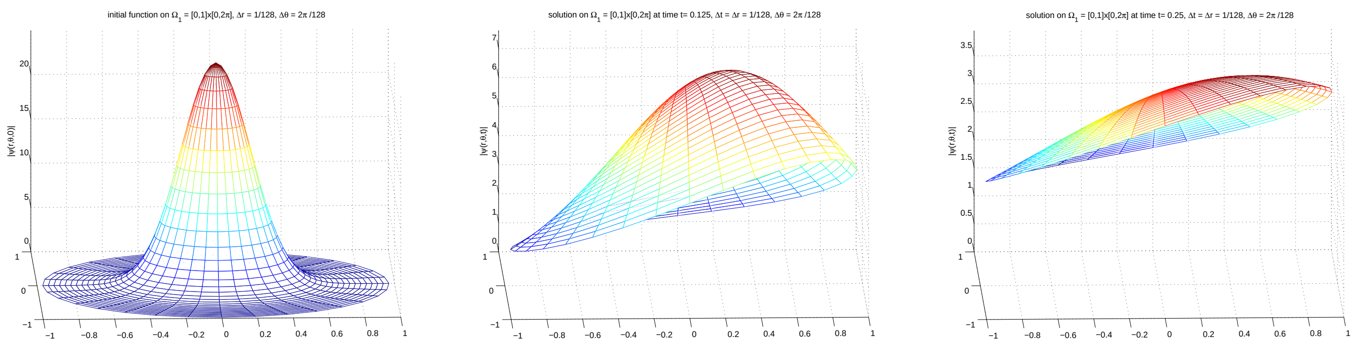
- calculation of the convolution coefficients for the DTBC
  $\longrightarrow$ "recursion from infinity"
- singularity at $r = 0$ $\longrightarrow$ not equidistant offset-grid $\tilde{r}_j = r_{j+\frac{1}{2}}$
- approximation of the convolution coefficients and the -sum

[A.Arnold, M. Ehrhardt, M. S., I. Sofronov (2006)]

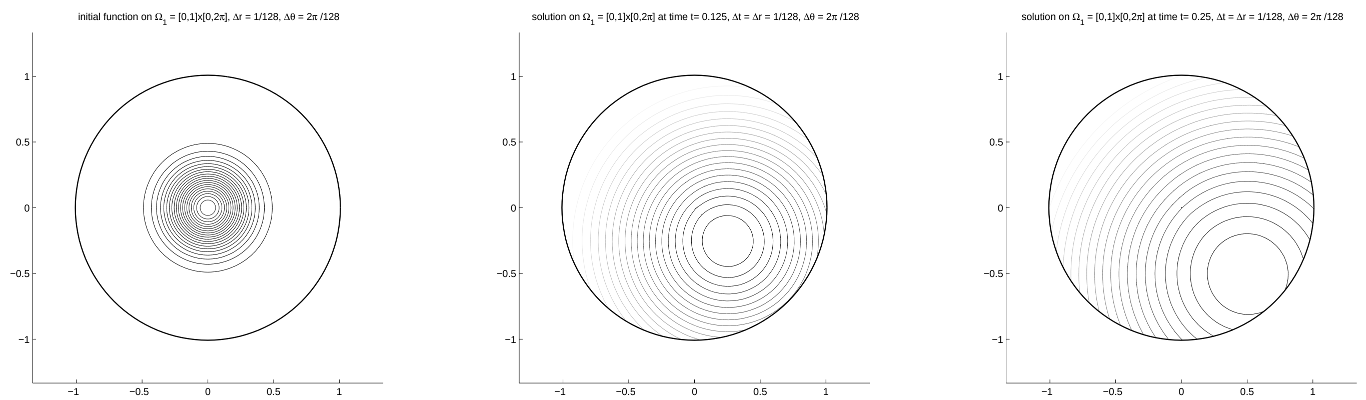
Example 4:

free Schrödinger equation on unit disc $\Omega_1 = [0,1] \times [0,2\pi]$

$$\psi^I(r,\theta) = \frac{1}{\sqrt{\alpha_x \alpha_y}} e^{2ik_x r\cos\theta + 2ik_y r\sin\theta - \frac{(r\cos\theta)^2}{2\alpha_x} - \frac{(r\sin\theta)^2}{2\alpha_y}}$$



initial function $\quad T = 0.125 \quad T = 0.25$



Error due to the scheme/TBC:

$$L(\psi, \varphi, t_n, \Omega) := \frac{||\psi(r_j, \theta_k, t_n) - \varphi(r_j, \theta_k, t_n)||_{\Omega,2}}{||\varphi(r_j, \theta_k, t_n)||_{\Omega,2}}$$

ψ: numerical solution

φ: exact solution or numerical reference solution