

# Spectral methods for nonlinear dispersive PDEs

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# Outline

- ♦ Introduction
- ♦ Multi-domain method, compactified domains
- ♦ nonlinear Schrödinger equations
- ♦ Korteweg-de Vries equations
- ♦ Helmholtz equations
- ♦ Benjamin-Ono equations
- ♦ Outlook

# Nonlinear dispersive PDEs

- ♦ nonlinearity against dispersion, stable structures (*solitons*)
- ♦ rapid oscillations (*dispersive shocks*)
- ♦ blow-up (loss of regularity in finite time), limit of applicability of the model
- ♦ most complete results for integrable equations, results generic?

# Hopf equation

- hyperbolic conservation law for  $u(x, t)$ ,  
initial data  $u_0(x)$

$$u_t + 6uu_x = 0, \quad u(x, 0) = u_0(x)$$

- solution with the method of characteristics

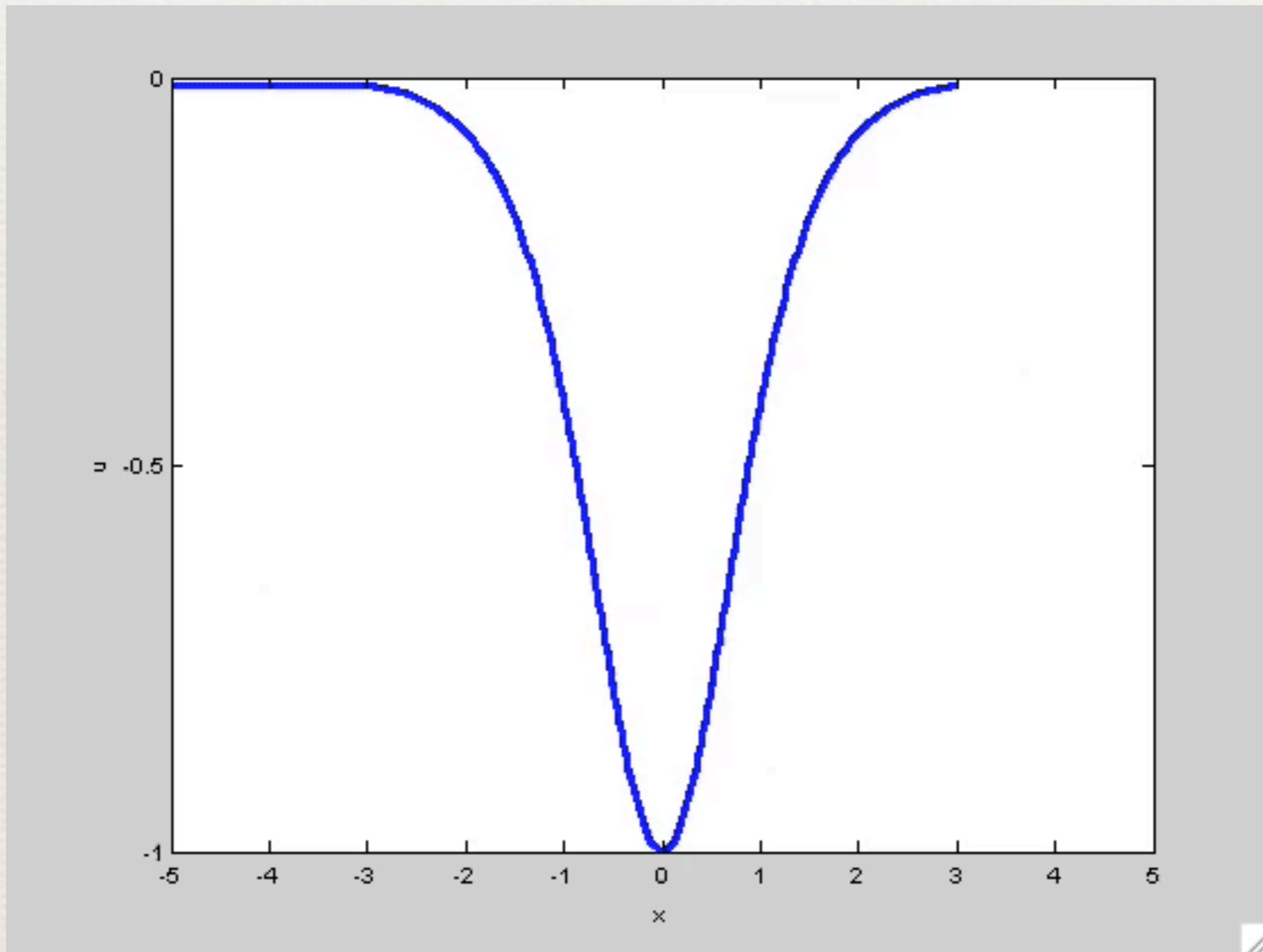
$$u(x, t) = u_0(\xi), \quad x = 6tu_0(\xi) + \xi$$

- critical time  $t_c = \frac{1}{\min_{\xi \in \mathbb{R}} [-6u'_0(\xi)]}$ ,

gradient catastrophe,

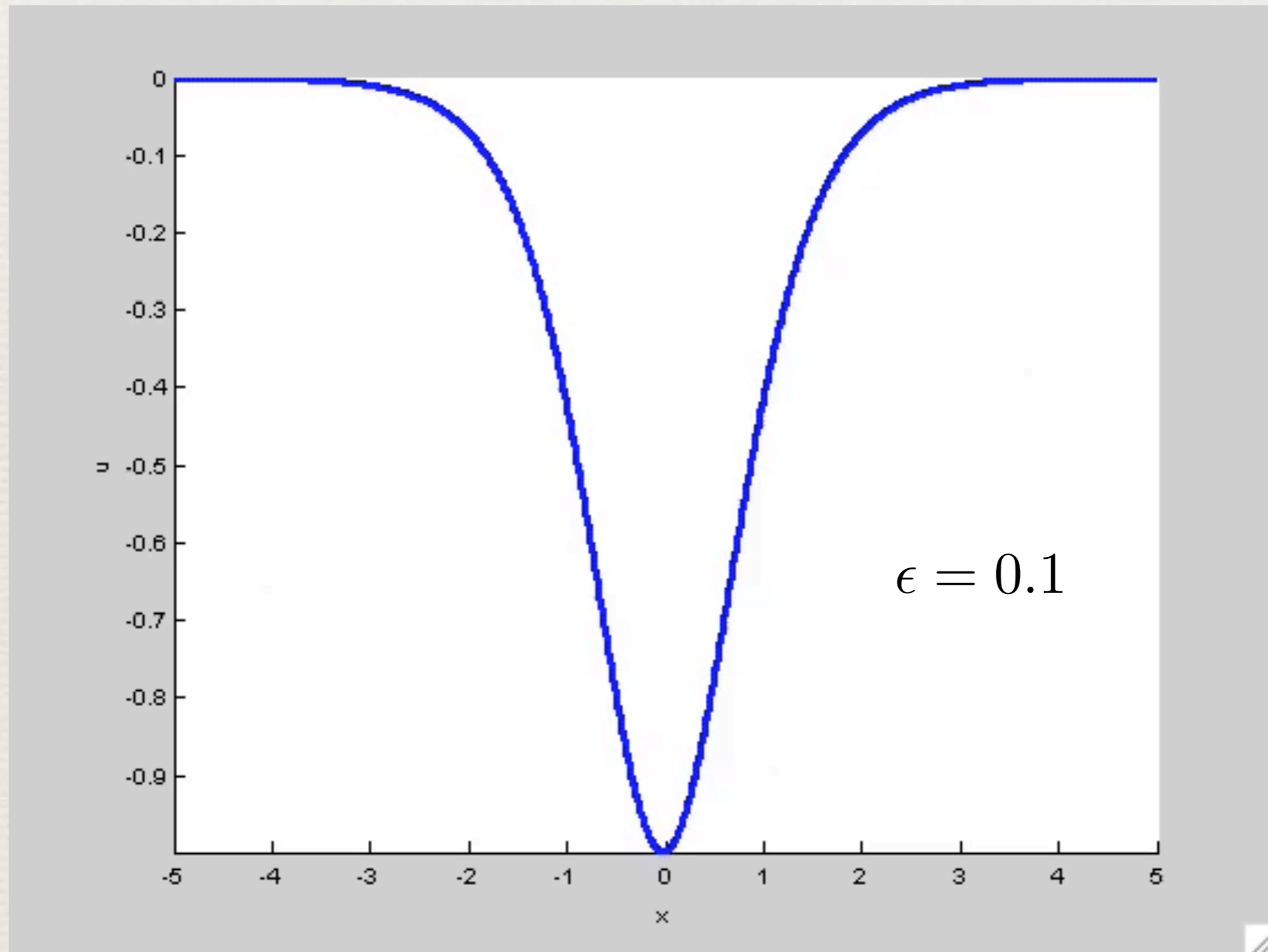
$t > t_c$ : solution multivalued (shock)

