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Open Boundary Conditions for Quantum Waveguide

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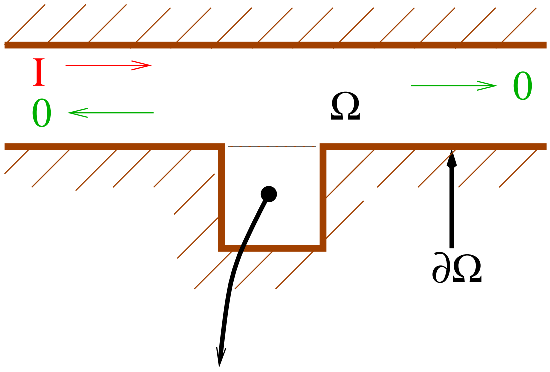
Outline

- Quantum Waveguides
  - Schrödinger model
- Transparent Boundary Conditions for Schrödinger Equation
  - discretization (nonlocal in t)
  - approximation (local in t)
  - waveguide simulation
  - circular geometry

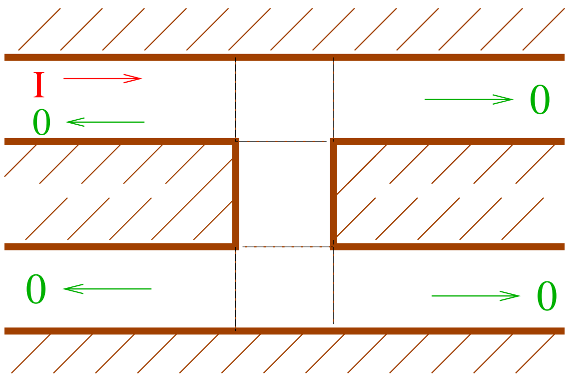
Quantum Waveguides

- Elements of future semiconductors:

Quantum interference transistor



Coupling of quantum wires



control potential V $\longrightarrow$ reflection/transmission

- 2D-electron gas . . . $\psi(x, y, t) \in \mathbb{C}$

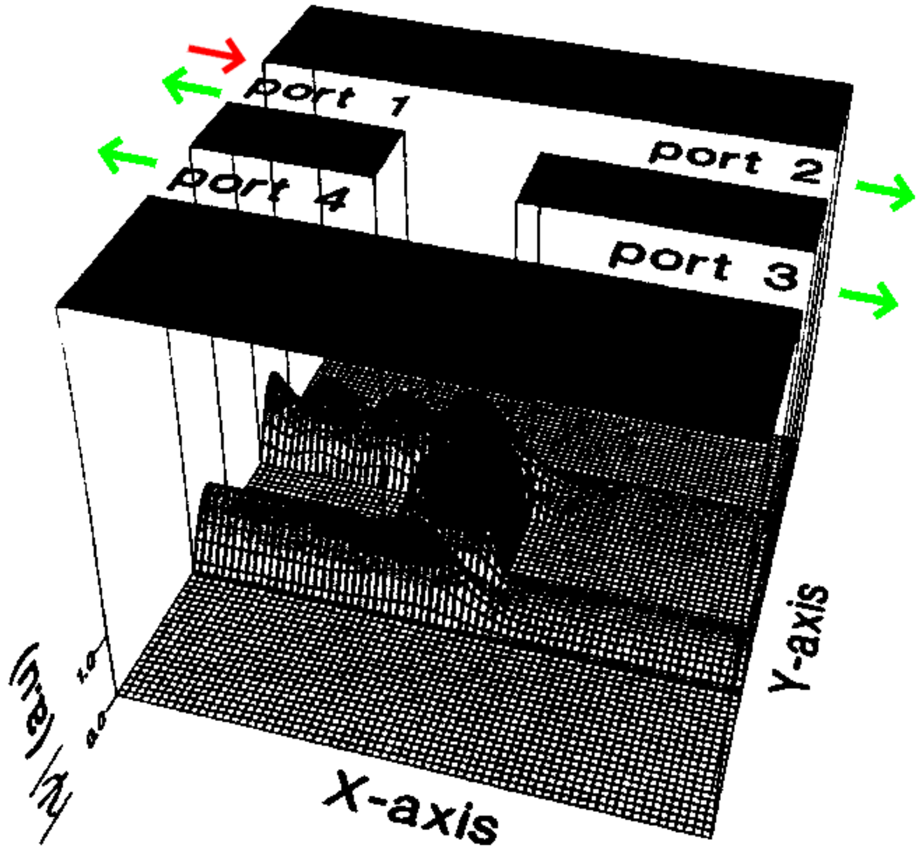
$$\begin{cases} i\hbar\psi_t = -\frac{\hbar^2}{2m_e}\Delta\psi + V(x,y,t)\psi, & \Omega \subseteq \mathbb{R}^2, t > 0 \\ \psi = 0, & \partial\Omega \\ + \text{“open” boundary conditions at } I, O \end{cases}$$

Goals:

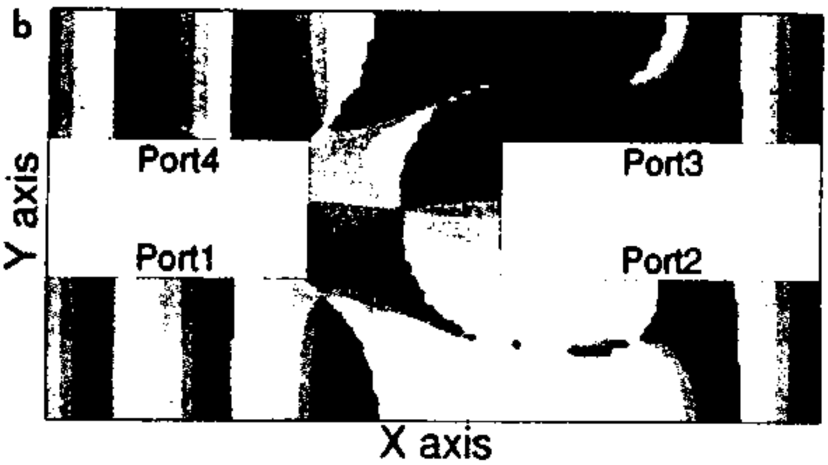
- stationary modes (with const. inflow)
- transient behavior (e.g. switching times)

Stationary Waves in a Quantum Waveguide

Electron density: modulus of wavefunction $|\psi(x,y)|$, interference in canal 1



phase of wavefunction: $\arg\psi(x,y)$



from: [Vanbésien, Burgnies, Lippens '95], IEMN-Lille

Question: Construction of *artificial* BCs for transient simulations for keeping the computational domain as small as possible

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Discretization of analytic TBC

left TBC for free 1D-Schrödinger equation $i\psi_t = -\psi_{xx}$:

