

Numerical inverse scattering for Korteweg–de Vries and nonlinear Schrödinger equations

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joint work with
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- We numerically solve the Cauchy problem for the focusing and defocusing nonlinear Schrödinger (NLS) equations

$$\begin{aligned}iu_t + u_{xx} \pm 2|u|^2 u &= 0 \\ u(0, x) &= u_0(x)\end{aligned}$$

and the Korteweg–de Vries (KdV) equation

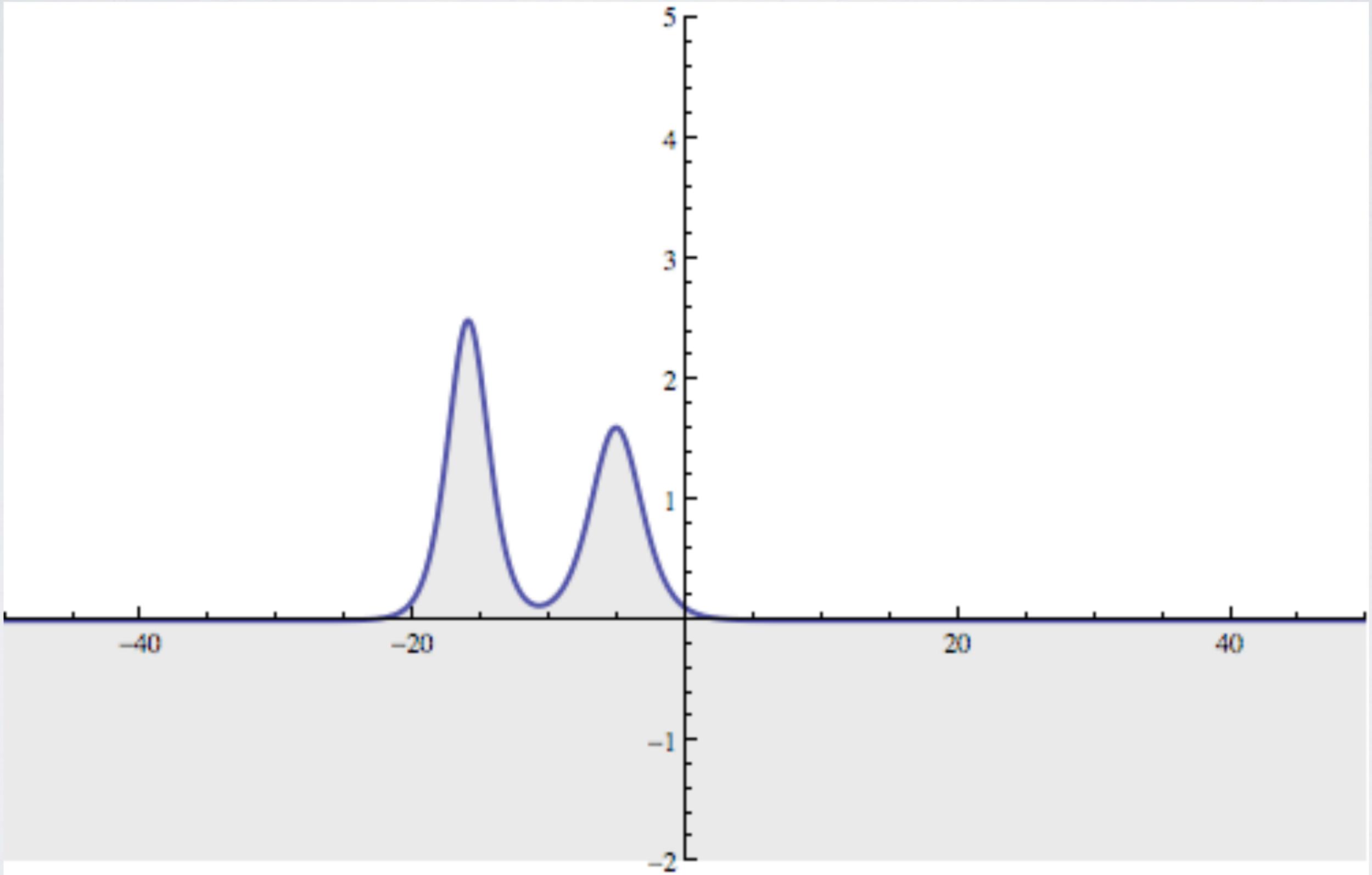
$$\begin{aligned}u_t + 6uu_x + u_{xxx} &= 0 \\ u(0, x) &= u_0(x)\end{aligned}$$

- We assume the initial condition is smooth and exponentially decaying
- We use **inverse scattering** numerically:
 - We compute the forward transform by utilizing **spectral methods**
 - We compute the inverse transform by solving **Riemann–Hilbert problems** numerically
 - By **deforming** the Riemann–Hilbert problem in the complex plane, we get representations which are numerically stable and accurate **uniformly** for all space and time

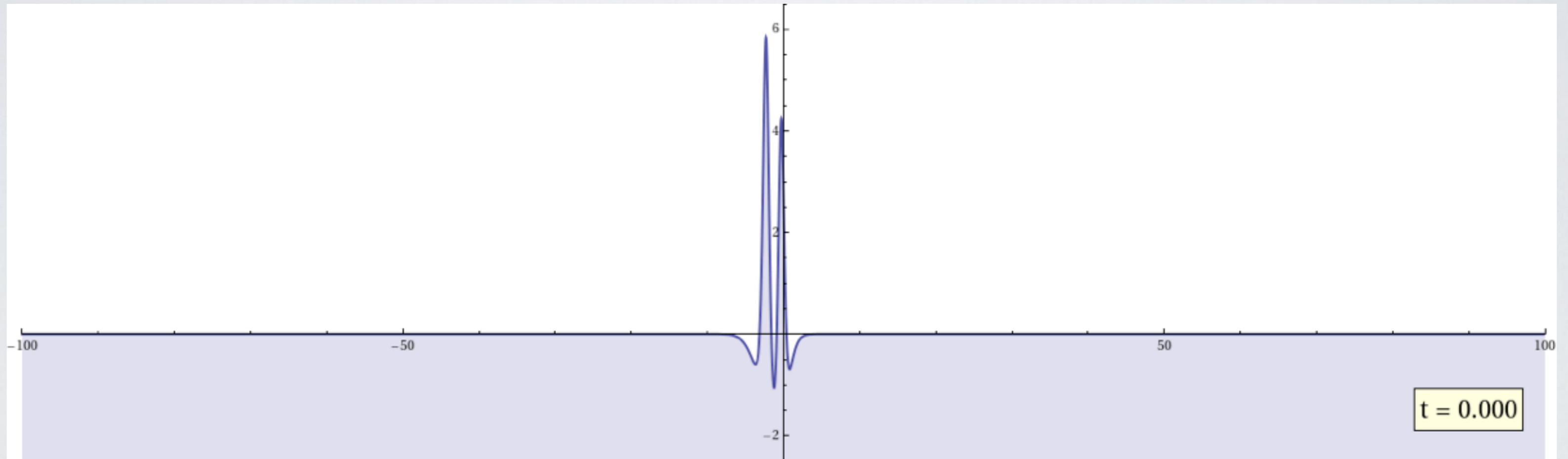
Why not use standard numerical methods?

- The standard numerical approach is to employ **pseudo-spectral methods**
 - Represent the solution by N evenly spaced points on, say, $[-L, L]$
 - Reduce the PDE to an ODE on how the solution evolves pointwise in time

KdV (Pure solitons)



A more generic solution to KdV



Why not use standard numerical methods?

- The standard numerical approach is to employ **pseudo-spectral methods**
 - Represent the solution by N evenly spaced points on, say, $[-L, L]$
 - Reduce the PDE to an ODE on how the solution evolves pointwise in time
- **Dispersion** causes this approach to quickly fail as time T increases
 - Dispersive waves travel **linearly with time**, so we must take $L = \mathcal{O}(T)$
 - Therefore, $N = \mathcal{O}(T)$
 - The CFL condition states that the time step must be $\Delta t = \mathcal{O}(N^{-1})$
 - The **total work** is at least

$$\mathcal{O}\left(N \log N \frac{T}{\Delta t}\right) = \mathcal{O}(T^3 \log T)$$

- The constant in front is initial condition dependent, and typically **very large!**

Review: Fourier solution of linear KdV

$$u_t + u_{xxx} = 0$$
$$u(0, x) = u_0(x)$$

$$u_0(x) \xrightarrow{\frac{1}{2\pi} \int_{-\infty}^{\infty} u_0(x) e^{-ikx} dx} \hat{u}_0(k)$$

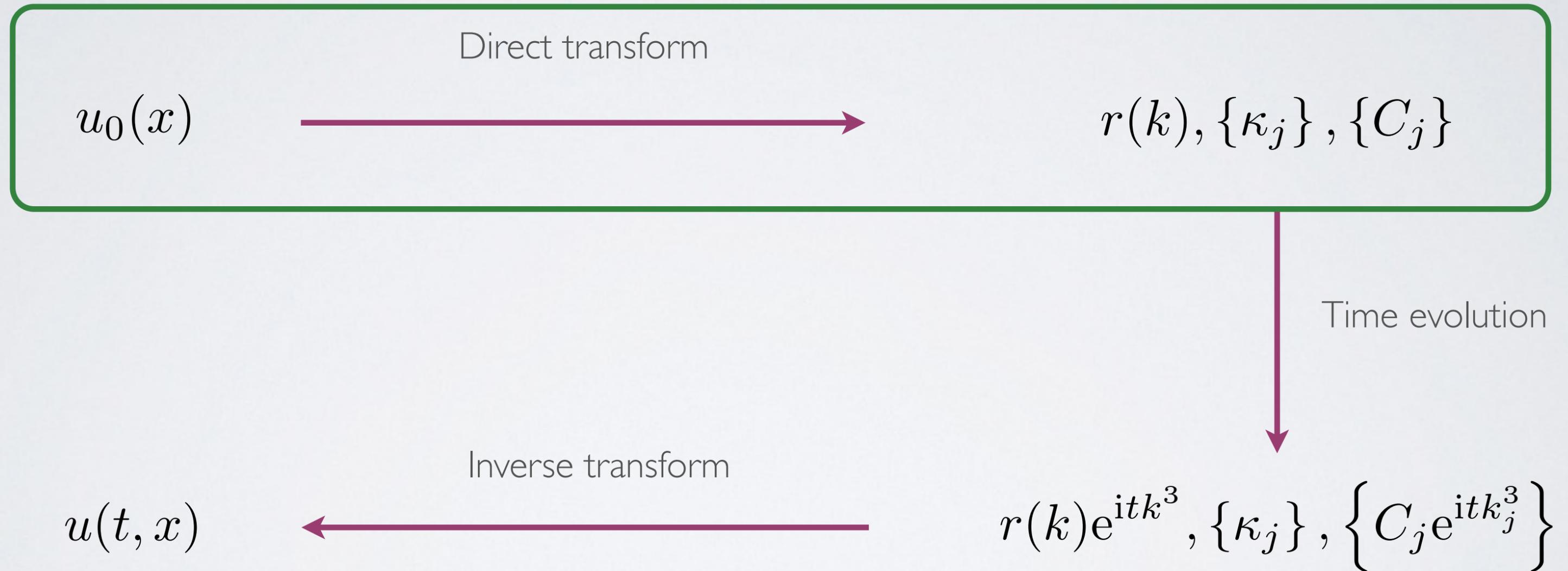
$$\hat{u}_0(k)$$

Time evolution

$$u(t, x) \xleftarrow{\int_{-\infty}^{\infty} \hat{u}_0(k) e^{i(tk^3 + kx)} dx} \hat{u}_0(k) e^{itk^3}$$

$$\hat{u}_0(k) e^{itk^3}$$

Inverse scattering for KdV



- Associated with an integrable PDE its Lax pair:

$$\mu_x = A(k, u, x)\mu \quad \text{and} \quad \mu_t = B(k, u, x)\mu$$

- The variable u must satisfy the relevant PDE for the pairs to be compatible
- For our purposes, we only need the $\mu_x = A\mu$ equations, which are:

- KdV (self-adjoint):

$$\mu_{xx} + (k^2 + u)\mu = 0$$

- defocusing NLS (self-adjoint):

$$\mu_x = \begin{pmatrix} -ik & u \\ \bar{u} & ik \end{pmatrix} \mu$$

- focusing NLS (not self-adjoint):

$$\mu_x = \begin{pmatrix} -ik & u \\ -\bar{u} & ik \end{pmatrix} \mu$$

- The direct scattering transform consists of spectral analysis of these equations

KdV Direct Scattering

- The direct scattering transform is a map

initial condition $u_0(x) \mapsto$ scattering data $r(k), \{\kappa_1, \dots, \kappa_N\}, \{C_1, \dots, C_N\}$

- The scattering data results from spectral analysis of

$$\mathcal{L} = \partial_x^2 + u_0(x)$$

- This operator has continuous spectra on $(-\infty, 0]$ and N discrete eigenvalues on the positive real axis at the points $\{\kappa_1, \dots, \kappa_N\}$:



- The discrete eigenvalues $\kappa_1, \dots, \kappa_N$ of

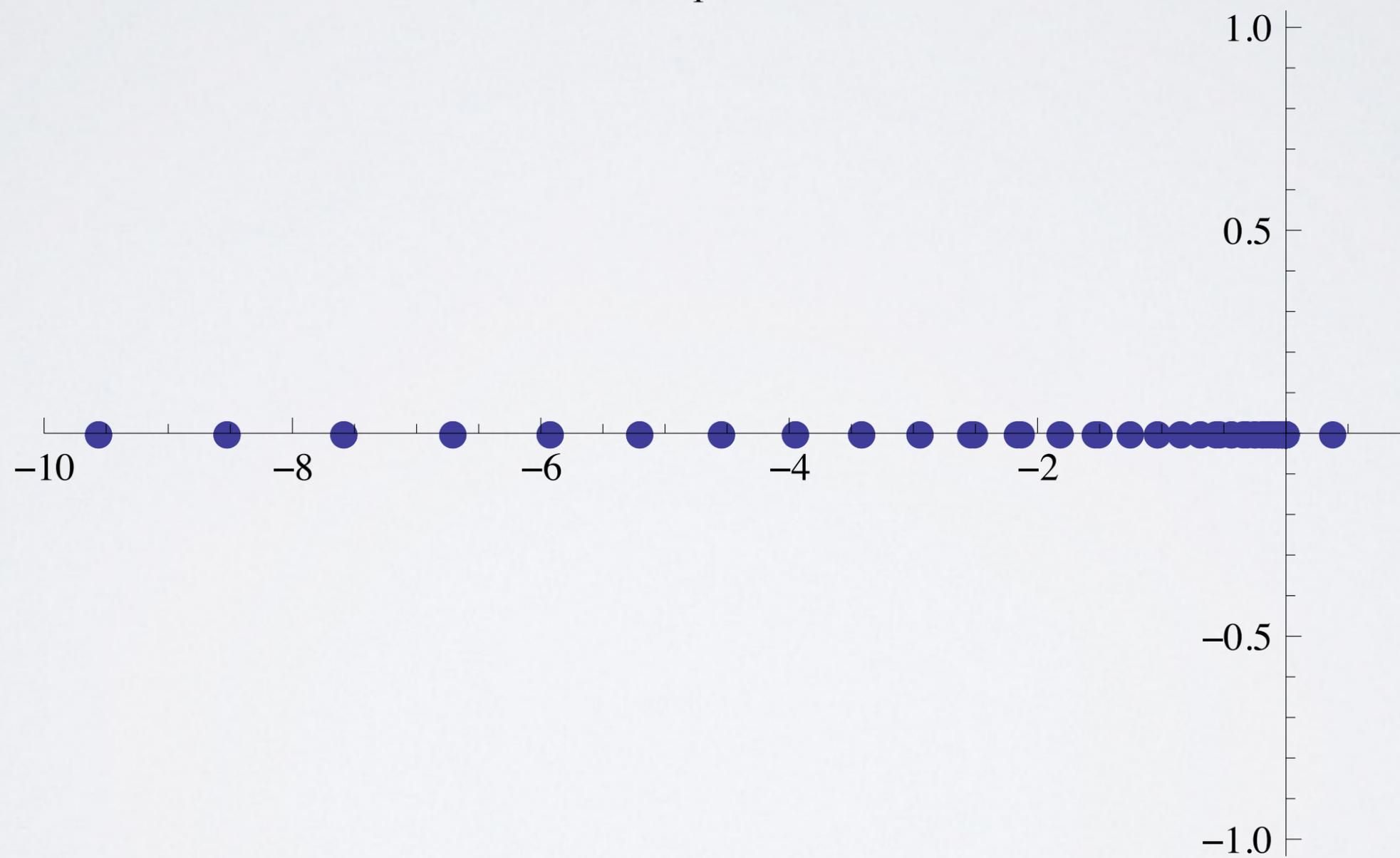
$$\mathcal{L} = \partial_x^2 + u_0(x)$$

correspond to the N -solitons of the solution

- These can be computed using Hill's method:
 - Map $(-\infty, \infty)$ to $[-\pi, \pi)$ using $\frac{2}{\pi} \arctan x$
 - Represent the mapped operator \mathcal{L} by its action on n Fourier coefficients
 - Calculate the positive eigenvalues of this discretized matrix
 - Verify the eigenvectors correspond to $L^2(-\infty, \infty)$ solutions

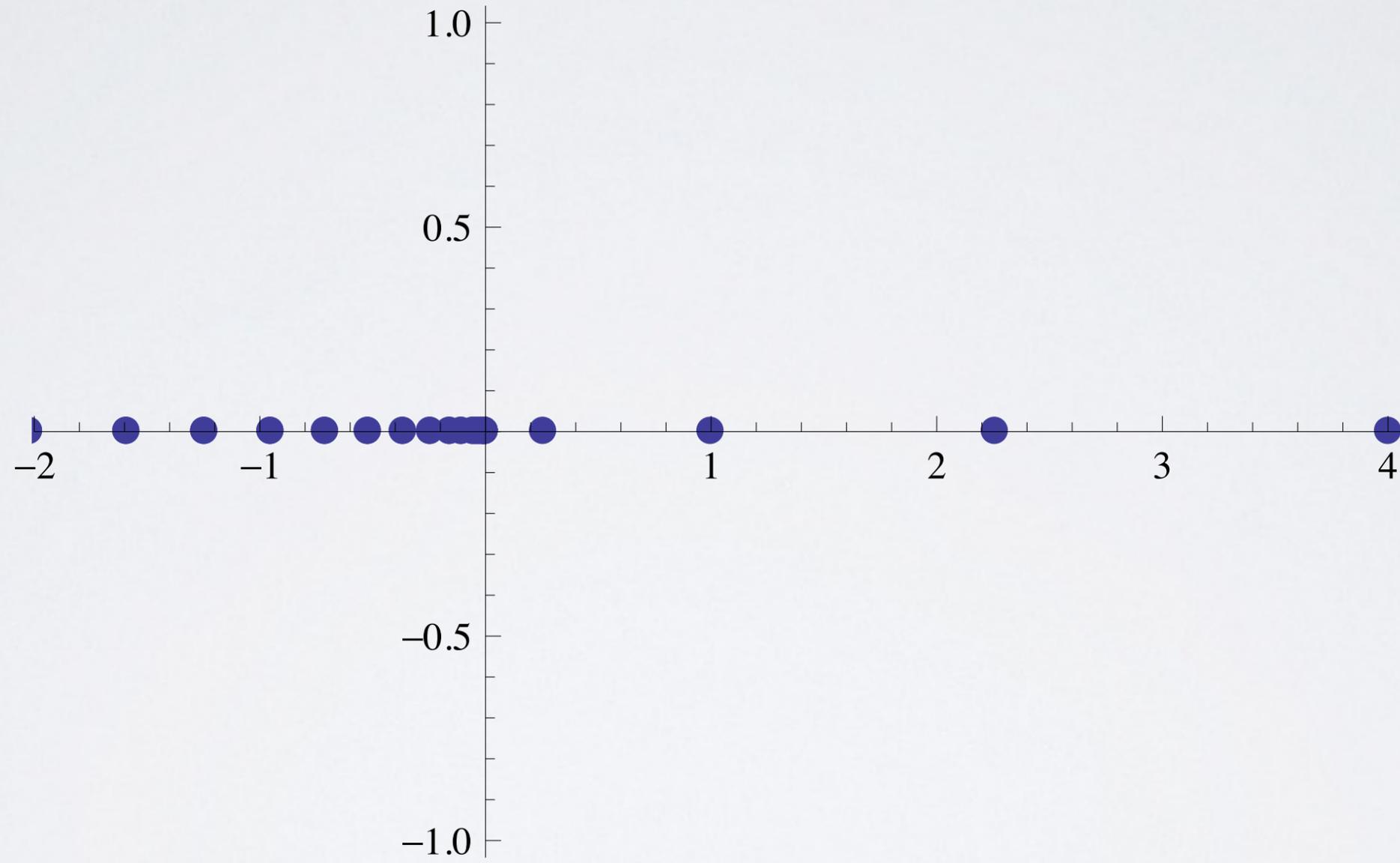
$$q_0(x) = \operatorname{sech}^2 x$$

$$n = 500 \quad \kappa_1 = 0.381966$$



Computed spectra for $u_0(x) = 5 \operatorname{sech}^2 \frac{x}{2}$

$$n = 300 \quad \kappa = \{4., 2.25, 1., 0.25, 2.66561 \times 10^{-13}\}$$



- The *reflection coefficient* $r(k)$ is defined for real k and corresponds to the continuous spectrum of the previous Schrödinger operator
- For each k , we can solve

$$\mu_{xx} + (u_0(x) + k^2)\mu = 0$$

with three initial conditions:

$$\phi(x) \sim e^{ikx}, \quad x \rightarrow -\infty$$

$$\psi^+(x) \sim e^{ikx} \quad \text{and} \quad \psi^-(x) \sim e^{-ikx}, \quad x \rightarrow \infty$$

- This is a *second order equation*: therefore there exists a and b so that

$$\phi(x) = a(k)\psi^+(x) + b(k)\psi^-(x)$$

- Then $r(k) = b(k)/a(k)$

- We need to solve

$$\phi''(x) + (u_0(x) + k^2)\phi(x) = 0, \quad \phi(x) \sim e^{ikx}, \quad x \rightarrow -\infty$$

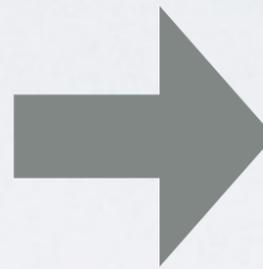
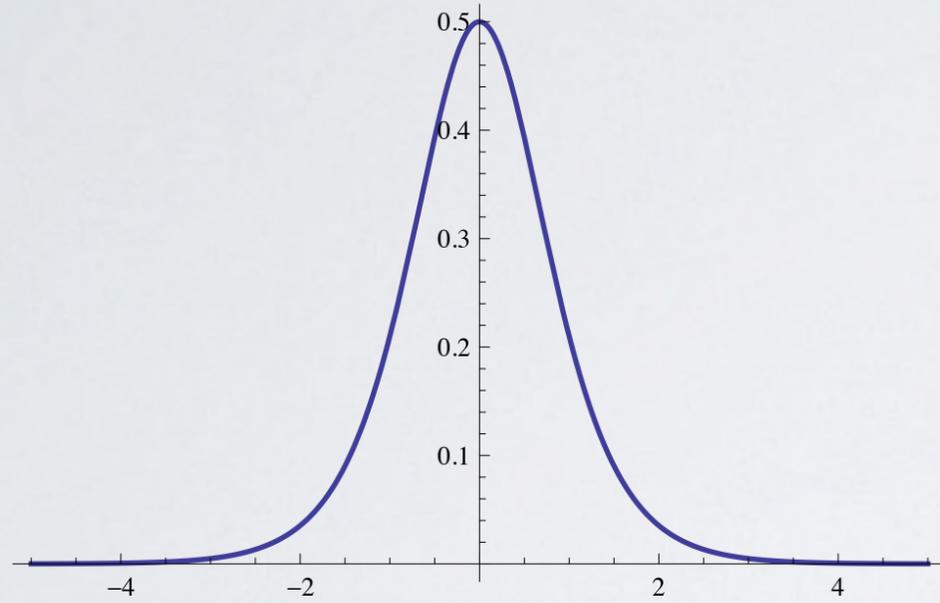
- We do a change of variables to **factor out oscillations**: $\phi = (1 + v)e^{ikx}$
- Plugging this in gives us an equation for v :

$$v'' + 2ikv' + u_0v = -u_0, \quad v(-\infty) = 0, \quad v'(-\infty) = 0$$

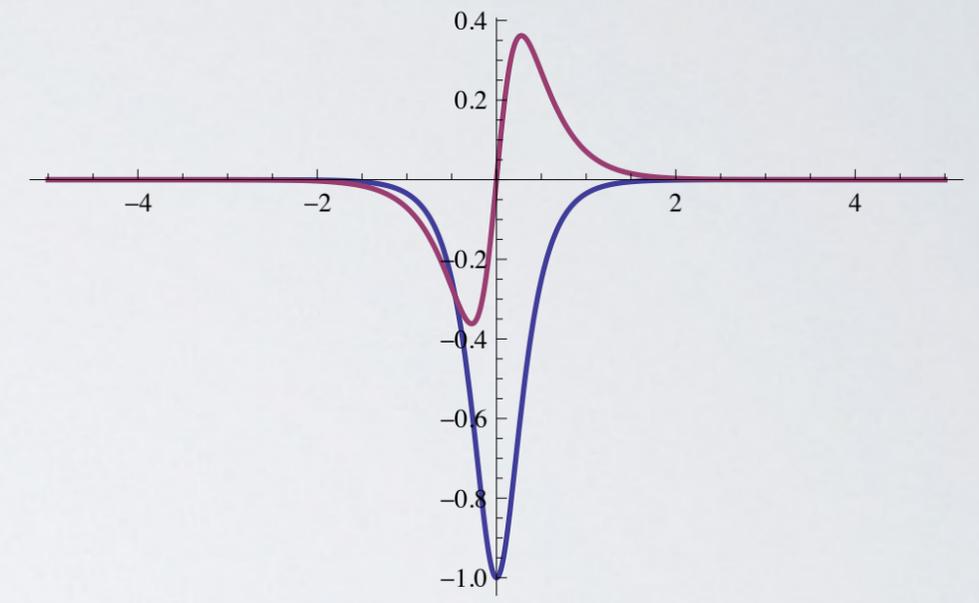
- We can easily solve this by mapping $(-\infty, 0)$ to the unit interval and using a **spectral method**
- Using the same approach, we can compute ψ^\pm on $(0, \infty)$
- We then solve

$$\begin{pmatrix} \psi^+(0) & \psi^-(0) \\ \psi_x^+(0) & \psi_x^-(0) \end{pmatrix} \begin{pmatrix} a(k) \\ b(k) \end{pmatrix} = \begin{pmatrix} \phi(0) \\ \phi_x(0) \end{pmatrix}$$

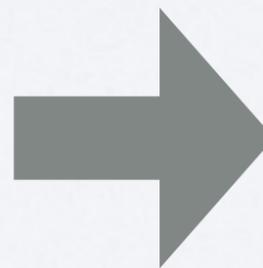
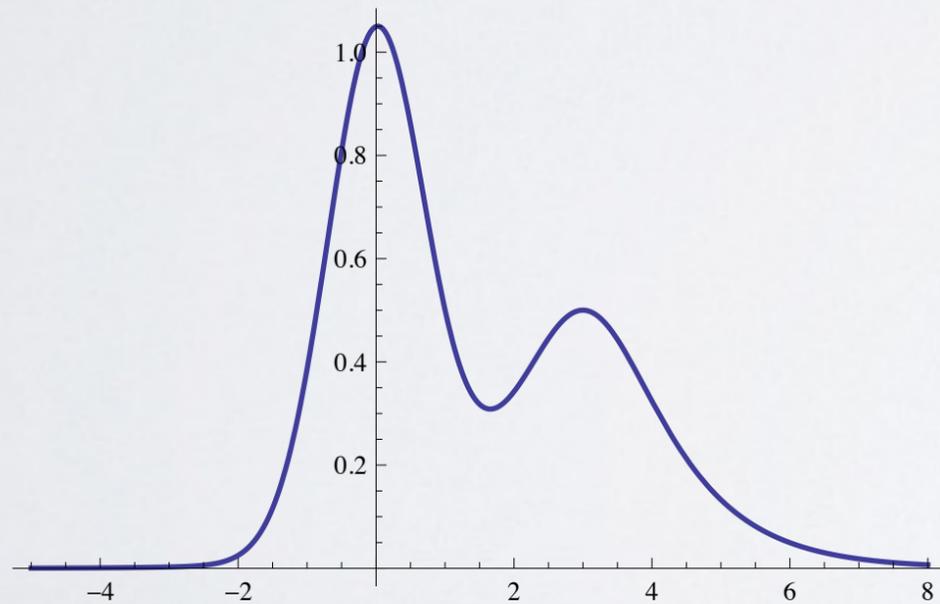
Initial condition