Example:  $u_0 = -\operatorname{sech}^2 x$



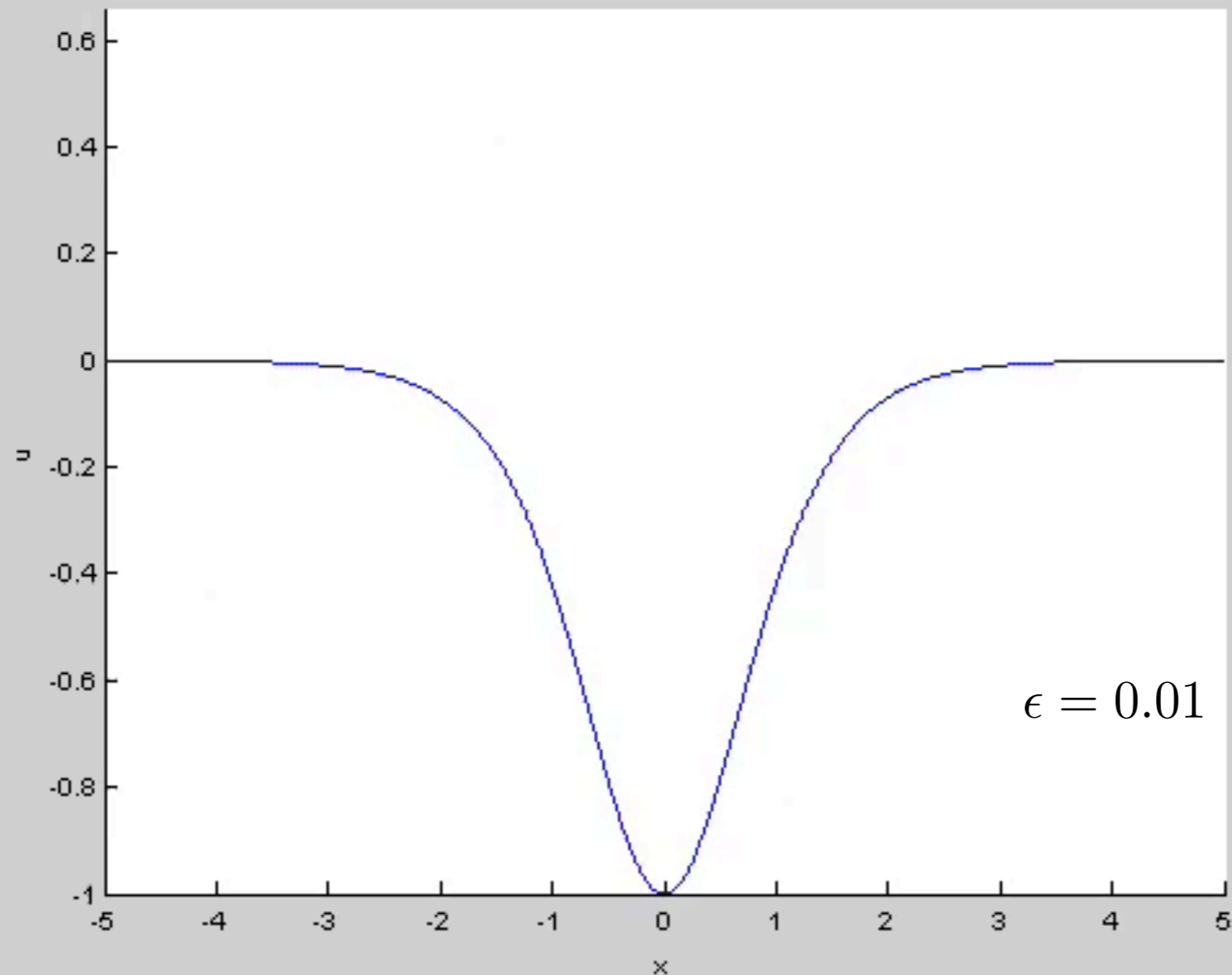
# Dissipative regularization

$$u_t + 6uu_x = \epsilon u_{xx}$$

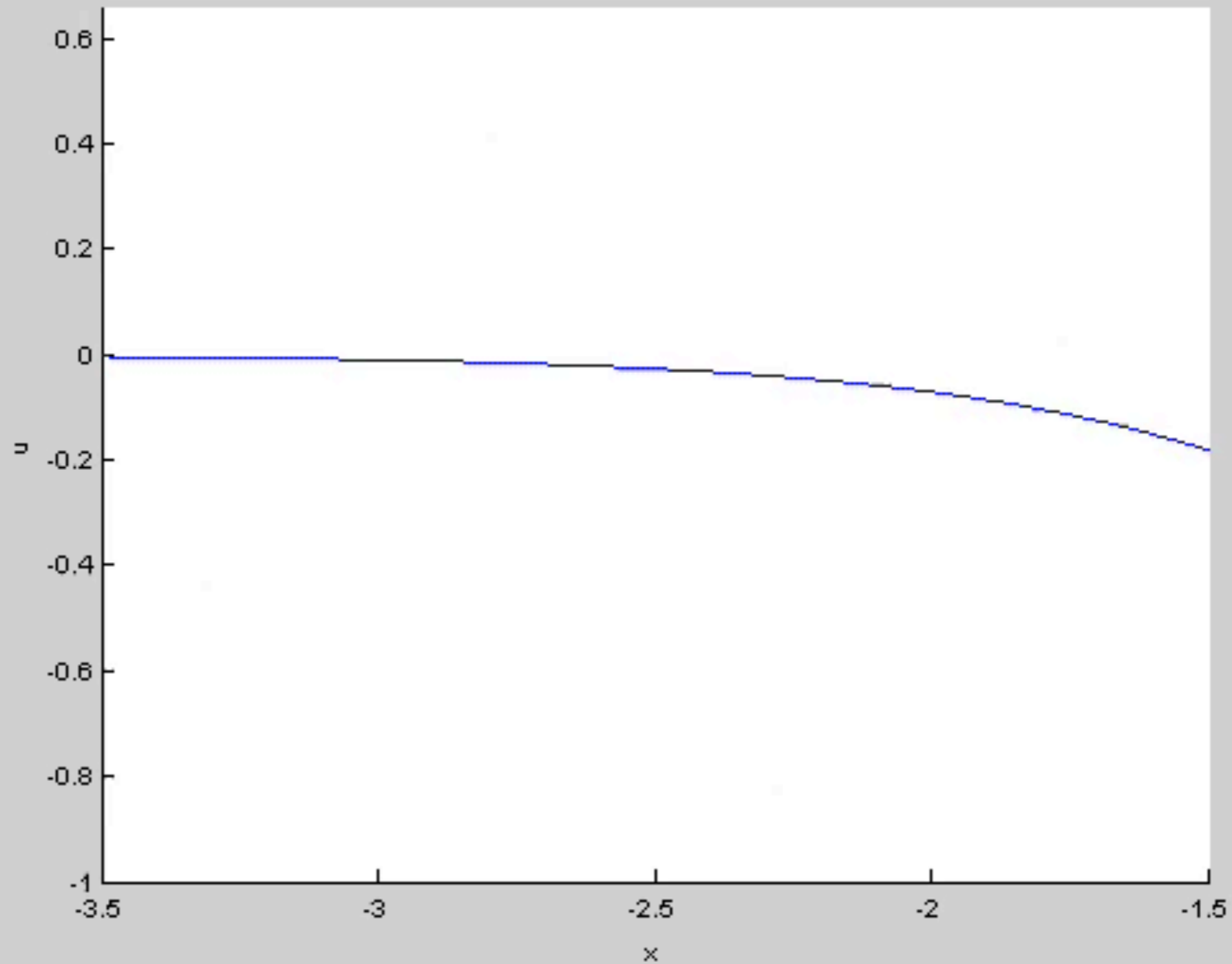


# Korteweg-de Vries equation

$$u_t + 6uu_x + \epsilon^2 u_{xxx} = 0 \quad u_0 = -\operatorname{sech}^2 x$$

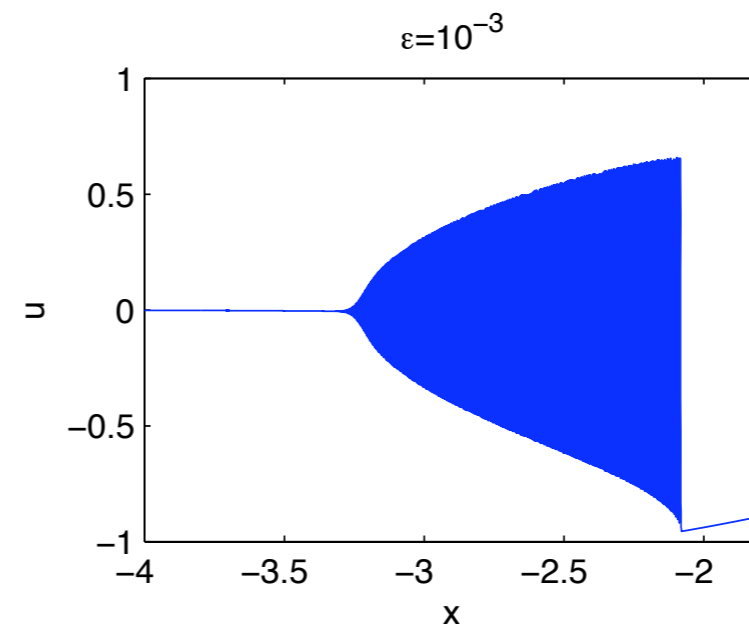
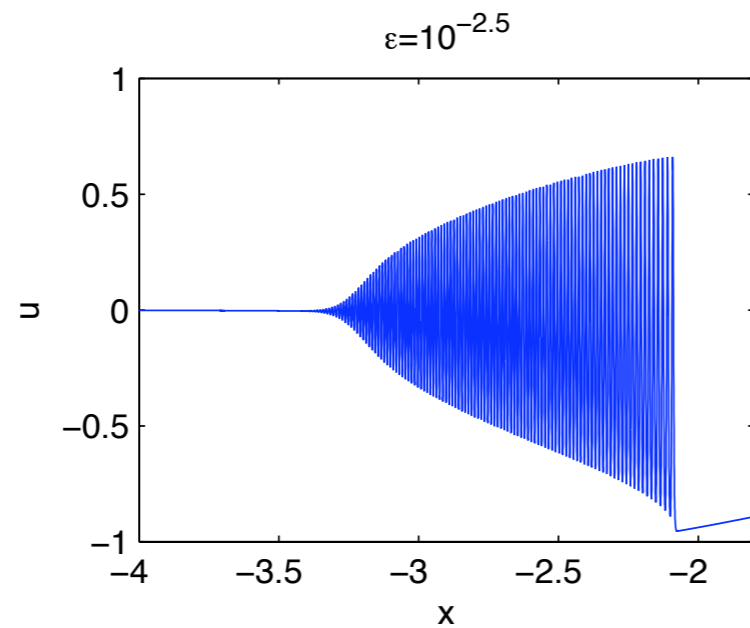
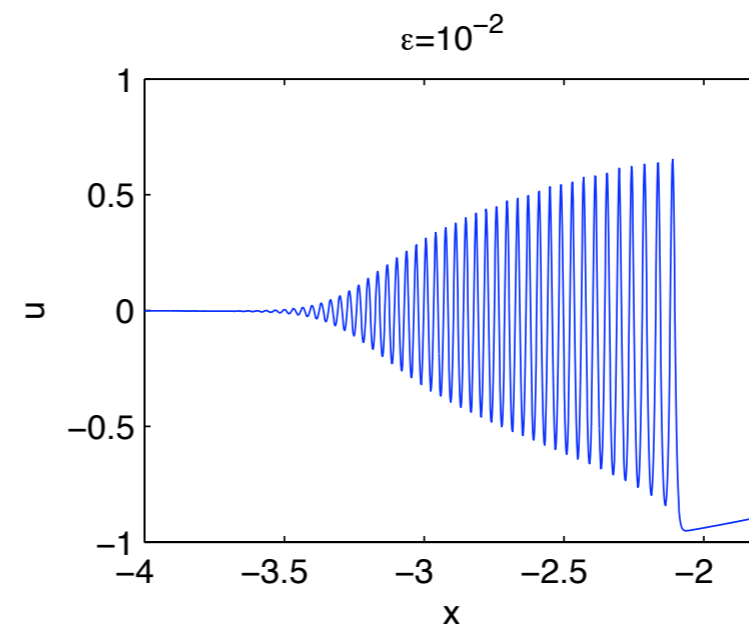
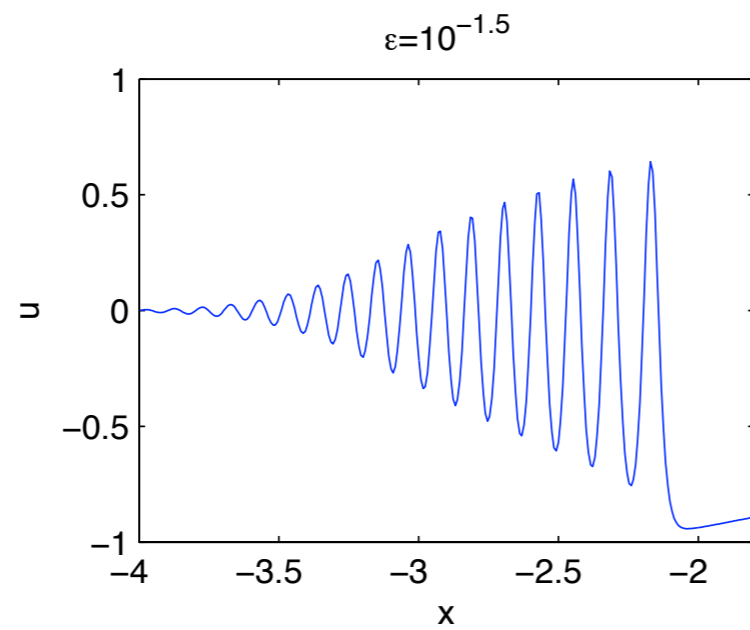


# Zoom in: dispersive shock





# Different values of $\varepsilon$



$t = 0.4$

# Blow-up

- generalized KdV equation

$$u_t + u^p u_x + \epsilon^2 u_{xxx} = 0, \quad p \in \mathbb{N}$$

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$$u_t + \epsilon^2 u_{xxx} = 0$$

(linear) and

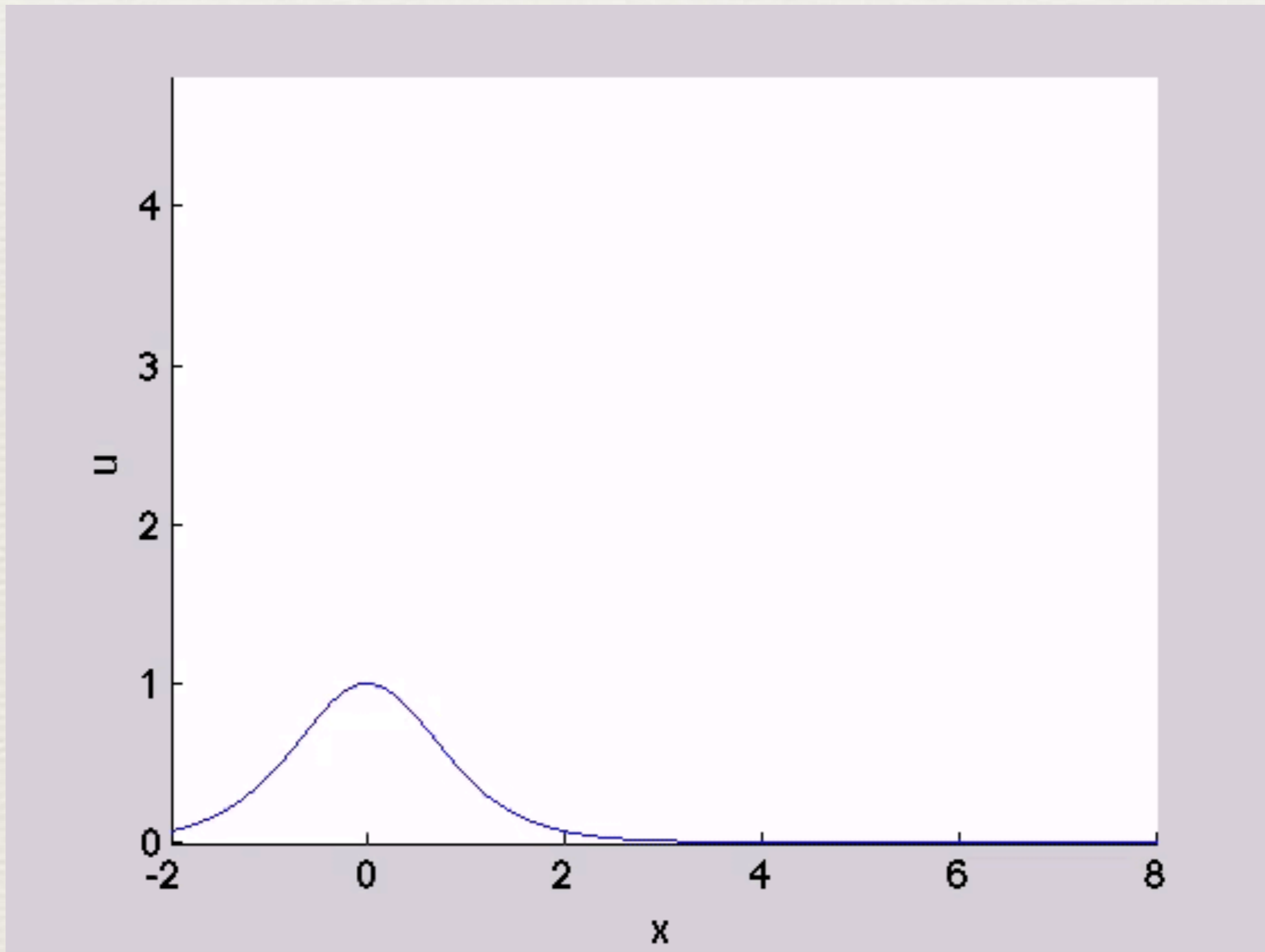
$$u_t + u^p u_x = 0$$

(shocks) do not have blow-up of the  $L_\infty$  norm of  $u$

- for  $p < 4$ : global existence in time,  
for  $p = 4$ : finite time blow-up (Martel, Merle, Raphaël: rescaled soliton),  
for  $p > 4$ : finite time blow-up, no theory yet.

