Solving Painléve II (and KdV) numerically with Riemann–Hilbert problems

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Anonymous referee report:

"[redacted embarrassing comments]. Reference [16] may serve as a wonderful example of a caring handling of complicated mathematical formulas."

(You can guess what reference [16] was...)

- We present a new method for computing solutions to matrix-valued Riemann–Hilbert problems:
  - It is a collocation method which converges spectrally (almost exponentially) quickly
- We investigate two applications:
  - Painlevé transcendents
  - KdV equation (joint work with Tom Trogdon)
- Other applications:
  - Integrable systems: nonlinear Schrödinger equation, Kadomtsev–Petviashvili equation, Benjamin–Ono equation etc.
  - Orthogonal polynomials
    - Can compute arbitrarily large order orthogonal polynomials for arbitrary weights
  - Random matrix theory
    - Can compute distributions for large but finite n

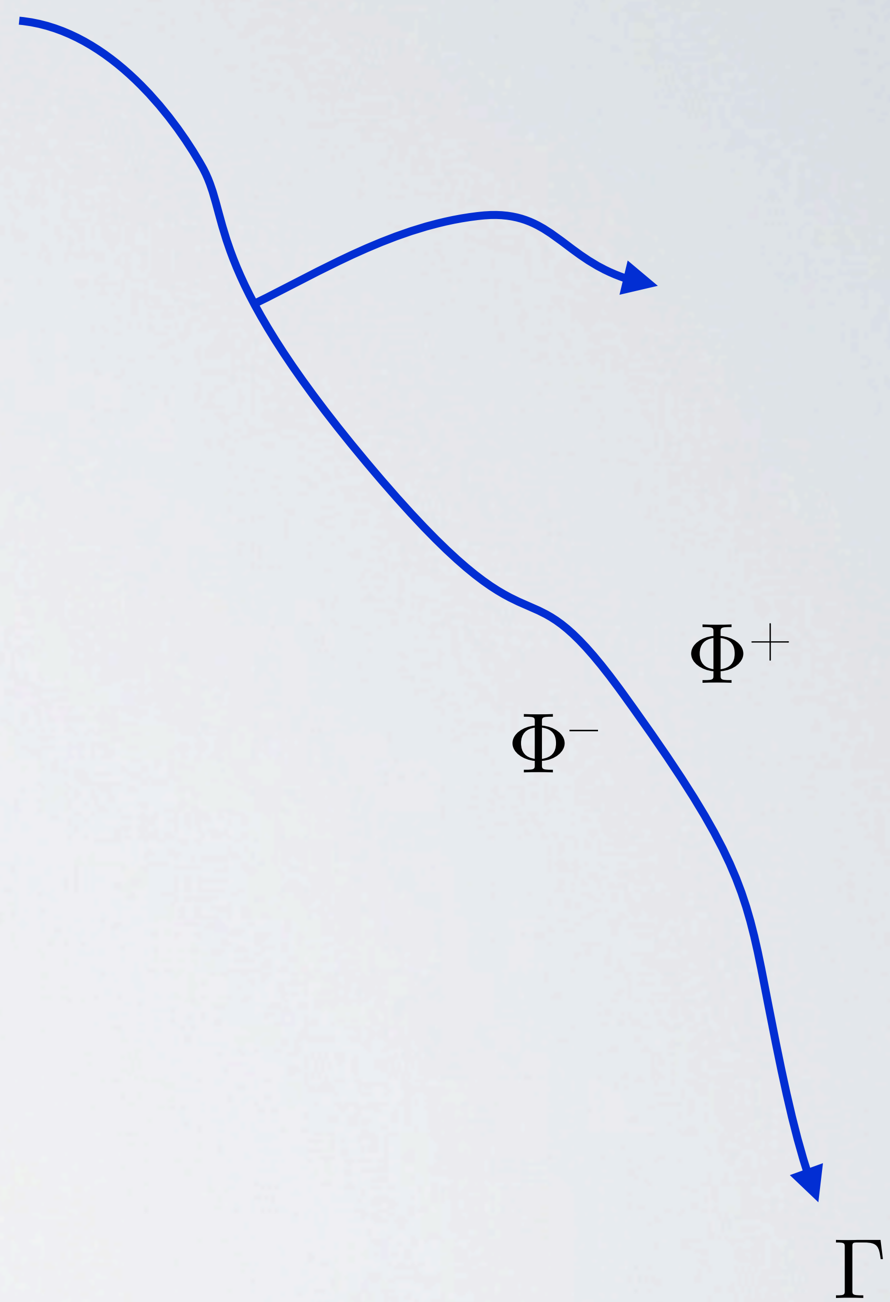
- A matrix-valued *Riemann–Hilbert problem* is the following:
  - Given an oriented contour Γ in the complex plane and a matrix-valued function G defined on Γ (here, all functions on Γ are analytic along each piece of Γ);
  - Find a matrix-valued function Φ that is analytic everywhere in the complex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

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

where

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

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



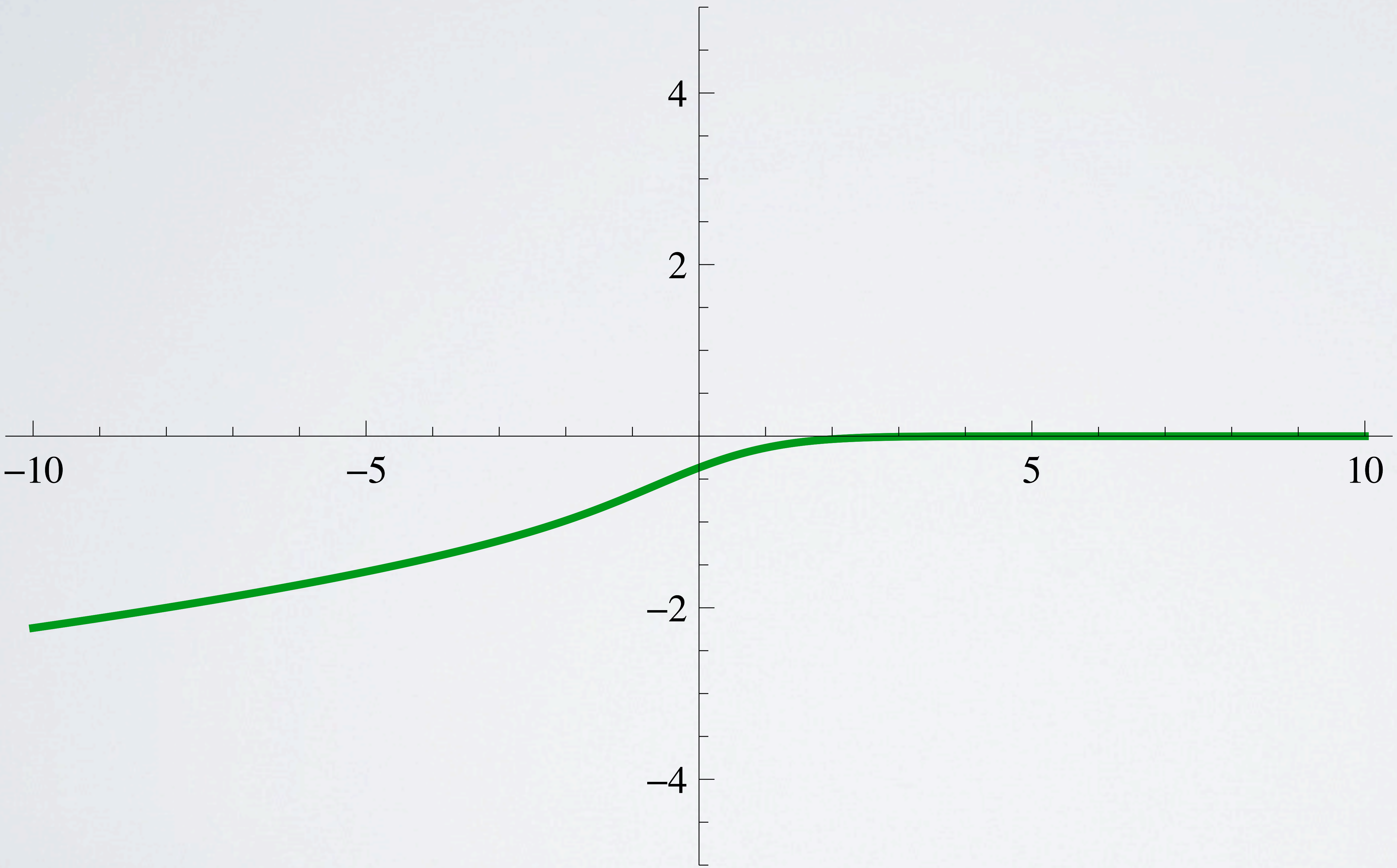
(see eg. Muskhelishvili 1953)

- 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 I have constructed, 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

Painlevé Transcendents

- Our preliminary application is computing solutions to Painlevé transcendents
- Applications of Painlevé transcendents
  - Asymptotics and special solutions of integrable systems
  - Random matrix distributions
  - Physical applications (quantum gravity, Bose gases, convective flows, general relativity, poly-electrolytes, nonlinear optics, etc.)
- In short: Painlevé equations are *nonlinear special functions*
- The computation of RH problems and Painlevé transcendents was an open problem (Deift 2008)
- We construct a black box routine for Painlevé II, which is reliable uniformly on the real axis

Hastings–McLeod solution to Painlevé II

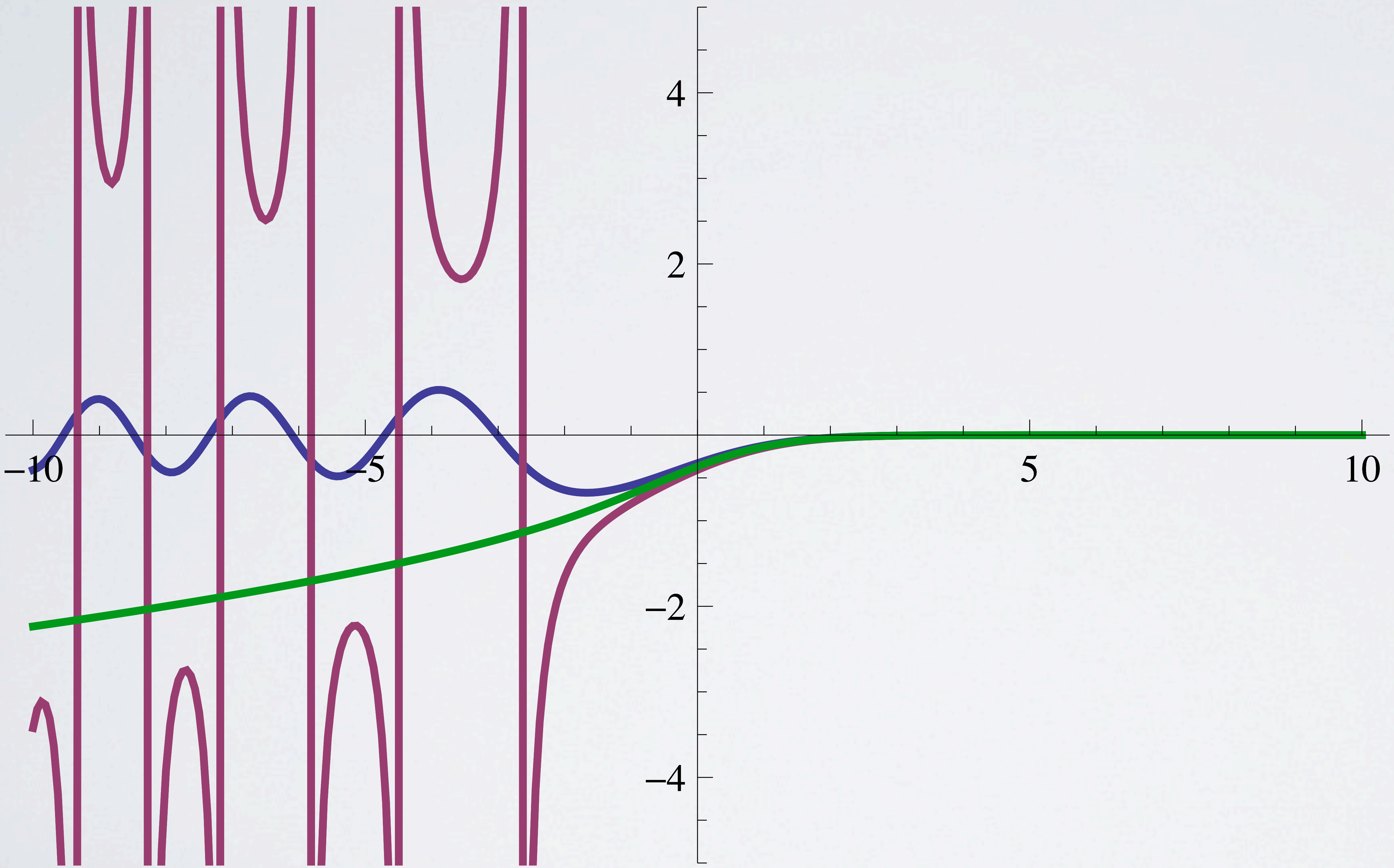


$$u'' = xu + 2u^3$$

$$u(x) \underset{x \to +\infty}{\sim} -\operatorname{Ai}(x)$$

$$u(x) \underset{x \to -\infty}{\sim} -\sqrt{\frac{|x|}{2}}$$

Hastings–McLeod solution to Painlevé II



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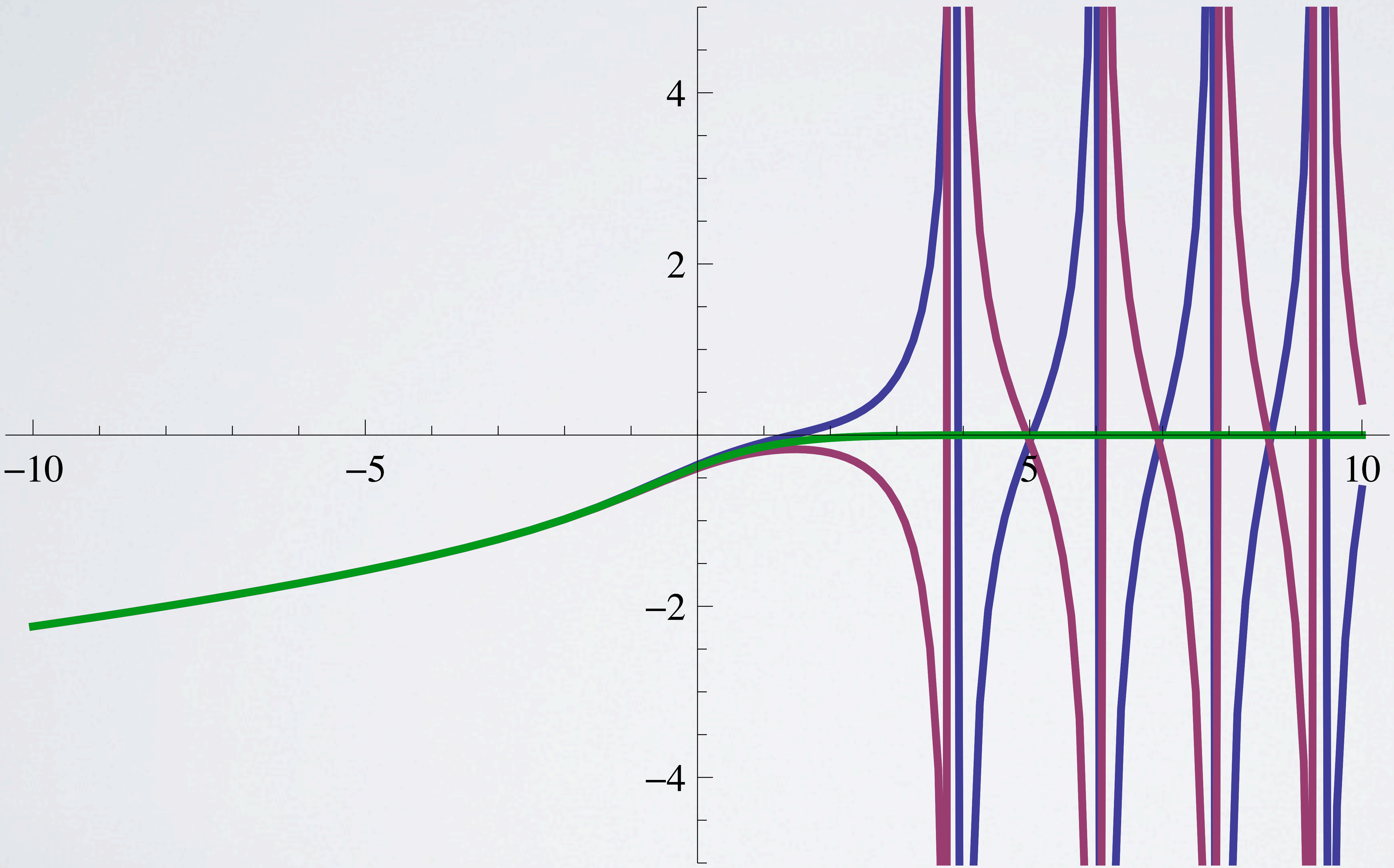