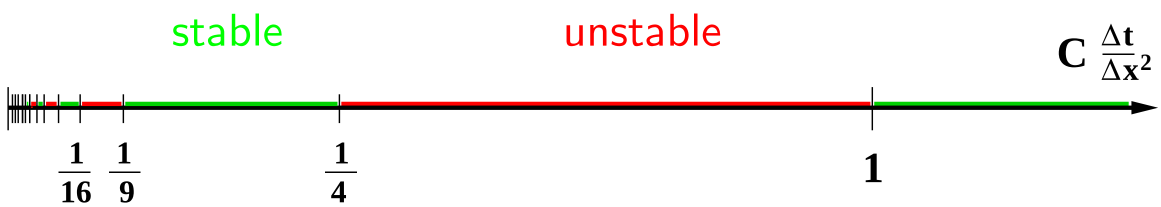
$$\sqrt{-i\partial_t}\,\psi = \psi_x \qquad \text{or} \qquad \psi(0,t) = \frac{1}{\sqrt{\pi}}\, e^{\frac{\pi}{4}i} \int_0^t \frac{\psi_x(0,\tau)}{\sqrt{t-\tau}}\, d\tau$$

previous discretization [Mayfield '89]:

$$\int_0^{t_N} \frac{\psi_x(0,t_N-\tau)}{\sqrt{\tau}} d\tau \approx \frac{1}{\Delta x} \sum_{n=0}^{N-1} (\underbrace{\psi_1^{N-n} - \psi_0^{N-n}}_{\text{left boundary of } [t_n, t_{n+1}]}) \int_{t_n}^{t_{n+1}} \frac{d\tau}{\sqrt{\tau}}$$

Theorem [Mayfield]: overall IBV–scheme (with Crank-Nicolson finite differences) is stable $\iff$

$$C\frac{\Delta t}{\Delta x^2} \in \bigcup_{j \in N_0} [(2j+1)^{-2}, (2j)^{-2}]$$



- Drawbacks of discretizing the analytic TBC:
  - destroys the unconditional stability of the CN–scheme !
  - numerical reflections at the boundary

New discrete TBC

STRATEGY:

- discretize whole space problem ($j \in \mathbb{Z}$)
- derivation of the discrete TBC (for discrete scheme)
  instead of: discretization of the analytic TBC

simple model discretization:
Crank-Nicolson FD-scheme for free Schrödinger equation:

$$i\frac{\psi_j^{n+1}-\psi_j^n}{\Delta t} = -D_{\Delta x}^2 \frac{\psi_j^{n+1}+\psi_j^n}{2}, \;\; D_{\Delta x}\,\psi_j^n = \frac{\psi_{j+\frac{1}{2}}^n - \psi_{j-\frac{1}{2}}^n}{\Delta x}$$

$\psi_j^n \approx \psi(j\Delta x, n\Delta t)$, unconditionally stable: $\|\psi^n\|_2 = \|\psi^0\|_2$

Z-transformed left exterior problem ($\psi_j^0 = 0,\; j \le 0$)
with $\mathcal{Z}\{\psi_j^n\} = \hat{\psi}_j(z) = \sum_{n=0}^{\infty} \psi_j^n\, z^{-n},\; z \in \mathbb{C}$:

$$\hat{\psi}_{j-1} - 2(1 - i\frac{\Delta x^2}{\Delta t}\frac{z-1}{z+1})\,\hat{\psi}_j + \hat{\psi}_{j+1} = 0, \quad j \le 1$$

$\longrightarrow$ transformed DTBC
(from decaying solution for $j \to -\infty$):

$$\hat{\psi}_1(z) = \alpha(z)\hat{\psi}_0(z), \quad |\alpha(z)| > 1$$

- inverse Z-transformation (explicit or numerical): $(s_n) := \mathcal{Z}^{-1}\{\frac{z+1}{z}\alpha(z)\}$
- discrete TBC: $\psi_1^n = \sum_{k=1}^{n} \psi_0^k s_{n-k} - \psi_1^{n-1}$
- 3-point recursion for (s_n)
- $s_n = O(n^{-3/2})$ ... cp. to (1)

Theorem [AA '95]: CN - FD scheme for Schrödinger equation with discrete TBC is unconditionally stable:

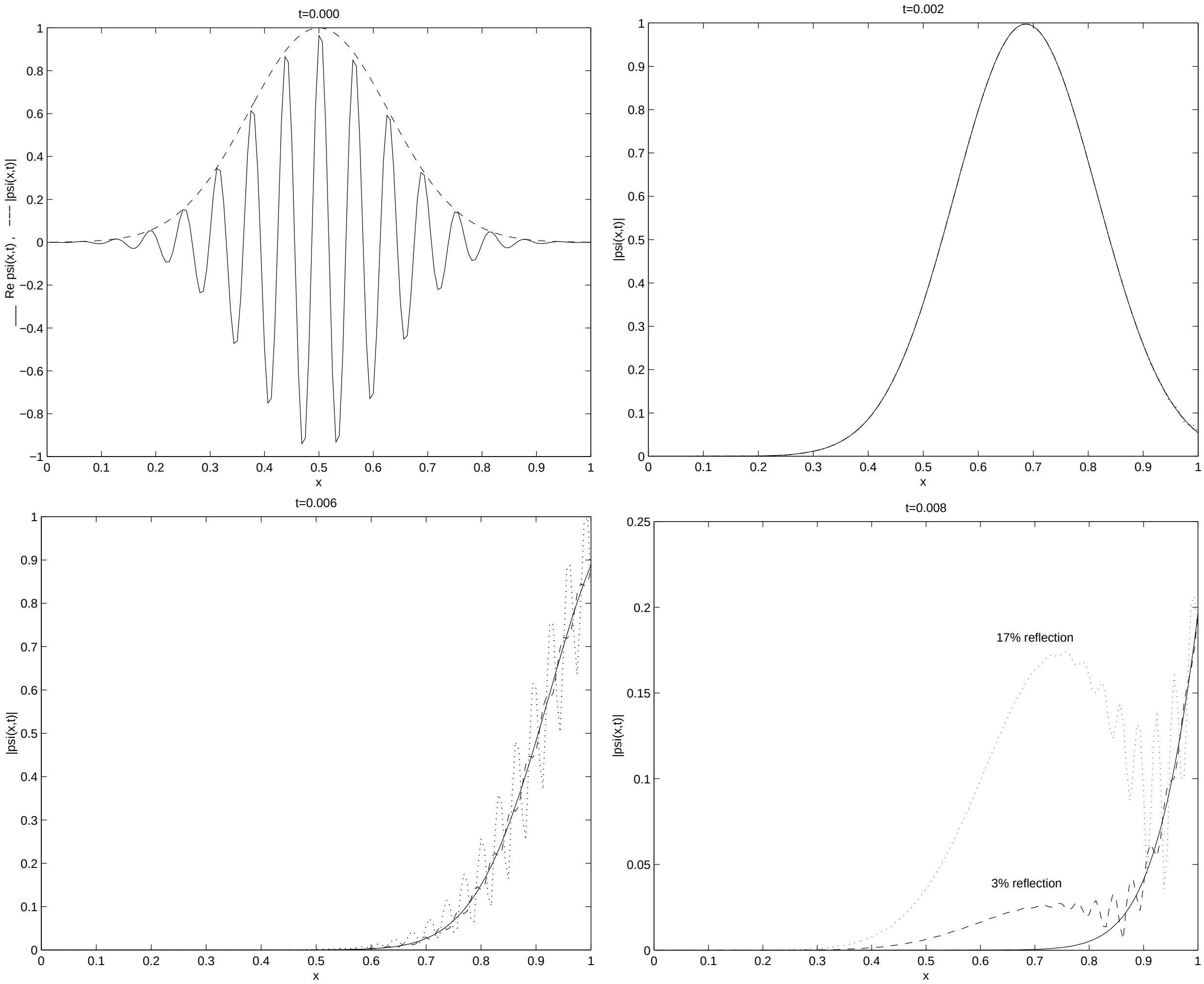
$$\|\psi^n\|_2^2 := \Delta x \sum_{j=1}^{J} |\psi_j^n|^2 \le \|\psi^0\|_2^2, \quad n \ge 1$$