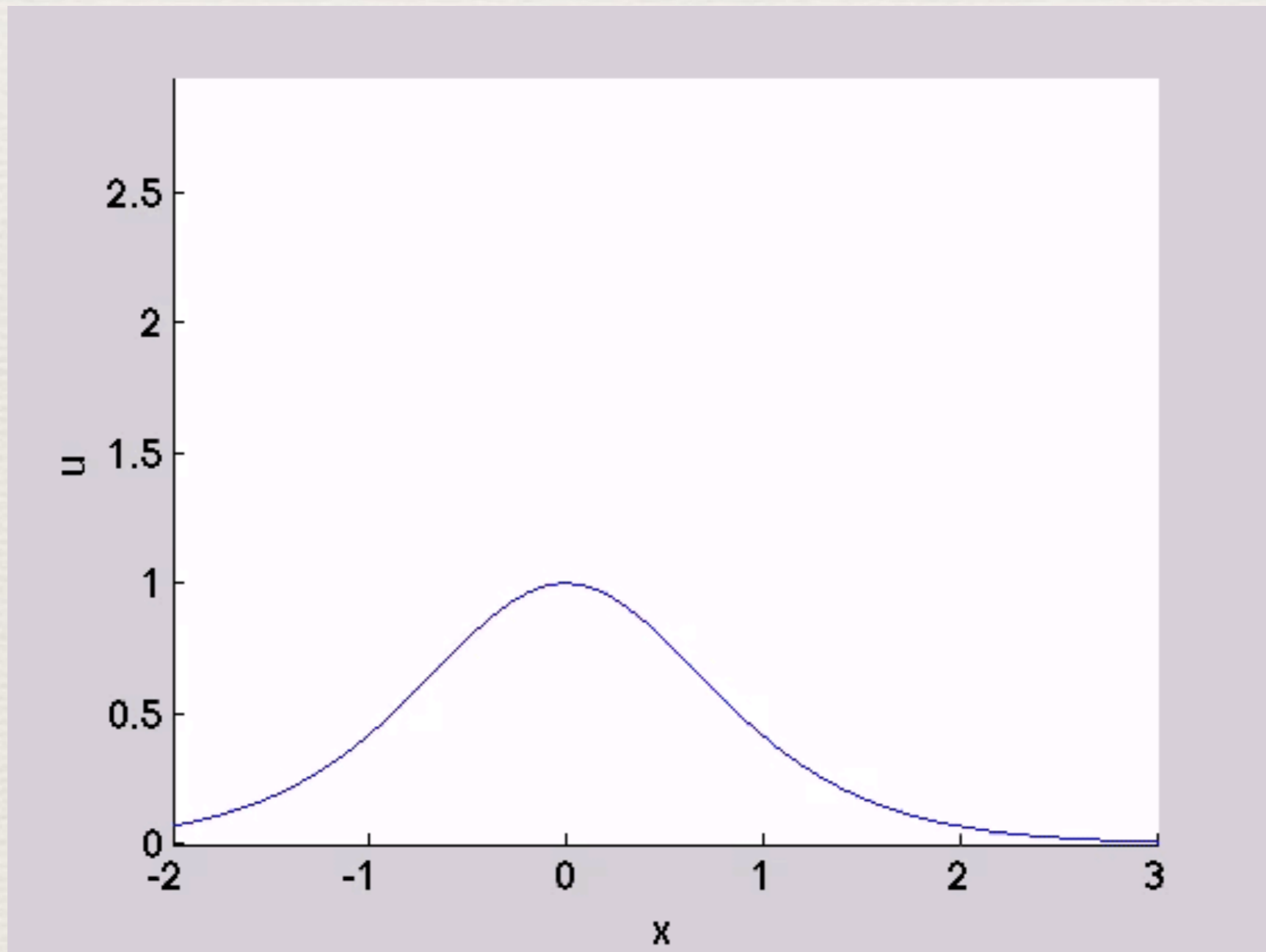
# gKdV, small dispersion

$$u_0 = \operatorname{sech}^2 x, \quad \epsilon = 0.1 \quad n = 4$$



# gKdV, small dispersion

$$u_0 = \operatorname{sech}^2 x, \quad \epsilon = 0.01 \quad n = 4$$




Applied Mathematical Sciences

Christian Klein  
Jean-Claude Saut

# Nonlinear Dispersive Equations

Inverse Scattering and PDE Methods

 Springer

# Spectral methods

- ♦ first success of spectral methods: Orszag 1971, Orr-Sommerfeld instability
- ♦ periodic problems: discrete Fourier series via *fast Fourier transform (fft)*
- ♦ exponential decrease of the Fourier coefficients for analytic functions: exponential decrease of the numerical error due to truncation of the series: *spectral convergence*
- ♦ non-periodic problems: polynomial interpolation

# Polynomial interpolation

- Chebychev collocation points (Runge phenomenon)

$$l_j = \cos\left(\frac{j\pi}{N}\right), \quad j = 0, \dots, N, \quad N \in \mathbb{N}$$

- Lagrange polynomial  $p(l)$  of order  $N$  for  $f : [-1, 1] \mapsto \mathbb{R}$ ,  
 $p(l_j) = f(l_j)$ ,  $j = 0, \dots, N$
- approximation of the derivative:  
 $f'(l_j) \approx p'(l_j) = \sum_{i=0}^N D_{ji} f(l_i)$ ,  $j = 0, \dots, N$ ;  $D$ : *differentiation matrix*
- spectral convergence for smooth  $f(l)$
- Clenshaw-Curtis algorithm:

$$\int_{-1}^1 f(l) dl \approx \int_{-1}^1 p(l) dl = \sum_{n=0}^N w_n f(l_n)$$

# Collocation method

- Chebychev polynomials

$$T_n(l) = \cos(n \arccos(l)), \quad n = 0, 1, \dots$$

- collocation method:  $f(l) \approx \sum_{n=0}^N a_n T_n(l)$ , on collocation points:

$$f(l_j) = \sum_{n=0}^N a_n T_n(l_j), \quad j = 0, \dots, N$$

relation to *fft* (*fast cosine transformation*, not precompiled in Matlab)

- spectral coefficients  $a_n$ , decrease exponentially with  $n$  for smooth  $f(l)$
- recurrence formula for Chebyshev polynomials, division by  $l$  in coefficient space

$$T_{n+1}(l) + T_{n-1}(l) = 2lT_n(x), \quad n = 1, 2, \dots$$



# Multidomain method

- spectral method of ‘infinite order’, but  $\text{cond}(D^2) = O(N^4)$ ; multi-domains to keep  $N$  small
- interval  $[x_l, x_r]$  mapped to  $[-1, 1]$ :

$$x = x_l \frac{1+l}{2} + x_r \frac{1-l}{2}, \quad l \in [-1, 1]$$

- compactified exterior domains (CED):  $s = 1/x$  local coordinate,

$$u_{xx} = s^4 u_{ss} + 2s^3 u_s$$

singular for  $s = 0$  (compactification with spectral methods first used by Grosch, Orszag 1977, popular in astrophysics)

# Schrödinger equations

- one dimensional Schrödinger equation

$$i\partial_t u + \partial_{xx} u + V(|u|^2, x)u = 0$$

- linear case: quantum mechanics, quantum semiconductors, in electromagnetic wave propagation, in seismic migration, lowest order one-way approximation (paraxial wave equation) to the Helmholtz equation, Fresnel equation in optics, underwater acoustics
- $V = \pm 2|u|^2$ : focusing (+) or defocusing (−) cubic nonlinear Schrödinger equation (NLS), completely integrable (Zakharov-Shabat)
- NLS: modulation of waves in hydrodynamics, nonlinear optics and plasma physics, Bose-Einstein condensates

# Choice of numerical approach

- (piecewise) smooth functions: use spectral methods
- rapidly decreasing or periodic functions: Fourier (additional advantage: diagonal differentiations matrices, well conditioned)
- solutions with algebraic decrease, compact support or a finite number of discontinuities: polynomial interpolation
- Galilei invariance:  $u(t, x)$  NLS solution, so is

$$\hat{u}(x, t) = u(x - ct, t)e^{icx/2 - ic^2t/4},$$

$c \in \mathbb{R}$  finite speed

# Rogue waves

- ♦ Giant waves on deep water, more than twice the average wave height
- ♦ NLS solutions?

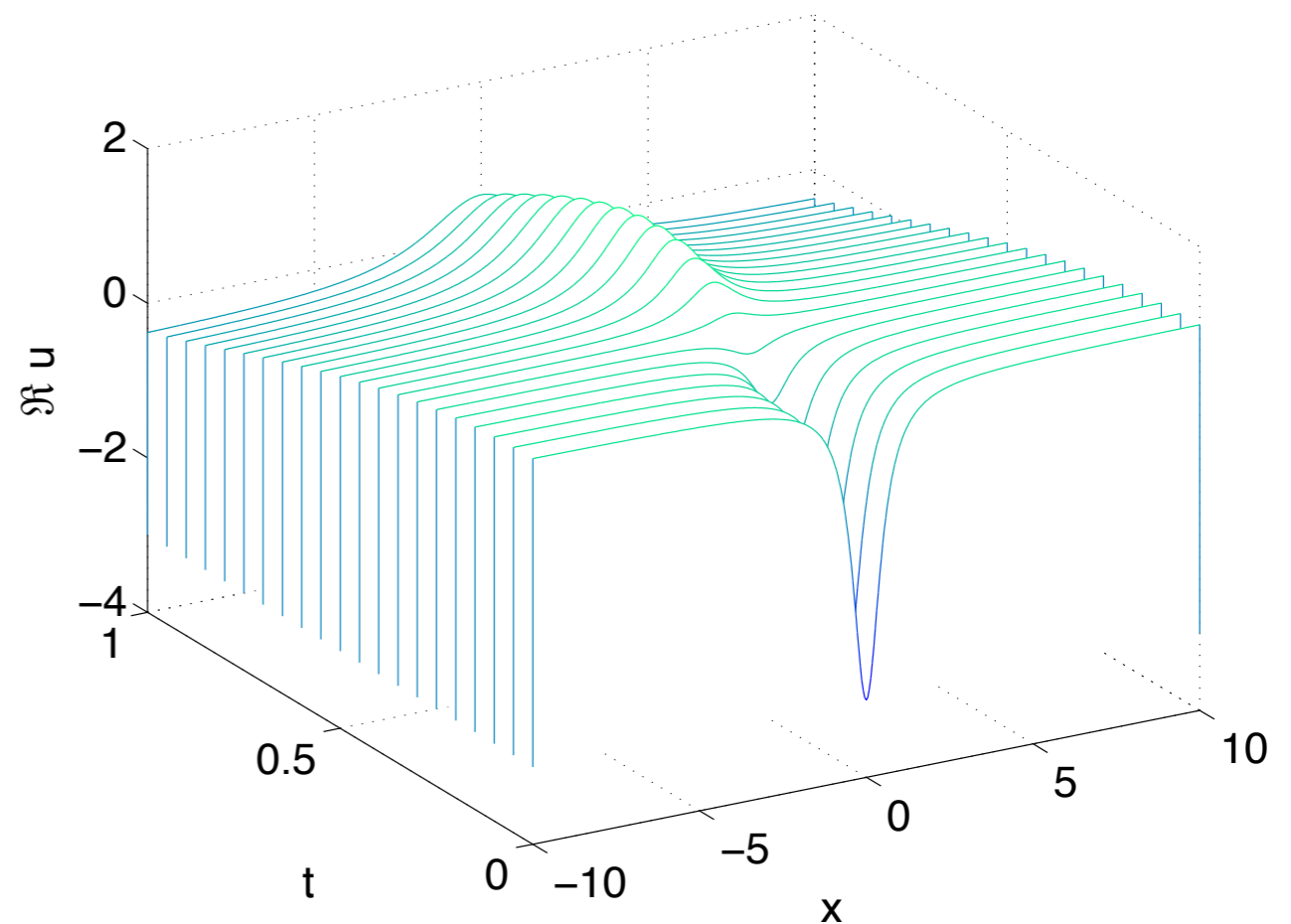
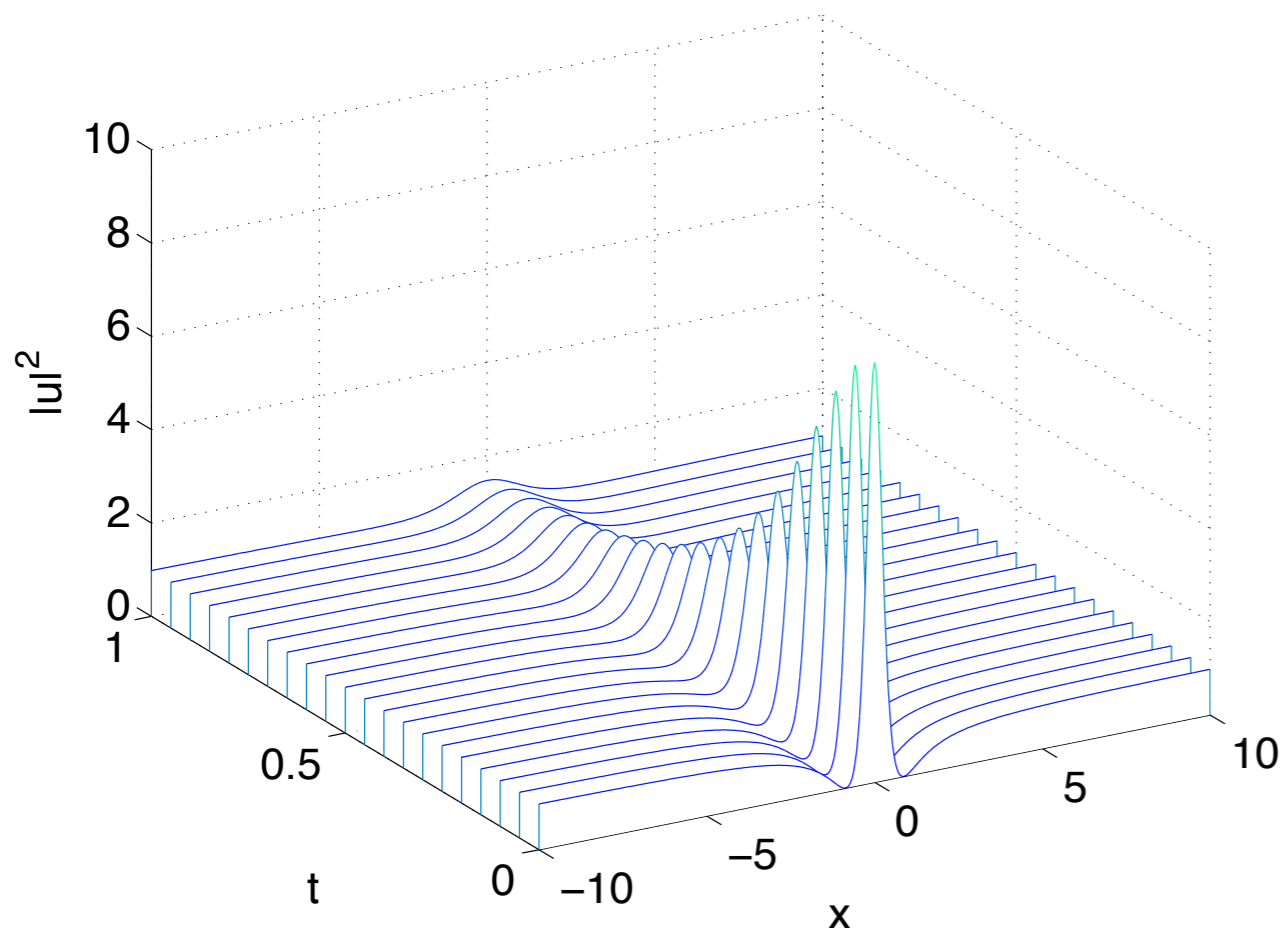