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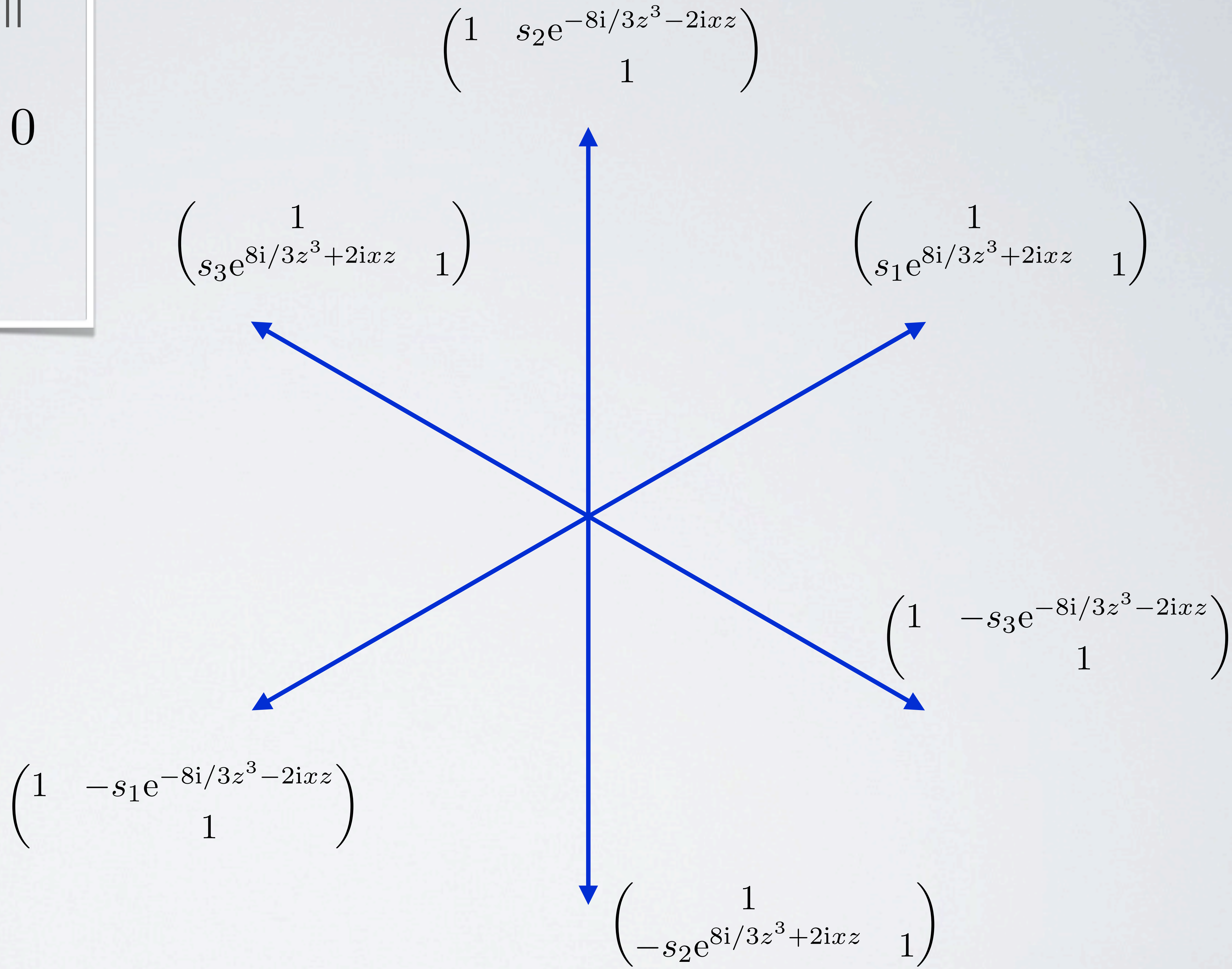
Homogeneous Painlevé II

$$u'' = xu + 2u^3$$

$$s_1 - s_2 + s_3 + s_1 s_2 s_3 = 0$$

$$\Phi^+(z) = \Phi^-(z) G(z)$$

$$u(x) = 2 \lim_{z \to \infty} z \Phi_{12}(z)$$



(see eg. Fokas et al 2006)

Where the RH formulation comes from (Rough sketch)

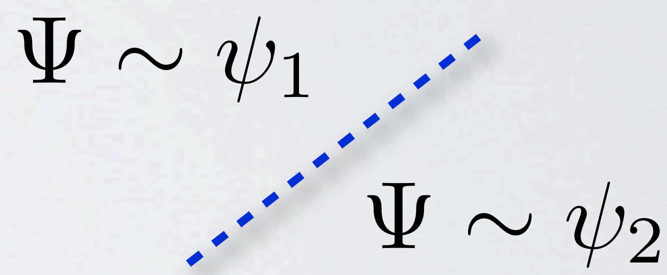
Nonlinear differential equation $$u'' = xu + 2u^3 - \alpha$$

⇕

Lax pair representation
$$\Psi_z(x,z) = A(u,x,z)\Psi(x,z)$$
$$\Psi_x(x,z) = U(u,x,z)\Psi(x,z)$$

⇕

Monodromy and Stokes data



⇕

Riemann–Hilbert problem $$\Phi^+(z) = \Phi^-(z)G(z)$$

(see eg. Fokas et al 2006)

Construction of a collocation method

- Consider the *Cauchy transform*

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

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

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

- 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 $\{\psi_1, \ldots, \psi_n\}$ of functions defined on Γ and set of nodes $\{z_1,\ldots,\ z_m\}$ on Γ
- Write

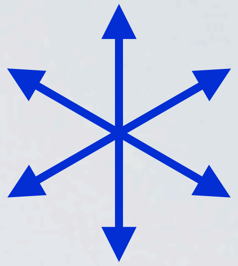
$$V = \sum \boldsymbol{c}_k \psi_k$$

- Solve the linear system

$$\boldsymbol{c}_1 \mathcal{M}\psi_1(z_1) + \cdots + \boldsymbol{c}_n \mathcal{M}\psi_n(z_1) = G(z_1) - I$$
$$\vdots$$
$$\boldsymbol{c}_1 \mathcal{M}\psi_1(z_m) + \cdots + \boldsymbol{c}_n \mathcal{M}\psi_n(z_m) = G(z_m) - I$$

Two remaining difficulties

- We must compute the Cauchy transform of our basis 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

For homogeneous Painlevé II, we need to compute $\mathcal{C}$ over the domain 

- But we can decompose the transform to a sum over each of Γ's parts:

$$\mathcal{C}_{\ast} = \mathcal{C}_{\swarrow} + \mathcal{C}_{\downarrow} + \mathcal{C}_{\searrow} + \mathcal{C}_{\nearrow} + \mathcal{C}_{\uparrow} + \mathcal{C}_{\nwarrow}$$

- Using a conformal map M_k from the unit interval to each ray Γ_k of the jump contour, the Cauchy transform is (due to Plemelj's lemma)

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

- Thus we have reduced the construction of our collocation method to one problem: the computation of the Cauchy transform over the unit interval $\mathcal{C}_{(-1,1)}$

- There are two standard numerical methods (cf., for eg. King 2009) for computing Cauchy/Hilbert transforms on the unit interval:
  - Standard quadrature, which blows up on the interval

$$\frac{1}{2\pi \mathrm{i}} \int_{-1}^{1} \frac{f(x)}{x-z} \, \mathrm{d}x \approx \frac{1}{2\pi \mathrm{i}} \sum_i w_i \frac{f(x_i)}{x_i - z}$$

  - Removal of the singularity (and higher order analogues) which is not defined off the interval

$$\frac{1}{2\pi \mathrm{i}} \int_{-1}^{1} \frac{f(x)}{x-z} \, \mathrm{d}x \approx \frac{1}{2\pi \mathrm{i}} \sum_i w_i \frac{f(x_i) - f(z)}{x_i - z} + \frac{f(z)}{2\pi \mathrm{i}} \int_{-1}^{1} \frac{1}{x-z} \, \mathrm{d}x$$

  (Higher order analogues of this discretization are standard in singular integral equations on the unit interval, used by Elliot 1982 and for RH problems in Dienstfrey 1998)

- Instead, we derived a method which is uniform for all z using Chebyshev polynomial moments:

$$\frac{1}{2\pi \mathrm{i}} \int_{-1}^{1} \frac{f(x)}{x-z} \, \mathrm{d}x \approx \sum \check{f}_k \frac{1}{2\pi \mathrm{i}} \int_{-1}^{1} \frac{T_k(x)}{x-z} \, \mathrm{d}x = \sum \check{f}_k \mathcal{C}_{(-1,1)} T_k(z)$$

  - These moments can be expressed in closed form using a very simple and stable one-term recurrence relationship and hypergeometric functions

- We include the origin as a collocation point to ensure that the computed solution is bounded. This is *crucial*, and the reason (Dienstfrey 1998) needed exponentially many points; to simulate boundedness
- At the origin, the Cauchy transforms over the individual rays blow up:

$$\mathcal{C}_{\Gamma_k} V_k(z) \underset{z\to 0}{\sim} -\frac{V_k(0)}{2\mathrm{i}\pi}\log(-\mathrm{e}^{\mathrm{i}\theta_k} z) + C_k$$

We define the finite part along a curve at angle t as the circled part:

$$\mathcal{C}_{\Gamma_k} V_k(z) \sim \boxed{C_k - \frac{V_k(0)}{2\mathrm{i}\pi}\mathrm{i}\arg(-\mathrm{e}^{\mathrm{i}(\theta_k+t)})} - \frac{V_k(0)}{2\mathrm{i}\pi}\log|z|$$

Whenever the limits of V along each ray sum to zero, this expression is an equality

$$\begin{aligned}\mathcal{C}_\Gamma V(z) &= \mathcal{C}_{\Gamma_1} V_1(z) + \cdots + \mathcal{C}_{\Gamma_6} V_6(z)\\ &= -\frac{1}{2\mathrm{i}\pi}(V_1(0) + \cdots + V_6(0))\log|z| + \text{bounded terms}\\ &\sim \text{bounded terms}\end{aligned}$$

- Final collocation method for the homogeneous Painlevé II equation:
  - Choose the basis of Chebyshev polynomials mapped to each ray
  - Using the Cauchy transform formulæ, construct the linear system, where we take the finite part as the definition of the Cauchy transform at zero
    - This will be justified because the collocation system itself ensures that the limits along each ray of the computed solution will always sum to zero whenever $s_1 s_3 - s_1 s_2 - s_2 s_3 \neq 9$
    - Otherwise, the linear system has an extra degree of freedom, and we can add as an extra condition that the contributions at the origin sum to zero

- We transform the RH problem to solution value:

$$u(x) \approx 2 \lim_{z \to \infty} z \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{V(t)}{t - z} \, \mathrm{d}t = -\frac{1}{2\pi \mathrm{i}} \int_\Gamma V(t) \, \mathrm{d}t$$

- The integral can be evaluated using *Clenshaw–Curtis quadrature*
- We can also apply this approach for computing the derivative of $u(x)$, reusing most of the computation
- This is the first reliable numerical method for computing the initial conditions for given Stokes' constants
    - And asymptotics are determined from the Stokes' constants

Painlevé II Examples

- Consider again the *Hastings–McLeod solution*, which is equivalent to the choice $(s_1, s_2, s_3) = (\mathrm{i}, 0, -\mathrm{i})$
- This solution is important in random matrix theory, in particular, the distribution of the largest eigenvalue of almost all random matrix ensembles is the *Tracy–Widom distribution*, which is expressed in terms of the Hastings–McLeod solution
- Numerical values of the Hastings–McLeod solution at a set of points are available (Prähofer and Spohn 2004)
  - Computed by using the known asymptotics to determine initial conditions for large x, then very high precision arithmetic with Taylor series methods: a very inefficient approach
  - As mentioned before, this computation is particularly difficult because a small perturbation of initial conditions can introduce oscillations or poles

Absolute Error

- Spectral convergence is evident
- The method takes less than 1.5 seconds per point for $n = 120$ (except the first evaluation, where it takes 5.5 seconds)
- For large x, we see the same instability issues as the ODE
- This will be resolved by deforming the RH problem