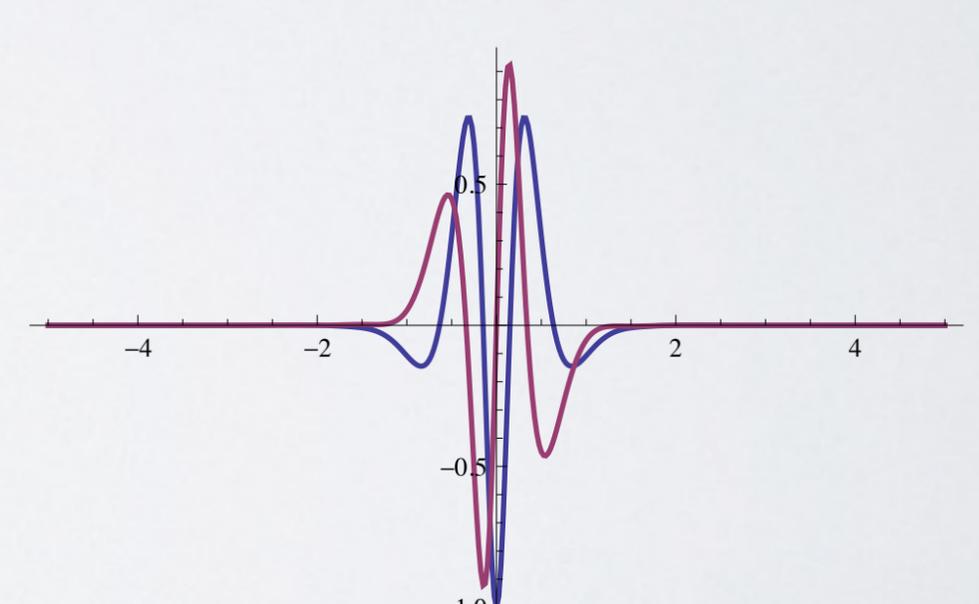
Reflection coefficient



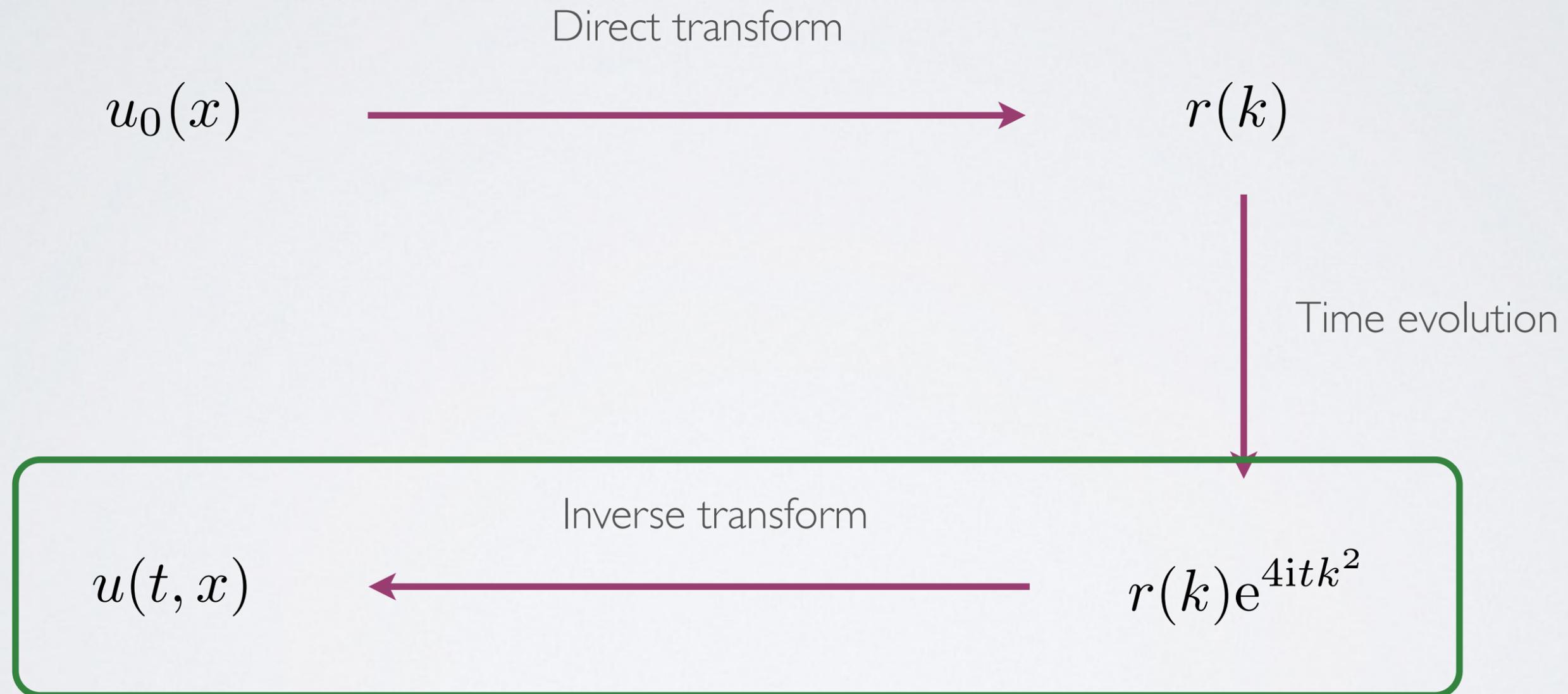
Initial condition



Reflection coefficient



Inverse scattering for defocusing NLS



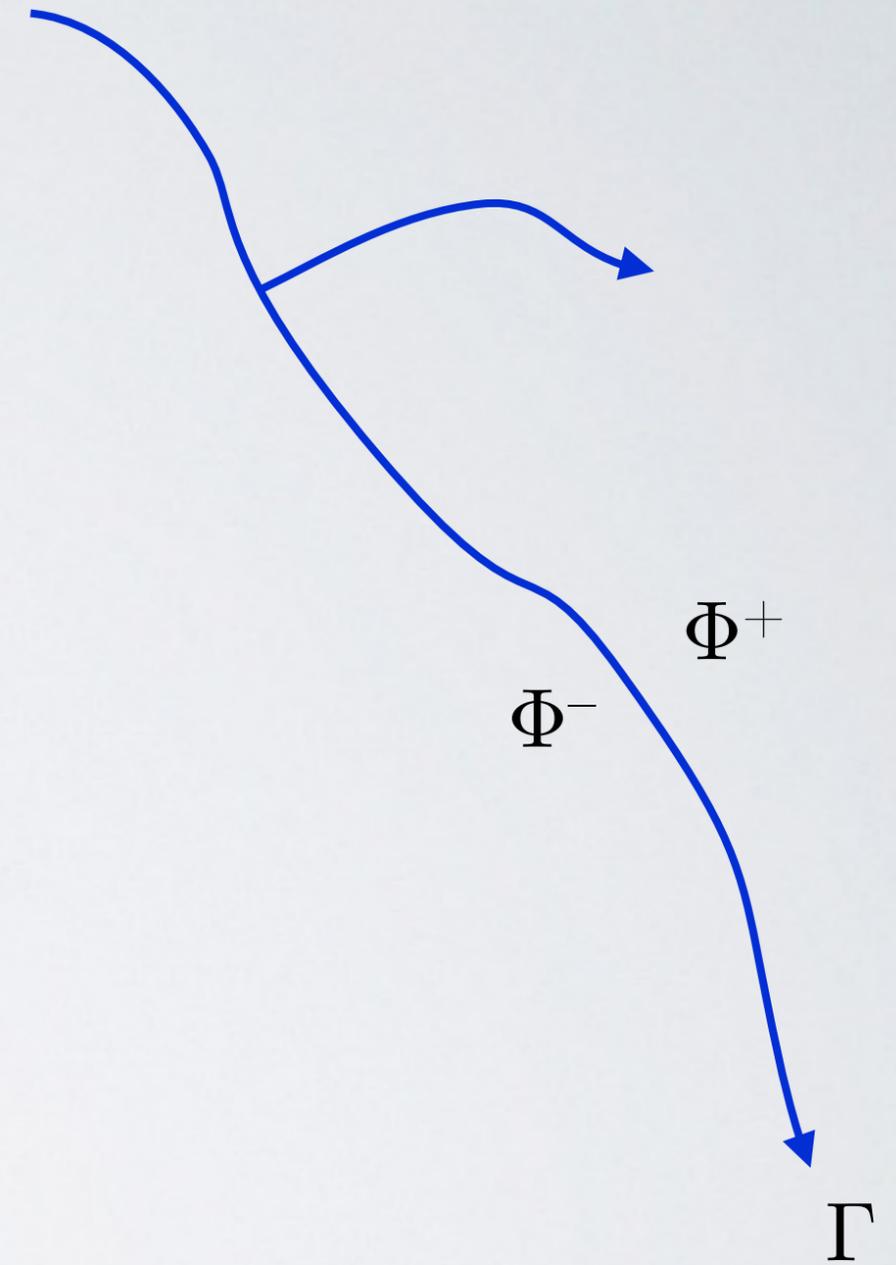
- A matrix-valued *Riemann–Hilbert problem* is the following:
 - Given an oriented contour Γ in the complex plane and a matrix-valued function G defined on Γ (here, all functions on Γ are analytic along each piece of Γ);
 - Find a matrix-valued function Φ that is analytic everywhere in the complex plane off of Γ such that

$$\Phi^+(z) = \Phi^-(z)G(z) \quad \text{for } z \in \Gamma \quad \text{and} \quad \Phi(\infty) = I$$

where

$$\Phi^+(z) = \lim_{x \rightarrow z} \Phi(x) \quad \text{where } x \text{ is left of } \Gamma$$

$$\Phi^-(z) = \lim_{x \rightarrow z} \Phi(x) \quad \text{where } x \text{ is right of } \Gamma$$



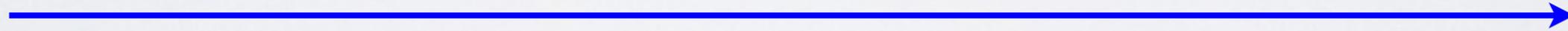
(see eg. Muskhelishvili 1953)

- Many linear differential equations have well-known **integral representations**
 - e.g., Airy equation, Bessel equation, Hypergeometric equation and heat and wave equations (via Fourier transform)
- Matrix-valued RH problems can be (loosely) viewed as an analogy of integral representations for *nonlinear equations*
- Importantly, RH problems can be used to determine asymptotics of solutions
 - This works similar to integral representations: the contour is deformed along the *path of steepest descent*
- Using a new approach, RH problems can now be used as a **numerical tool**
- Previous method: the Sine kernel RH problem (on the unit interval) and a special solution to Painlevé V were computed in ([Dienstfrey 1998](#)), by adapting standard **singular integral equation** (SIE) methods
 - Required **exponentially clustered collocation points** near the endpoints
 - Not applicable to more complicated domains

Inverse transform

- The inverse transform is a Riemann–Hilbert problem on the real line:

$$\Phi^+(z) = \Phi^-(z) \begin{pmatrix} 1 - |r(z)|^2 & -\bar{r}(z)e^{-2i(2tz^2+xz)} \\ r(z)e^{2i(2tz^2+xz)} & 1 \end{pmatrix}$$



- Then the solution to dNLS is

$$u(t, x) = 2i \lim_{z \rightarrow \infty} z \Phi(z)_{12}$$

Construction of a collocation method

- Consider the *Cauchy transform*

$$\mathcal{C}_\Gamma f(z) = \frac{1}{2i\pi} \int_\Gamma \frac{f(t)}{t-z} dt.$$

This map defines a one-to-one correspondence between a function defined on Γ and a function which is analytic everywhere off Γ which decays at ∞

- Let

$$\Phi = I + \mathcal{C}V$$

- The RH problem $\Phi^+ = \Phi^- G$ becomes

$$\mathcal{C}^+ V(x) - \mathcal{C}^- V(x) G(x) = G(x) - I \quad \text{for } x \in \Gamma$$

- Having a method to compute the Cauchy transform and its left and right limits allows us to apply the linear operator

$$\mathcal{M}V = \mathcal{C}^+ V - (\mathcal{C}^- V)G$$

(similar to Dienstfrey 1998)

- We want to construct an approximation to V which satisfies

$$\mathcal{M}V = G - I$$

at a sequence of points; i.e., we construct a **collocation method**:

- For some basis $\{\psi_1, \dots, \psi_n\}$ of functions defined on Γ and set of nodes $\{z_1, \dots, z_m\}$ on Γ

- Write

$$V_n = \sum_{k=1}^n \mathbf{c}_k \psi_k$$

- Solve the **linear system**

$$\begin{aligned} \mathbf{c}_1 \mathcal{M}\psi_1(z_1) + \dots + \mathbf{c}_n \mathcal{M}\psi_n(z_1) &= G(z_1) - I \\ &\vdots \\ \mathbf{c}_1 \mathcal{M}\psi_1(z_m) + \dots + \mathbf{c}_n \mathcal{M}\psi_n(z_m) &= G(z_m) - I \end{aligned}$$

- Consider the map

$$M^{-1}(z) = \frac{i - z}{i + z}$$

- This maps the real line to the unit circle
 - More precisely: it conformally maps the upper half plane to the interior of the circle



- It also conformally maps the lower half plane to the exterior of the circle

- The inverse

$$M(z) = i \frac{1 - z}{z + 1}$$

conformally maps the unit circle to the real line

- The Cauchy transform is (due to Plemelj's lemma)

$$\mathcal{C}_{(-\infty, \infty)} f(z) = \mathcal{C}_{\circlearrowleft} [f \circ M](M^{-1}(z)) - \mathcal{C}_{\circlearrowleft} [f \circ M](-1)$$

- Thus we have reduced the construction of our collocation method to one problem: the computation of the Cauchy transform over the unit circle

- We know

$$\mathcal{C}_{\circ}[\diamond^k](z) = \begin{cases} z^k & |z| < 1 \text{ and } k \geq 0 \\ -z^k & |z| > 1 \text{ and } k < 0 \\ 0 & \text{otherwise} \end{cases}$$

- Thus we know the Cauchy transform exactly on the real line:

$$\mathcal{C}_{(-\infty, \infty)}[M^{-1}(\diamond)^k](z) = \begin{cases} M^{-1}(z)^k - (-1)^k & \Im z > 0 < 1 \text{ and } k \geq 0 \\ (-1)^k - M^{-1}(z)^k & \Im z < 0 \text{ and } k < 0 \\ 0 & \text{otherwise} \end{cases}$$

- We use this basis in the collocation system, with mapped evenly spaced points

- Finally, we recover the solution to dNLS:

$$\begin{aligned} u(t, x) &= 2i \lim_{z \rightarrow \infty} z \Phi(z)_{12} = 2i \lim_{z \rightarrow \infty} z \mathcal{C}V(z)_{12} \\ &= \frac{1}{\pi} \lim_{z \rightarrow \infty} \int_{-\infty}^{\infty} \frac{z V(x)_{12}}{x - z} dx \\ &= -\frac{1}{\pi} \int_{-\infty}^{\infty} V(x)_{12} dx \\ &\approx -\frac{1}{\pi} \int_{-\infty}^{\infty} V_n(x)_{12} dx \end{aligned}$$