# Peregrine solution

- exact solution

$$u_{Per} = \left( 1 - \frac{4(1 + 4it)}{1 + 4x^2 + 16t^2} \right) e^{2it}$$

- $|u|$  asymptotically decaying to 1 (both in  $x$  and  $t$ ), maximum three times the asymptotic value

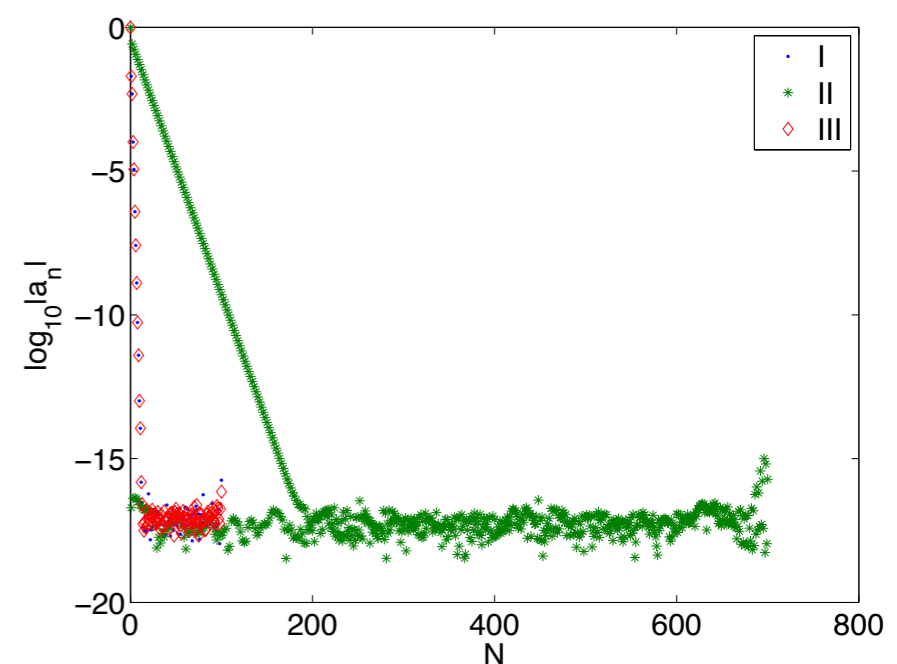
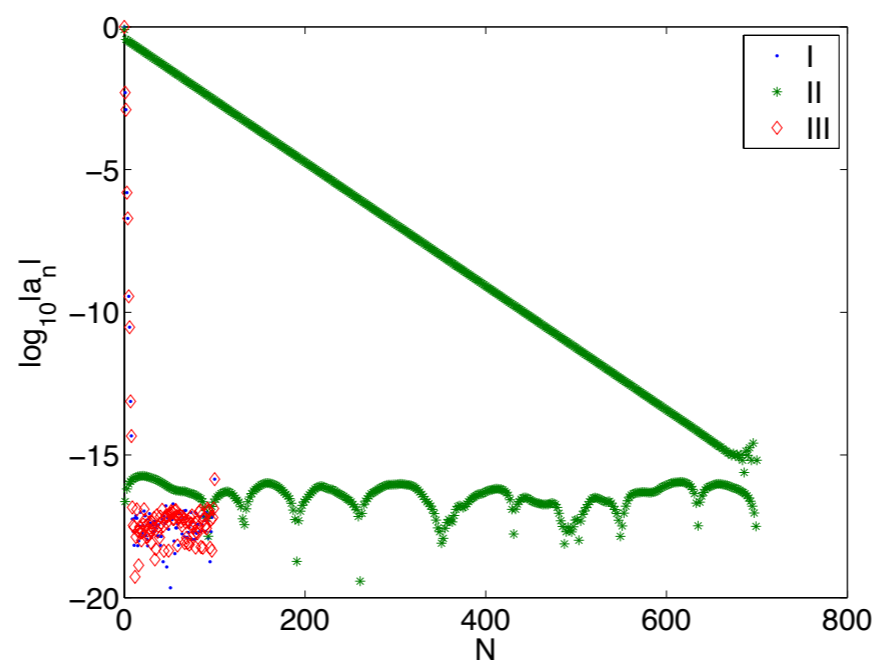
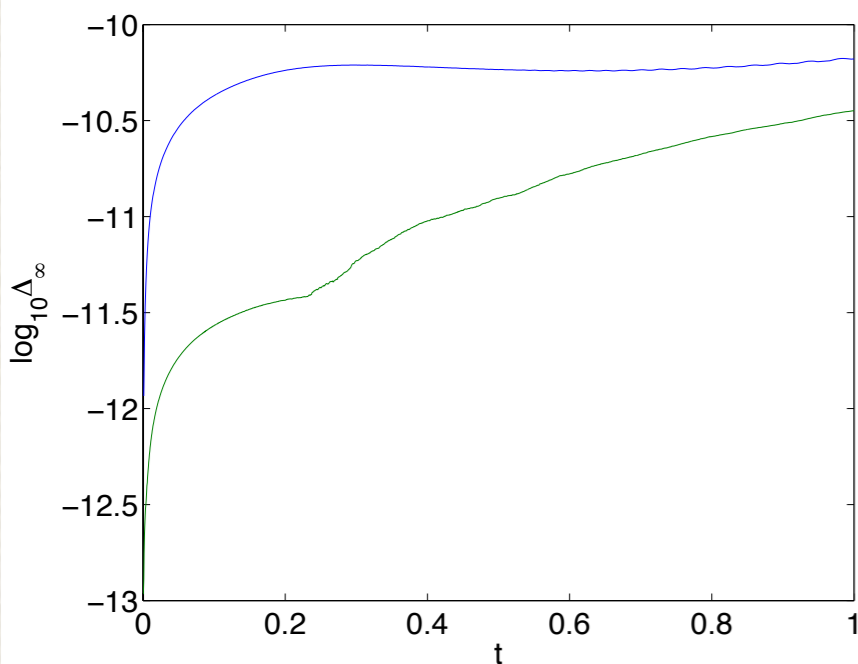


# Fourth order method

- $x_r = -x_l = 10$
- $N^I = N^{III} = 50, N^{II} = 700$
- $N_t = 1000, 2000$

$t = 0$

$t = 1$



# „Benjamin-Feir instability“

- linearization:  $u = u_{Per}(1 + \tilde{v})$

$$i\tilde{v}_t + \tilde{v}_{xx} + 2(\ln u_{Per})_x \tilde{v}_x + 4|u_{Per}|^2 \Re \tilde{v} = 0,$$

numerically problematic for  $u_{Per} \approx 0$

- $u_{Per} \rightarrow e^{2it}$  for  $x \rightarrow \infty$  or  $t \rightarrow \infty$ ,  $\tilde{v} = \alpha + i\beta$

$$\alpha_t + \beta_{xx} = 0, \quad -\beta_t + \alpha_{xx} + 4\alpha = 0$$

- Fourier transform in  $x$ , eigenvalues

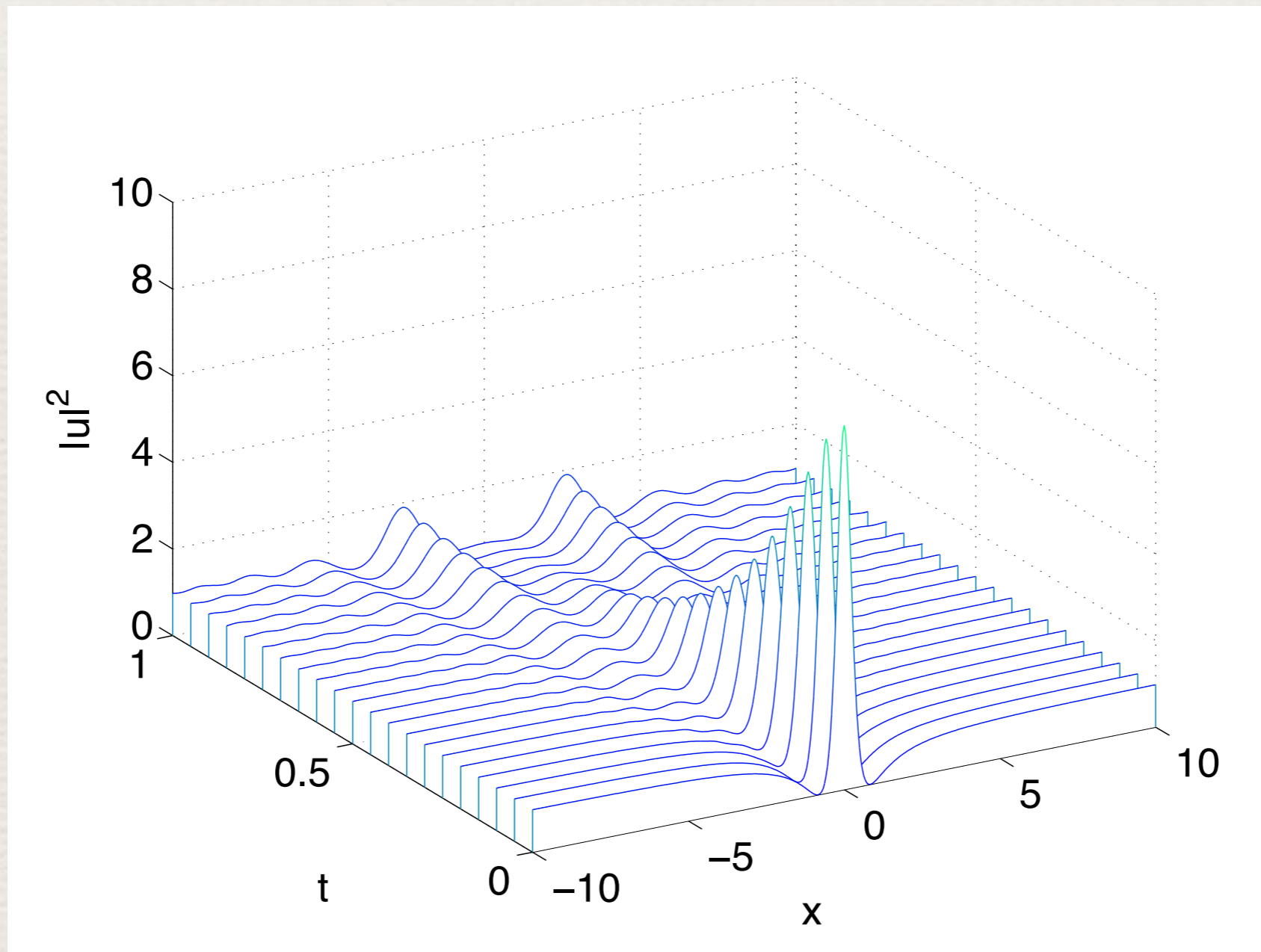
$$\lambda_{1,2}(k) = \pm |k| \sqrt{4 - k^2}$$