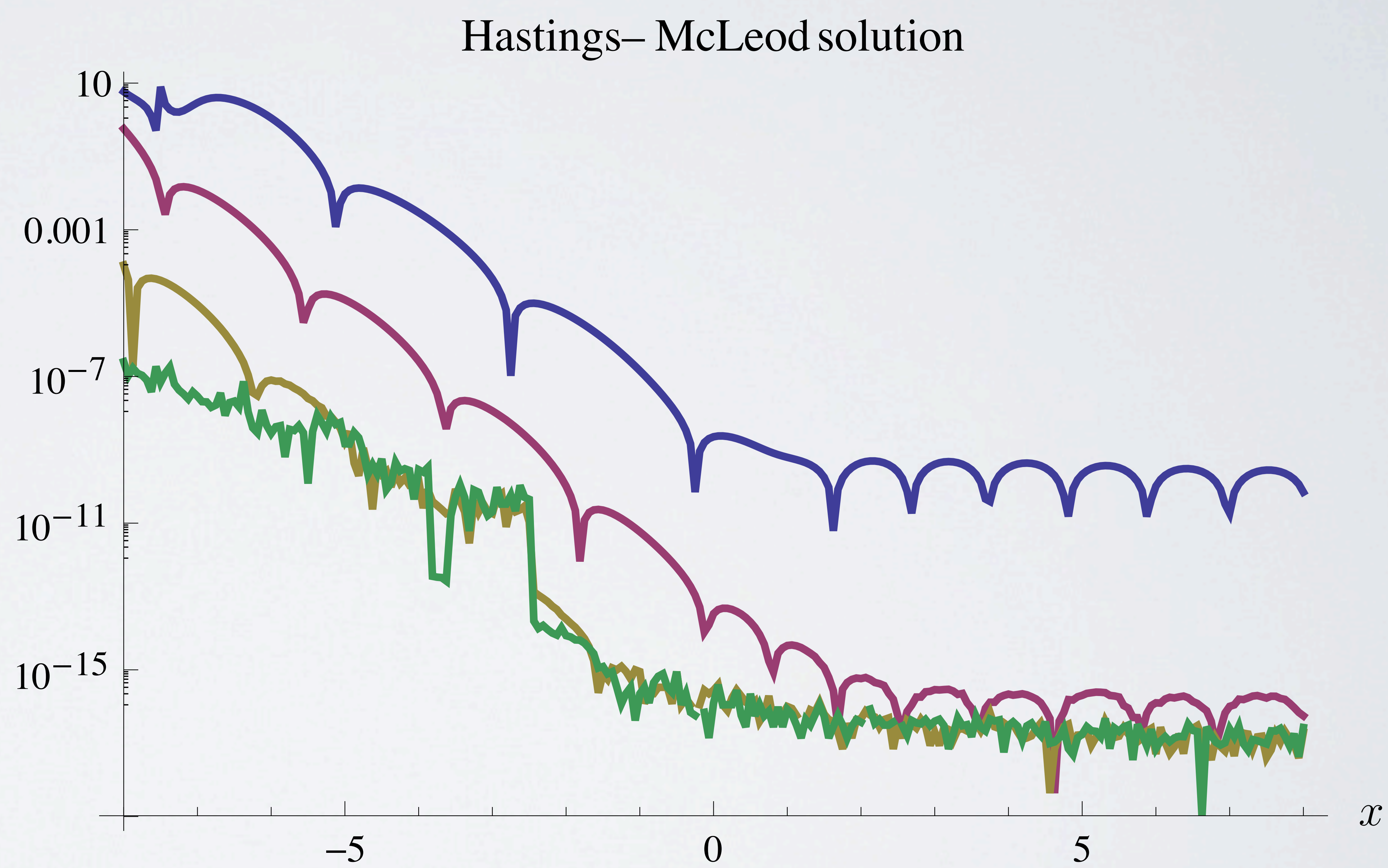
\# collocation points per ray

40

80

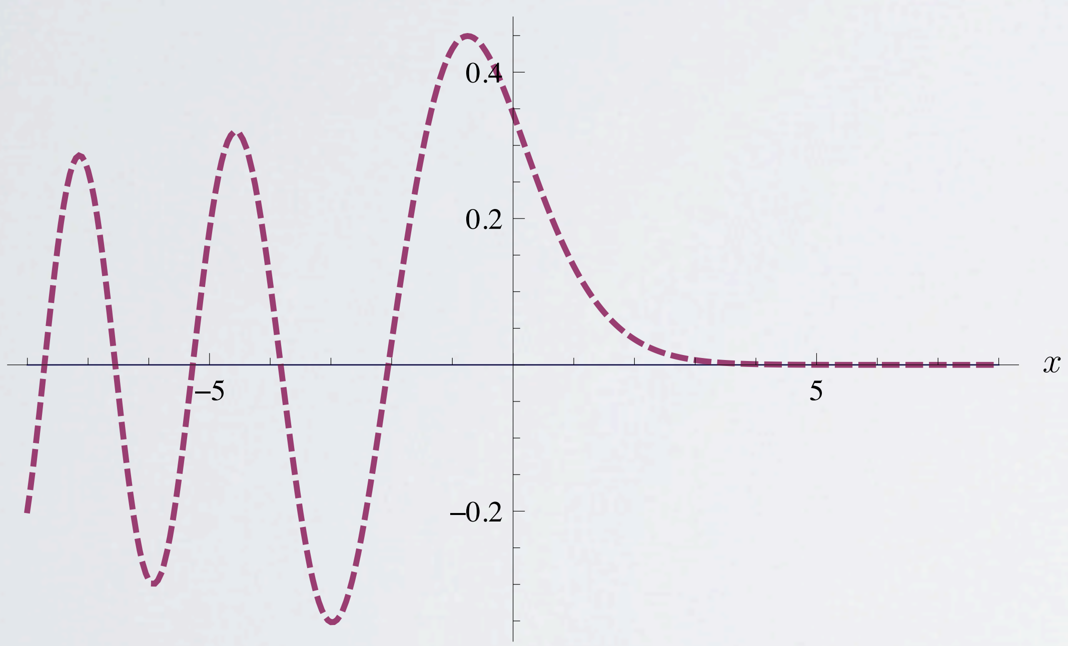
120

160

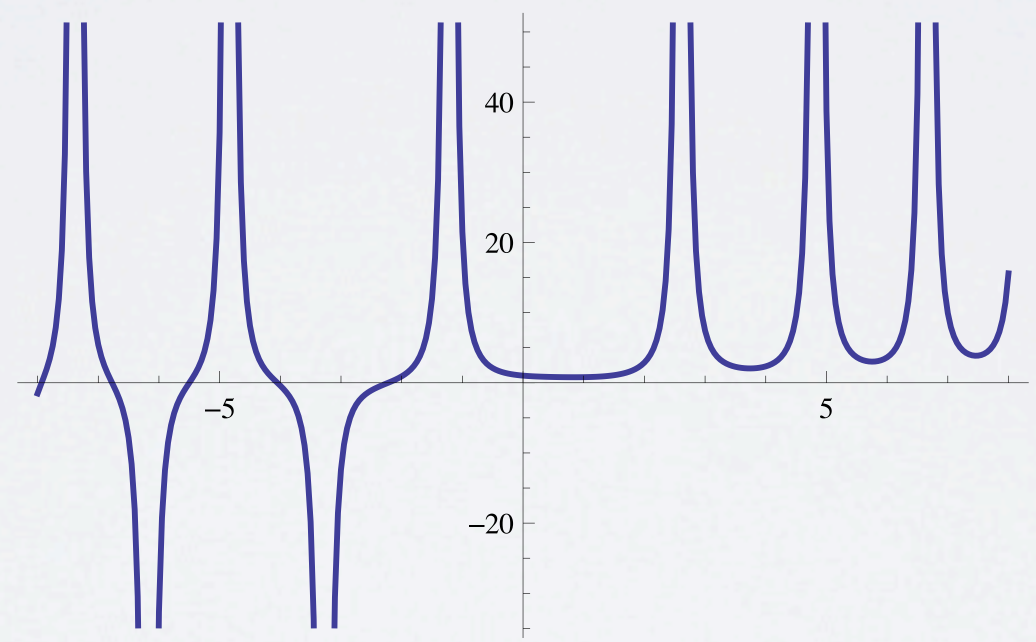


Other solutions

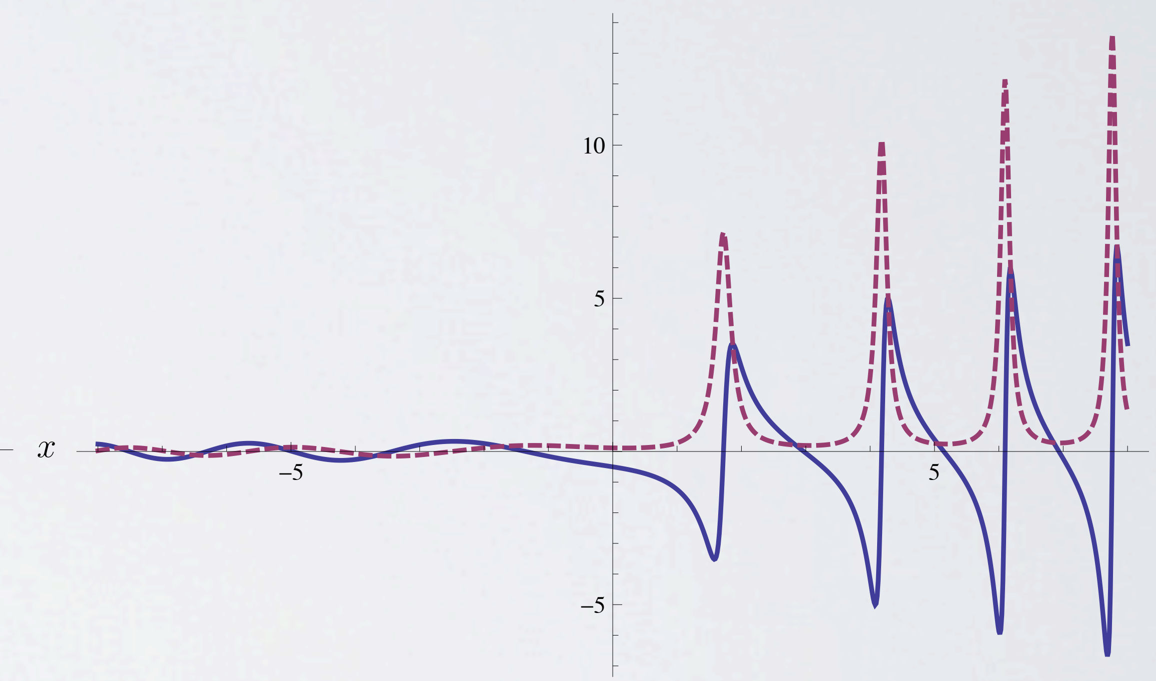
$(s_1, s_2, s_3) = (1,0,-1)$



$(1 + \mathrm{i}, -2, 1 - \mathrm{i})$



$(1,2,1/3)$

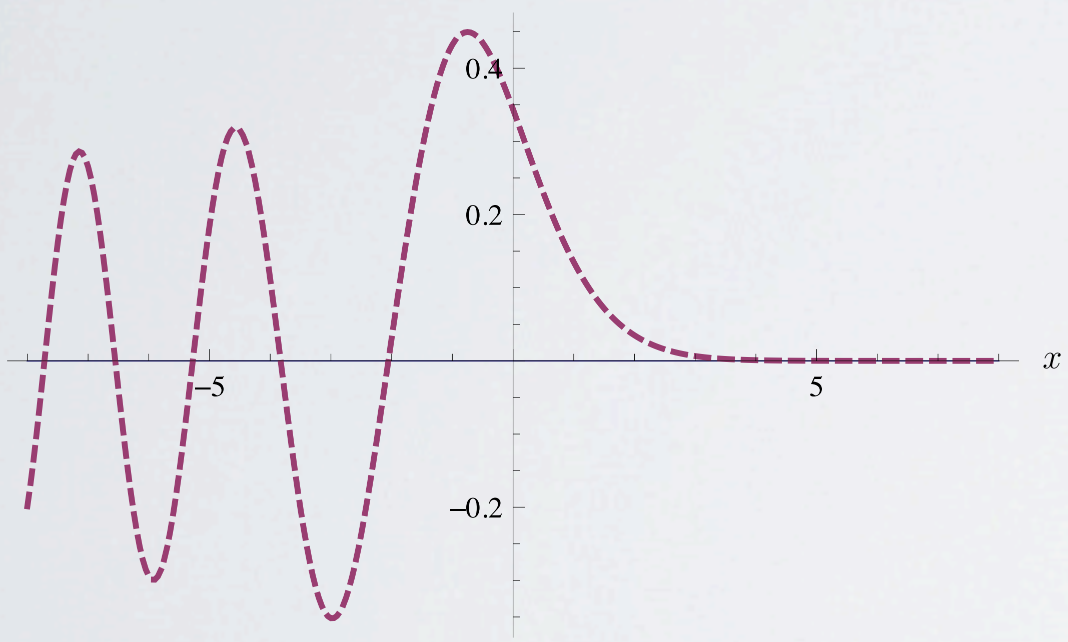


Real and imaginary parts

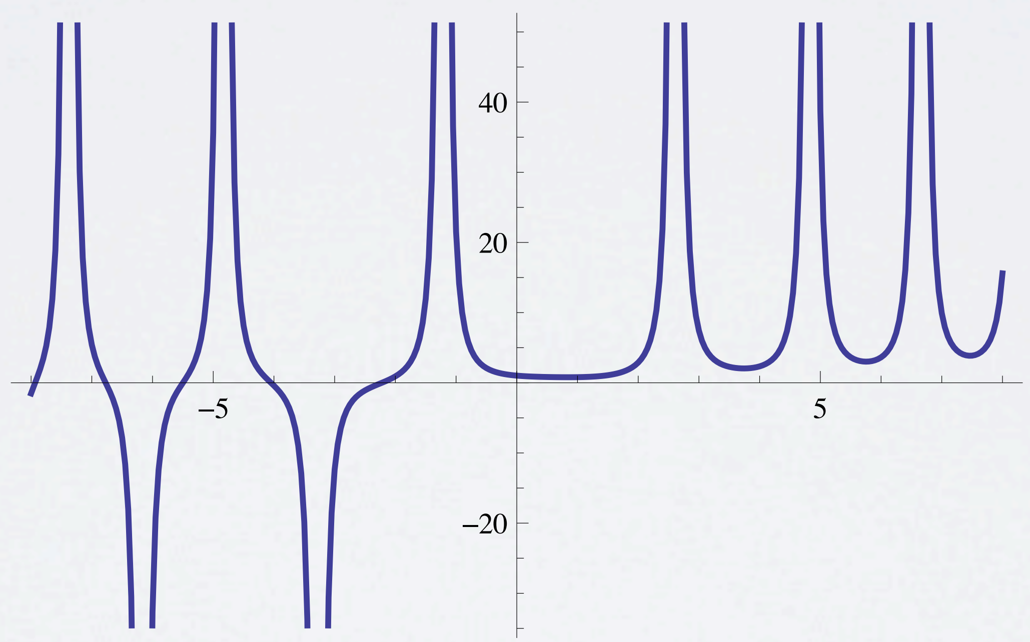
Other solutions

Spectral system becomes badly conditioned at poles (can be used to compute location of poles)

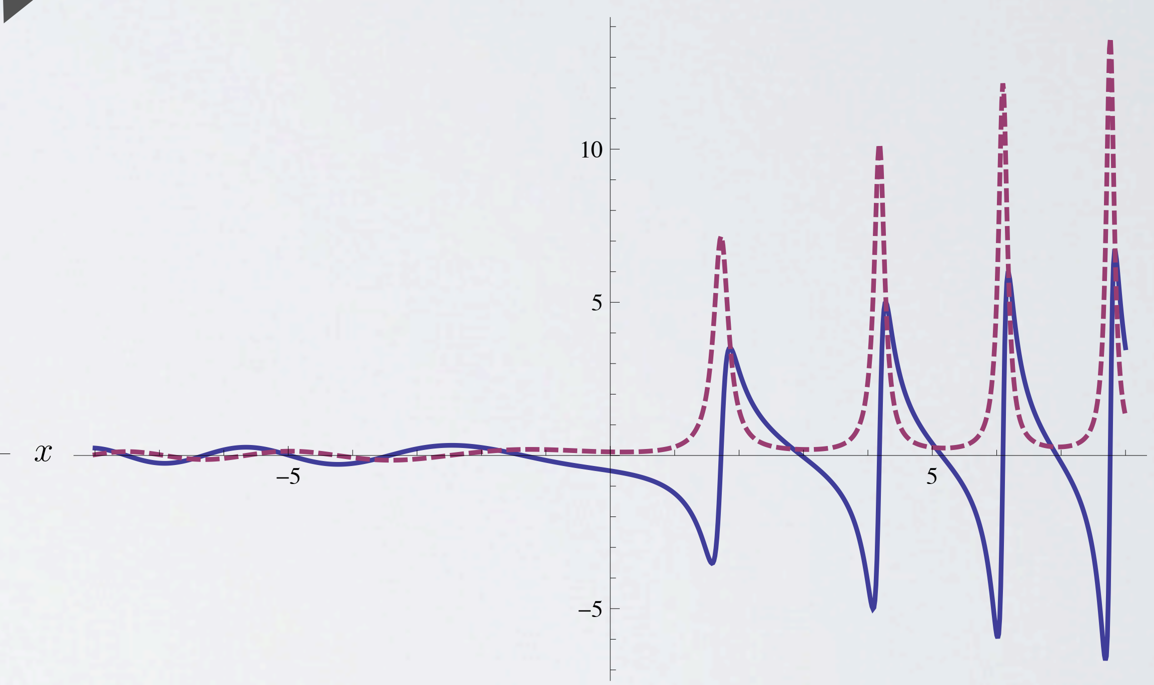
$$(s_1, s_2, s_3) = (1, 0, -1)$$



$$(1 + \mathrm{i},\ -2,\ 1 - \mathrm{i})$$



$$(1, 2, 1/3)$$



Real and imaginary parts

NONLINEAR STEEPEST DESCENT

- As x becomes large, the $\mathrm{e}^{\pm(8\mathrm{i}/3z^3+2\mathrm{i}xz)}$ terms in the jump matrix G becomes increasingly oscillatory
  - Resolving oscillations requires more collocation points
  - The representation on six rays is also inherently badly conditioned
- We use three tools from the asymptotic analysis to remove the oscillations (Deift & Zhou 1995):
  - Deformation along the path of steepest descent
  - Matrix factorization and lensing
  - Replace the oscillator with a similar oscillator

Numerical nonlinear steepest descent: negative x

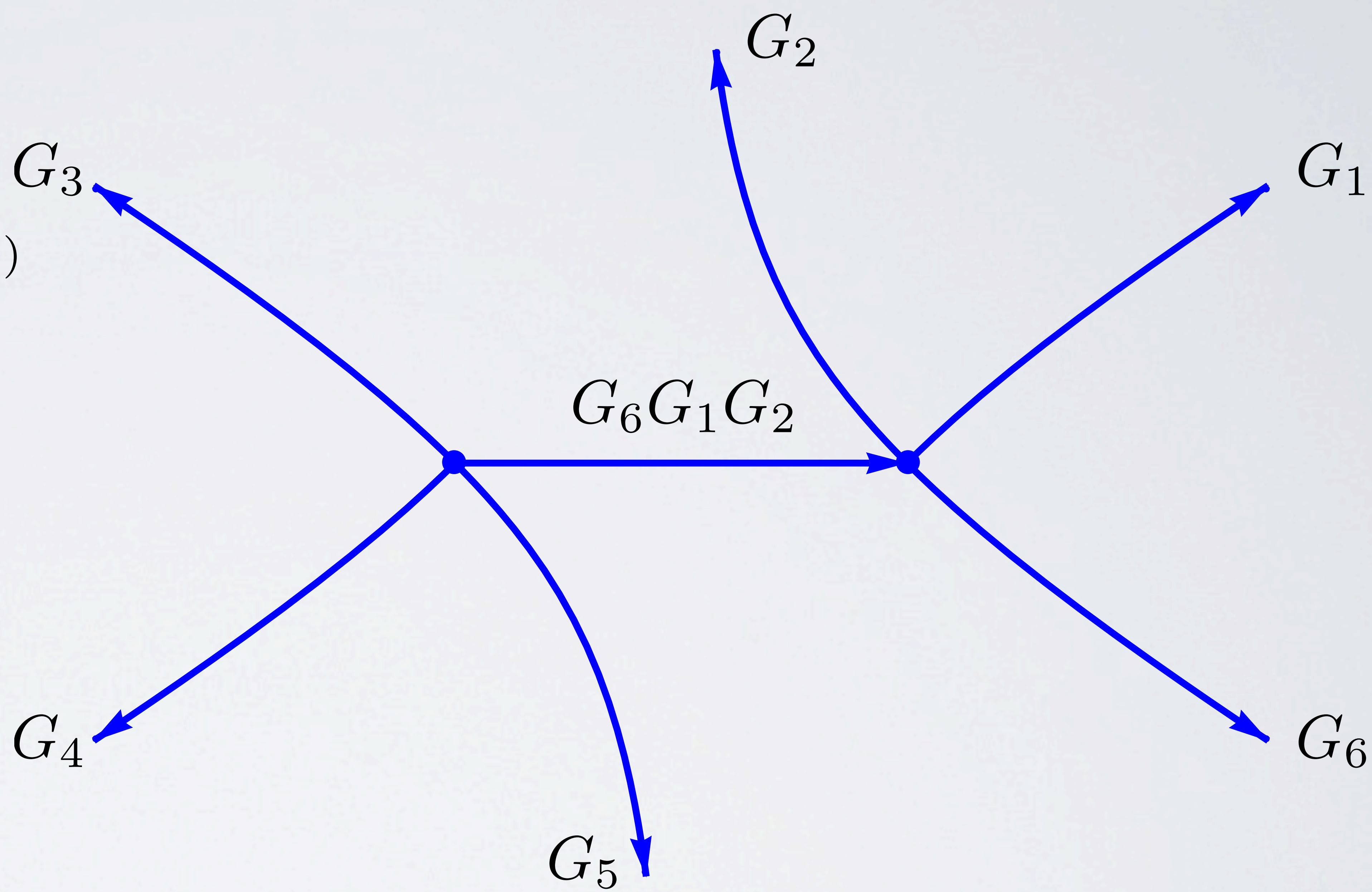
- We first do the transformation

$$z \mapsto \sqrt{-x}\,z$$

so that

$$\mathrm{e}^{\pm(8\mathrm{i}/3z^3+2\mathrm{i}xz)} \mapsto \mathrm{e}^{\pm\mathrm{i}(-x)^{3/2}(8/3z^3-2z)}$$

- This has two stationary points at $\pm 1/2$, thus we deform the contour to obtain the Riemann–Hilbert problem:



(based on Deift & Zhou 1995 and Fokas et al 2006)

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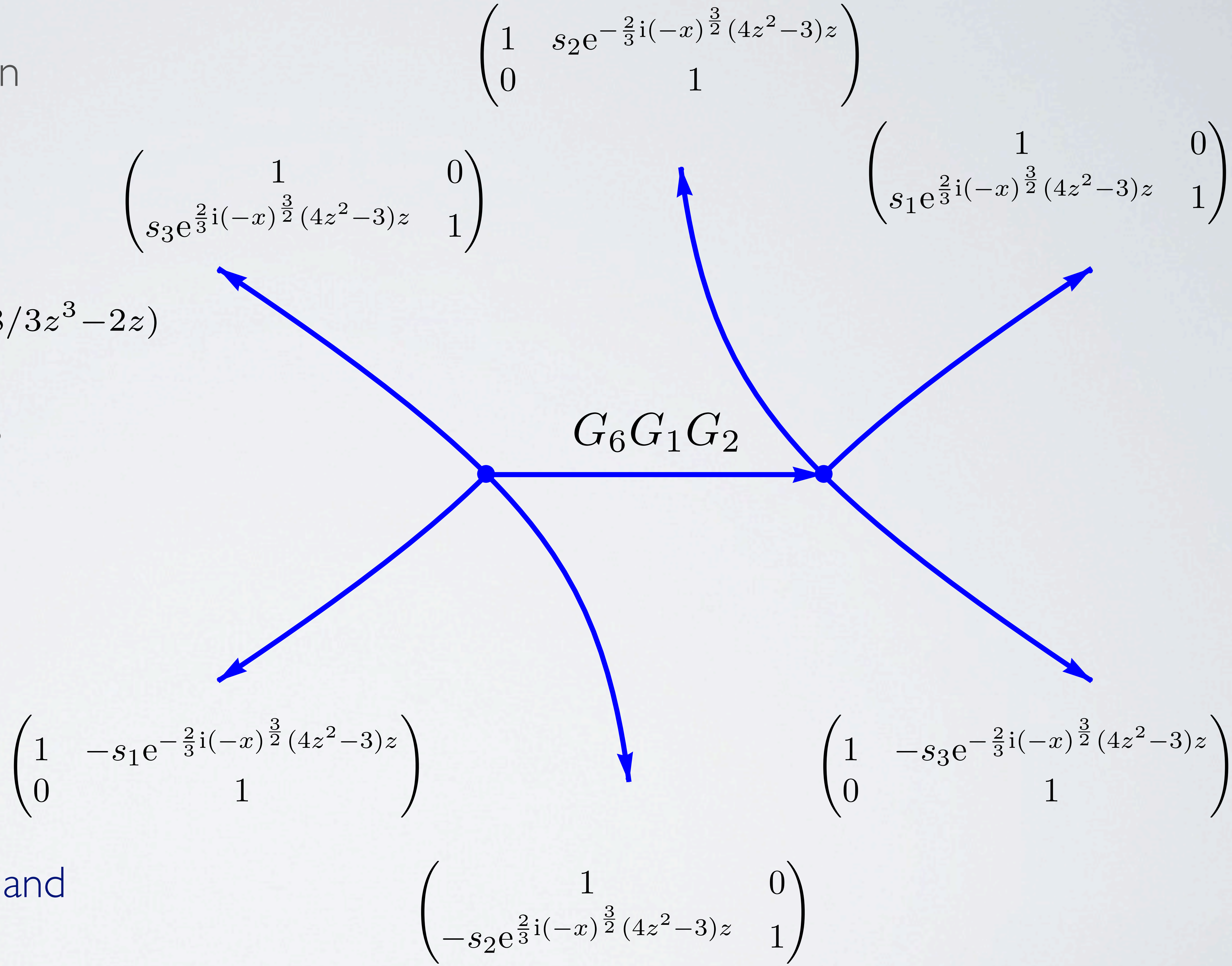