$\longrightarrow$ no numerical reflections

$\longrightarrow$ same numerical effort as 'ad-hoc' discretization of

$$\psi_x(0,t) = C \frac{d}{dt} \int_0^t \frac{\psi(0,\tau)}{\sqrt{t-\tau}} d\tau \qquad (1)$$

free Schrödinger equation ($V = 0$)



Gaussian beam, right-traveling [AA, VLSI Design '98]

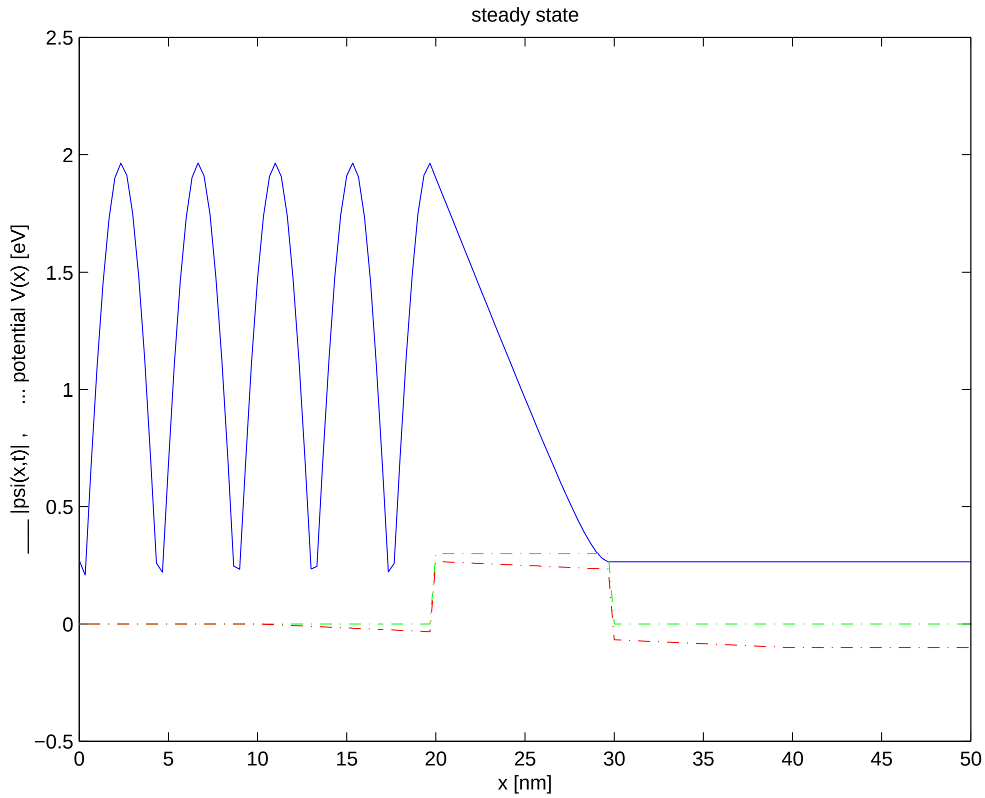
$$\psi^I(x) = \exp[100ix - 30(x-0.5)^2], \quad x \in \mathbb{R}$$

$\Delta x = \frac{1}{160}$, $\Delta t = 0.00002$

$\cdots$	B. Mayfield	discretization of the analytic TBC
- - -	Baskakov & Popov	
——	AA	new discrete TBC

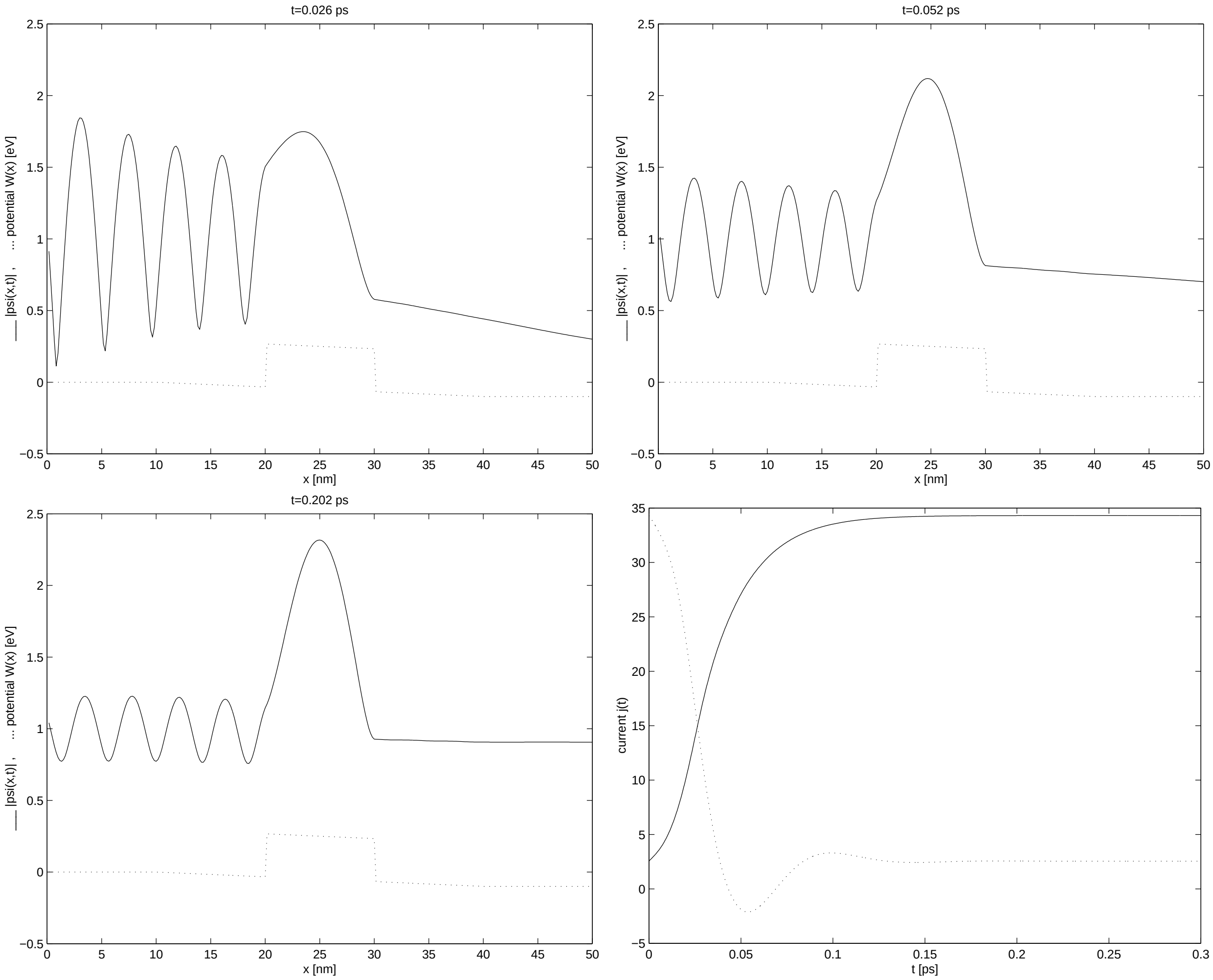
Scattering at potential barrier

- incoming plane wave ψ^{in} (from left) with 0.3 eV
- potential barrier $V(x)$: 0.3 eV
- at $t = 0$: applied bias of -0.1 eV switched on:



- *important:* inhomogeneous discrete TRB at $x = 0$ [AA, TTSP 2001]

$$(\partial_x - \sqrt{-i\partial_t})\,(\psi(0,t) - \psi^{in}(0,t)) = 0$$



$\longrightarrow$ $\psi(x,t)$ converges to new steady state corresp. to $W(x)$

$\longrightarrow$ switching current $j(t)$ stationary from $t \approx 0.2$ ps on

2D Schrödinger equation - waveguide

$$\psi_{xx} = -\psi_{yy} - i\psi_t + V\psi$$

- TBC at $x = 0$ is non-local (pseudo-differential) in t and y:

$$\psi_x(0, y, t) = \sqrt{-\partial_{yy} - i\partial_t + V}\ \psi$$

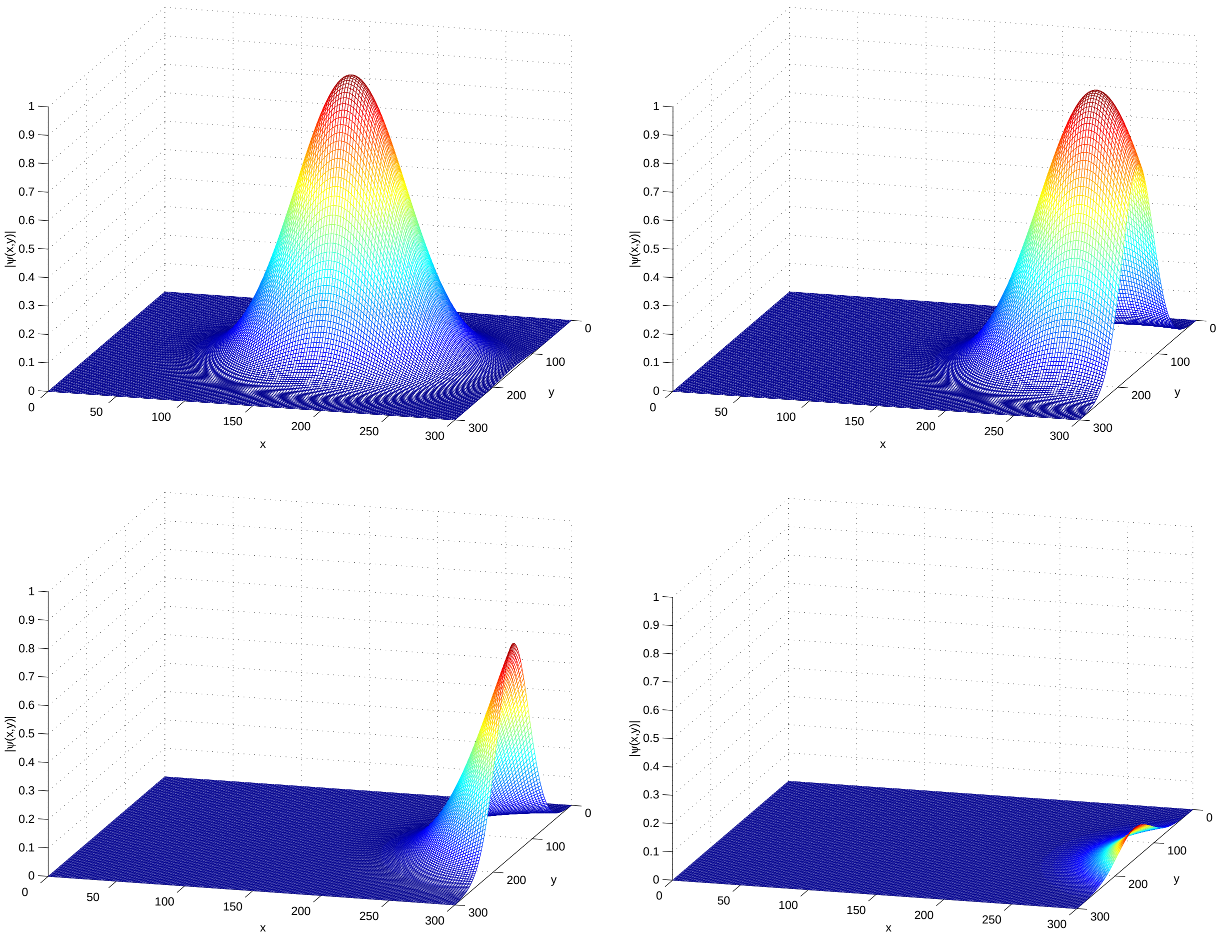
- for waveguides: $\psi(x, 0, t) = \psi(x, Y, t) = 0$:

- TBC is local for each sine-mode in y:

$$\begin{aligned} \hat{\psi}_x^m(0, t) &= \sqrt{-i\partial_t + V^m}\ \hat{\psi}^m \\ &= \sqrt{\frac{-i}{\pi}\frac{d}{dt}}\, e^{-iV^m t} \int_0^t \frac{\hat{\psi}^m(0, \tau) e^{iV^m \tau}}{\sqrt{t-\tau}} d\tau \\ V^m &= V_0 + \left(\frac{m\pi}{Y}\right)^2, \qquad m \in \mathbb{N} \end{aligned}$$