Convergence

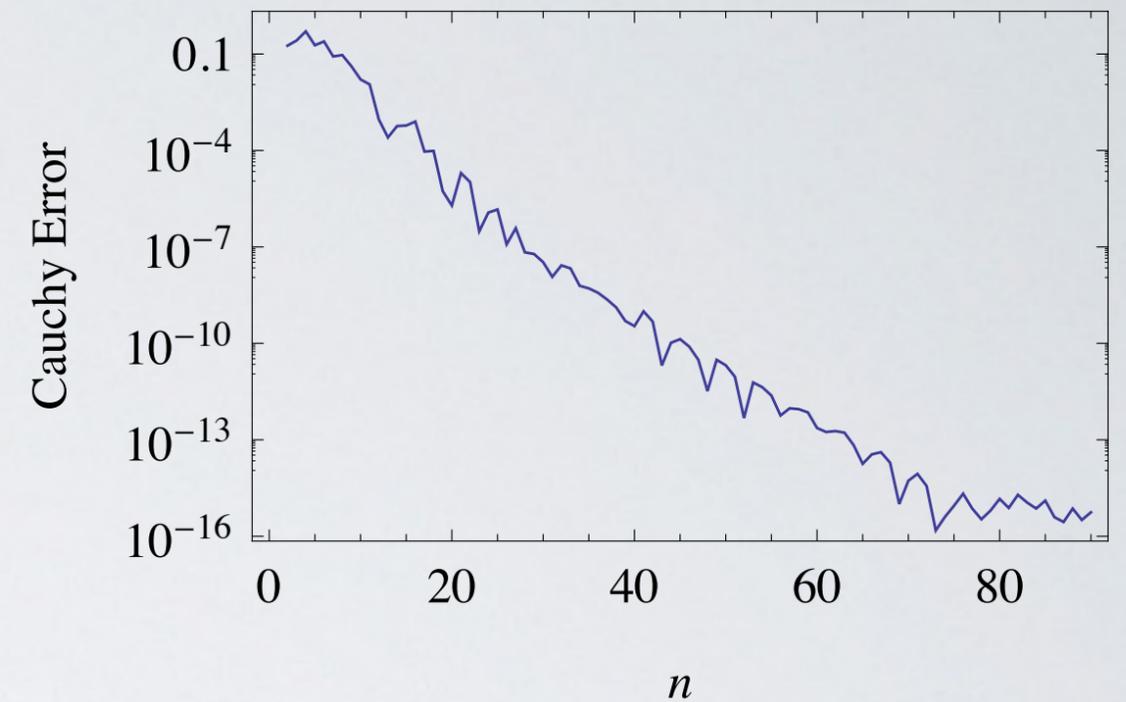
- The error in approximation is bounded by

$$\|V - V_n\| \leq [1 + C \log n \|M_n^{-1}\| \|\mathcal{M}\|] \|V - \mathcal{P}_n V\|$$

Number of
collocation points n

Collocation matrix
(Grows logarithmically)

Interpolation of
solution by basis
(Converges spectrally)

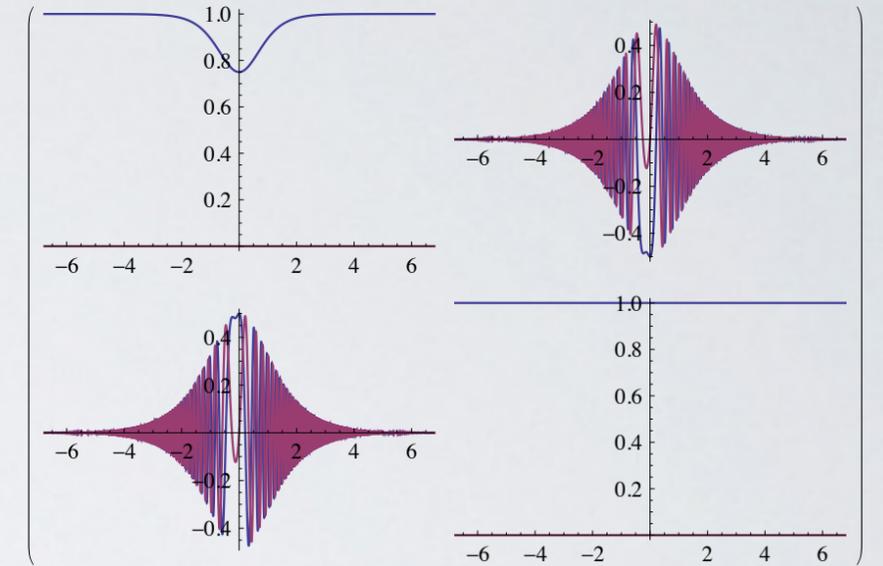


Nonlinear steepest descent

- The previous method works well for small x and t
- But as x and t become large the jump matrix

$$\begin{pmatrix} 1 - r(z)r(-z) & -\bar{r}(z)e^{-2i(2tz^2+xz)} \\ r(z)e^{2i(2tz^2+xz)} & 1 \end{pmatrix} =$$

becomes oscillatory



- We overcome this by deforming the Riemann–Hilbert problem into the complex plane
 - This converts oscillations into exponential decay
 - We must deform through the stationary points:

$$k_0 = -\frac{x}{4t}$$

- There are two ways we use to **factor** the jump matrix:

$$\begin{aligned} \begin{pmatrix} \tau & \bar{r}e^{-\theta} \\ re^{\theta} & 1 \end{pmatrix} &= LDU = \begin{pmatrix} 1 & \\ \frac{r}{\tau}e^{\theta} & 1 \end{pmatrix} \begin{pmatrix} \tau & \\ & \frac{1}{\tau} \end{pmatrix} \begin{pmatrix} 1 & \frac{\bar{r}}{\tau}e^{-\theta} \\ & 1 \end{pmatrix} \\ &= MP = \begin{pmatrix} 1 & \bar{r}e^{-\theta} \\ & 1 \end{pmatrix} \begin{pmatrix} 1 & \\ re^{\theta} & 1 \end{pmatrix} \end{aligned}$$

- The key now is that we can **lens** the jump contours without altering behaviour at infinity:

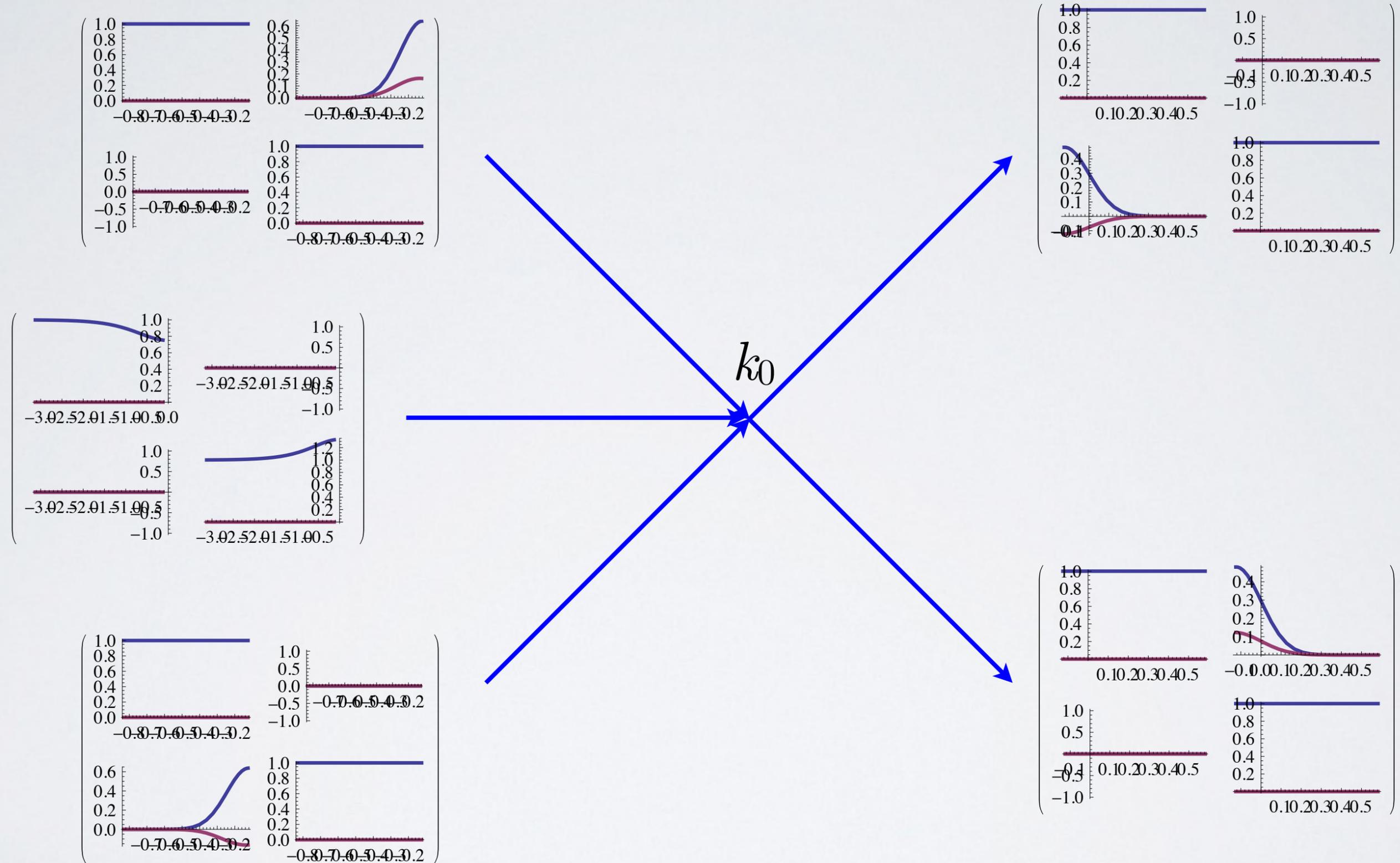


(based on Deift & Zhou 2003)

G



Jump matrices after truncation



Algorithm for computation

- We must choose a basis and **compute the Cauchy transform** over Γ
 - By splitting the domain and using **conformal maps**, this can be reduced to computing the Cauchy transform over the **unit interval**
 - The Cauchy transform for **Chebyshev polynomials** over the unit interval can be found in closed form!
- We must include the **junction points** of Γ in the collocation system
 - This is needed to ensure that the approximation is **bounded**
 - The Cauchy transform of our basis explodes there; therefore, we assign it a **special value** corresponding to the value if the singularities were to cancel

- We use the fact that the Cauchy transform of Chebyshev polynomials

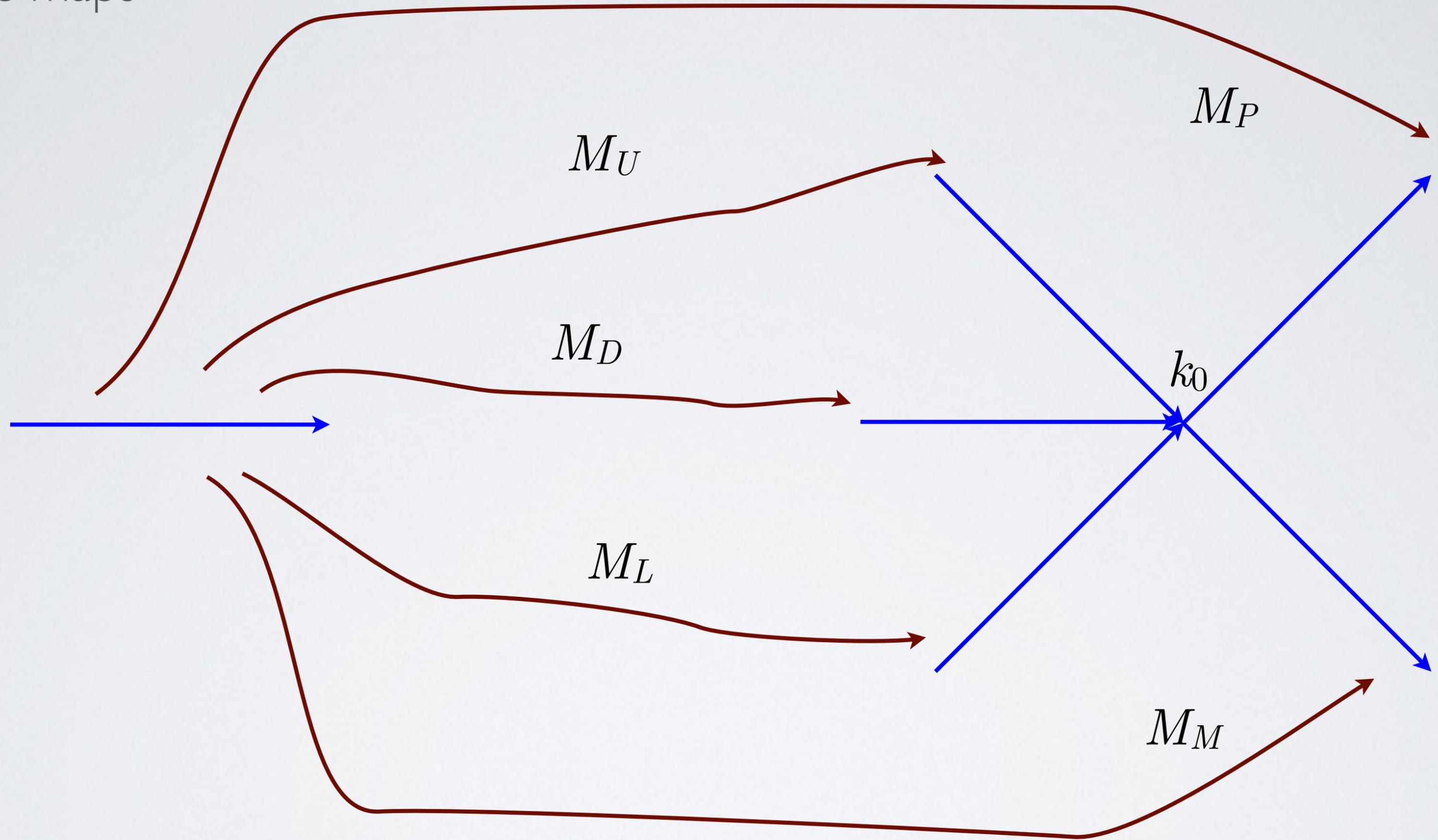
$$\mathcal{C}_{(-1,1)}T_k(z) = \frac{1}{2\pi i} \int_{-1}^1 \frac{T_k(x)}{x-z} dx$$