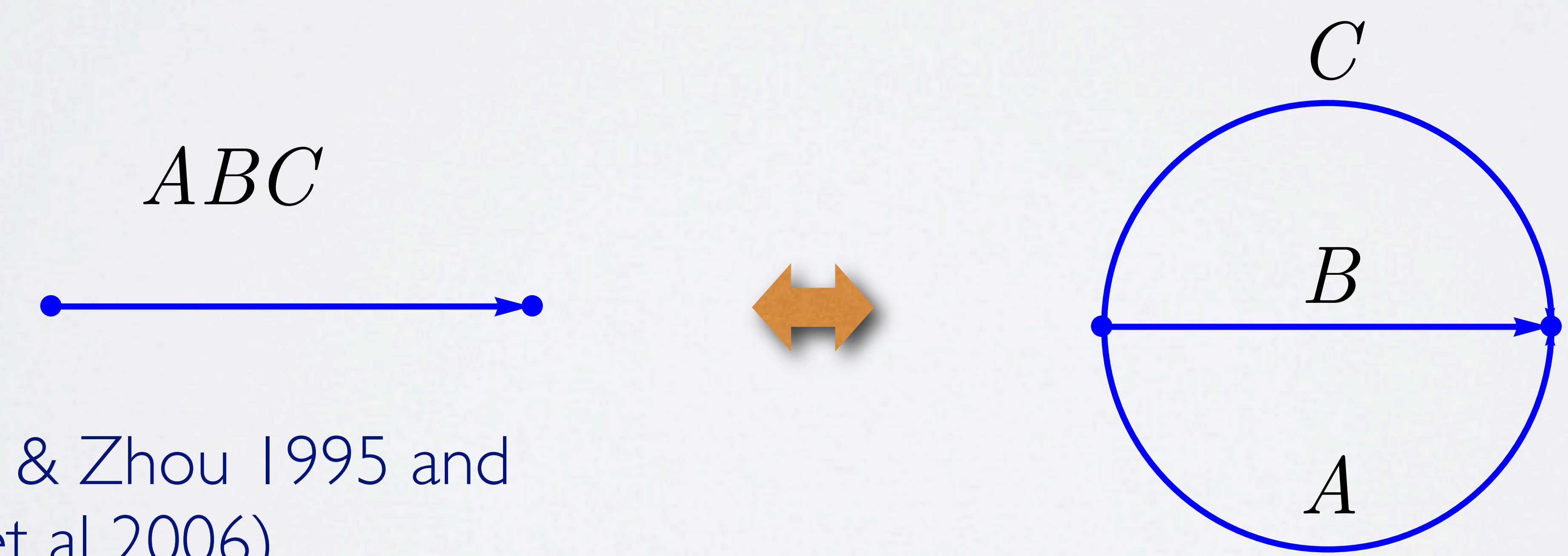
(based on Deift & Zhou 1995 and Fokas et al 2006)

- Each of the paths to infinity have no oscillations and super-exponential decay
- But the path connecting $\pm 1/2$ is still oscillatory:

$$G_6 G_1 G_3 = \begin{pmatrix} 1 & -s_3 \mathrm{e}^{-\frac{2}{3}\mathrm{i}(-x)^{\frac{3}{2}}(4z^2-3)z} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ s_1 \mathrm{e}^{\frac{2}{3}\mathrm{i}(-x)^{\frac{3}{2}}(4z^2-3)z} & 1 \end{pmatrix} \begin{pmatrix} 1 & s_2 \mathrm{e}^{-\frac{2}{3}\mathrm{i}(-x)^{\frac{3}{2}}(4z^2-3)z} \\ 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 - s_1 s_3 & \mathrm{e}^{-\frac{2}{3}\mathrm{i}(-x)^{\frac{3}{2}}(-3+4z^2)z} s_1 \\ \mathrm{e}^{\frac{2}{3}\mathrm{i}(-x)^{\frac{3}{2}}(-3+4z^2)z} s_1 & 1 + s_1 s_2 \end{pmatrix}$$

- The key now is that we can split jump contours:



(based on Deift & Zhou 1995 and Fokas et al 2006)

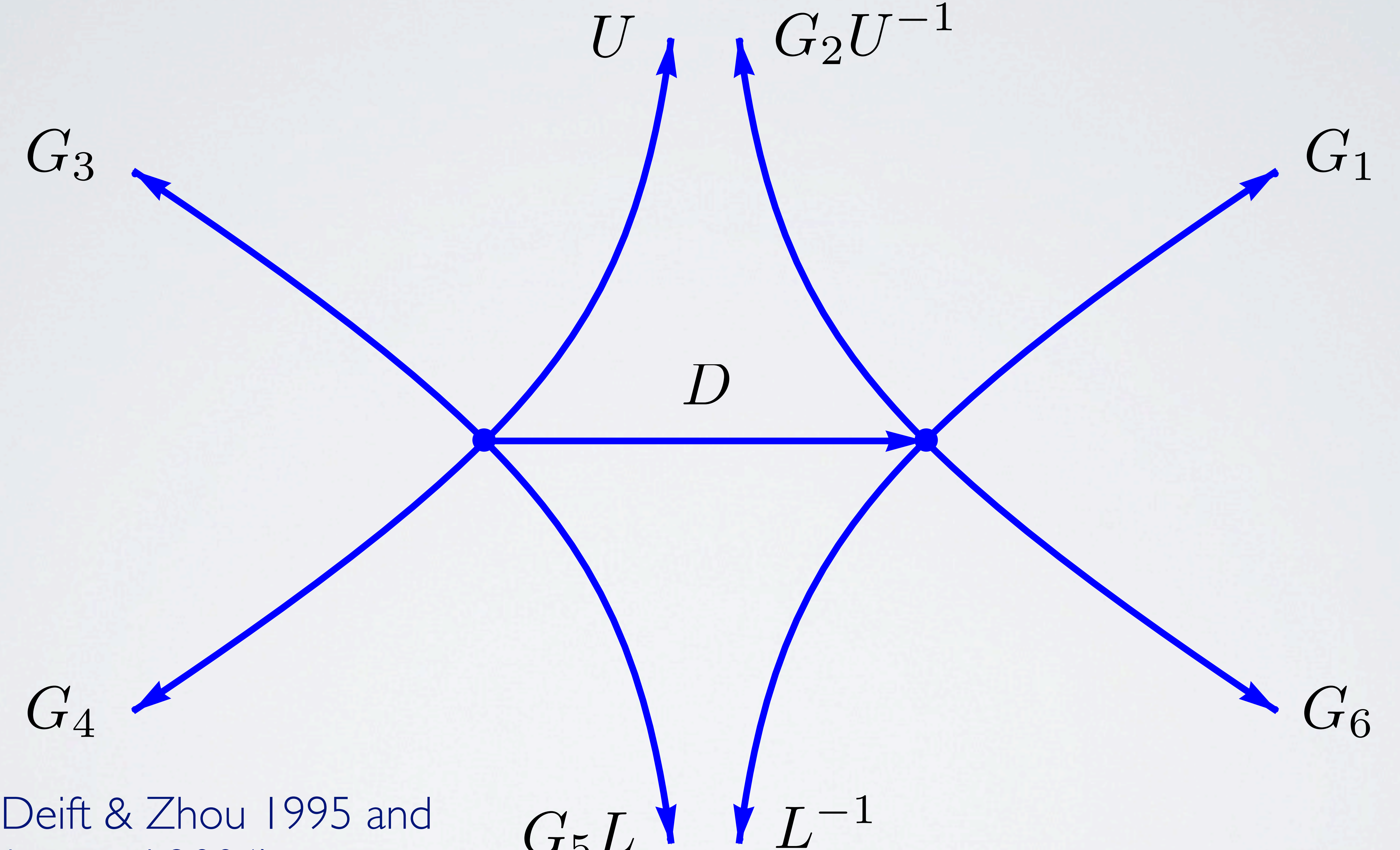
- We want to write $G_6 G_1 G_2$ as ABC where A goes to the identity matrix near the negative imaginary axis, B is nonoscillatory and C goes to the identity matrix near the positive imaginary axis
- This happens to be satisfied by the LDU factorization:

$$G_6 G_1 G_2 = LDU = \begin{pmatrix} 1 & 0 \\ \frac{s_1}{1-s_1 s_3} e^{\frac{2}{3} i(-x)^{\frac{3}{2}}(-3+4z^2)z} & 1 \end{pmatrix} \begin{pmatrix} 1 - s_1 s_3 & \\ & \frac{1}{1-s_1 s_3} \end{pmatrix} \begin{pmatrix} 1 & \frac{s_1}{1-s_1 s_3} e^{-\frac{2}{3} i(-x)^{\frac{3}{2}}(-3+4z^2)z} \\ 0 & 1 \end{pmatrix}$$

- Note that we must restrict our attention to the case where $s_1 s_3 \neq 1$
  - This excludes the Hastings–McLeod solution
  - Though a different factorization can be used in this case (will touch on later)

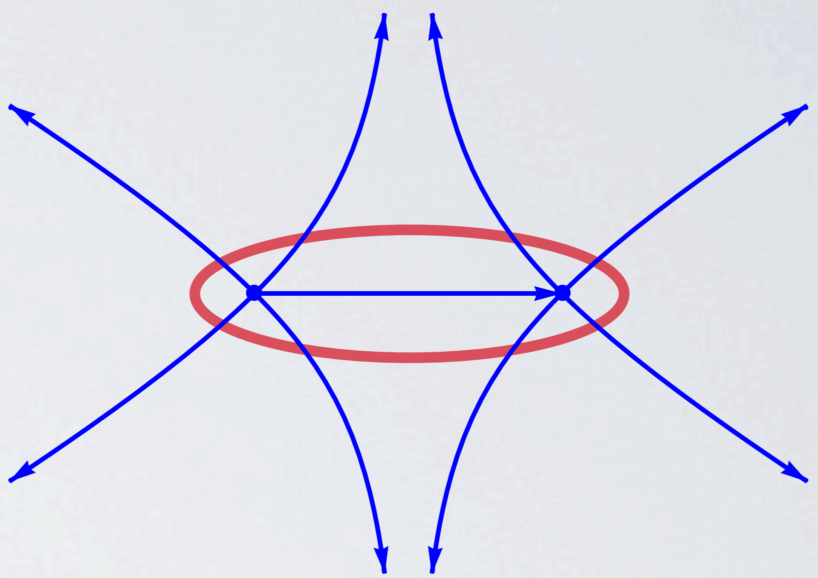
(based on Deift & Zhou 1995 and
Fokas et al 2006)

The RH problem for negative x and $s_1 s_3 \neq 1$



(based on Deift & Zhou 1995 and Fokas et al 2006)

- We can implement a spectral method for this Riemann–Hilbert problem just as we did for the canonical six rays case
- The problem:
  - The solution is oscillatory along circled connecting curve
  - Fortunately, we have a closed form solution (parametrix) for the contribution from that curve from the analytic development:

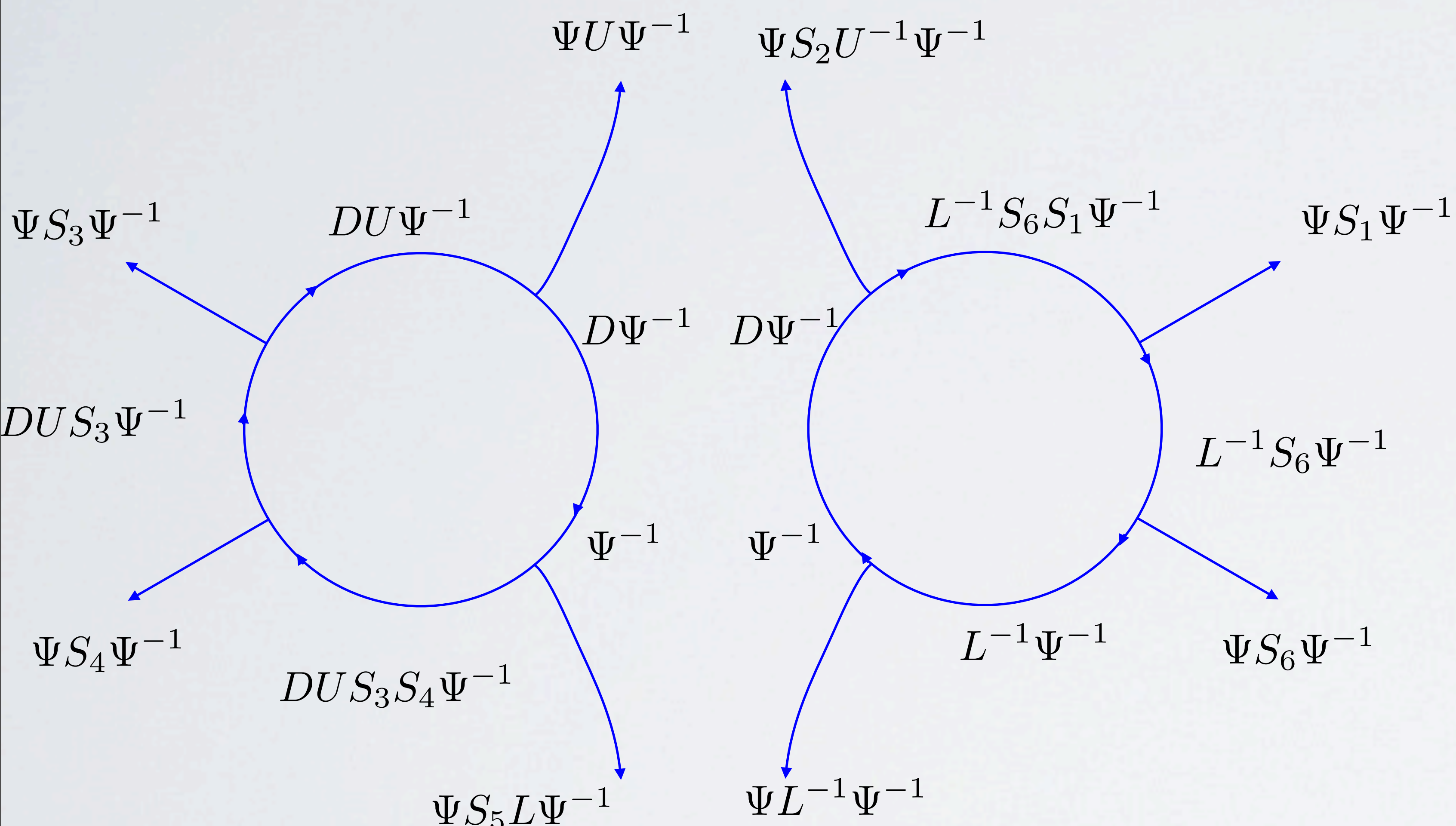


$$\Psi^+ = \Psi^- D$$

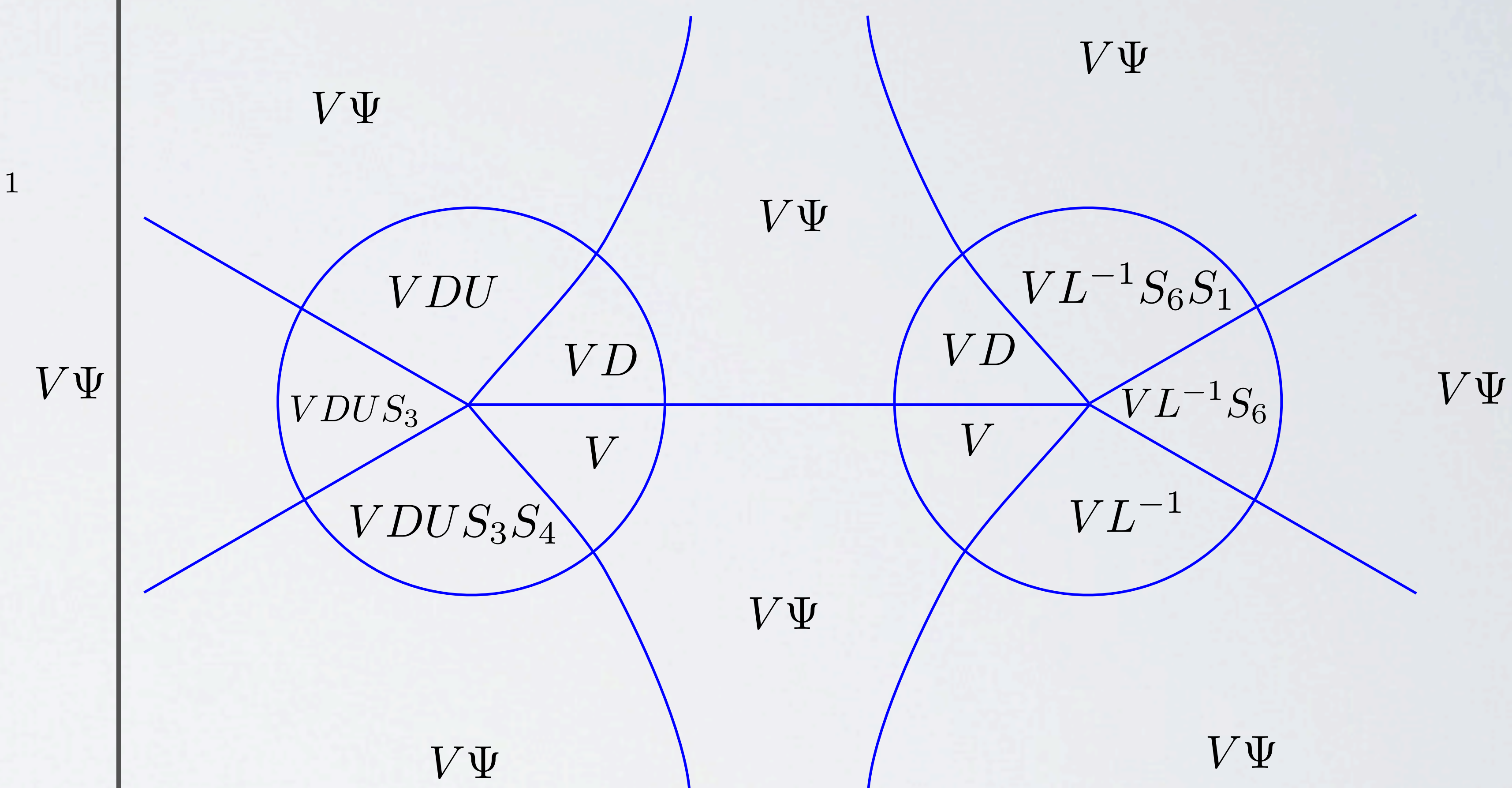
$$\Psi(z) = \begin{pmatrix} \left(\frac{1+2z}{2z-1}\right)^{\frac{\mathrm{i}}{2\pi}\log D_{11}} & \\ & \left(\frac{1+2z}{2z-1}\right)^{\frac{\mathrm{i}}{2\pi}\log D_{22}} \end{pmatrix}$$

(based on Deift & Zhou 1995 and Fokas et al 2006)

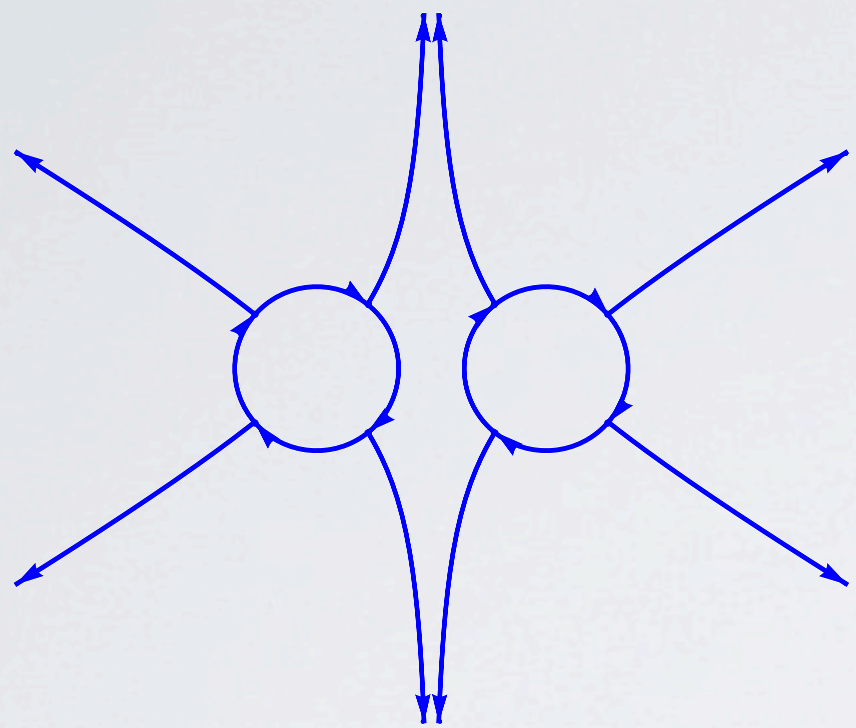
- V satisfies the RH problem:



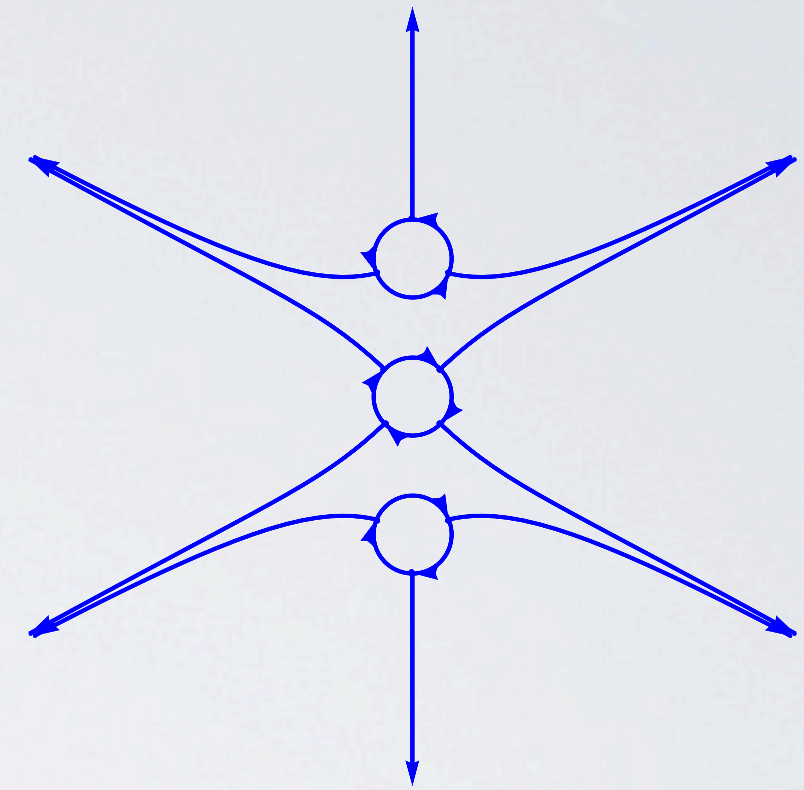
We recover the solution by:



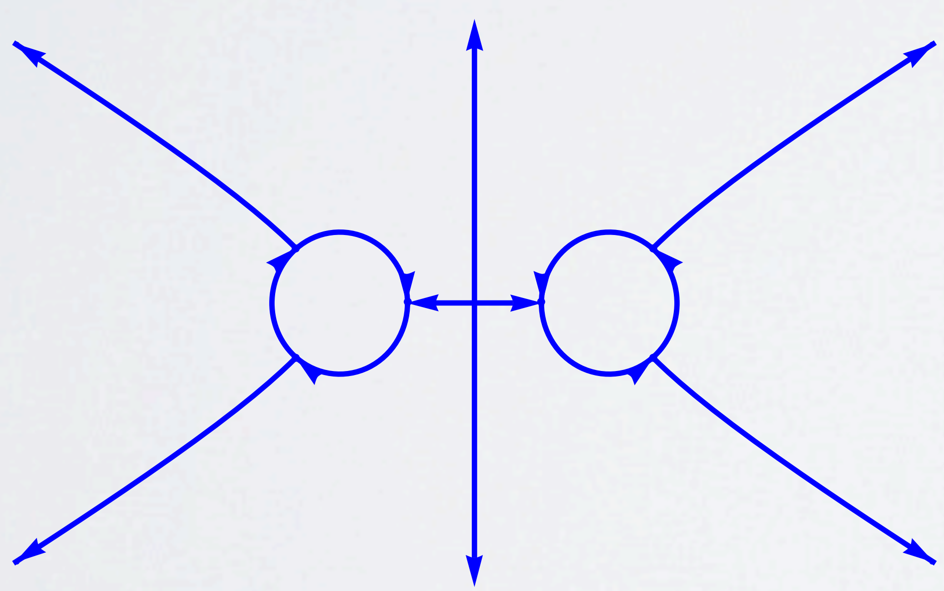
Negative x with $s_1 s_3 \neq 1$



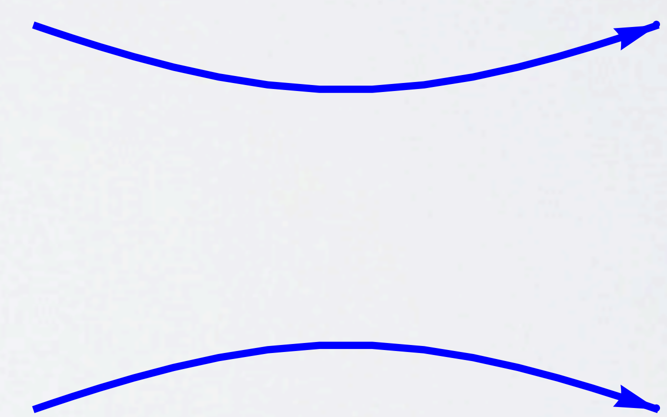
Positive x with $s_2 \neq 0$



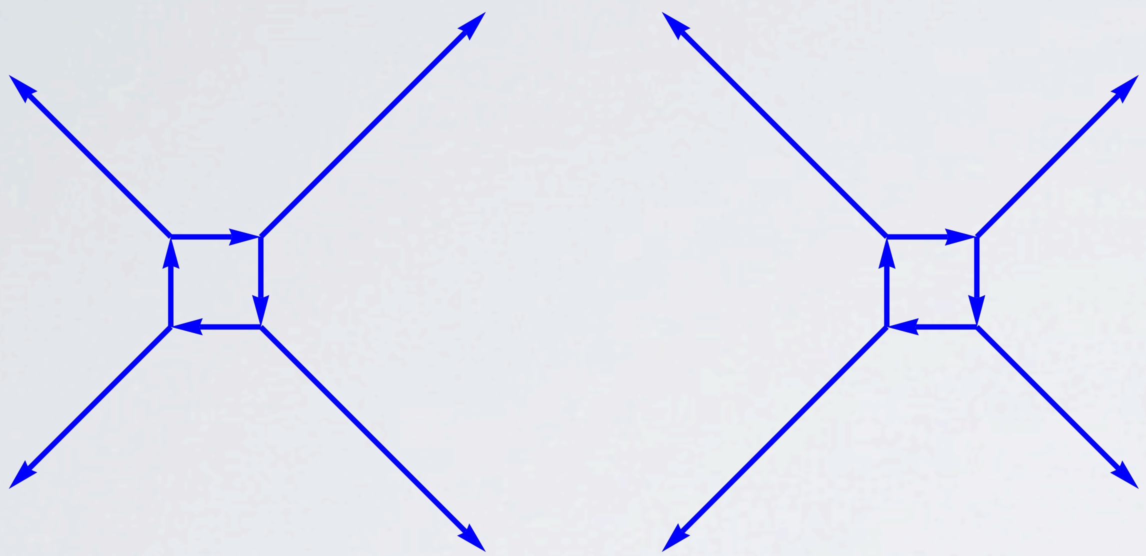
Negative x with $s_1 s_3 = 1$



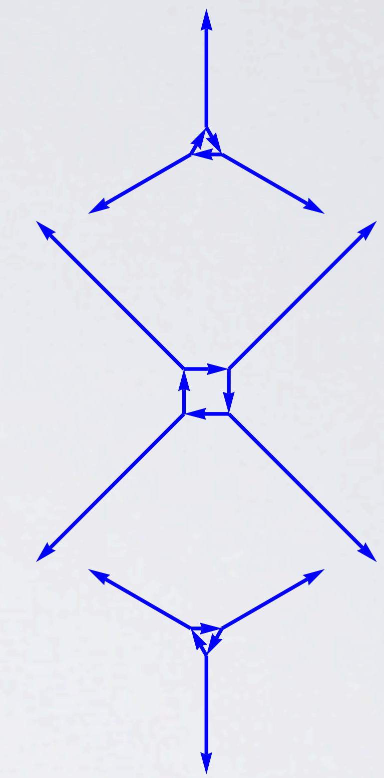
Positive x with $s_2 = 0$



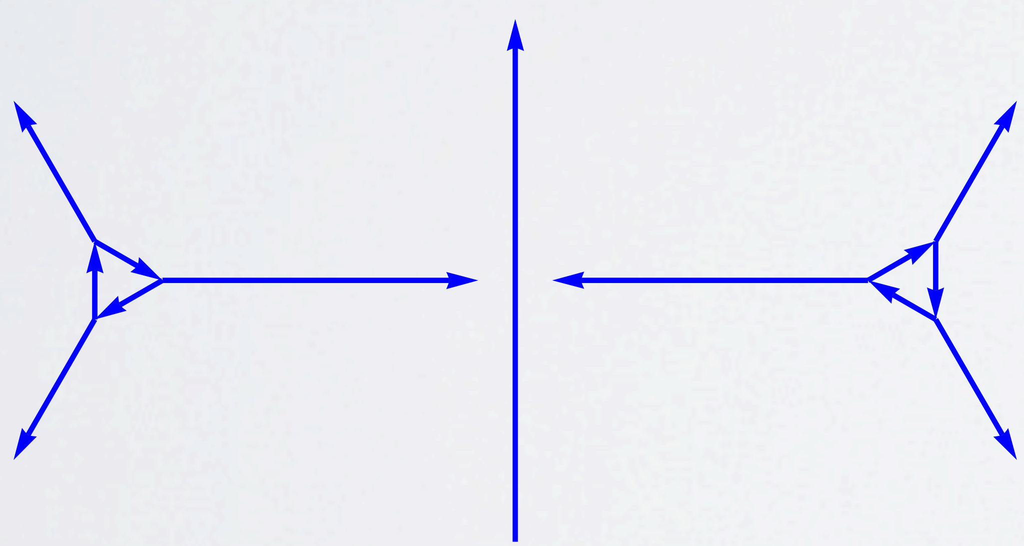
Negative x with $s_1 s_3 \neq 1$



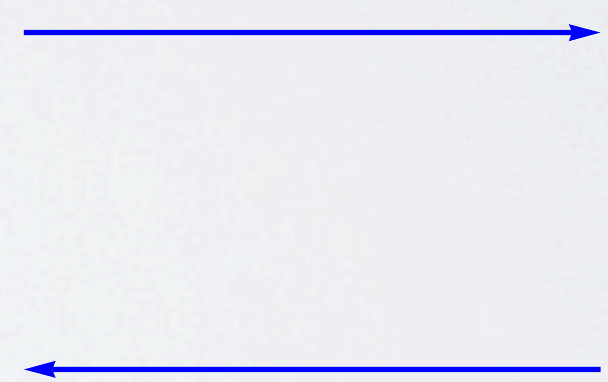
Positive x with $s_2 \neq 0$



Negative x with $s_1 s_3 = 1$

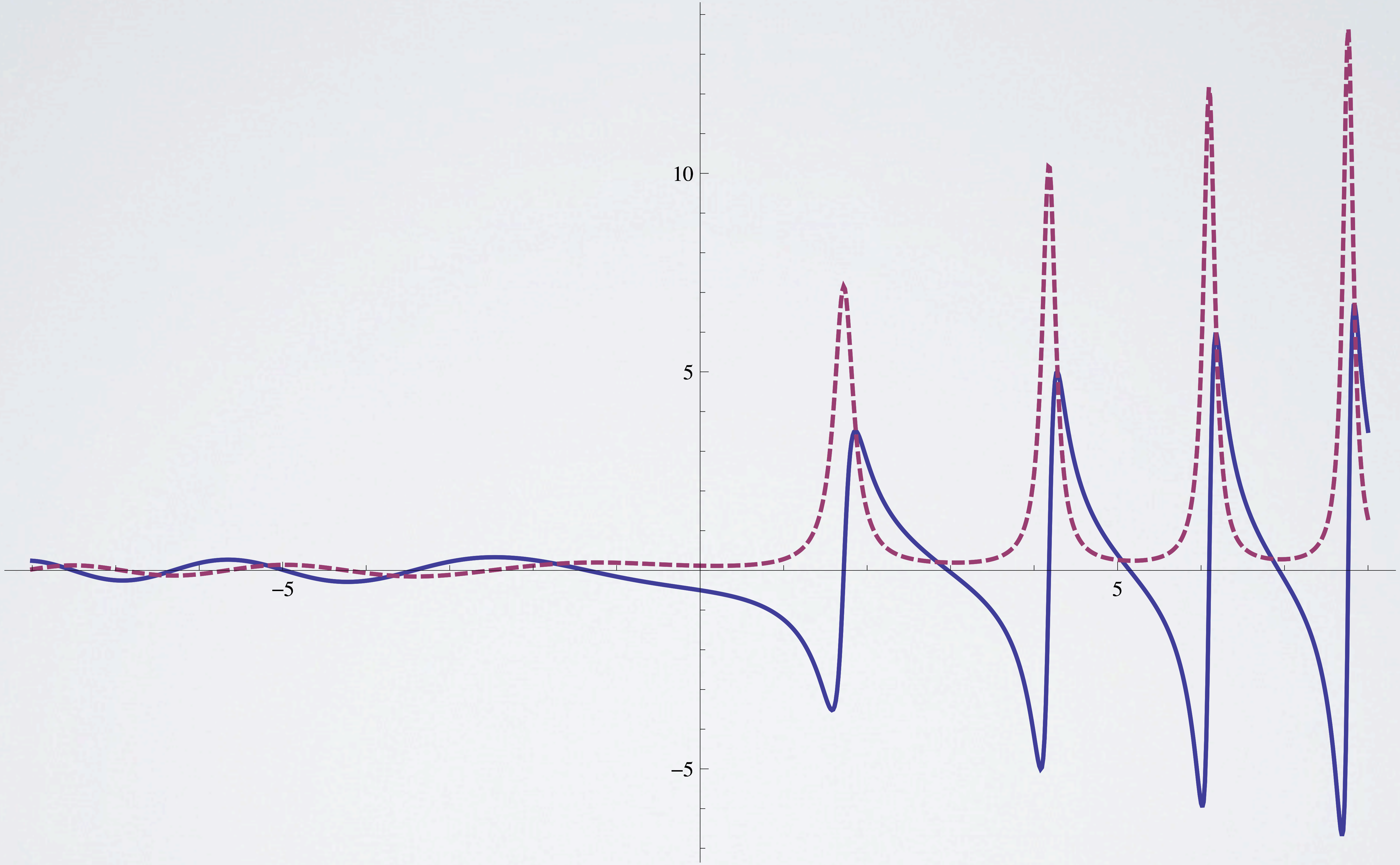


Positive x with $s_2 = 0$



(joint work with G. Wechslburger)

We can now extend the graph for $(s_1, s_2, s_3) = (1, 2, 1/3)$



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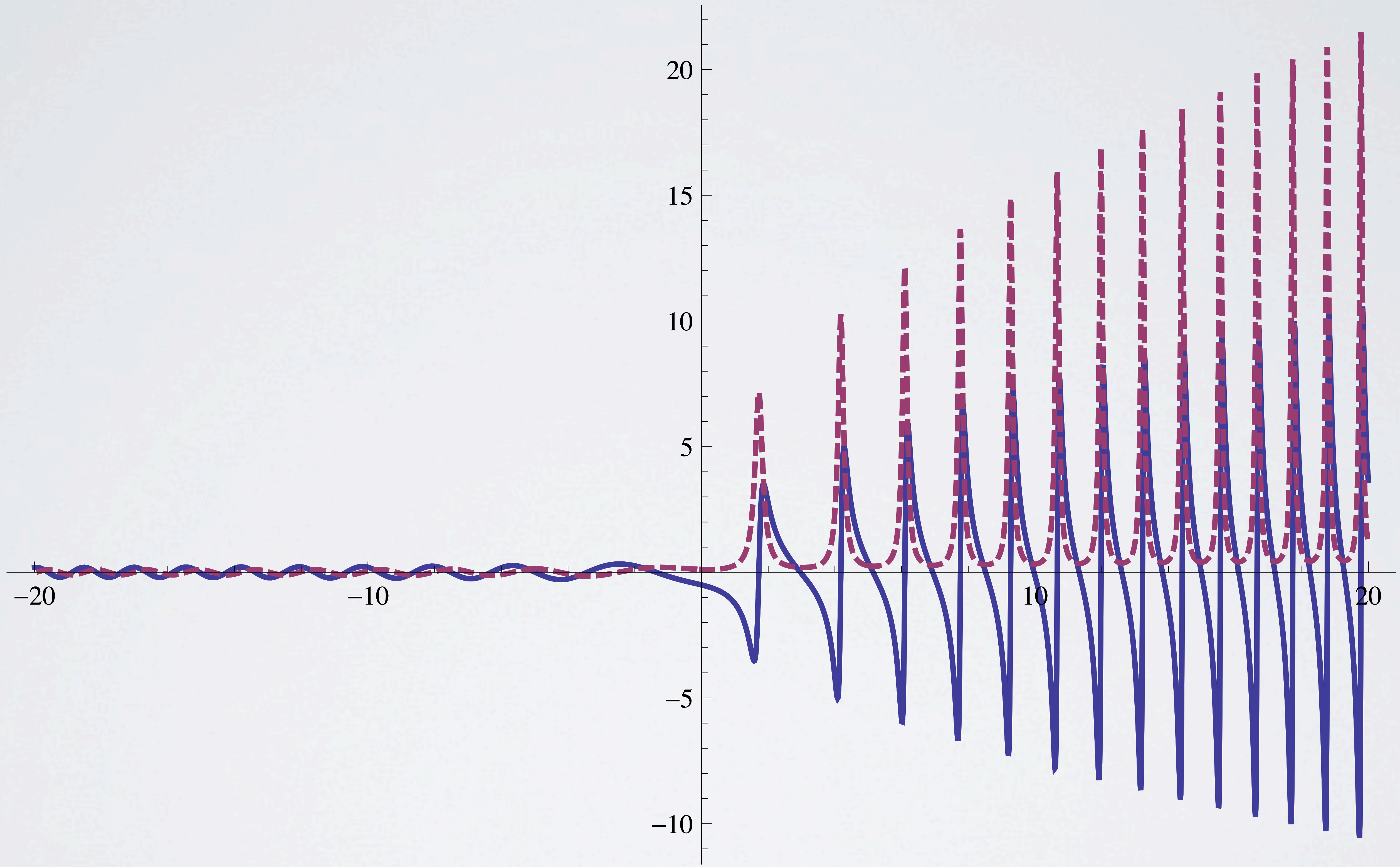