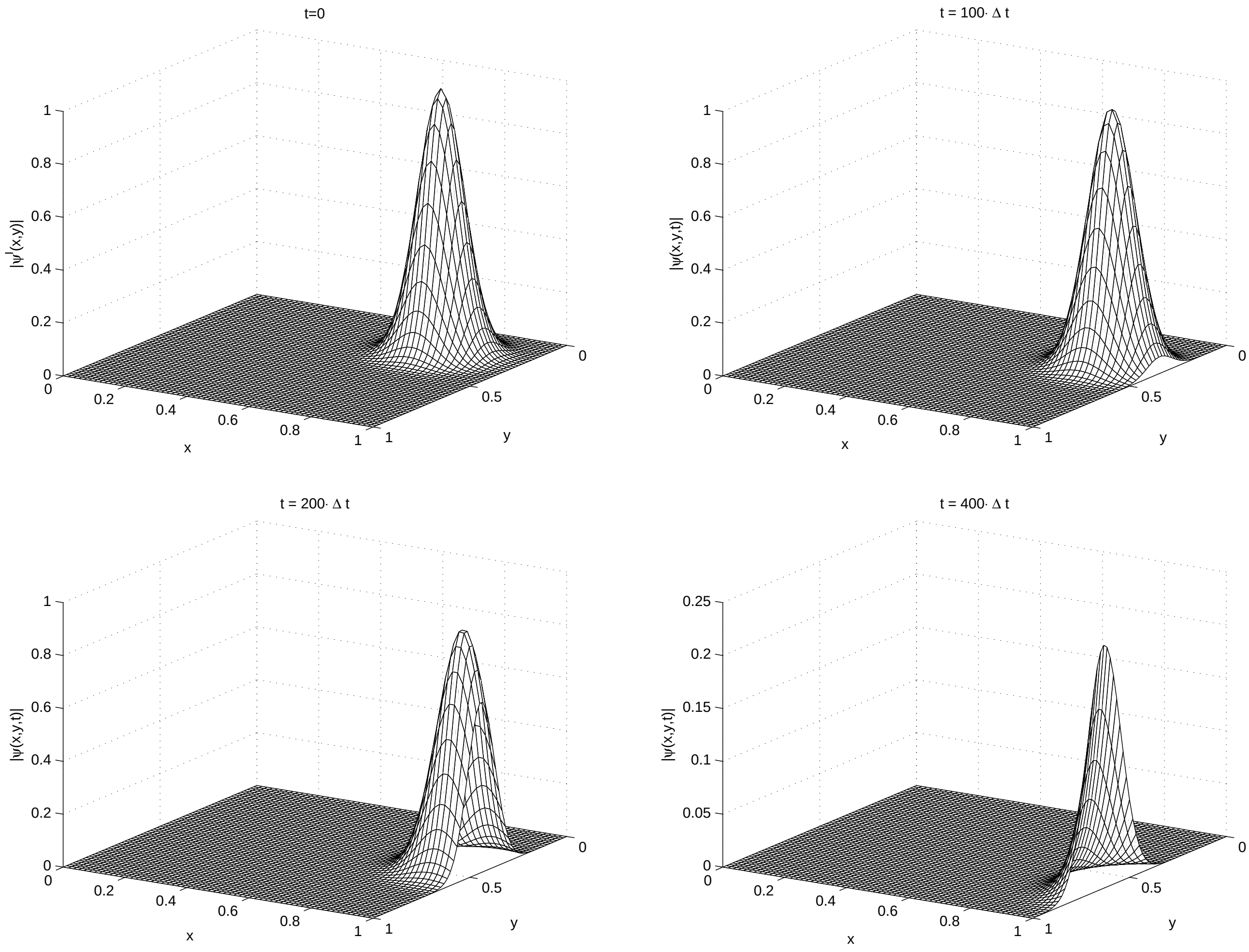
- rigorous derivation for Schrödinger-Poisson: [Ben Abdallah-Méhats-Pinaud '04]
- discrete derivation: [AA-Ehrhardt-Sofronov '03]

2D Schrödinger equation ($V = 0$) – orthogonal incident



- right-traveling Gaussian beam, TBC at $x{=}300$ [Schulte-AA '07]
- implementation of discrete TBC in y-Fourier space (since nonlocal in y and t)

2D Schrödinger equation ($V = 0$) – non-orthogonal incident

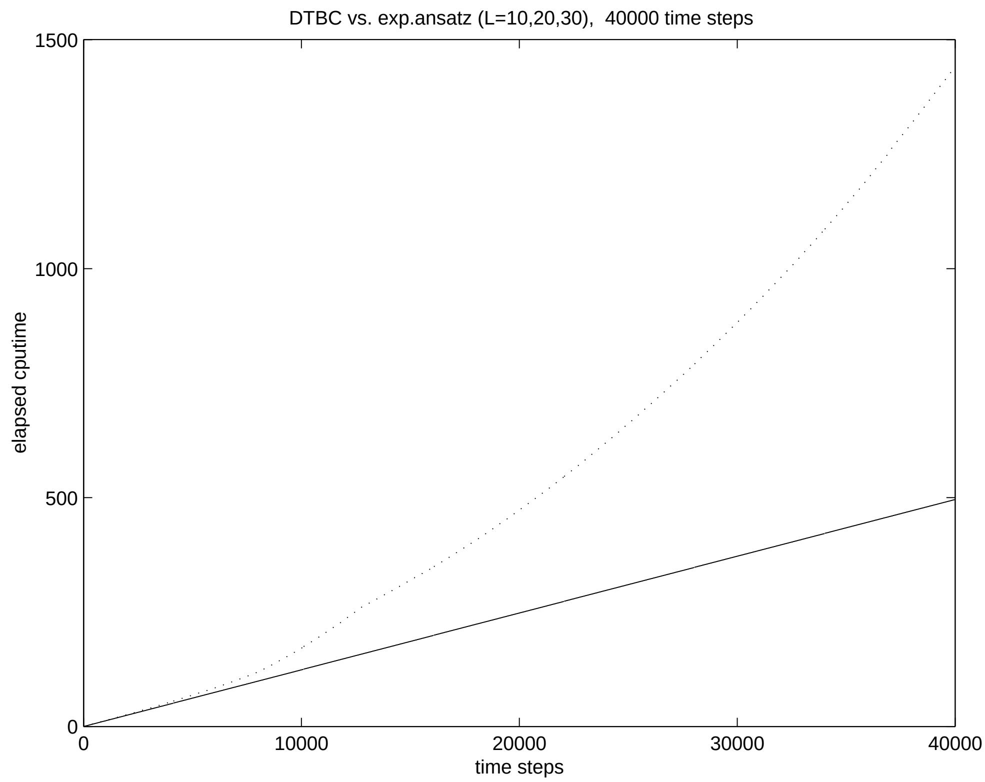


- right-traveling Gaussian beam hits boundary at 45°
- result impossible with *absorbing layer* – can only be tuned for 1 wavenumber

- advantage of TBCs:
  - absolutely reflection–free
  - unconditionally stable

- disadvantage (for long–time calculations):
  numerical effort $O(N^2)$; N...# of time steps
  TBC-evaluation (discrete convolution) dominates PDE-solution

- goal:
  approximate convolution kernel $(s_n) \longrightarrow O(N)$–effort



cpu–time for TBC $(\cdots)$ and approximative TBC (—)

Approximative TBCs – Fast evaluation of convolutions

- Idea: approximation of s_n by sum of exponentials; $s_n = O(n^{-3/2})$ — discrete analogue of [Grote-Keller '95]:

$$s_n \approx \tilde{s}_n = \sum_{l=1}^{L} b_l q_l^{-n}, \quad n \in \mathbb{N}, \; |q_l| > 1, \; L \sim 20$$

$$\mathcal{Z}\{\tilde{s}_n\} = s_0 + \sum_{l=1}^{L} \frac{b_l}{q_l z - 1}, \quad |z| \geq 1.$$

- b_l, q_l from Padé approximation of

$$f(x) = \sum_{n=0}^{2L-1} s_n x^n, \quad x = \frac{1}{z}$$

- Advantage for long-time calculations:

– reduction of numerical costs: $O(N^2) \to O(L \cdot N)$
– reduction of memory: $O(N) \to O(L)$

- recursion:

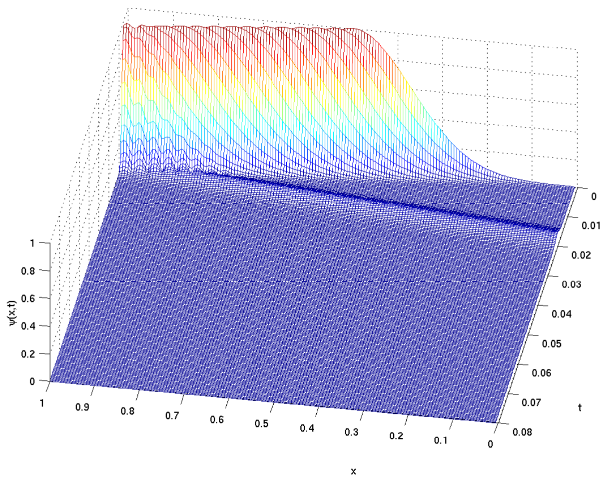
$$\sum_{k=0}^{n-1} u_k \tilde{s}_{n-k} = \sum_{l=1}^{L} C_l^{(n)},$$

with

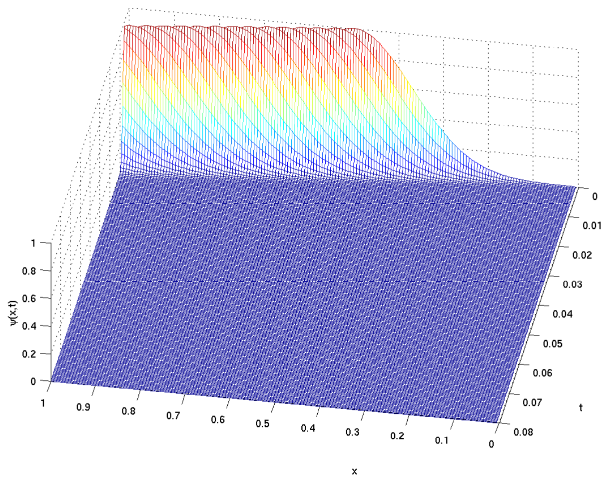
$$C_l^{(n)} = q_l^{-1} C_l^{(n-1)} + b_l q_l^{-1} u_{n-1}; \quad n = 1, \ldots, N$$

$$C_l^{(0)} \equiv 0.$$

free Schrödinger equation (1D, $V = 0$)

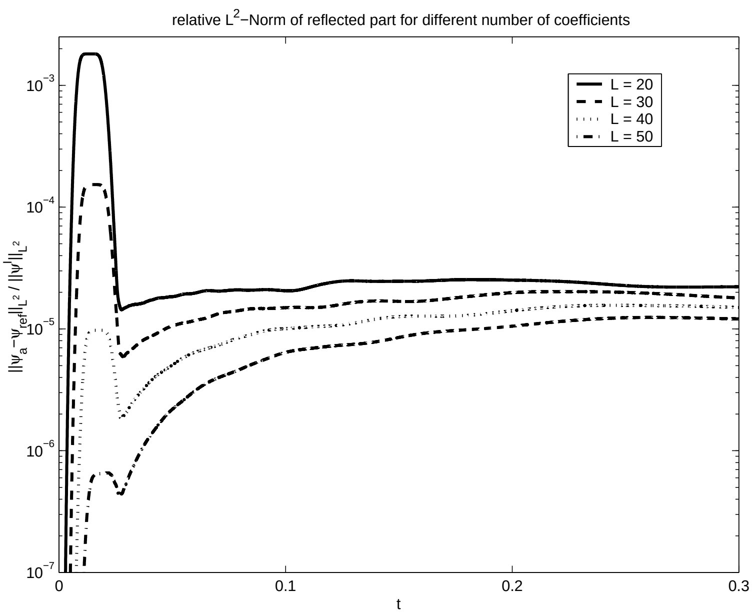


solution with $L = 10$

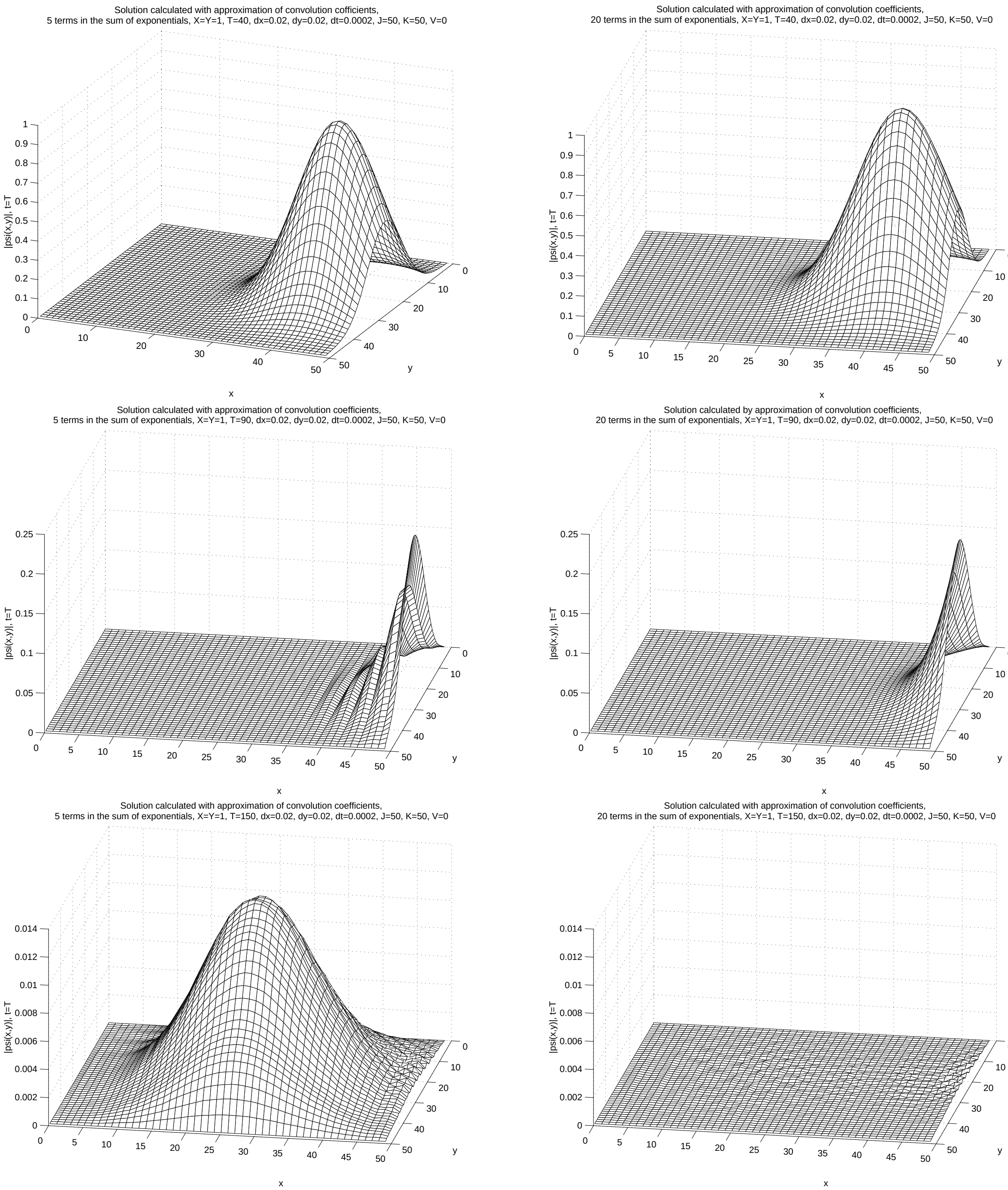


solution with $L = 20$

relative L^2-error with approximate TBCs, up to 15.000 time steps



2D Schrödinger equation ($V = 0$)