modulational instability

# NLS, localized perturbation

- Gaussian perturbation

$$u(x, 0) = u_{Per}(x, 0) + 0.1 \exp(-x^2)$$





# Localized perturbation

- conserved quantity

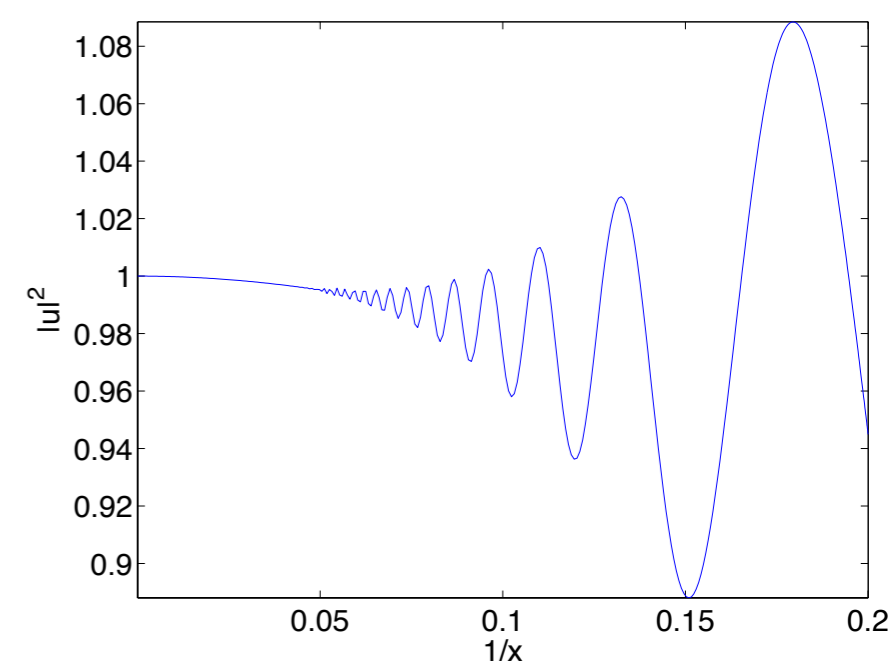
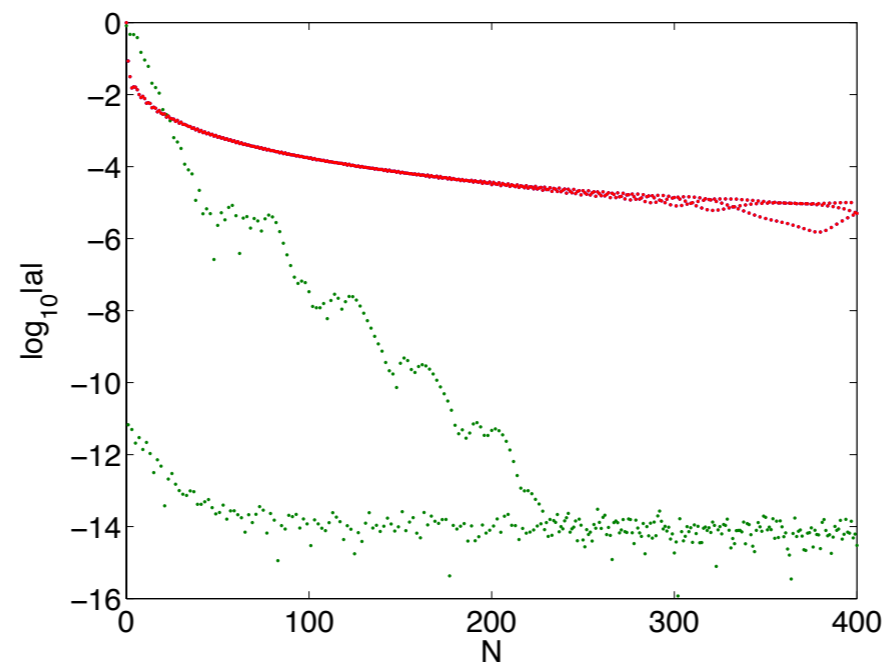
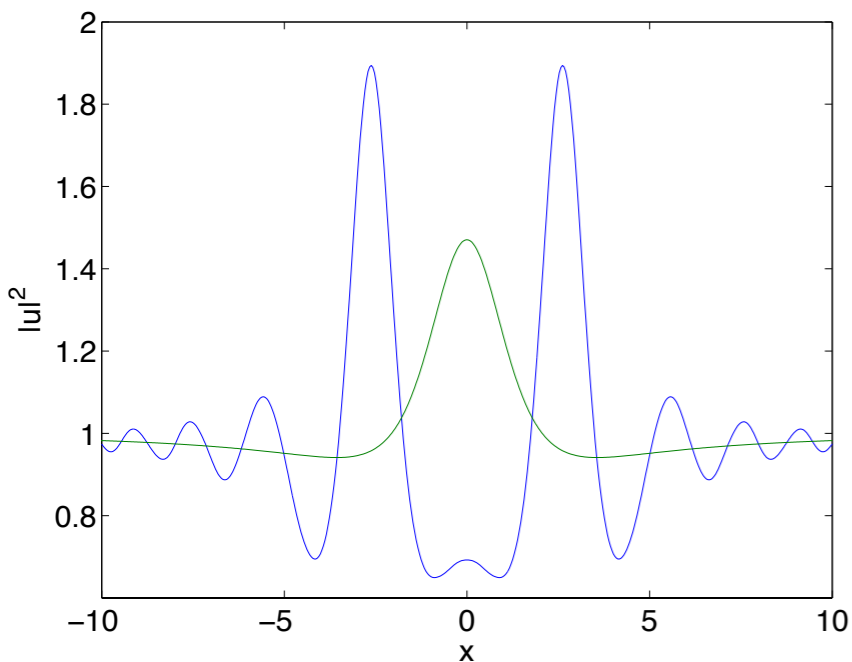
$$E = \frac{1}{2} \int_{\mathbb{R}} \{ |u_x|^2 - |u|^2 (|u|^2 - 1) \} dx$$

relative conservation better than  $10^{-3}$

$t=1$

Chebyshev  
coefficients

compactified zone



# Transverse stability

C. Klein, N. Stoilov, Numerical study of the transverse stability of the Peregrine solution, Stud Appl Math. 145 (2020) 36–51. <https://doi.org/10.1111/sapm.12306>

- 2d NLS

$$i\partial_t u + \partial_{xx} u + \partial_{yy} u + 2|u|^2 u = 0$$

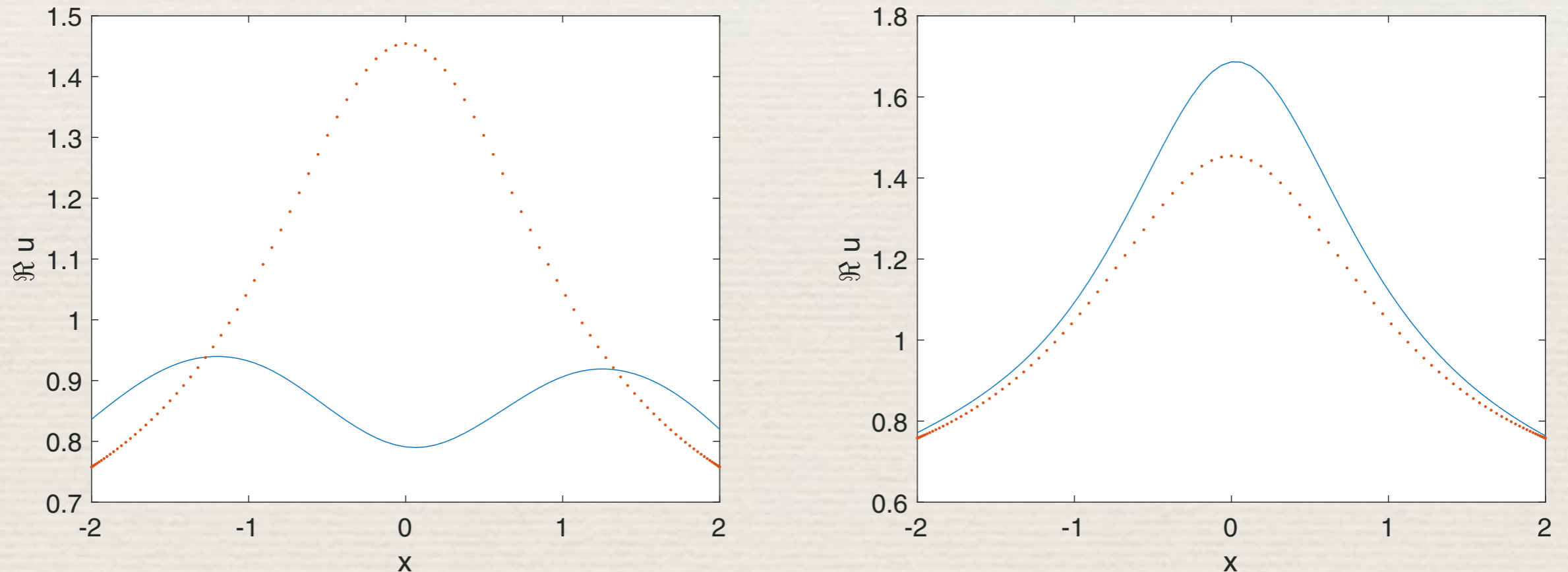
- hypothesis: periodic in  $y$  (this includes data rapidly decreasing in  $y$ )
- Fast Fourier transform (FFT) techniques in  $y$  (diagonal differentiation matrices),  $x \in \mathbb{R}$  as before (2 domains, one compactified)
- inexact 4th order splitting technique (linear step integrated with IRK4) fully explicit,