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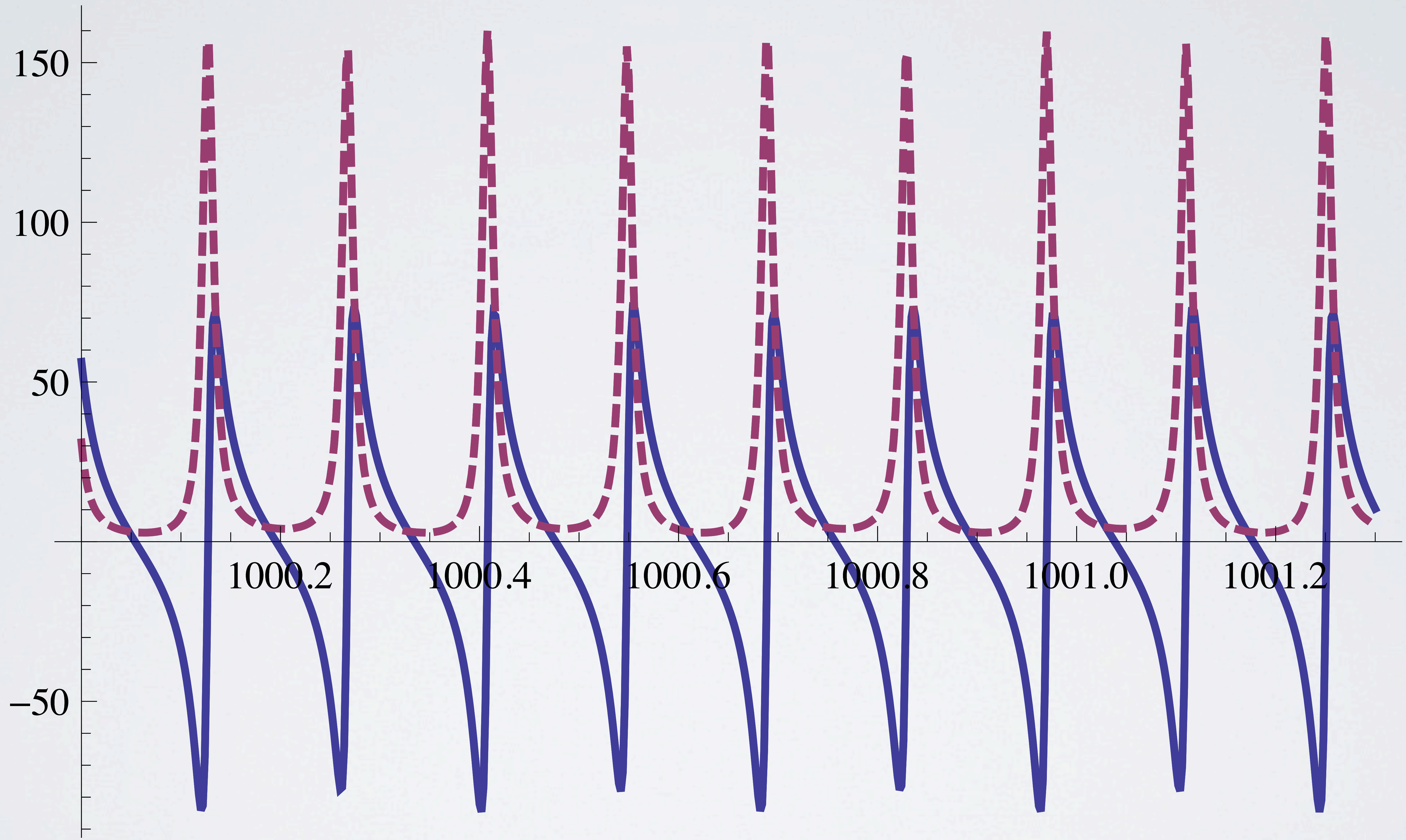


Hastings–McLeod $(s_1, s_2, s_3) = (\mathrm{i}, 0, -\mathrm{i})$

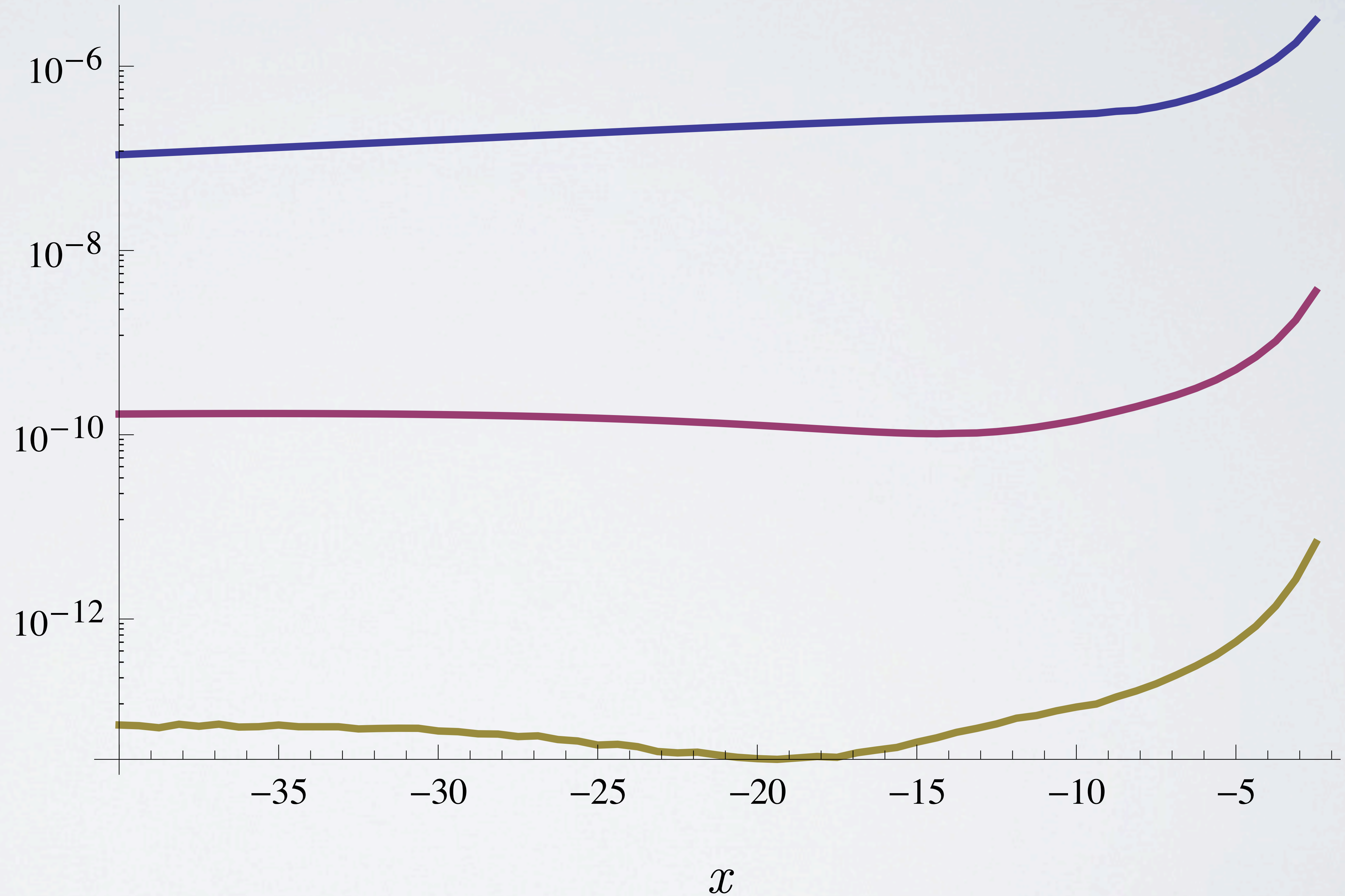
Relative error compared to (Prähofer and Spohn 2004)

Total # collocation points

186

310

436



Integrable Systems

- Many integrable systems can be written as RH problems
  - Here, RH problems are generalizations of the Fourier transform solutions to linear PDEs, such as the heat, wave, linear Schrödinger and linear KdV equations
- Examples include
  - Nonlinear Schrödinger (NLS) equation $$\mathrm{i}u_t + u_{xx} + |u|^2 u = 0$$
    - Davey–Stewartson (DS) I equation $$\mathrm{i}u_t + \frac{1}{2}(u_{xx} + u_{yy}) = u\phi - |u|^2 u$$ $$\phi_{xx} - \phi_{yy} = 2\left(|u|^2\right)_{xx}$$
  - Shallow water waves:
    - Korteweg–de Vries (KdV) equation $$u_t + 6uu_x + u_{xxx} = 0$$
    - Kadomtsev–Petviashvili (KP) I equation $$(u_t + 6uu_x + u_{xxx})_x - 3u_{yy} = 0$$

KdV equation

- We want to find Φ which satisfies the following jump on the real axis:

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

  where r is the *reflection coefficient* (essentially, a generalization of the Fourier transform)

- Given a reasonable initial condition, we can efficiently compute r numerically by solving an oscillatory, time-independent linear Schrödinger equation
  - But here we will just assume r is given
- Now Φ is not analytic, but rather meromorphic, with simple poles (depending on the initial condition)
- We can transform the poles to small circles surrounding the pole (suggested by J. DiFranco)

(joint work with T. Trogden, U. Washington)