can be expressed exactly in terms of hypergeometric functions

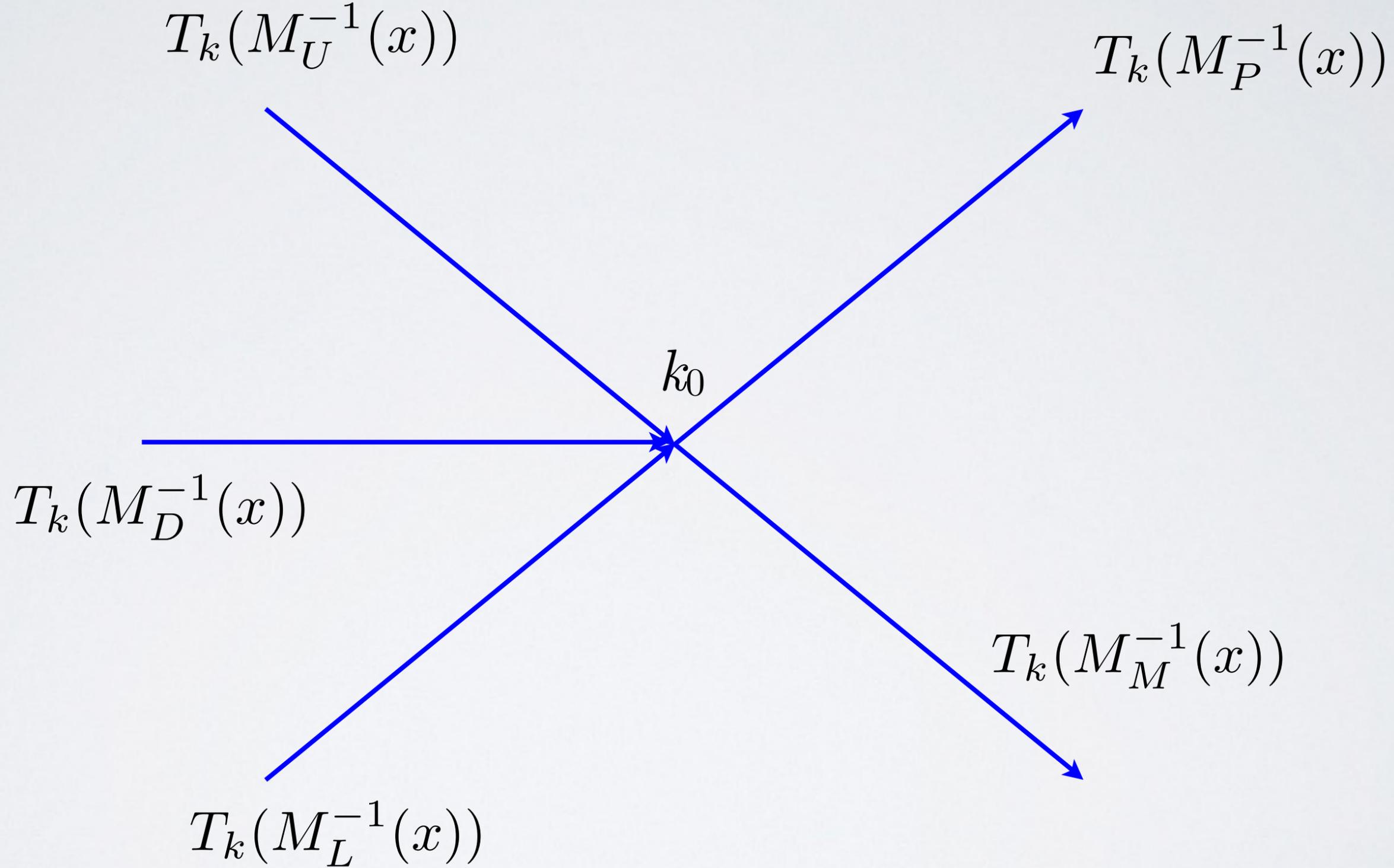
- And calculated rapidly, **uniformly accurate** in z using a one-term recurrence relationship
- If M is an affine transformation, then we have (from Plemelj's lemma)

$$\mathcal{C}_{M((-1,1))}f(z) = \mathcal{C}_{(-1,1)}[f \circ M](M^{-1}(z))$$

Affine maps



Piecewise collocation basis



- For our choice of basis and each affine transformation M , we can calculate

$$\mathcal{C}_{M((-1,1))}[T_k \circ M^{-1}](z) = \mathcal{C}_{(-1,1)}T_k(M^{-1}(z))$$

exactly

- The problem:

$$\mathcal{C}_{M((-1,1))}[T_k \circ M^{-1}](k_0) = \mathcal{C}_{(-1,1)}T_k(1) = \infty$$

- However, the solution V lies in a special space \mathcal{Z} that implies its Cauchy transform is **bounded** at k_0
- We therefore assume that our numerical approximation $V_n \in \mathcal{Z}$, allowing us to assign a value

$$\mathcal{C}_{M((-1,1))}[T_k \circ M^{-1}](k_0) = \mathcal{C}_{(-1,1)}T_k(1) \approx \alpha_k$$

- The resulting linear system imposes that the approximation V_n is indeed in \mathcal{Z}

$$\psi_1(z), \dots, \psi_n(z) = T_0(M_L^{-1}(x)), \dots, T_k(M_D^{-1}(x)), \dots, T_p(M_P^{-1}(x))$$


$$\mathbf{c}_1 \mathcal{M} \psi_1(z_1) + \dots + \mathbf{c}_n \mathcal{M} \psi_n(z_1) = G(z_1) - I$$

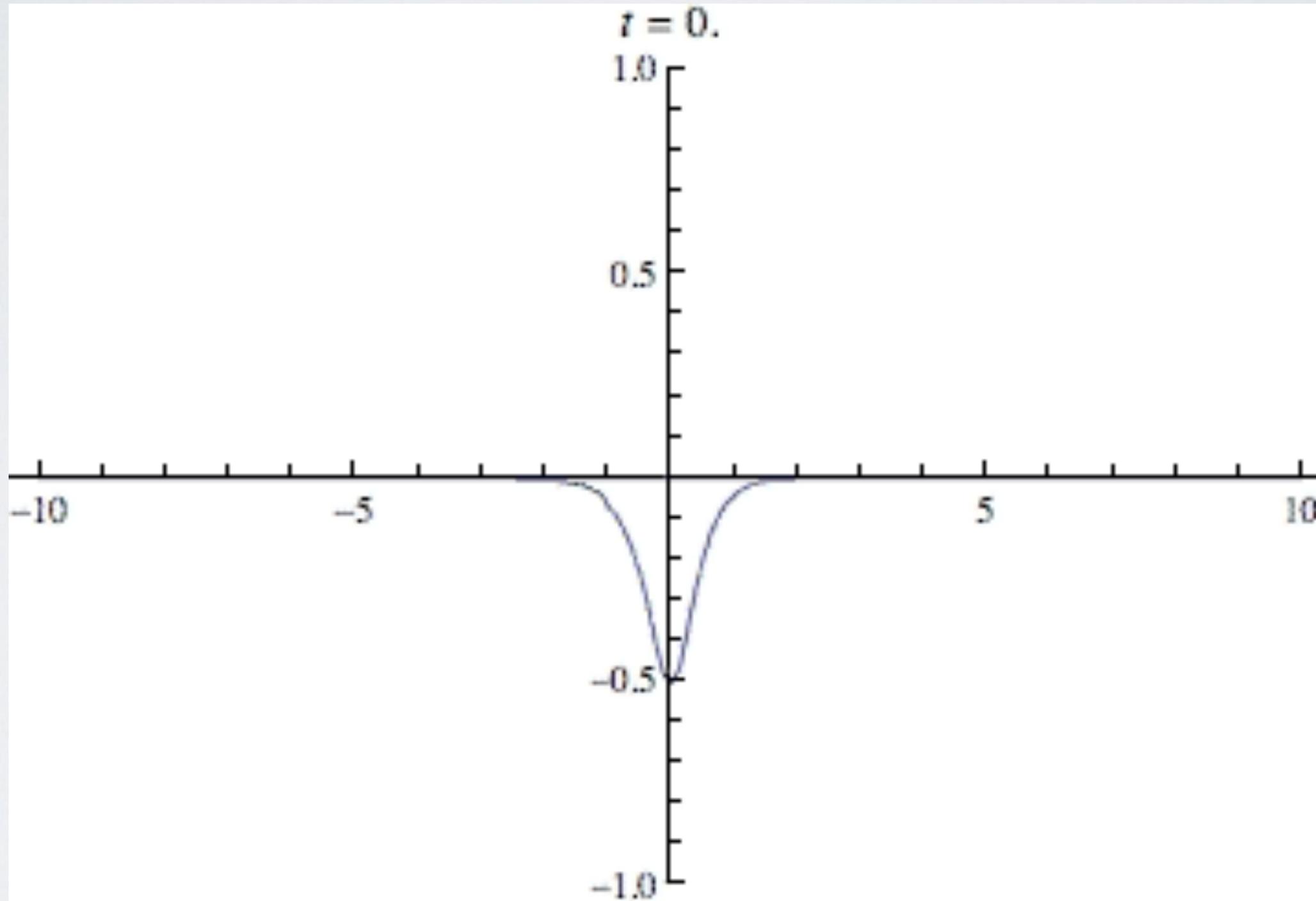
$$\vdots$$

$$\mathbf{c}_1 \mathcal{M} \psi_1(z_m) + \dots + \mathbf{c}_n \mathcal{M} \psi_n(z_m) = G(z_m) - I$$

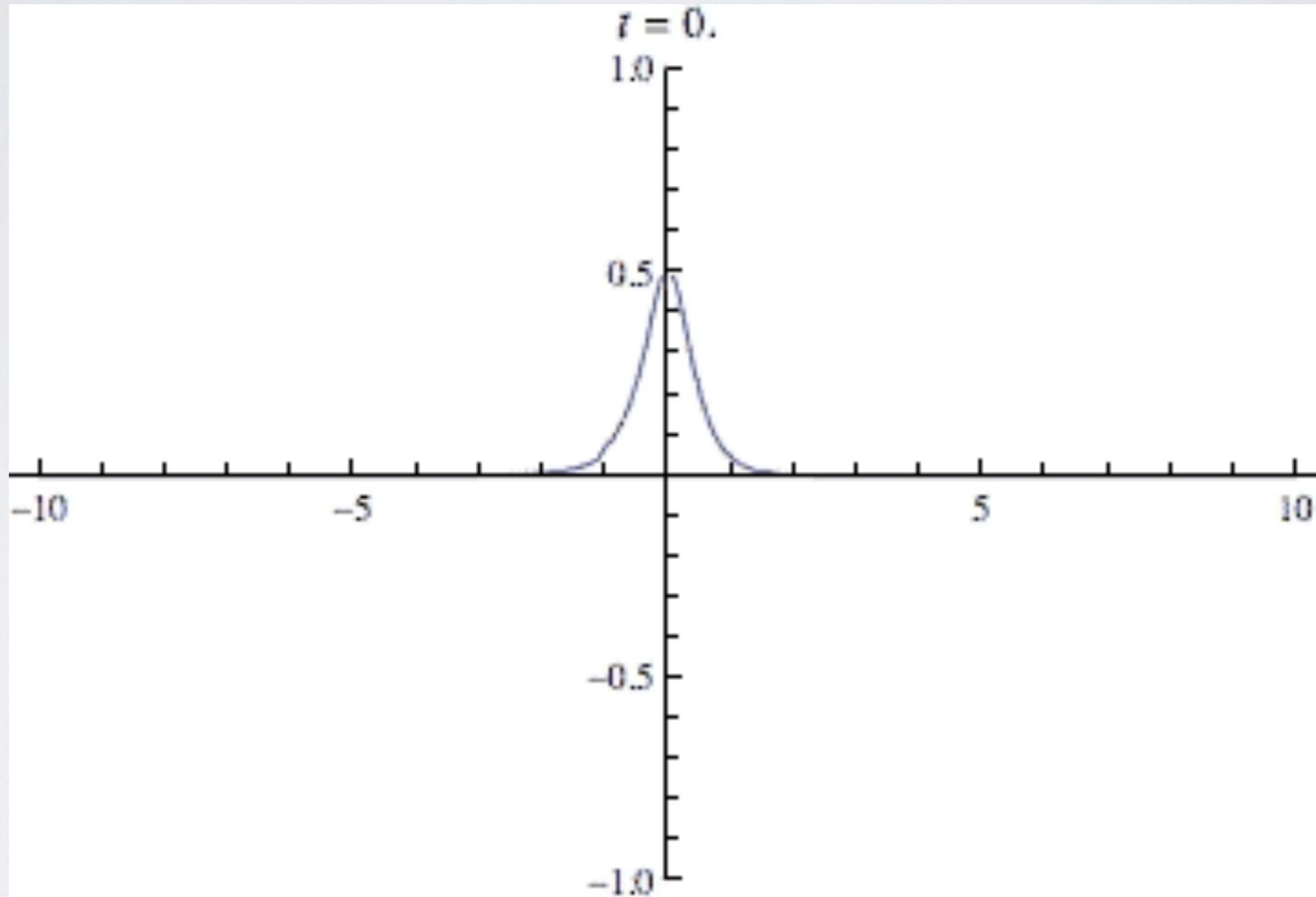

$$z_1, \dots, z_m =$$



Evolution of defocusing NLS



Evolution of defocusing NLS (Absolute value)

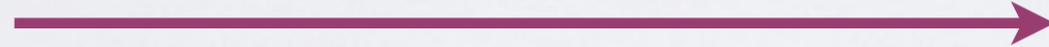


KdV

Inverse scattering for KdV

$$u_0(x)$$

Direct transform



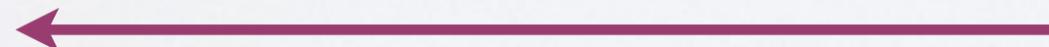
$$r(k), \{\kappa_j\}, \{C_j\}$$

Time evolution



$$u(t, x)$$

Inverse transform



$$r(k)e^{itk^3}, \{\kappa_j\}, \left\{C_j e^{itk_j^3}\right\}$$

Reflection data

$$r(k), \{\kappa_j\}, \{C_j\}$$

Undeformed RH Problem

$$\begin{pmatrix} 1 - r(z)r(-z) & -r(-z)e^{-2i(4tz^3+xz)} \\ r(z)e^{2i(4tz^3+xz)} & 1 \end{pmatrix}$$



$$\circlearrowleft \begin{pmatrix} 1 & \\ -C_1 \frac{e^{\theta(\kappa_1)}}{k - \kappa_1} & 1 \end{pmatrix}$$

$$\circlearrowright \begin{pmatrix} 1 & -C_1 \frac{e^{\theta(\kappa_1)}}{k + \kappa_1} \\ & 1 \end{pmatrix}$$