$$\mathcal{L}_+ \mathcal{L}_- (K_1 + K_2) = 2i\Delta U(t_n),$$

where  $\mathcal{L}_\pm = \hat{1} - h(0.25i \pm 0.25/\sqrt{3})\Delta$

- perturbation localised in  $x$  and  $y$ ,  $t \leq 0.5$

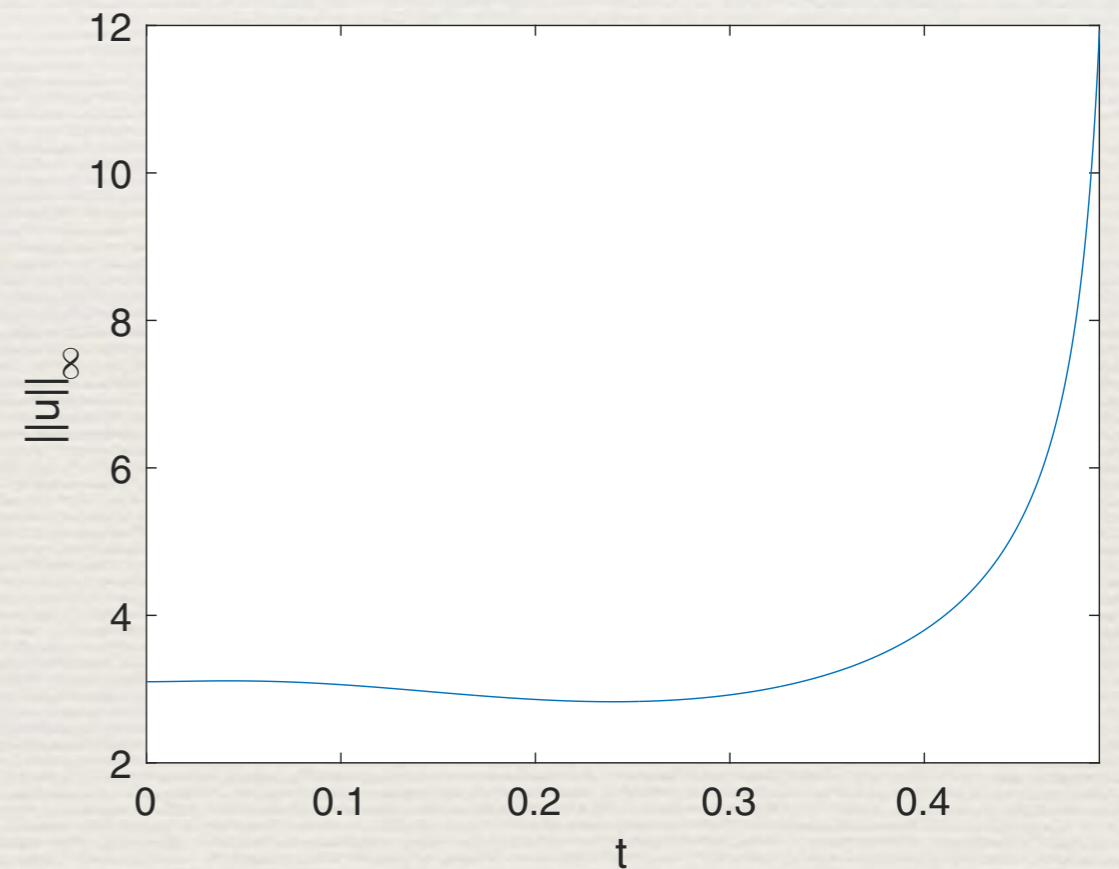
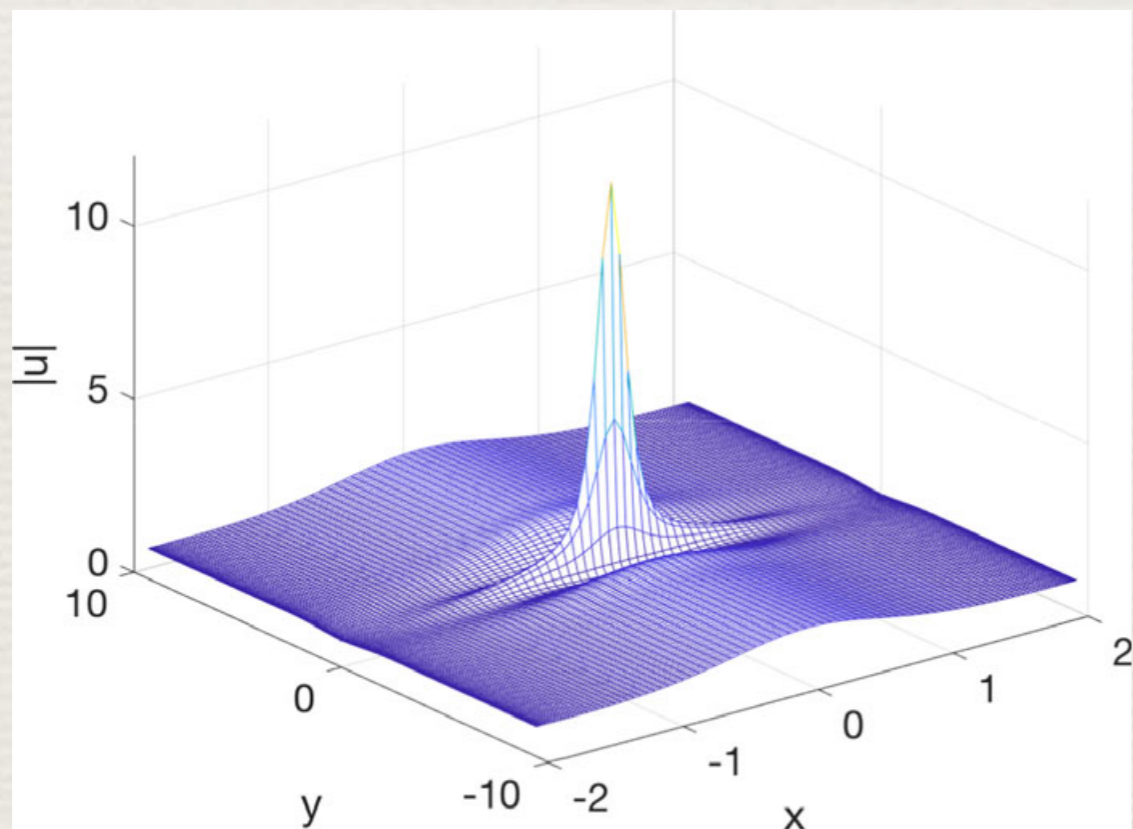
$$u(x, y, 0) = u_{Per} + 0.1 \exp(-(x + 1)^2 - y^2)$$



**FIGURE 4** Real part of the solution to the 2D NLS equation for the initial data  $u(x, y, 0) = u_{Per}(x, t_0) + 0.1 \exp(-(x + 1)^2 - y^2)$  for  $t = 0.5$ , on the left for  $y = 0$ , on the right for  $y = 1.6199$ ; the Peregrine solution for the same time is shown as a dotted line

- perturbation localised in  $x$  and  $y$ ,  $t \leq 0.5$

$$u(x, y, 0) = u_{Per} + 0.1 \exp(-x^2 - y^2)$$



**FIGURE 8** Solution to the 2D NLS equation for the initial data  $u(x, y, 0) = u_{Per}(x, t_0) - 0.1 \exp(-x^2 - y^2)$  for  $t = 0.49$  on the left and the  $L^\infty$  norm of the solution in dependence of time on the right

# Generalized KdV equations

C. Klein, N. Stoilov, Spectral approach to Korteweg-de Vries equations on the compactified real line, App. Num. Math., <https://doi.org/10.1016/j.apnum.2022.02.015>

- $$u_t(x, t) + u_{xxxx}(x, t) + u(x, t)^{p-1}u_x(x, t) = 0, \quad p = 2, 3, \dots$$

- inverse scattering if Faddeev decay condition holds,

$$\int_{\mathbb{R}} (1 + |x|)|u_0(x)|dx < \infty,$$

- exotic blow-up
- compactification

$$x = c \tan \frac{\pi l}{2}, \quad l \in [-1, 1], \quad c = \text{const}$$

- boundary conditions

$$u(l, t) \Big|_{l=1} = 0, \quad u(l, t) \Big|_{l=-1} = 0, \quad u_l(l, t) \Big|_{l=-1} = 0.$$

$$u(x, 0) = \frac{1}{(1 + x^2)^a}, \quad a = \frac{1}{2}, 1.$$

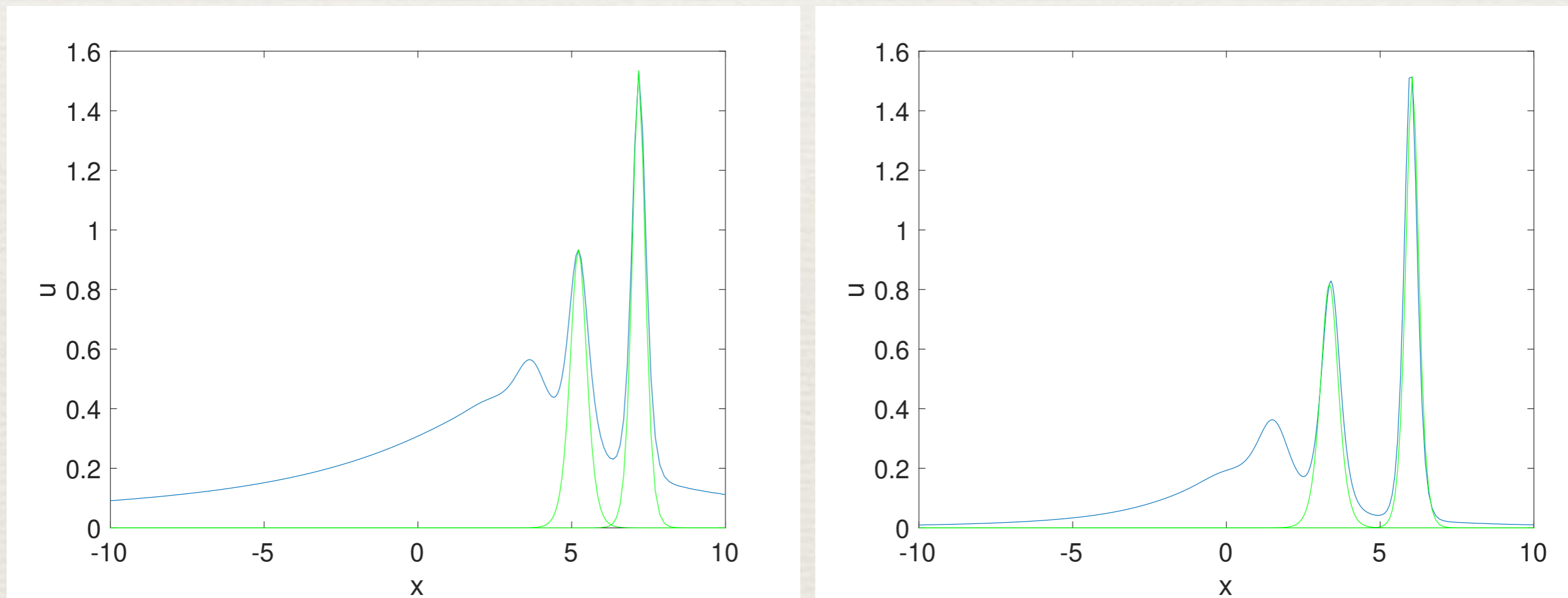


FIGURE 10. Solution to the KdV equation (1) with  $p = 2$  for the initial data (22) for  $t = 10$ , on the left for  $a = 1/2$ , on the right for  $a = 1$ ; in green fitted solitons (4).

# Maxwell equations

- wave equation for each component of the electric field, vector Helmholtz equation after Fourier transform in time

$$\nabla \times \nabla \times \mathbf{E} - \omega^2 \epsilon(r, \omega) \mathbf{E} = 0$$

$\epsilon(r, \omega)$  piecewise constant function

- axial symmetry, spherical coordinates,  $\mathbf{E} = (E^\rho(\rho, \theta), E^\theta(\rho, \theta), E^\phi(\rho, \theta))$

$$\rho E_{\rho\theta}^\theta - E_{\theta\theta}^\rho + \cot(\theta) E^\theta - \epsilon(\omega, \rho) \rho^2 \omega^2 E^\rho - \cot(\theta) E_\theta^\rho + E_\theta^\theta + \rho \cot(\theta) E_\rho^\theta = 0,$$

$$\rho E_{\rho\rho}^\theta - E_{\rho\theta}^\rho + \epsilon(\omega, \rho) \rho \omega^2 E^\theta + 2E_\rho^\theta = 0,$$

$$\rho^2 E_{\rho\rho}^\phi + E_{\theta\theta}^\phi + E^\phi (-\csc(\theta)^2 + \rho^2 \omega^2 \epsilon(\omega, \rho)) + \cot(\theta) E_\theta^\phi + 2\rho E_\rho^\phi = 0,$$

$E^\phi$  decouples, can be put equal to zero in the axisymmetric case

# Sommerfeld condition

C. Klein, N. Stoilov, Multidomain spectral approach with Sommerfeld condition for the Maxwell equations, J. Comp. Phys., <https://doi.org/10.1016/j.jcp.2021.110149>

- no incoming radiation from infinity

$$\lim_{\rho \rightarrow \infty} \rho \left( \frac{\partial}{\partial \rho} + ik \right) \mathbf{E}(\rho, \theta) = 0$$