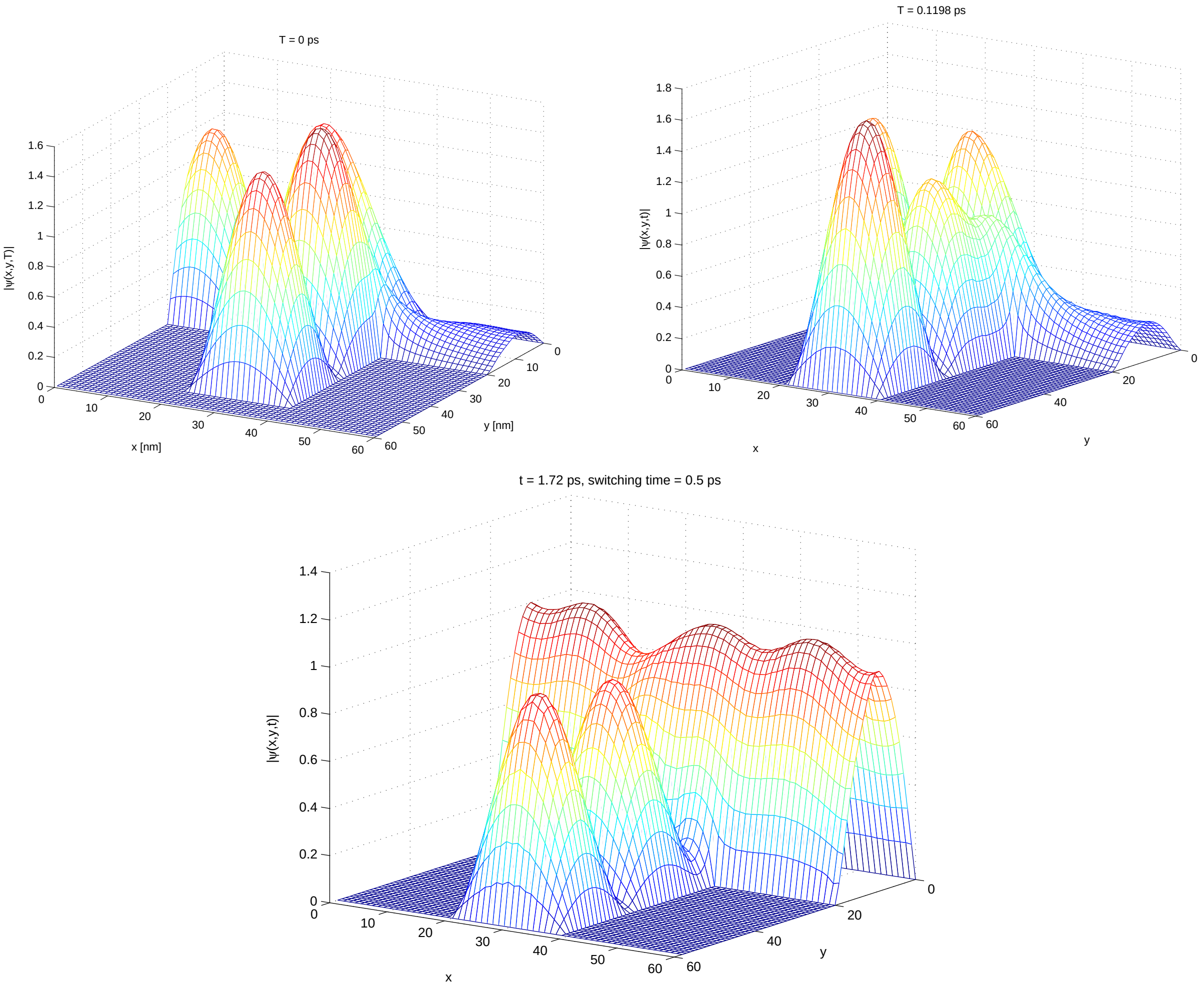


solution with $L = 5$ solution with $L = 20$

TBC at $x = 50$; Gaussian beam, right-traveling [Schulte-AA 07]

Quantum waveguide with resonator - switching

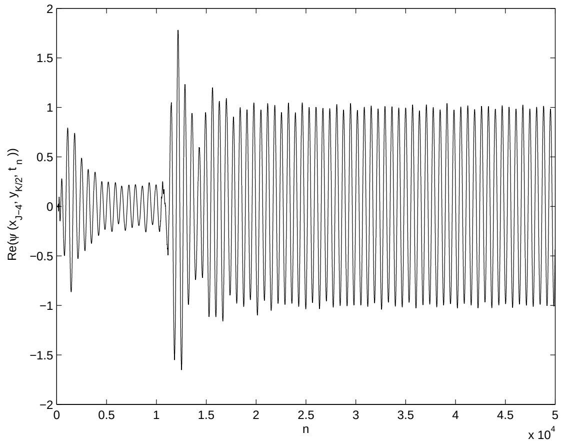
- incoming plane wave ψ^{in} (from left) with 0.03 eV
- resonator size: 20×32 nm / 20×39 nm



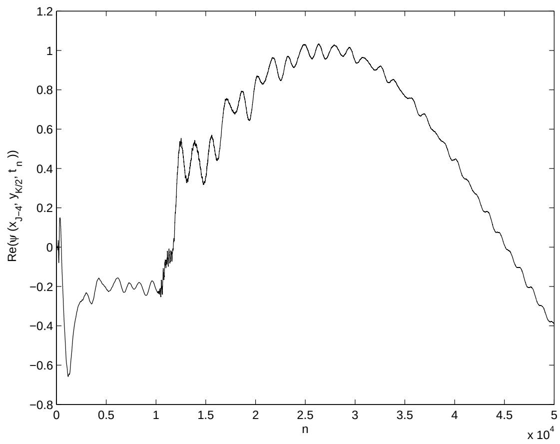
- inhomogeneous TBC essential
- advantage over existing strategies (damping potential, e.g.): ψ^{in} is *not* restricted to 1 transversal mode