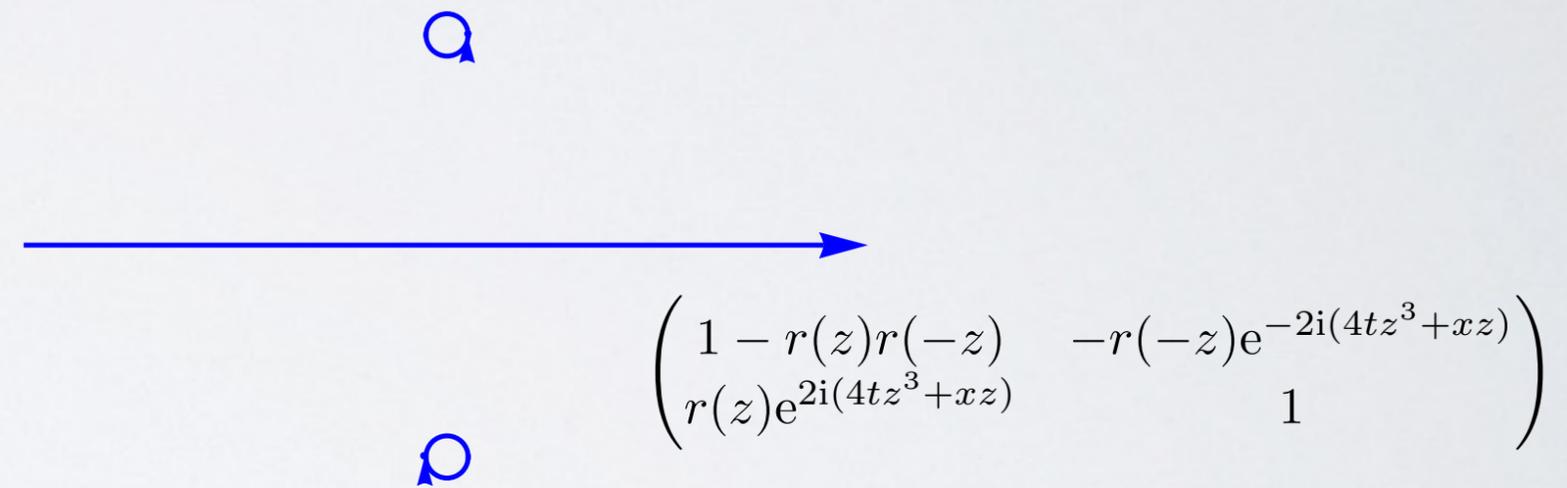
Deformations

- We have two stationary points at

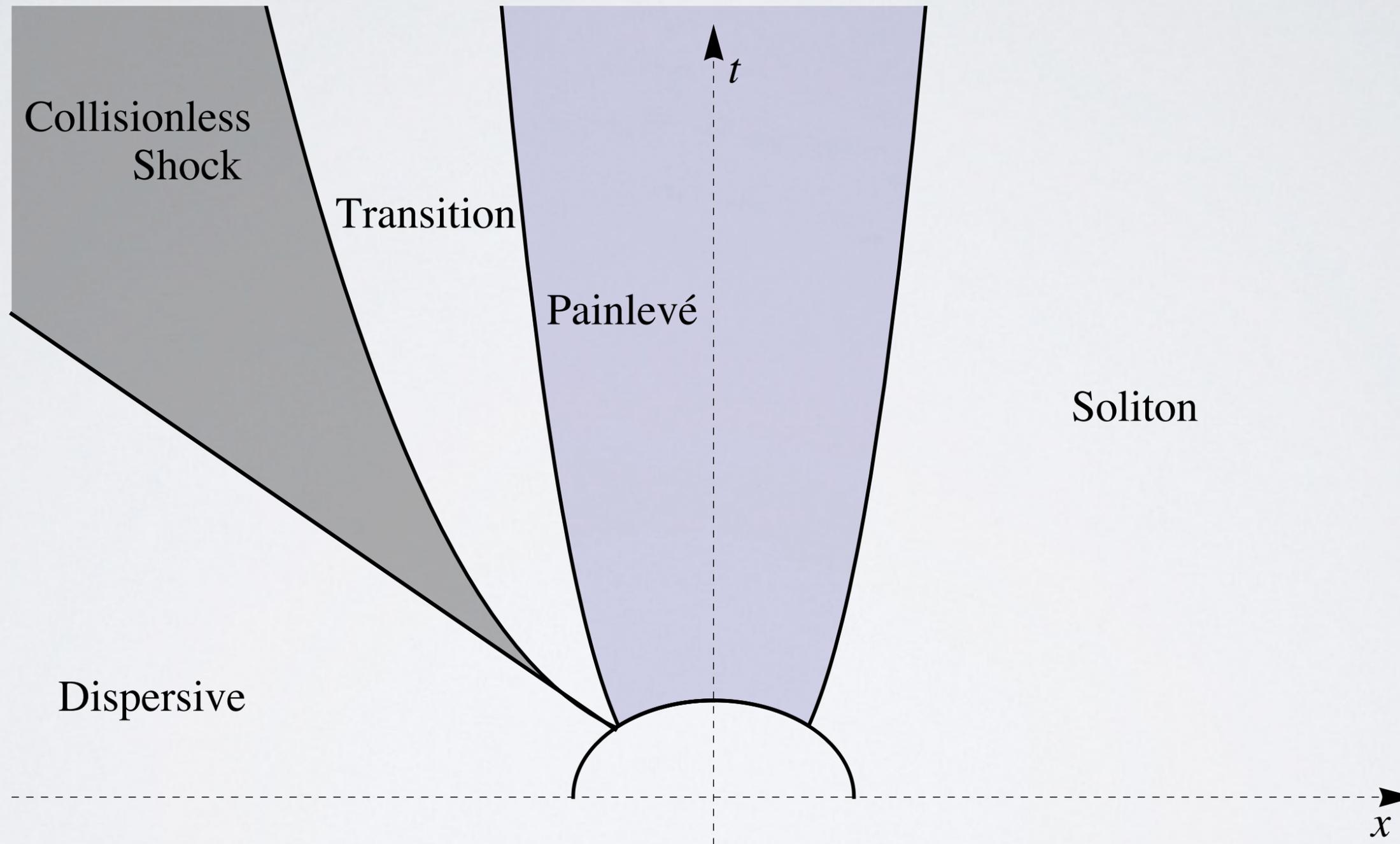
$$\pm k_0 = \pm \sqrt{-\frac{x}{12t}}$$

- We will deform the contour through these stationary points along the paths of steepest descent
- Different regimes of x and t require different *lensings*
 - Added difficulty: the lensing introduces a **pole**
- Deformations based on [Deift & Zhou 1993](#), [Deift, Zhou & Venakides 1994](#), [Grunert & Teschl 2008](#)