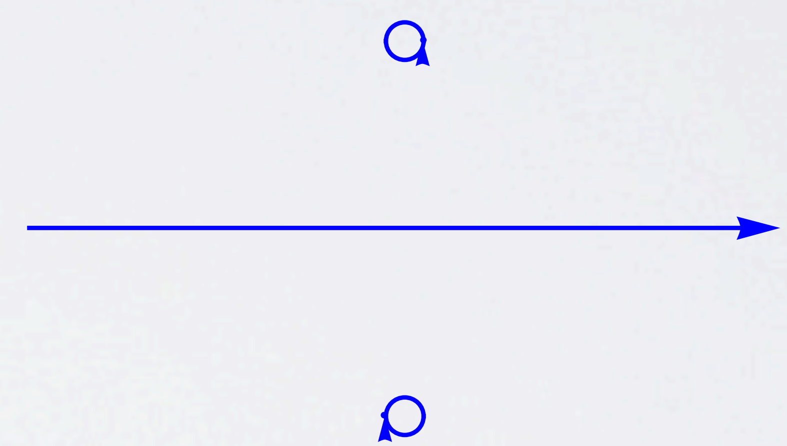
Deformations

- We have two stationary points at

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

- 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

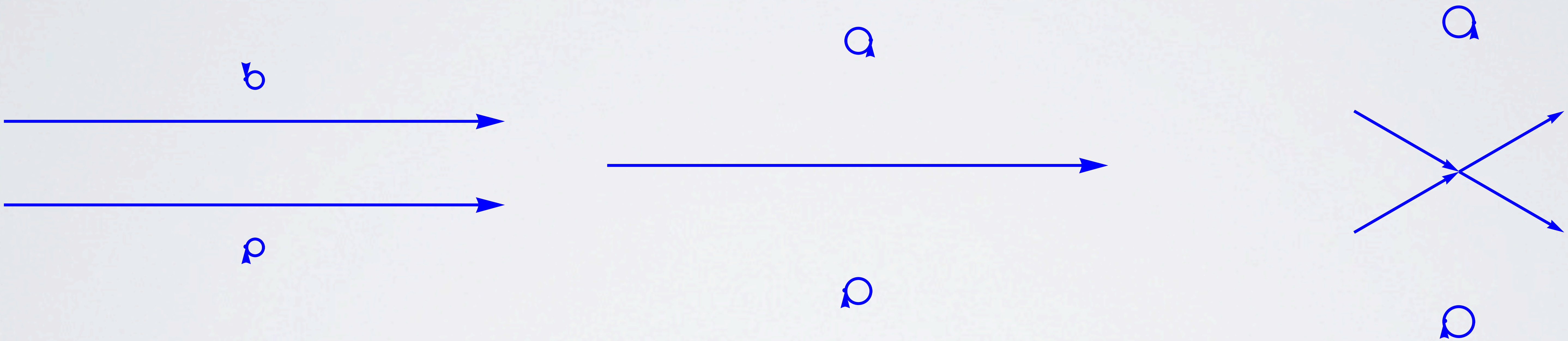
Undeformed



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

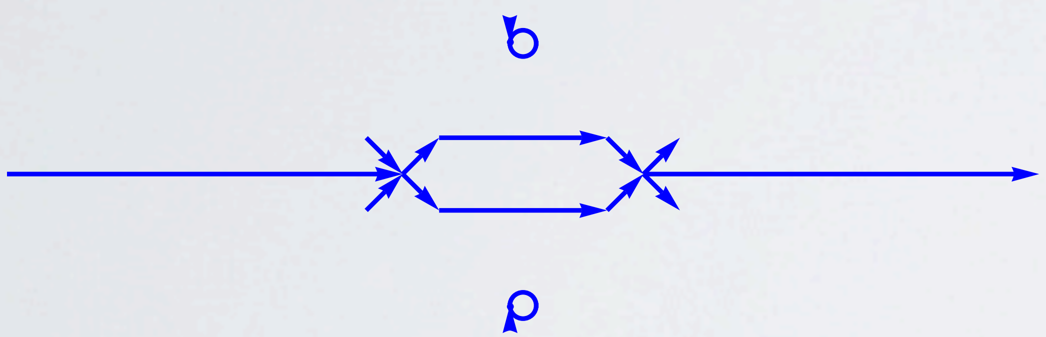
$$t = 0$$

$x \leq 0$ $x = 0$ $0 \leq x$

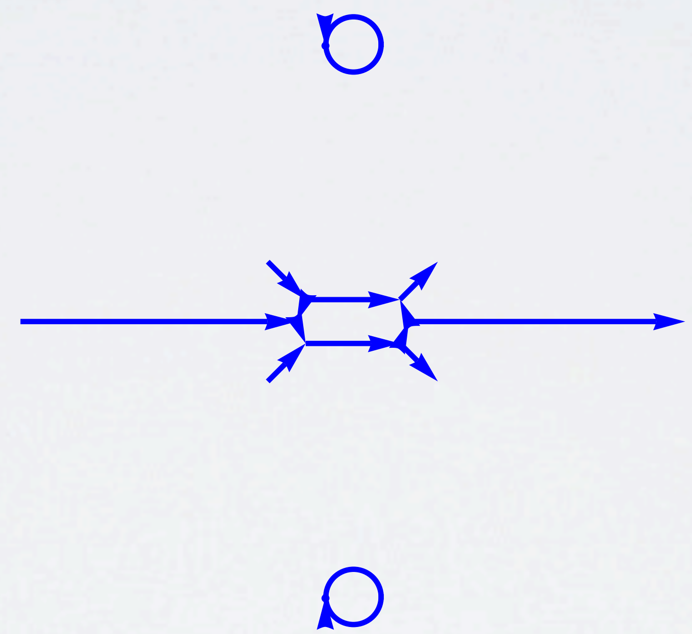


$$t > 0$$

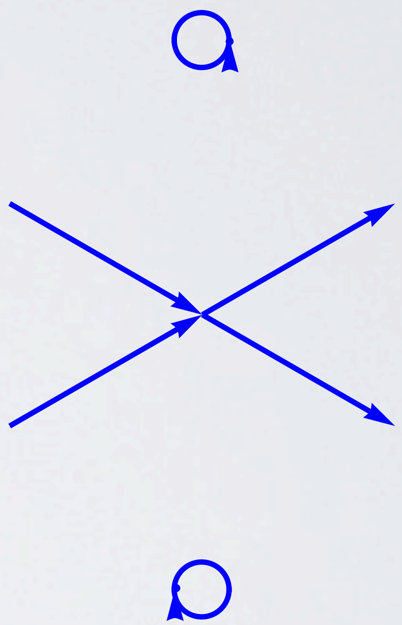
$x < -t$



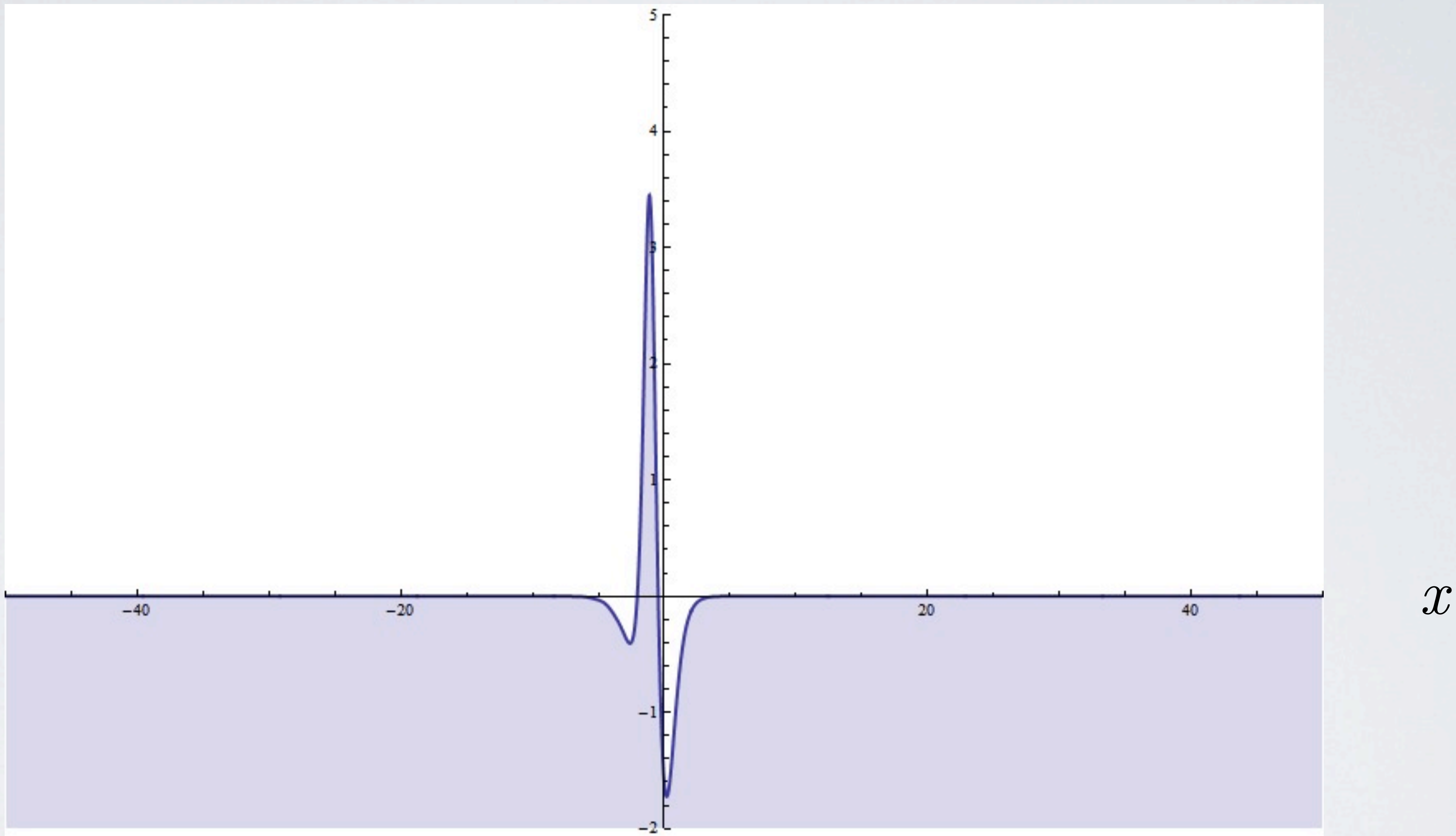
$-t \leq x < 0$



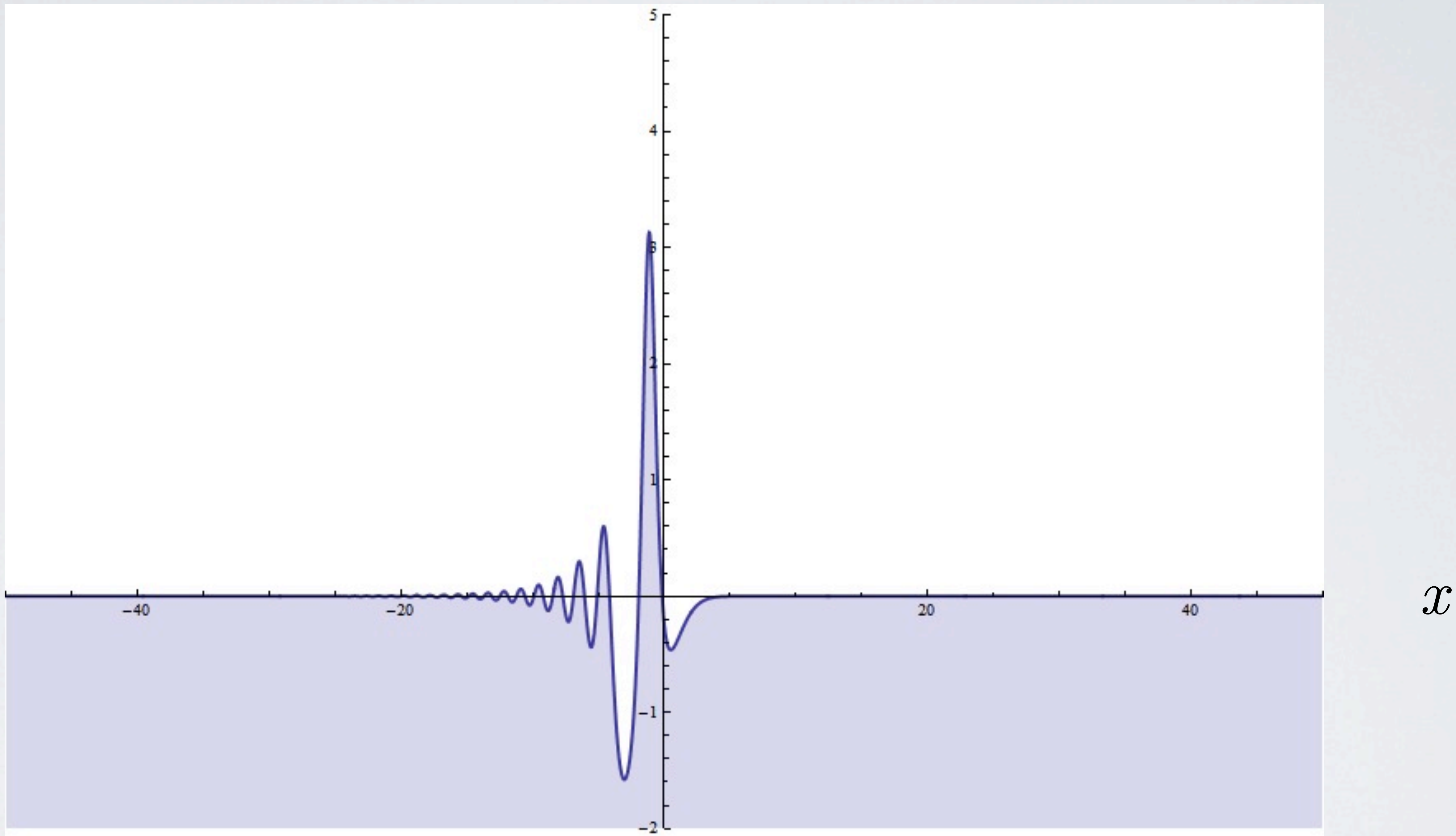