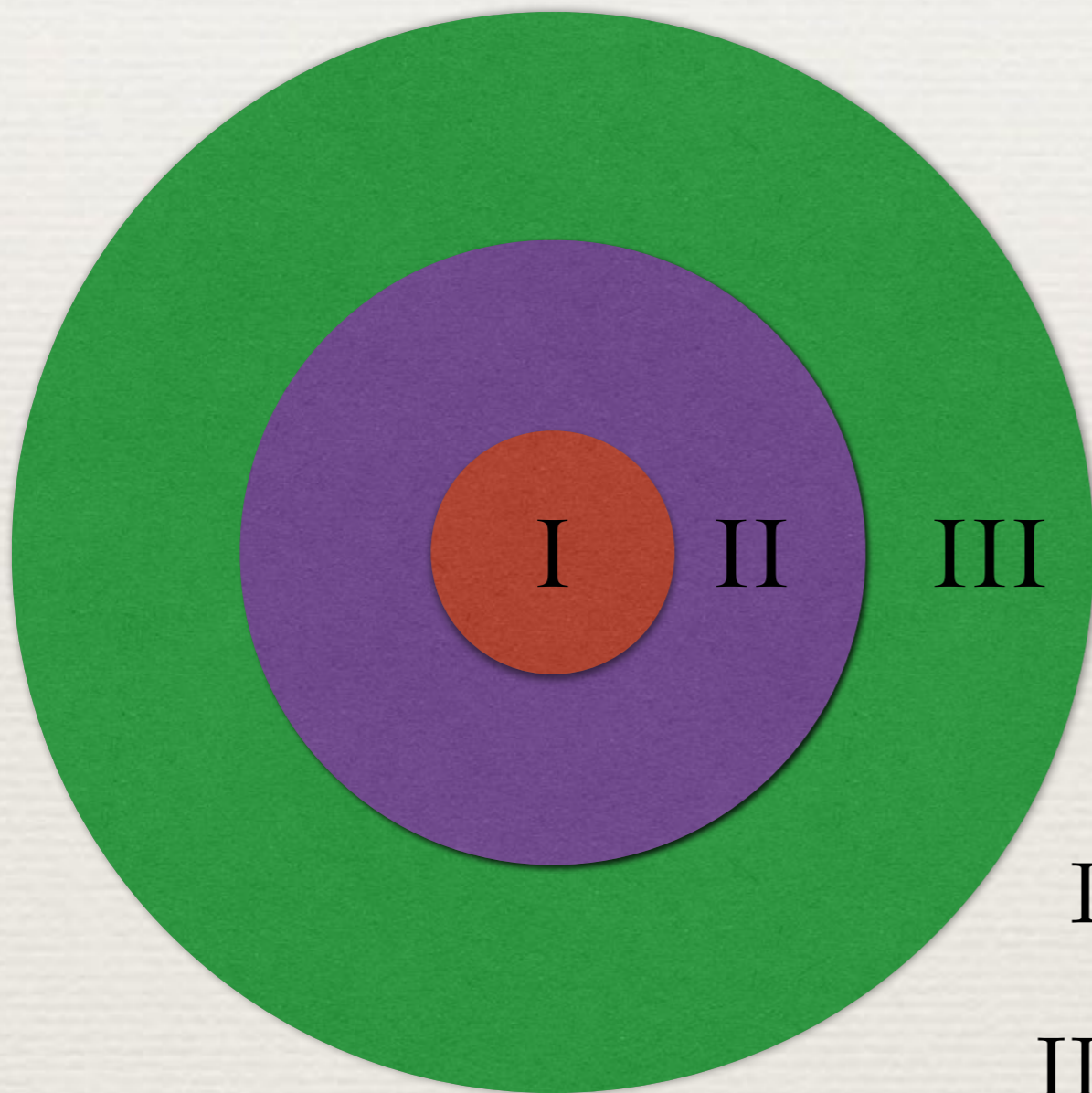
thus

$$\mathbf{E} = \tilde{\mathbf{E}} e^{-ik\rho}, \quad \tilde{\mathbf{E}} = O(1/\rho)$$

- assumption  $\tilde{\mathbf{E}}$  is a smooth function in  $s = 1/\rho$  in the vicinity of infinity



# Multi-domain approach



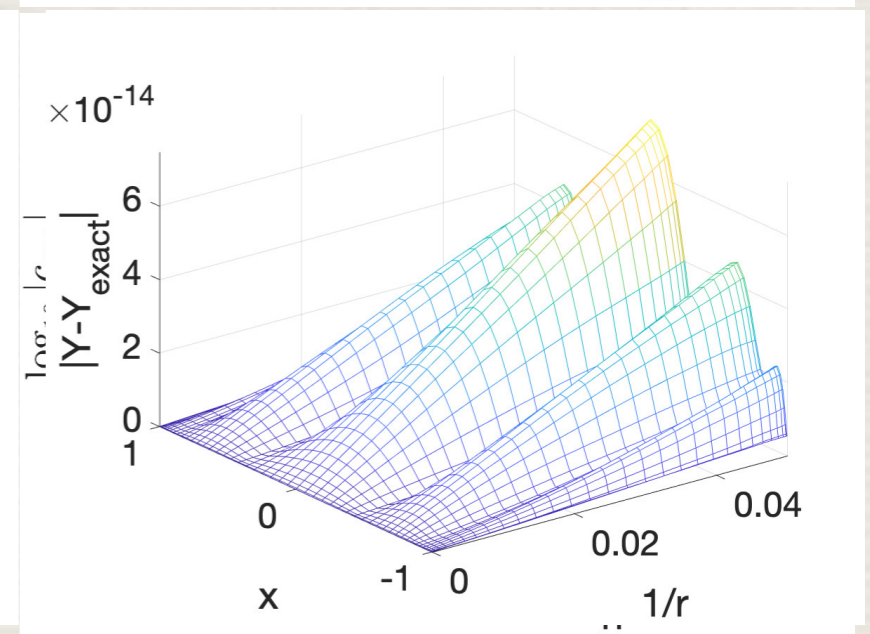
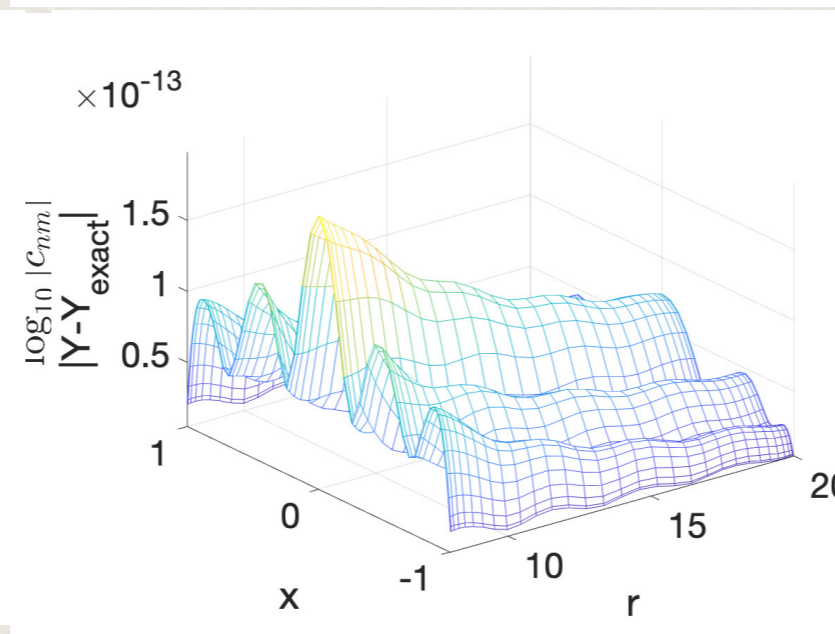
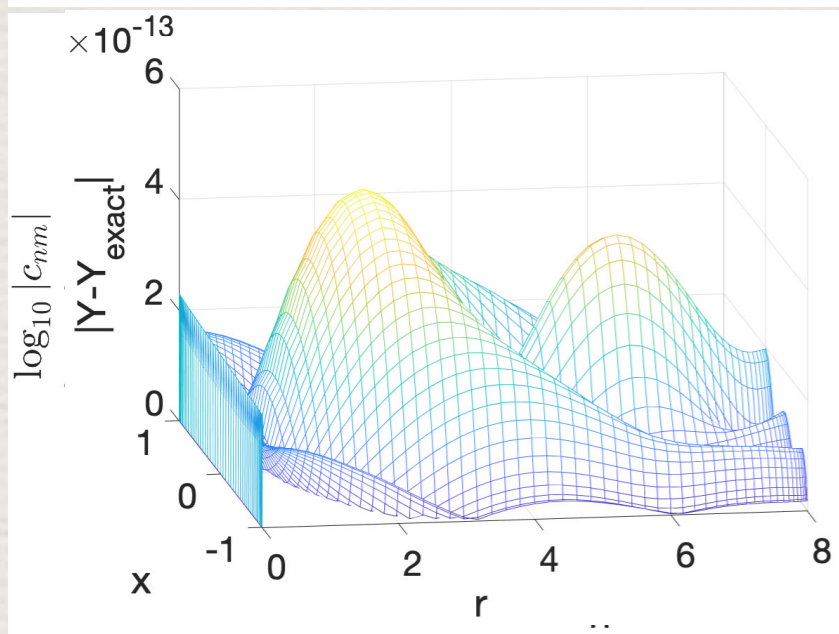
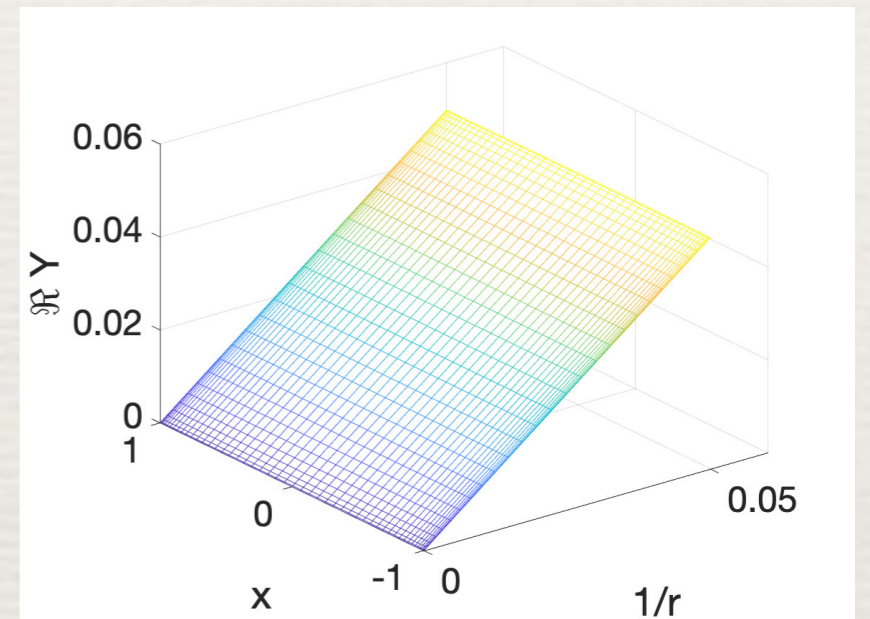
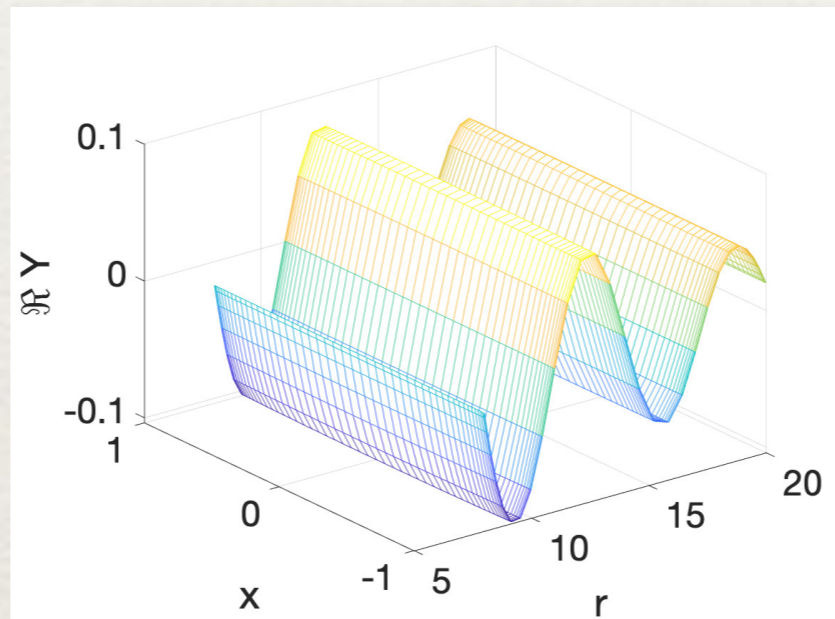
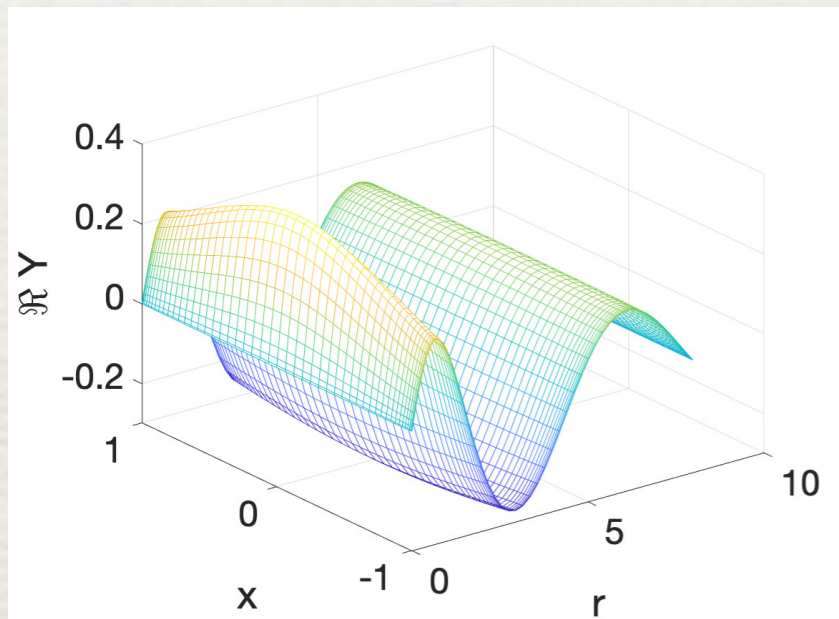
$$\text{I} \quad \rho = r_I(1 + l)/2$$

$$\text{II} \quad \rho = r_I(1 - l)/2 + r_{II}(1 + l)/2$$

$$\text{III} \quad \rho = 2r_{II}/(1 + l)$$

$$l \in [-1, 1]$$

# Example



# Benjamin-Ono equations

C. Klein, J. Riton, N. Stoilov, Multi-domain spectral approach for the Hilbert transform on the real line, SN Partial Differential Equations and Applications (2:36) (2021) <https://doi.org/10.1007/s42985-021-00094-8>