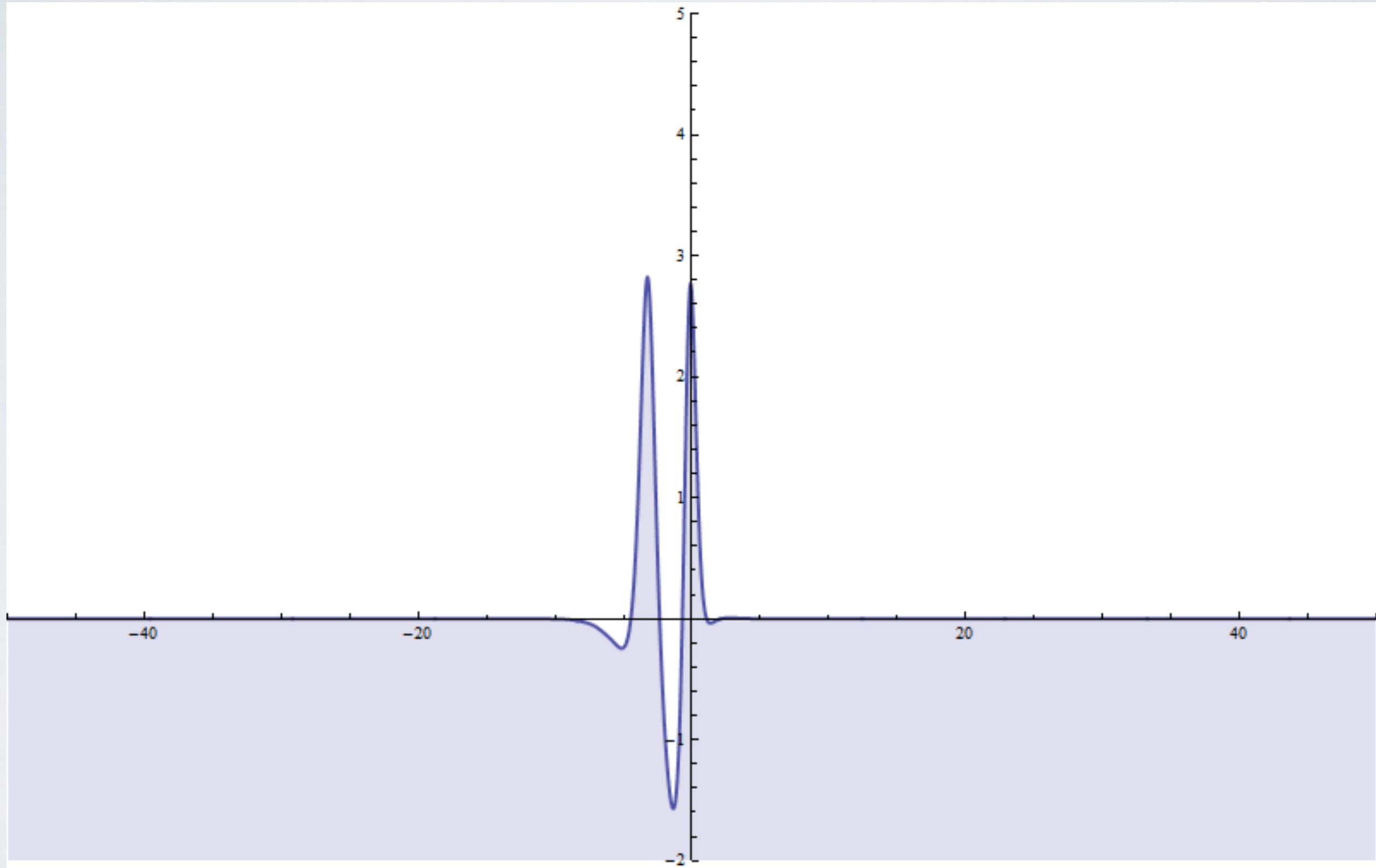
Undeformed



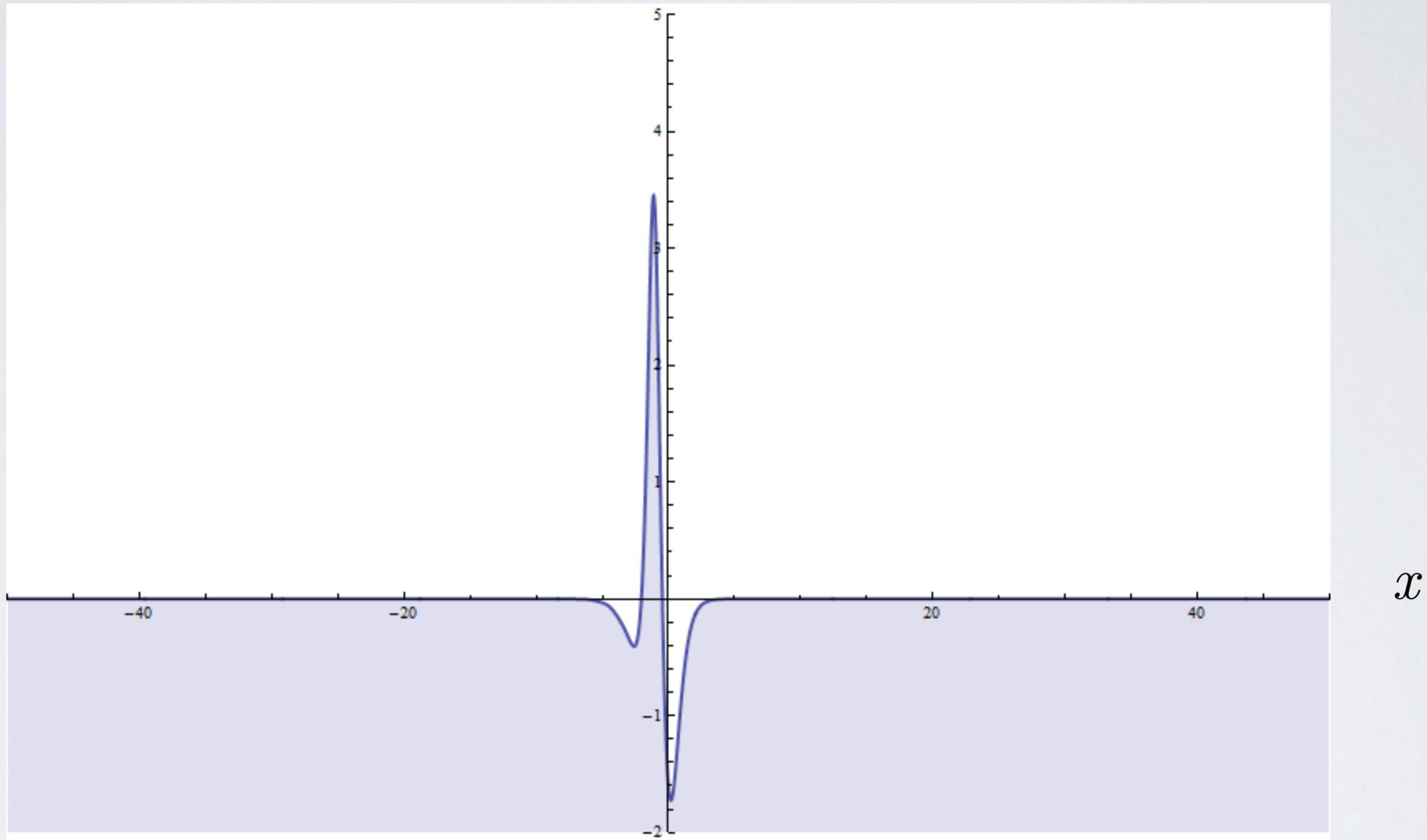
Different regions for deformations



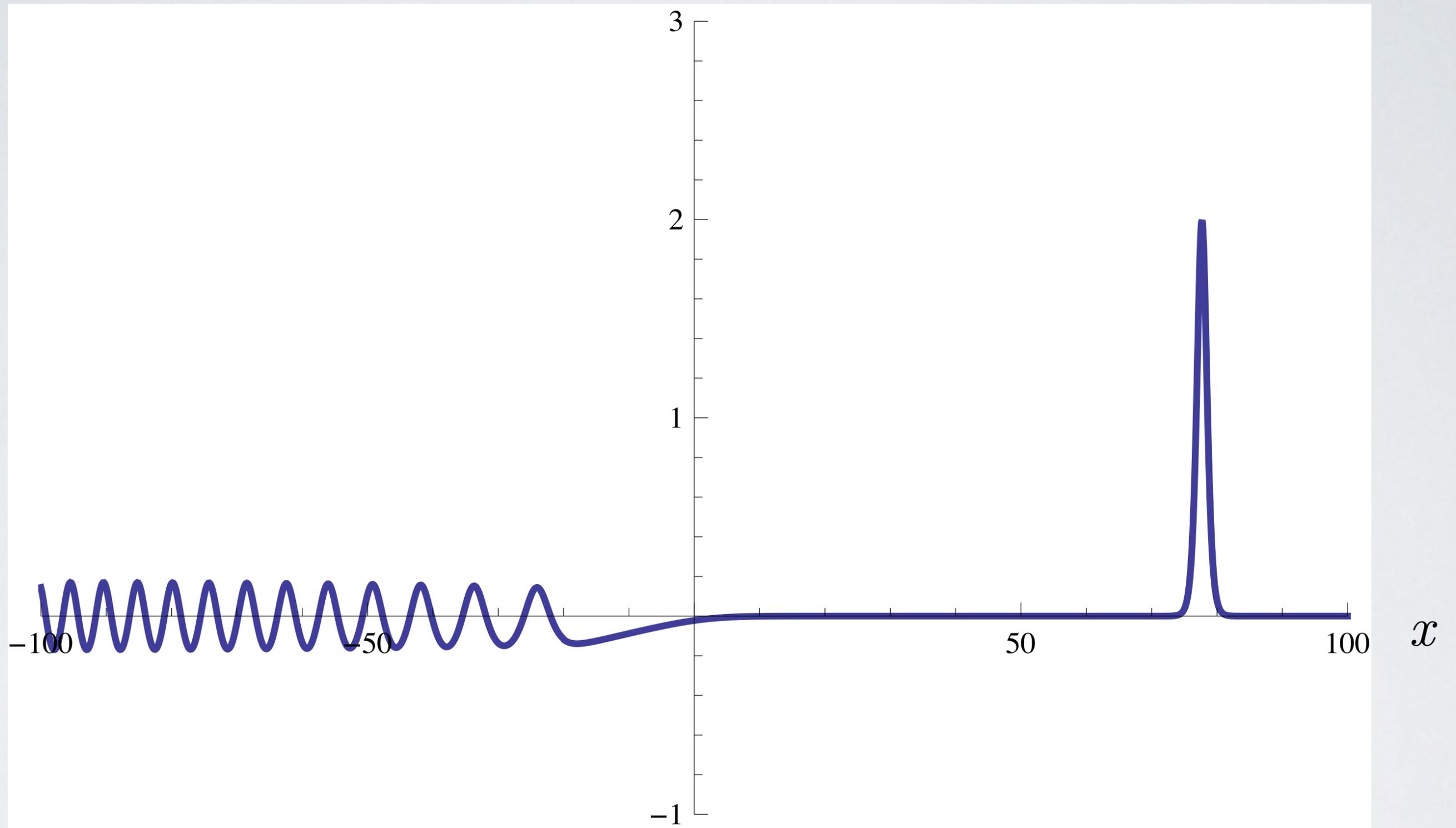
KdV (Generic)



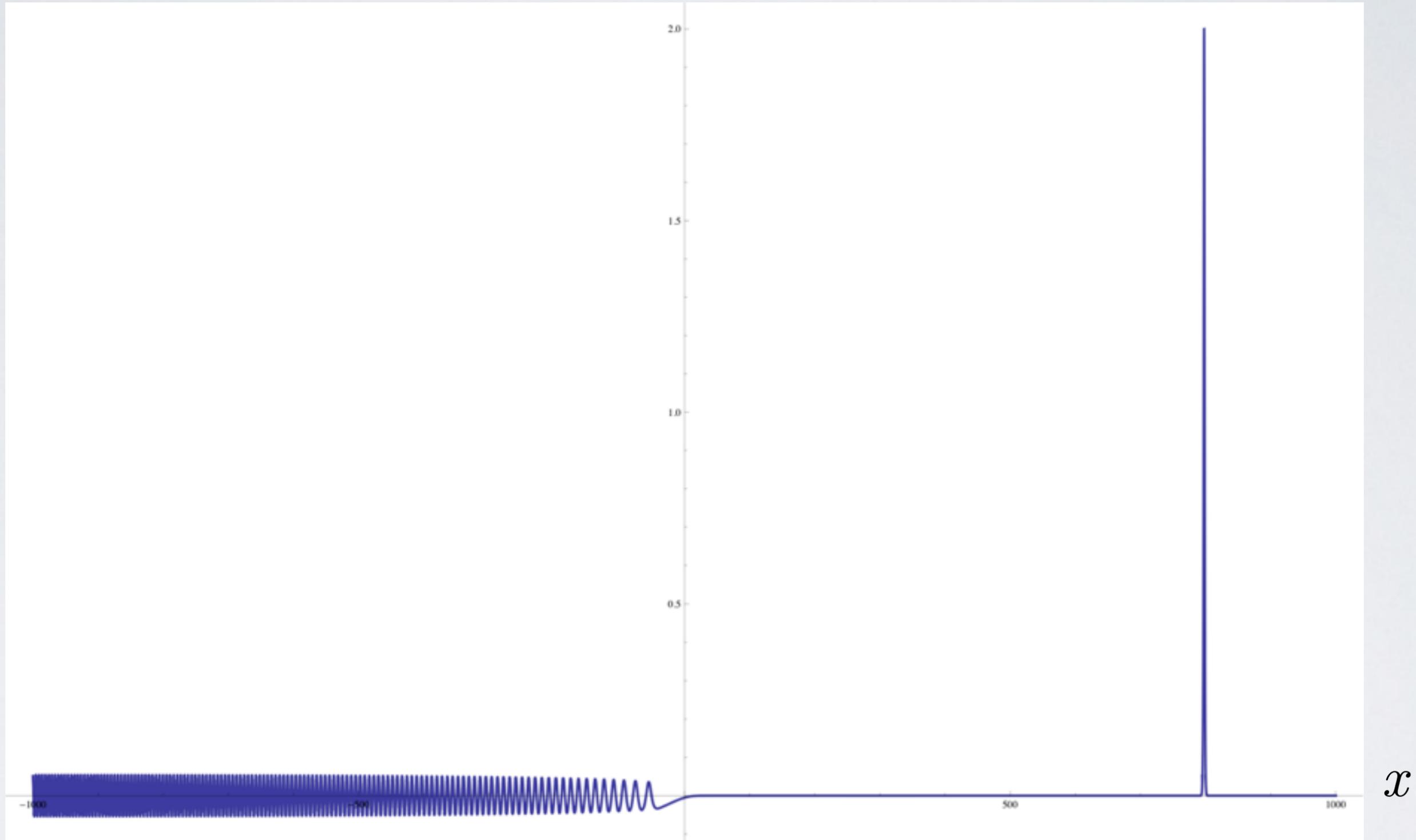
KdV One soliton



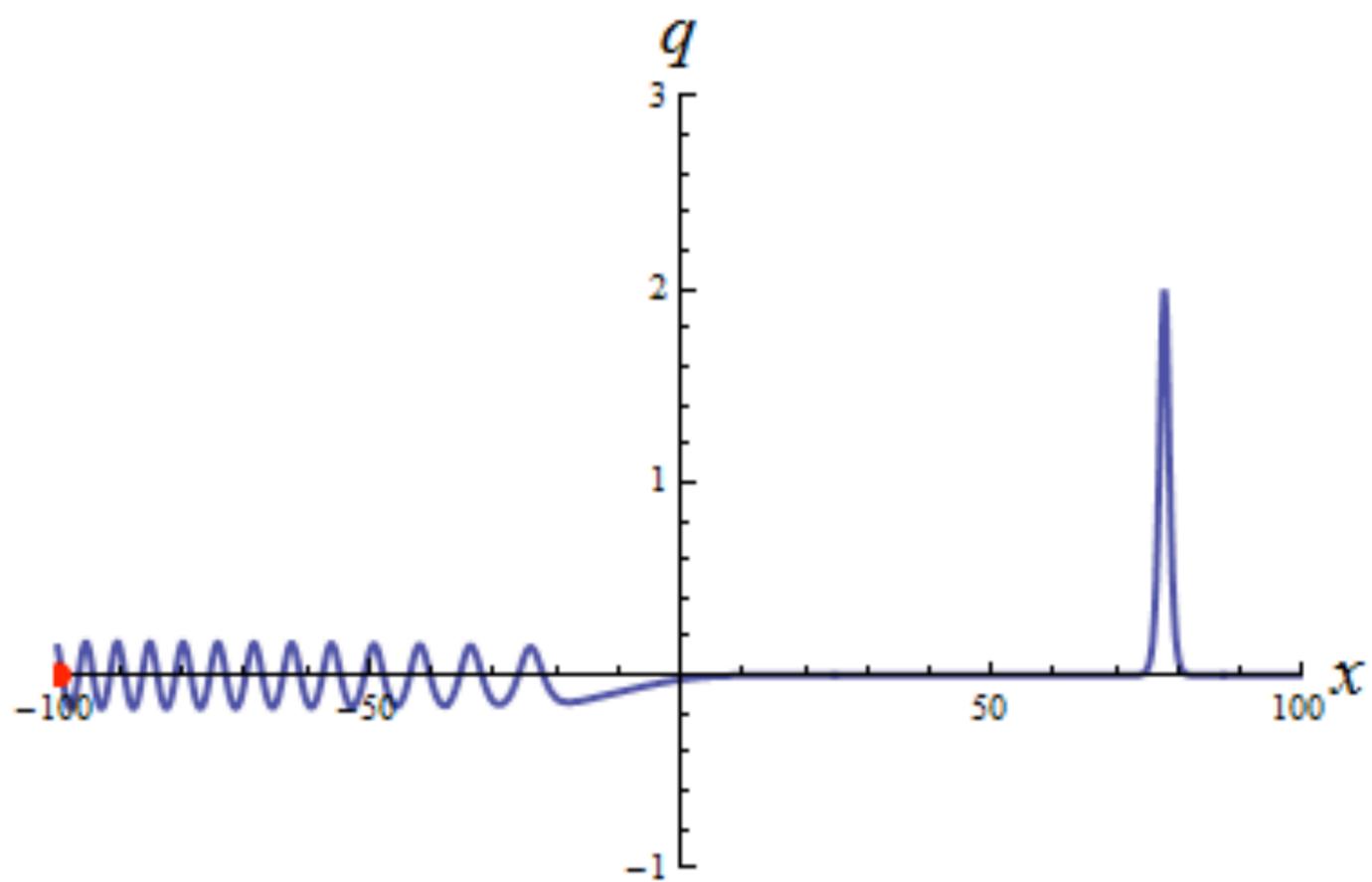
Plot for $t = 20$



Plot for $t = 200$, $-1000 < x < 1000$



Change of contour



Focusing NLS

Focusing NLS

- The undeformed jump contour is very similar to defocusing NLS:

$$\begin{pmatrix} 1 - |r(z)|^2 & -\bar{r}(z)e^{-2i(2tz^2+xz)} \\ r(z)e^{2i(2tz^2+xz)} & 1 \end{pmatrix} \longrightarrow \begin{pmatrix} 1 + |r(z)|^2 & \bar{r}(z)e^{-2i(2tz^2+xz)} \\ r(z)e^{2i(2tz^2+xz)} & 1 \end{pmatrix}$$

- The deformations are the exact same as well!
- Except now we have discrete spectra, which may be anywhere in the complex plane
- For numerical examples, we just specify simple discrete spectra

Reflection data

$$r(k), \{\kappa_j\}, \{C_j\}$$

Undeformed RH Problem

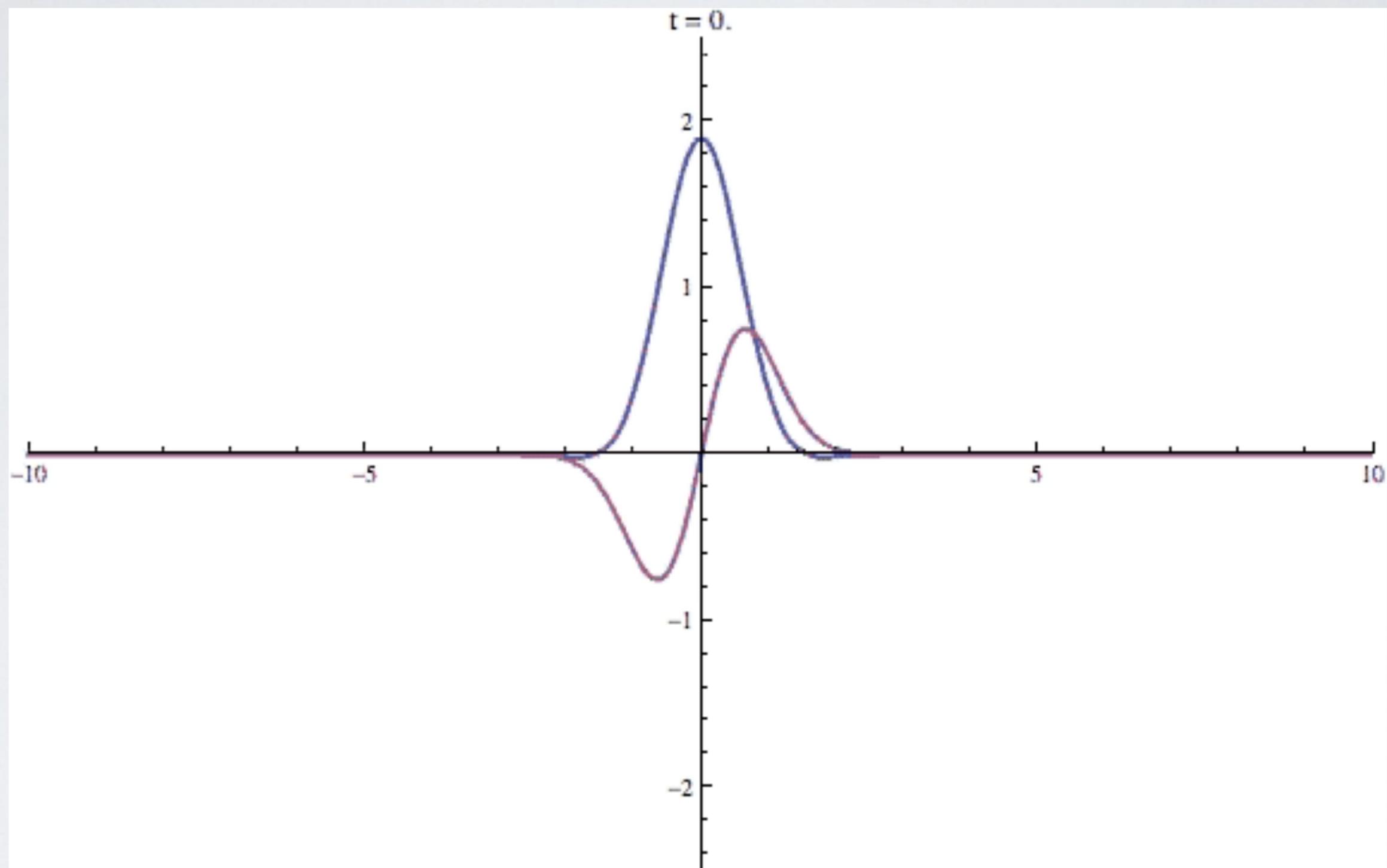
$$\begin{pmatrix} 1 + |r(z)|^2 & \bar{r}(z)e^{-2i(2tz^2+xz)} \\ r(z)e^{2i(2tz^2+xz)} & 1 \end{pmatrix}$$