Quantum waveguide – reduction of oscillations

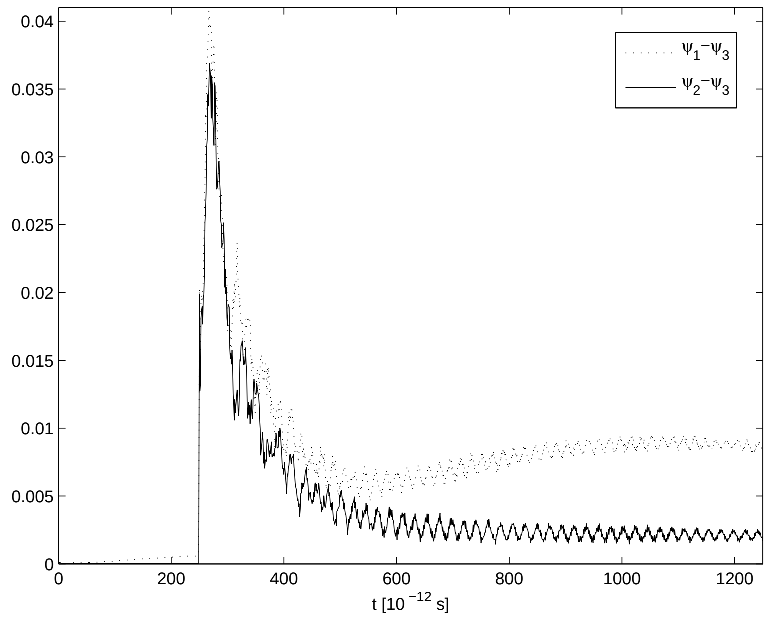
solution $\psi_1(x, y, t)$ highly oscillatory in t
$\longrightarrow$ transformation $\varphi(x, y, t) := e^{-i\omega t}\psi_1(x, y, t)$ for numerics,
$\psi_2(x, y, t) = e^{i\omega t}\varphi(x, y, t)$



$\psi_1(x_0, y_0, t)$



$\varphi(x_0, y_0, t)$



$\Rightarrow$ error reduction (in $\|\cdot\|_{L^2(\Omega)}$) up to 75%

2D Schrödinger equation - circular domain

free 2D Schrödinger equation in polar coordinates:

$$i\psi_t = -\frac{1}{2}\left(\frac{1}{r}(r\psi_r)_r + \frac{1}{r^2}\psi_{\theta\theta}\right)$$

- uniform radial off-set grid $r_j = (j + \frac{1}{2})\Delta r$,
  uniform angular grid: $\psi^n_{j,k} \approx \psi(r_j, \theta_k, t_n)$
- discrete Fourier transform in θ_k, Z-transform in $t \Rightarrow$ finite difference equation for each mode m – *variable* coefficients:

$$a_j\hat{\psi}_{j-1}(z) + b^m_j(z)\hat{\psi}_j(z) + c_j\hat{\psi}_{j+1}(z) = 0,\ j \geq J-1 \tag{2}$$

- Z-transformed TBC: $\hat{\ell}_{J+1}(z) = \frac{\hat{\psi}_{J+1}(z)}{\hat{\psi}_J(z)}$
  for *decaying* solution $\hat{\psi}_j(z)$ as $j \to \infty$
- for stability: solve (2) from $j =$ "∞" back to $j = J$;
  initial condition at $j =$ "∞": 1D–TBC
- numerical / discrete inverse Z-transformation of $\hat{\ell}_{J+1}(z)$:
  $\to$ convolution coefficients

computational domain: unit disc $\Omega_1 = [0,1] \times [0,2\pi]$

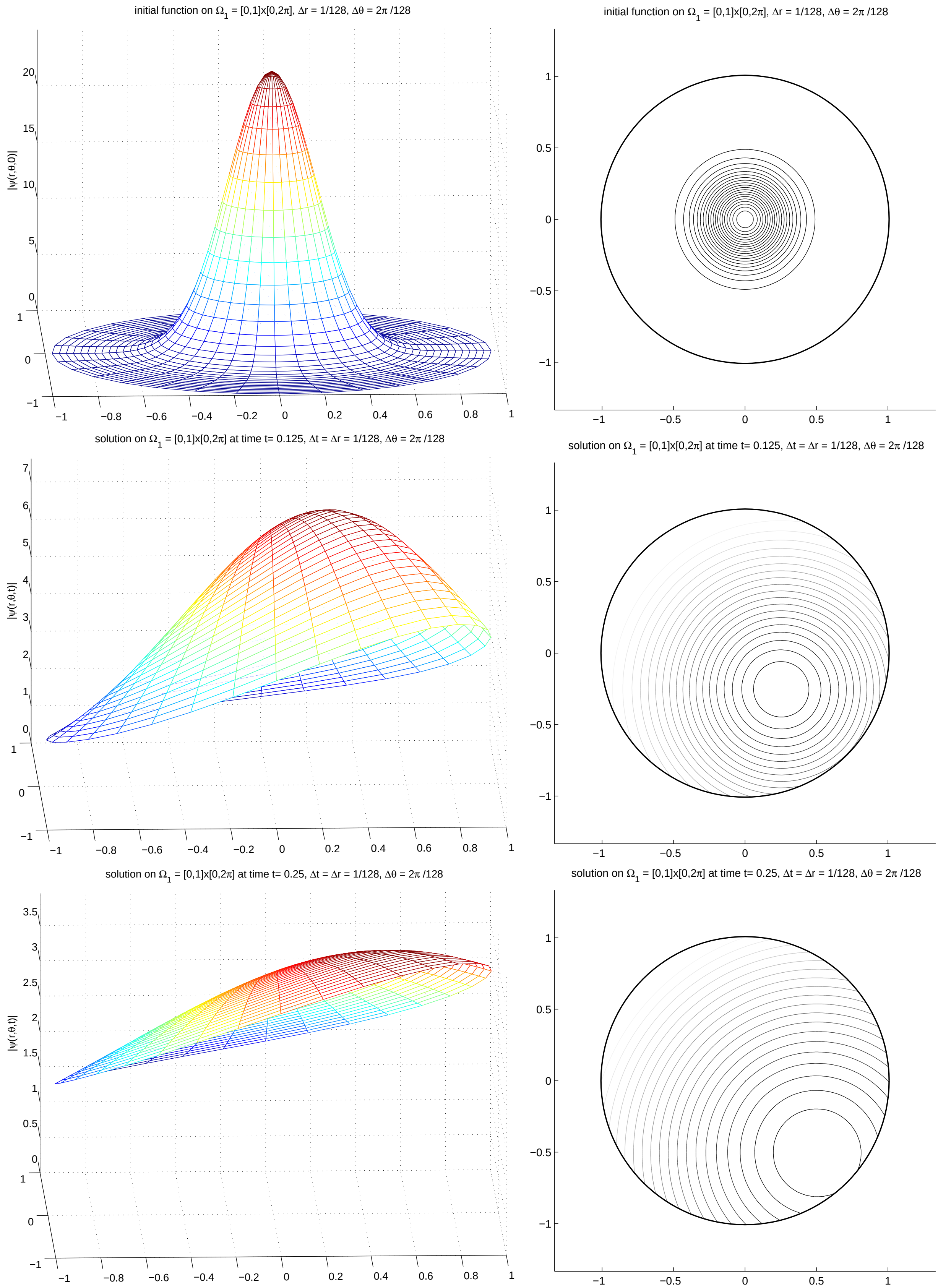
initial condition: Gaussian beam, traveling in direction $\vec{k} = (2.5, -2.5)$:

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

$\alpha_x = \alpha_y = 0.04$

symmetric polar grid: $\Delta r = \frac{1}{128}$, $\Delta\theta = \frac{2\pi}{128}$; $J = K = 128$; $\Delta t = \frac{1}{128}$

CIRCULAR DOMAIN



sol. at $t = 0,\ 0.125,\ 0.25$ [AA-Ehrhardt-Schulte-Sofronov]

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

ψ: numerical solution
φ: exact solution or numerical reference solution on Ω_2