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$$u_t + u^{m-1}u_x - \mathcal{H}u_{xx} = 0,$$

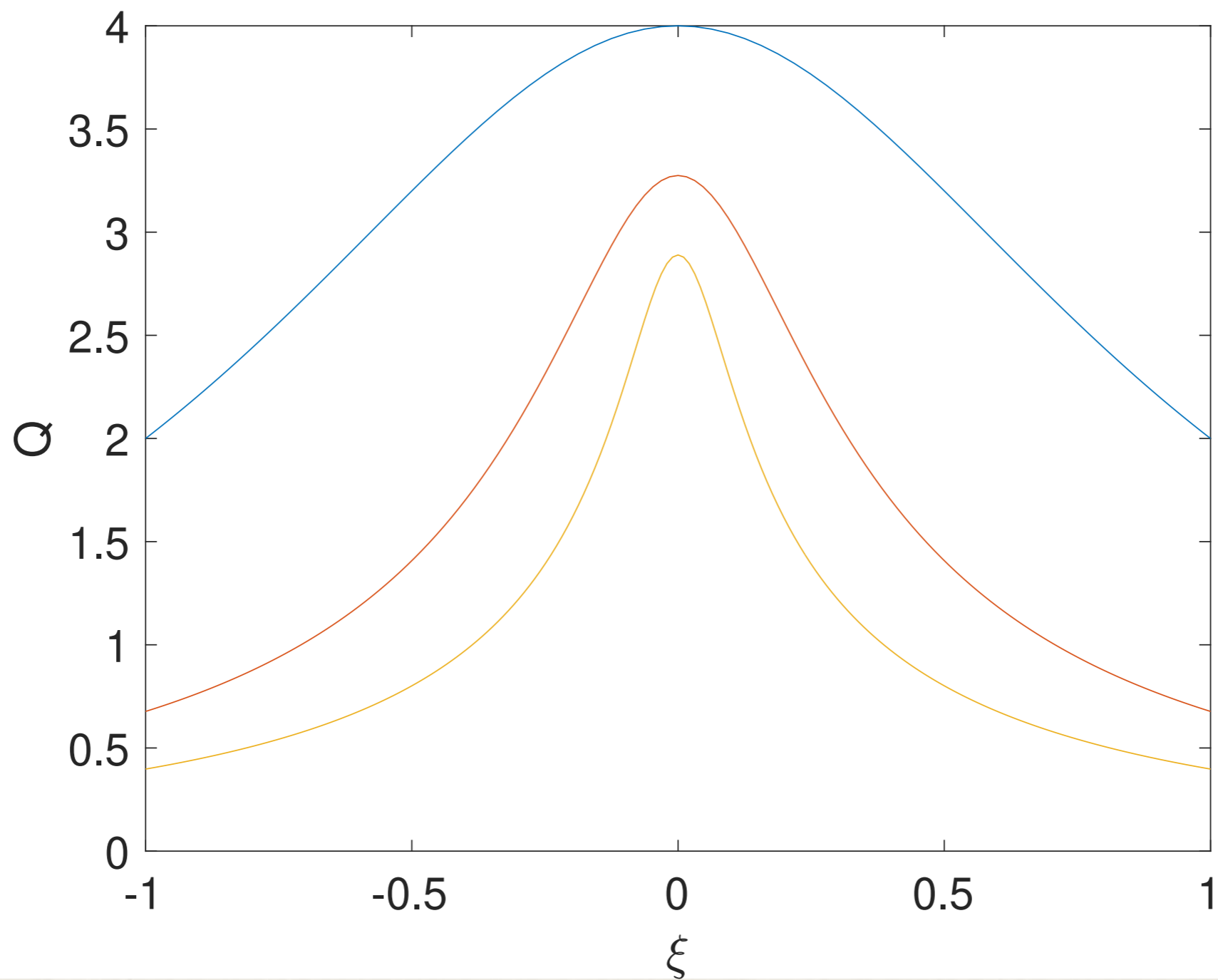
- Hilbert transform

$$\mathcal{H}[f](x) := \frac{1}{\pi} \mathcal{P} \int_{\mathbb{R}} \frac{f(y)}{x-y} dy$$

- solitary wave solutions

$$-cQ_c(\xi) - HQ'_c(\xi) + \frac{1}{m}Q_c^m(\xi) = 0$$

# Newton iteration



# Fourier transforms

- ♦ diagonal differentiation matrices, efficient for time integration
- ♦ not well approximated by DFT for slowly decreasing and discontinuous functions
- ♦ integration in the complex plane on contours motivated by steepest descent

# Step initial data for Airy equation

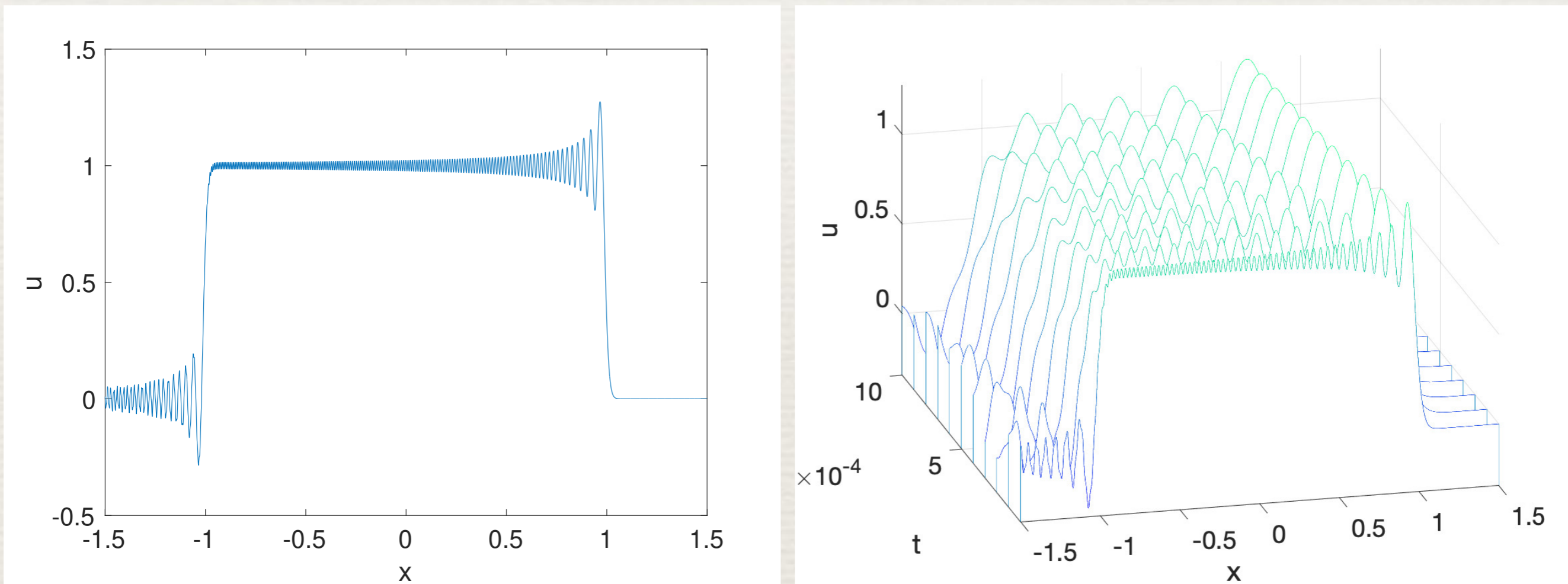


FIGURE 5. Solution for the Airy equation (2) and step initial data (7): on the left for  $t = 10^{-6}$ , on the right for several values of  $t \in [10^{-5}, 10^{-3}]$ .

# Integration path

$$F(\eta) = \int_{\mathbb{R}} \frac{dk}{k} \exp(ik^3 + ik\eta)$$

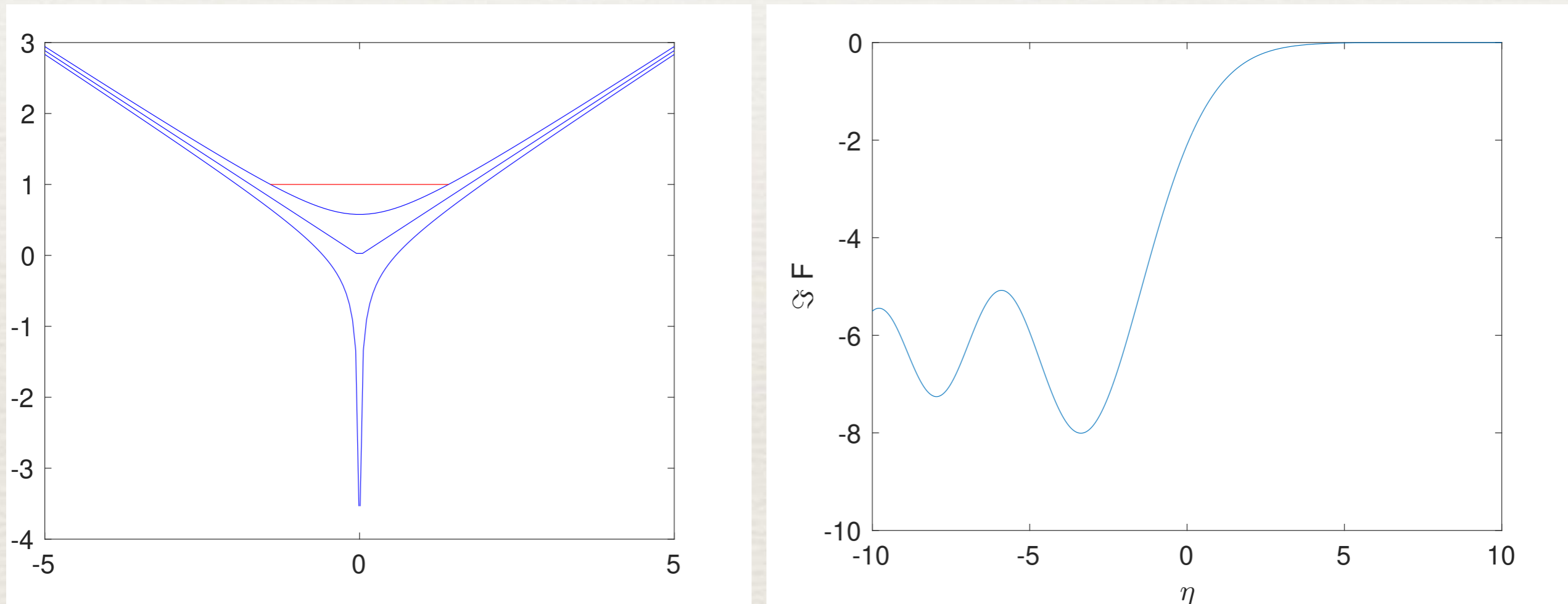


FIGURE 6. On the left the integration contours in the complex  $k$ -plane for  $\eta = 1$  (top),  $\eta = 0$  (middle) and an open contour for  $\eta = -1$  (in red the contour bridging between the blue arcs for  $\eta = 1$  to address the pole at the origin), on the right the function  $F(\eta)$ .

# Outlook

- ♦ adapted time integrators
- ♦ matching conditions for higher order PDEs
- ♦ fractional derivatives
- ♦ Fourier transforms



# References

- C. Klein, N. Stoilov, Multi-domain spectral approach to rational order fractional derivatives, *Stud. App. Maths.*, (2024) DOI: 10.1111/sapm.12671
- C. Klein, J. Prada-Malagon, N. Stoilov, On numerical approaches to non-linear Schrödinger and Korteweg-de Vries equations for piecewise smooth and slowly decaying initial data, *Physica D* 454 (2023) 133885
- C. Klein, N. Stoilov, Spectral approach to Korteweg-de Vries equations on the compactified real line, *App. Num. Math.*, (2022) <https://doi.org/10.1016/j.apnum.2022.02.015>
- C. Klein, N. Stoilov, Numerical study of break-up in solutions to the dispersionless Kadomtsev-Petviashvili equation, *Lett. Math. Phys.* (2021) 111:113 <https://doi.org/10.1007/s11005-021-01454-6>
- C. Klein, J. Riton, N. Stoilov, Multi-domain spectral approach for the Hilbert transform on the real line, *SN Partial Differential Equations and Applications* (2:36) (2021) <https://doi.org/10.1007/s42985-021-00094-8>
- C. Klein, N. Stoilov, Numerical study of the transverse stability of the Peregrine solution, *Stud Appl Math.* 145 (2020) 36–51. <https://doi.org/10.1111/sapm.12306>
- C. Klein, N. Stoilov, Multidomain spectral approach with Sommerfeld condition for the Maxwell equations, *J. Comp. Phys.*, <https://doi.org/10.1016/j.jcp.2021.110149>
- M. Birem and C. Klein, *Multidomain spectral method for Schrödinger equations*, *Adv. Comp. Math.*, 42(2), 395-423 DOI 10.1007/s10444-015-9429-9 (2016)