$$\circlearrowleft \begin{pmatrix} 1 & \\ -C_1 \frac{e^{\theta(\kappa_1)}}{k - \kappa_1} & 1 \end{pmatrix}$$

$$\circlearrowright \begin{pmatrix} 1 & \overline{-C_1 \frac{e^{\theta(\kappa_1)}}{k - \kappa_1}} \\ & 1 \end{pmatrix}$$

fNLS Soliton + Dispersion



Focusing NLS with boundary conditions

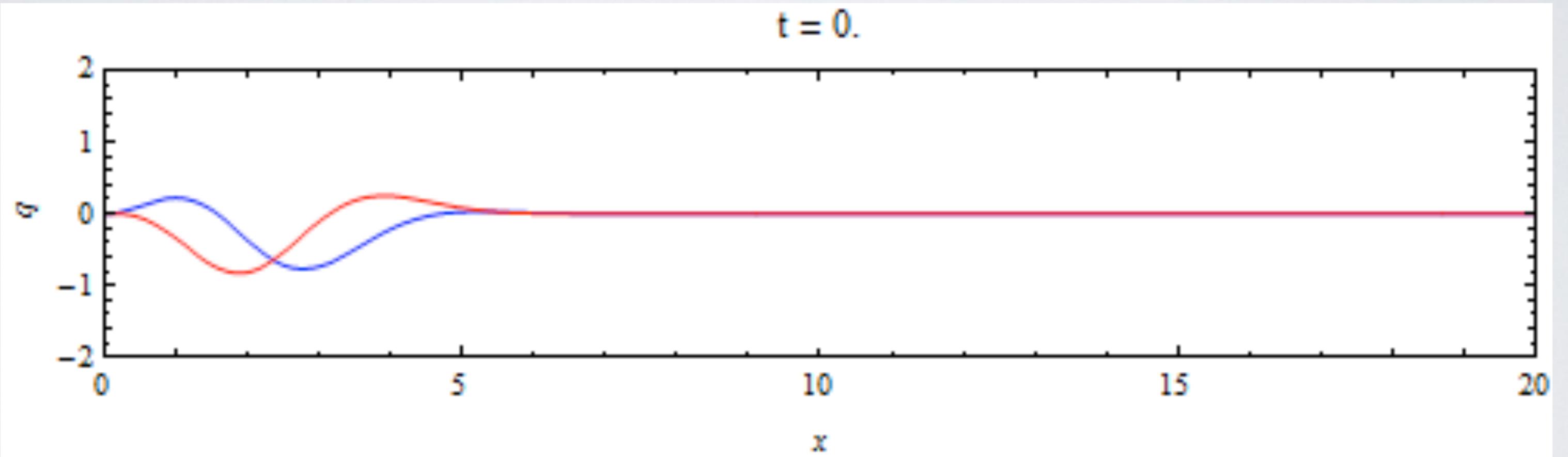
- We can use a similar approach to solve NLS on the half line with Robin boundary conditions:

$$\begin{aligned}iu_t + u_{xx} \pm 2|u|^2 u &= 0, \\ \alpha u(0, t) + u_x(0, t) &= 0 \quad \text{and} \\ u(x, 0) &= u_0(x)\end{aligned}$$

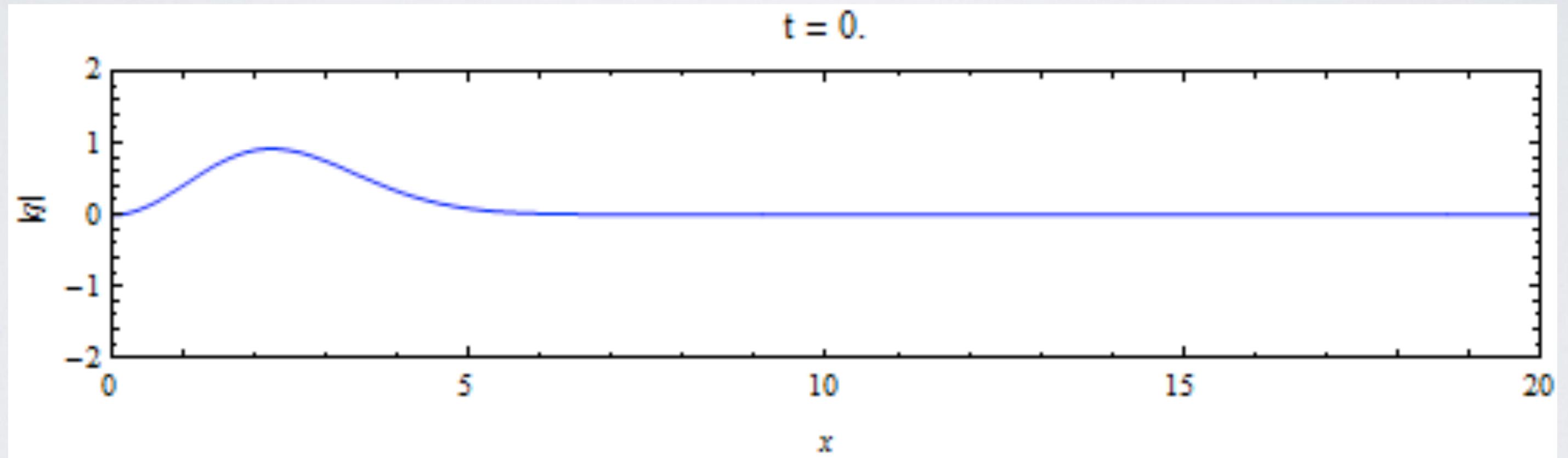
- The basic idea: use a Darboux transformation to extend $u_0(x)$ to the entire real line
 - For Neumann $\alpha = 0$ it is the even extension $u_0(-x) = u_0(x)$
 - For Dirichlet $\alpha = \infty$, it is the odd extension $u_0(-x) = -u_0(x)$
 - In general, the extension results from solving a linear ODE.
- The extension can have a discontinuity in derivatives at zero. However, our method for computing the direct scattering transform is not affected!

(based on Biondini & Bui 2012)

fNLS with Neumann conditions



fNLS with Neumann conditions (Absolute value)

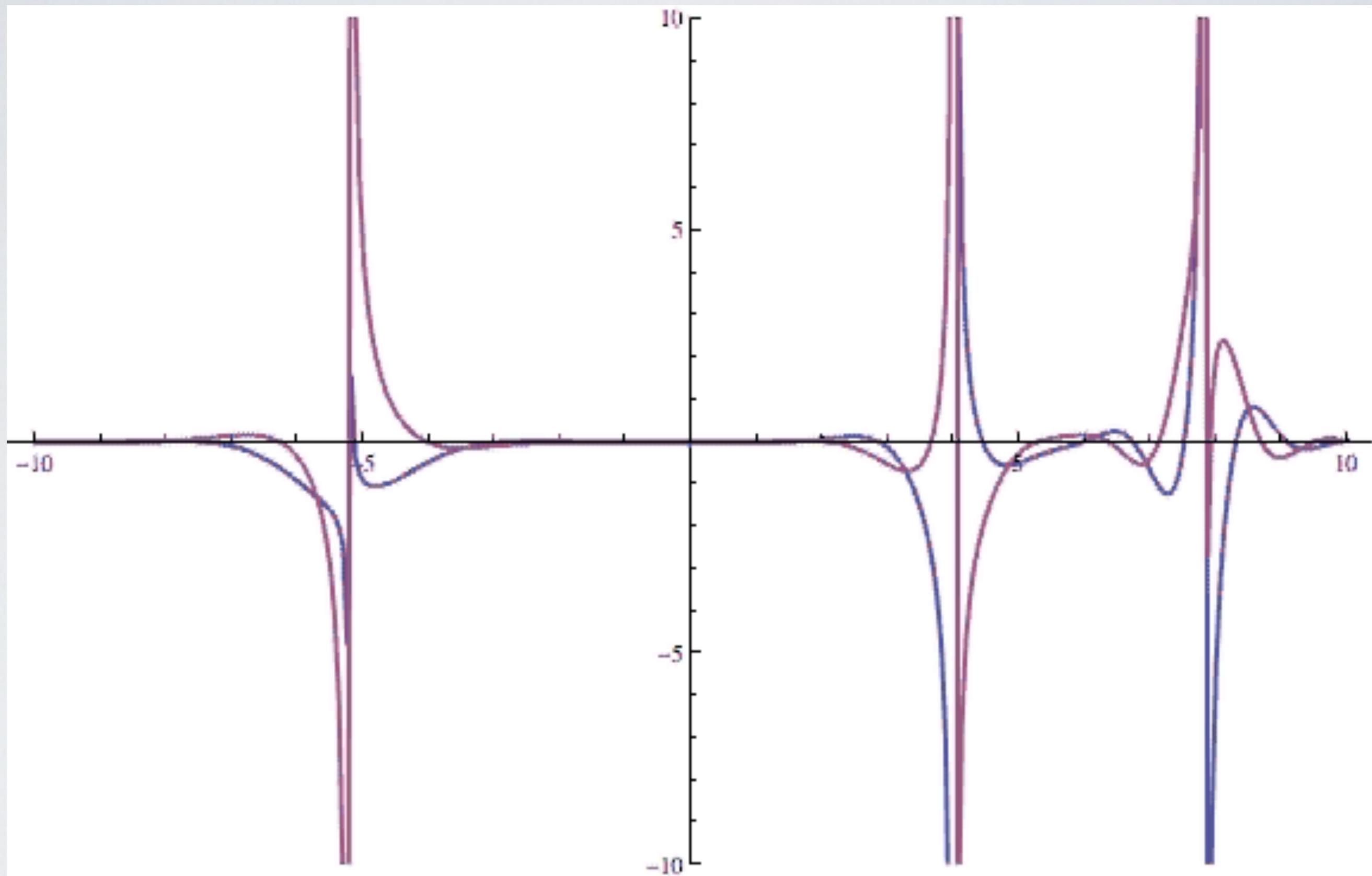


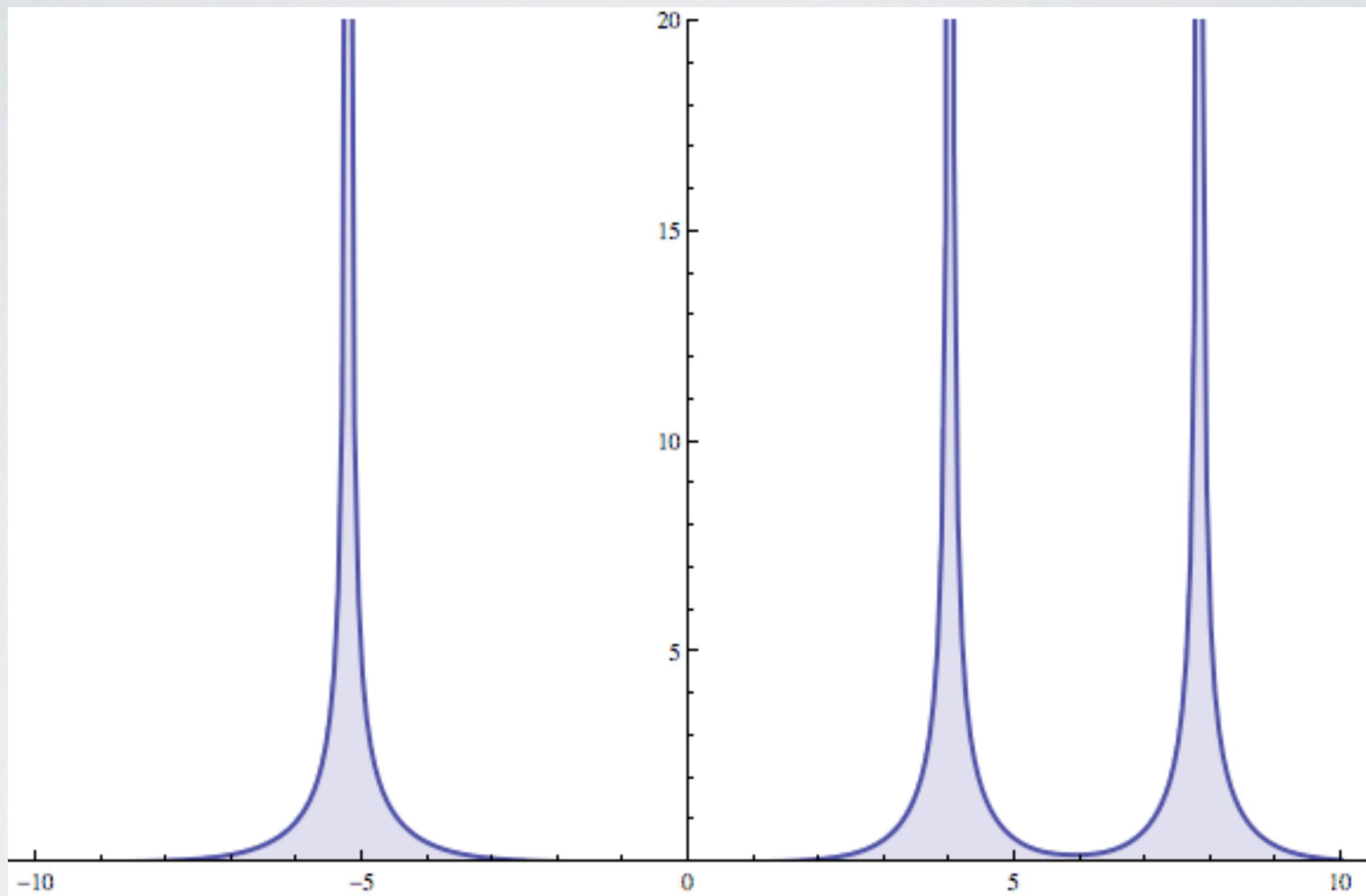
Defocusing solitons

- Suppose we switch the sign in the jump matrix for the focusing solitons

$$\begin{pmatrix} 1 & \overline{-C_1 \frac{e^{\theta(\kappa_1)}}{k - \kappa_1}} \\ & 1 \end{pmatrix} \rightarrow \begin{pmatrix} 1 & \overline{C_1 \frac{e^{\theta(\kappa_1)}}{k - \kappa_1}} \\ & 1 \end{pmatrix}$$

- Then the solution satisfies **defocusing NLS**
- Thus we get “solitons”
- How can this be? Doesn't defocusing NLS have no solitons (except dark solitons)?
- The answer: these solitons have poles!





Happy “Birthday” Dad!