$0 \leq x$



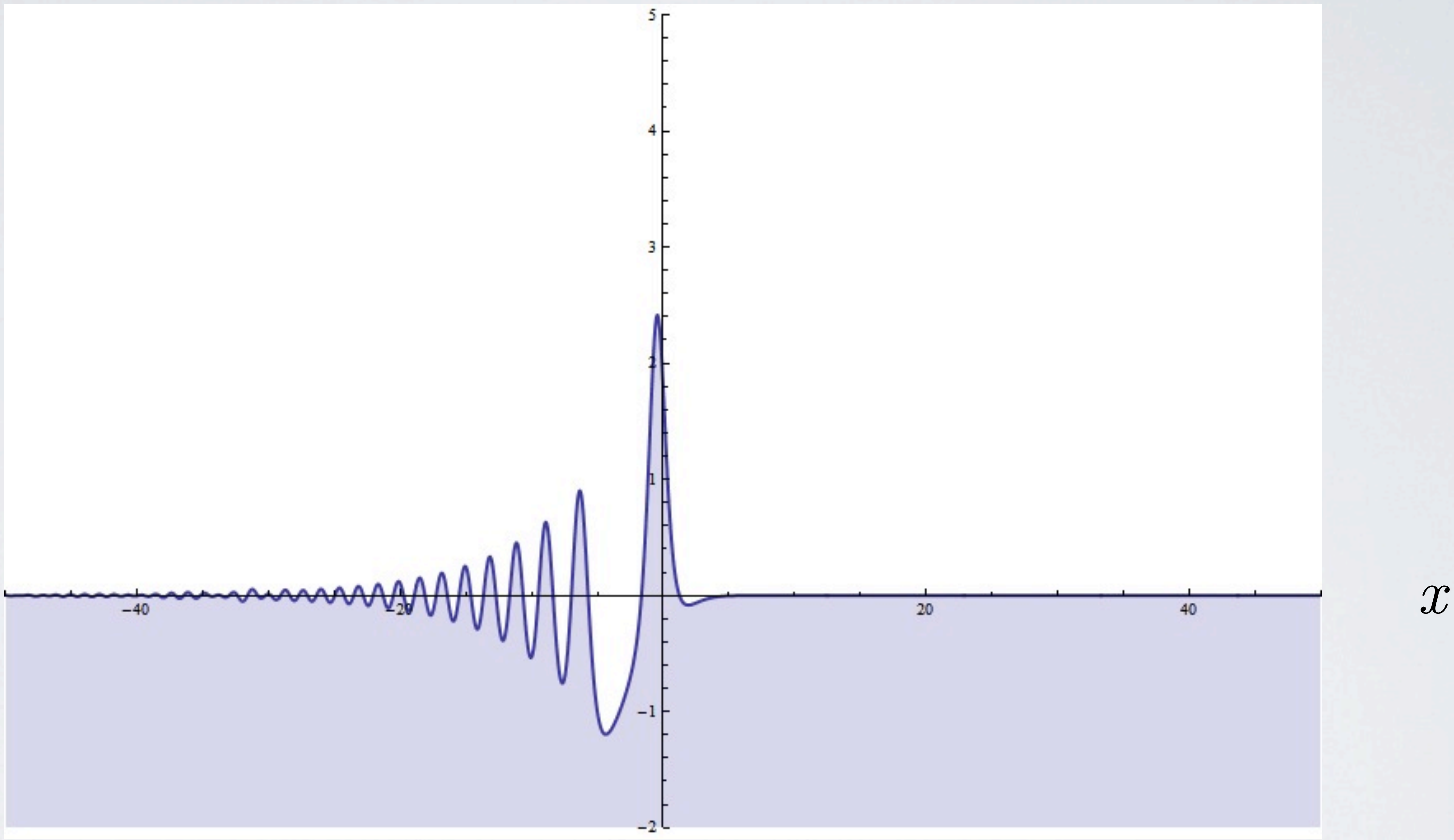
One soliton



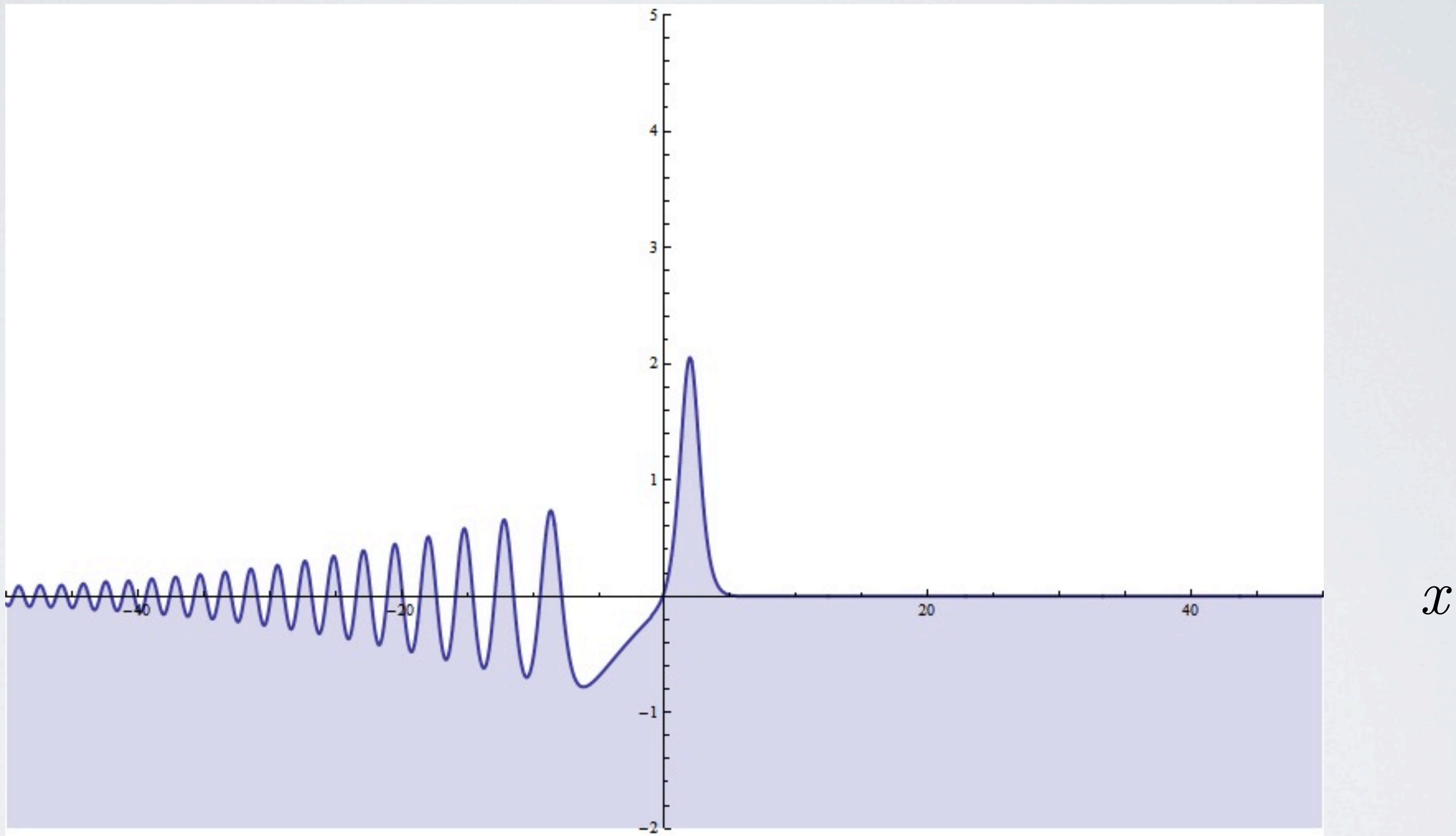
One soliton



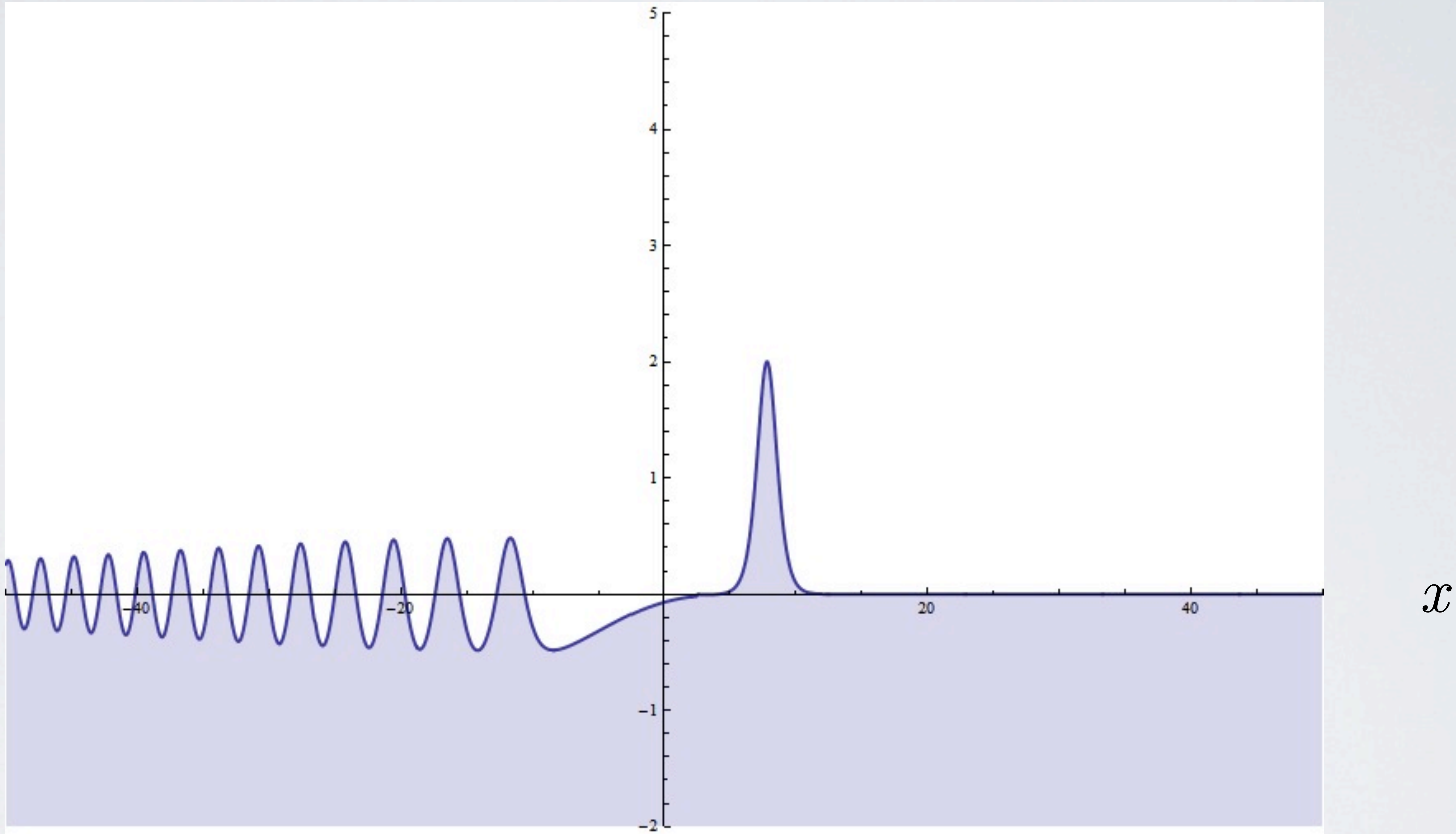
One soliton



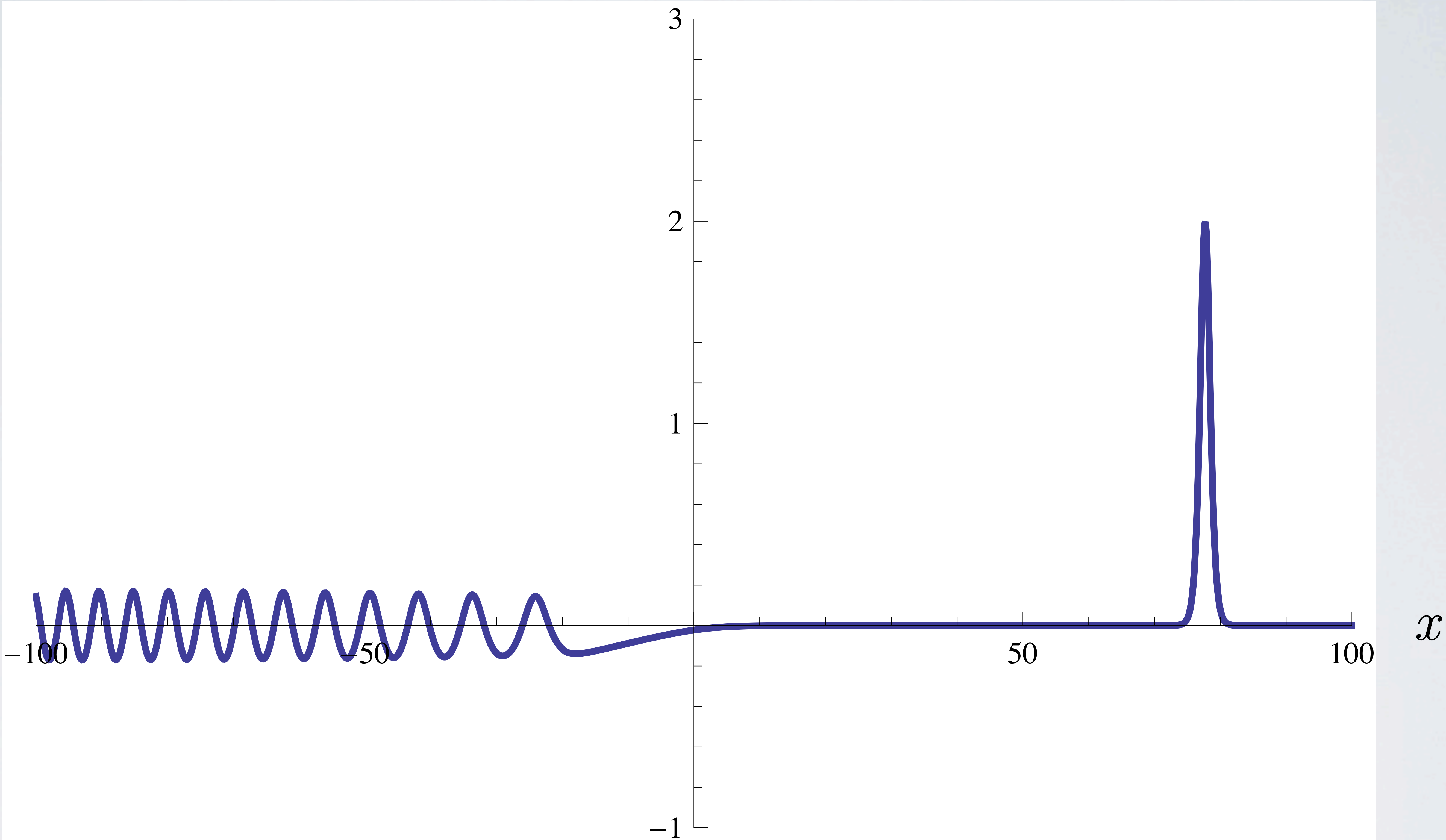
One soliton



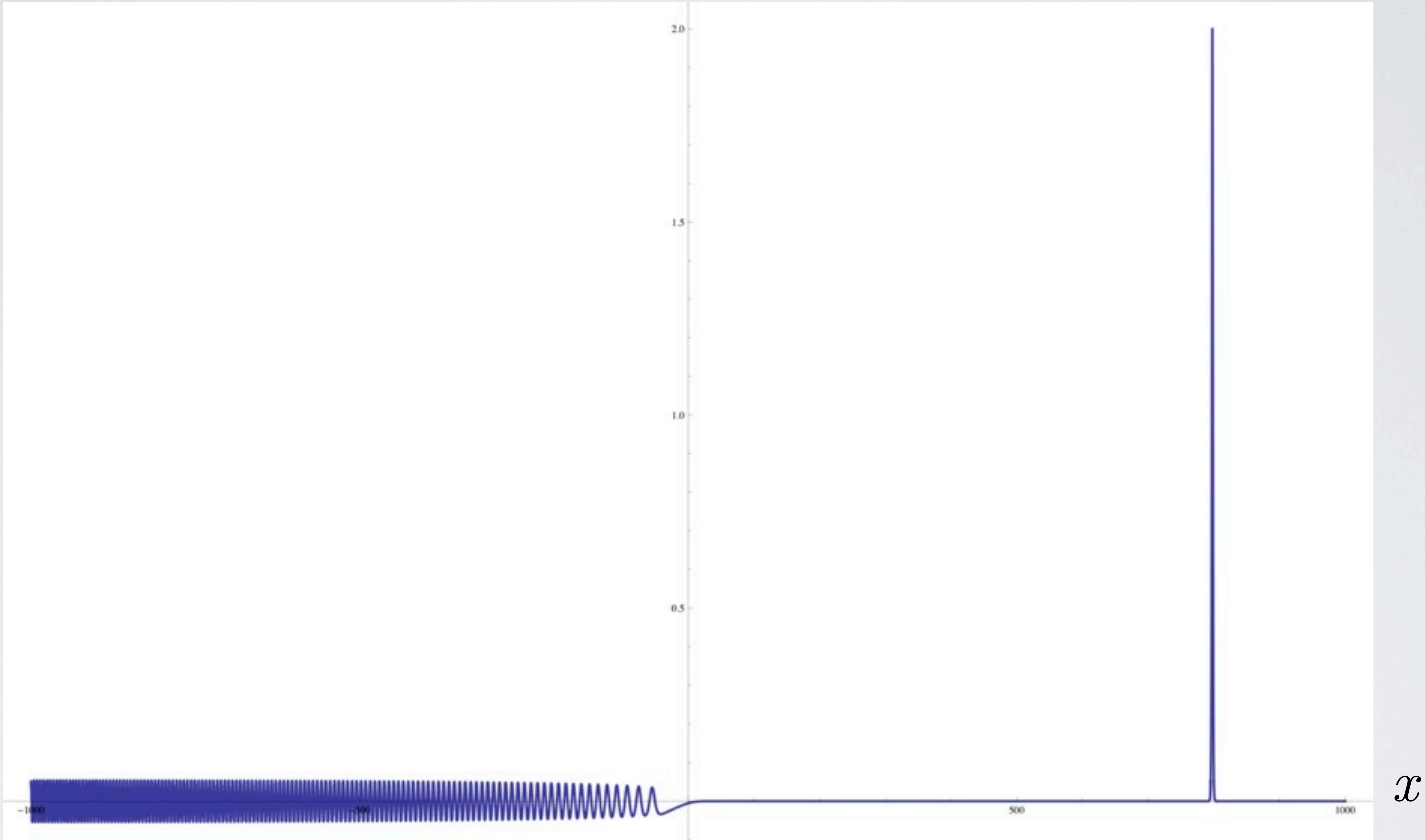
One soliton



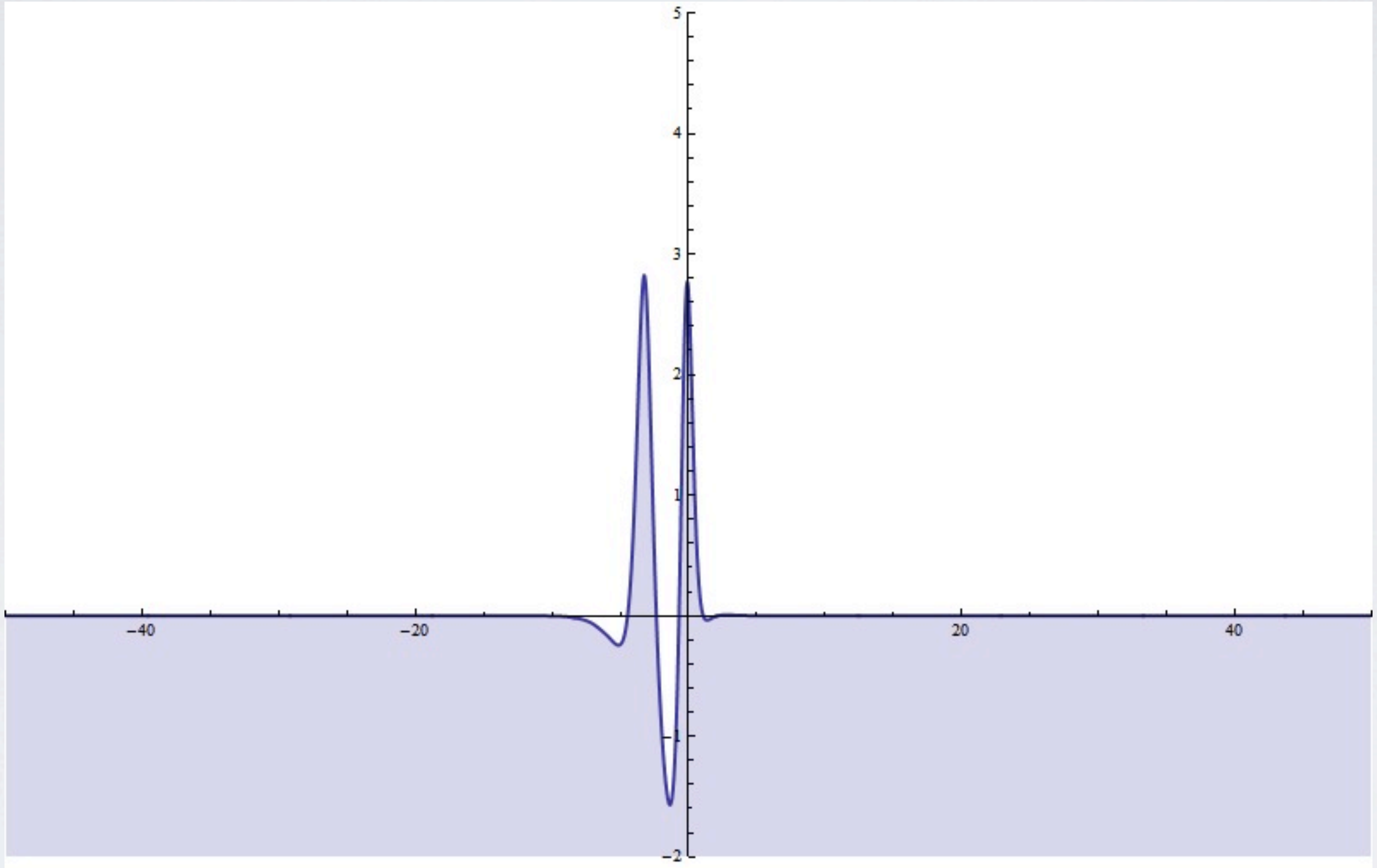
Plot for $t = 20$



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

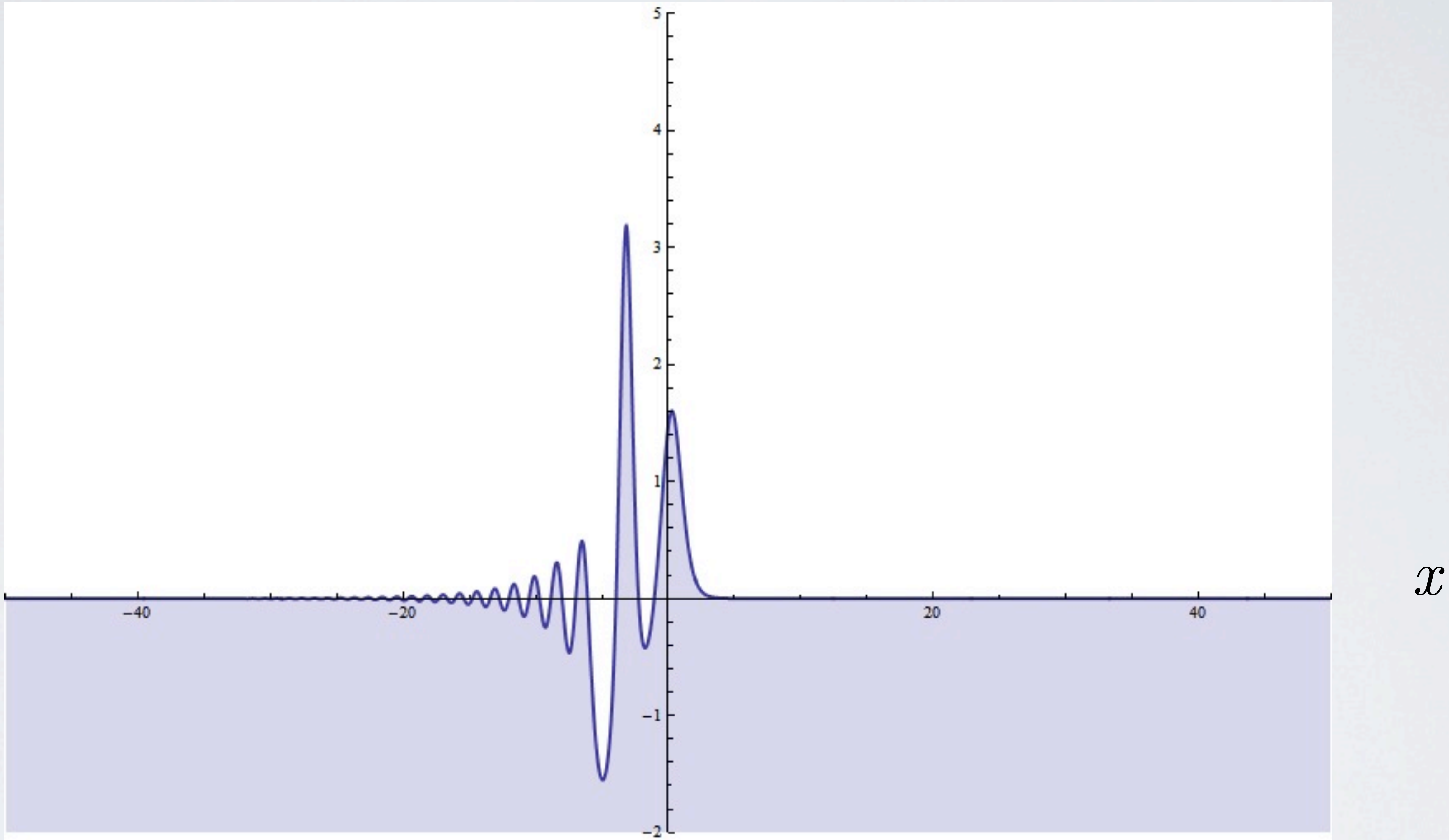


Two solitons

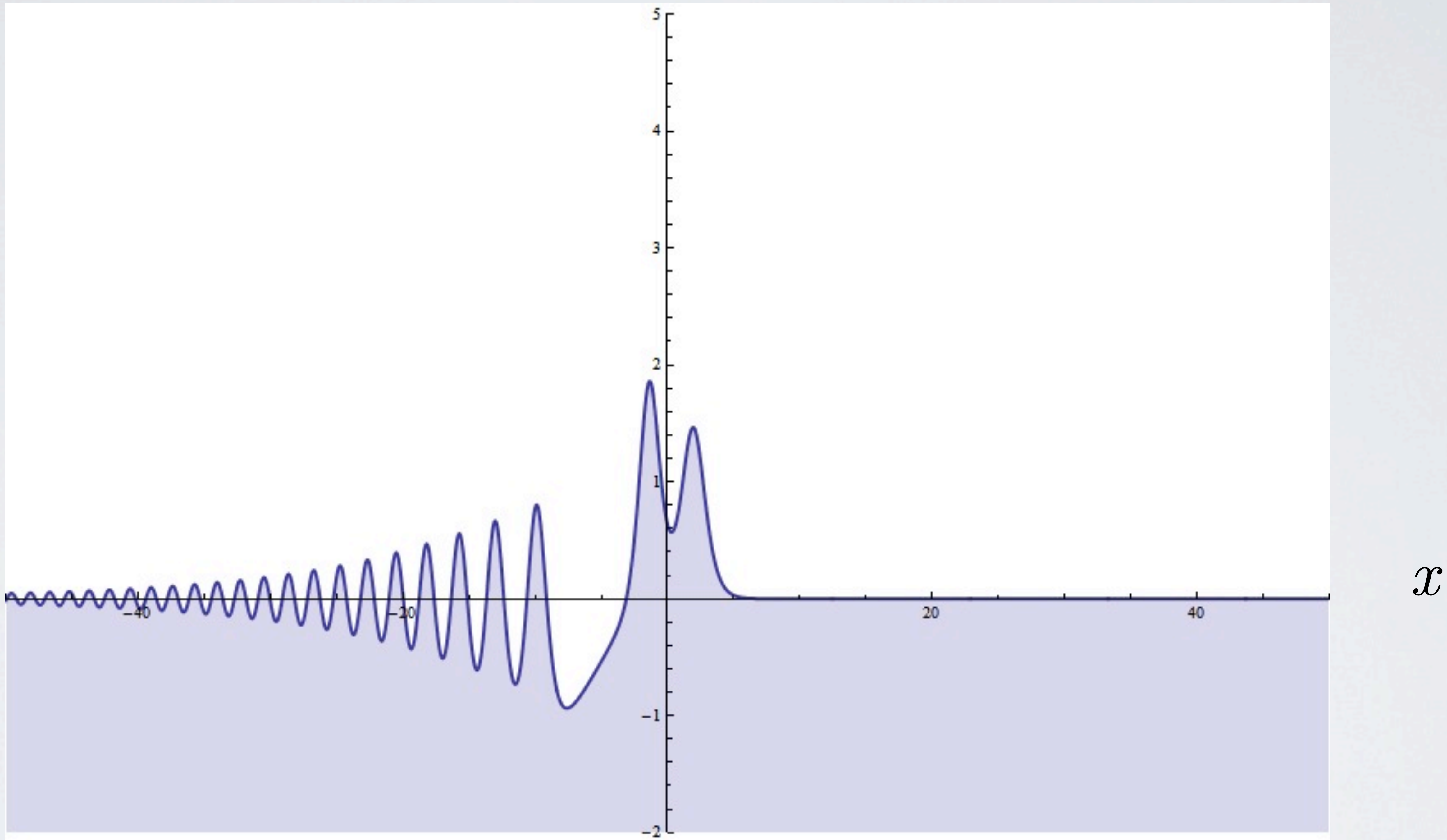


x

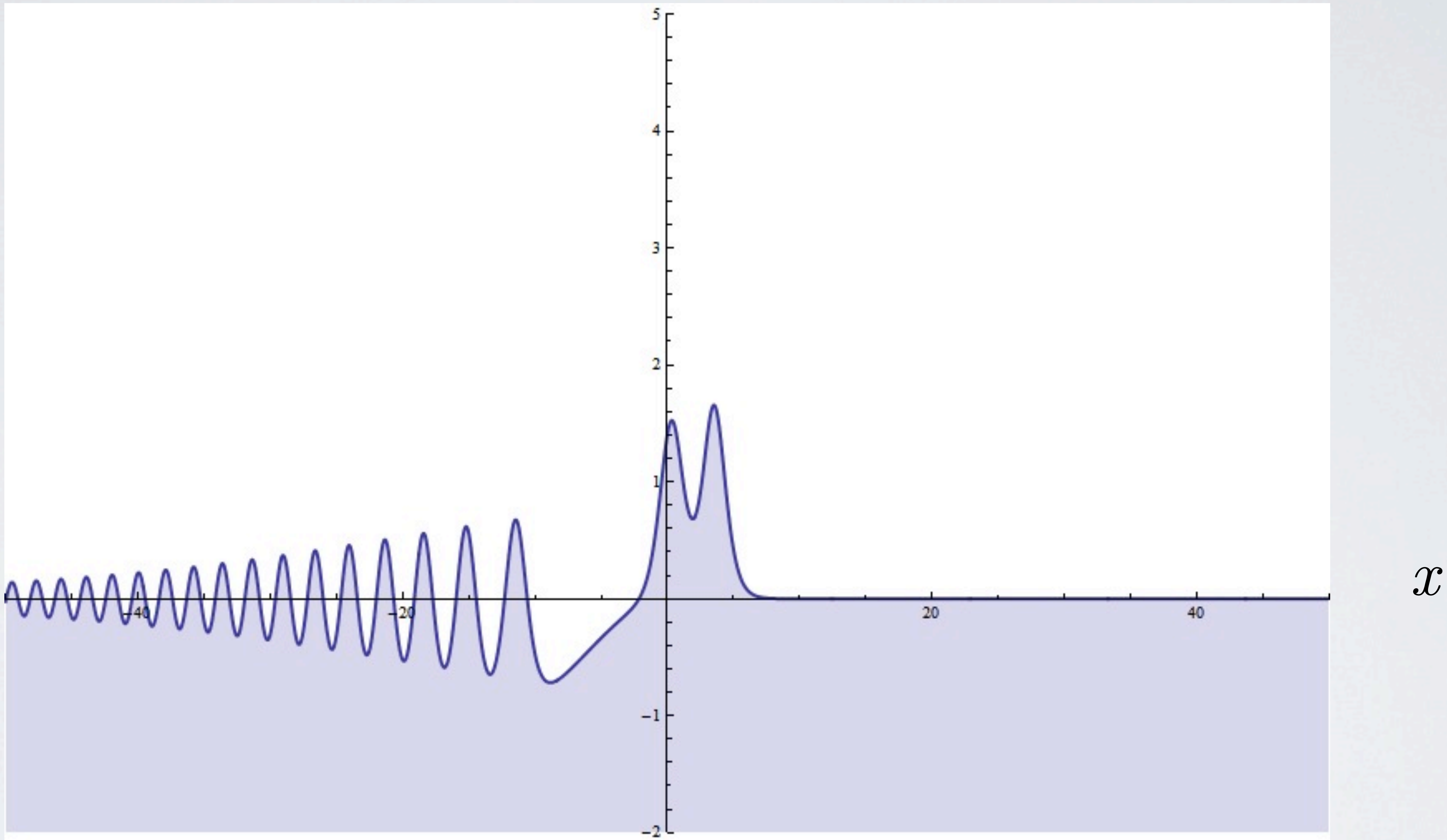
Two solitons



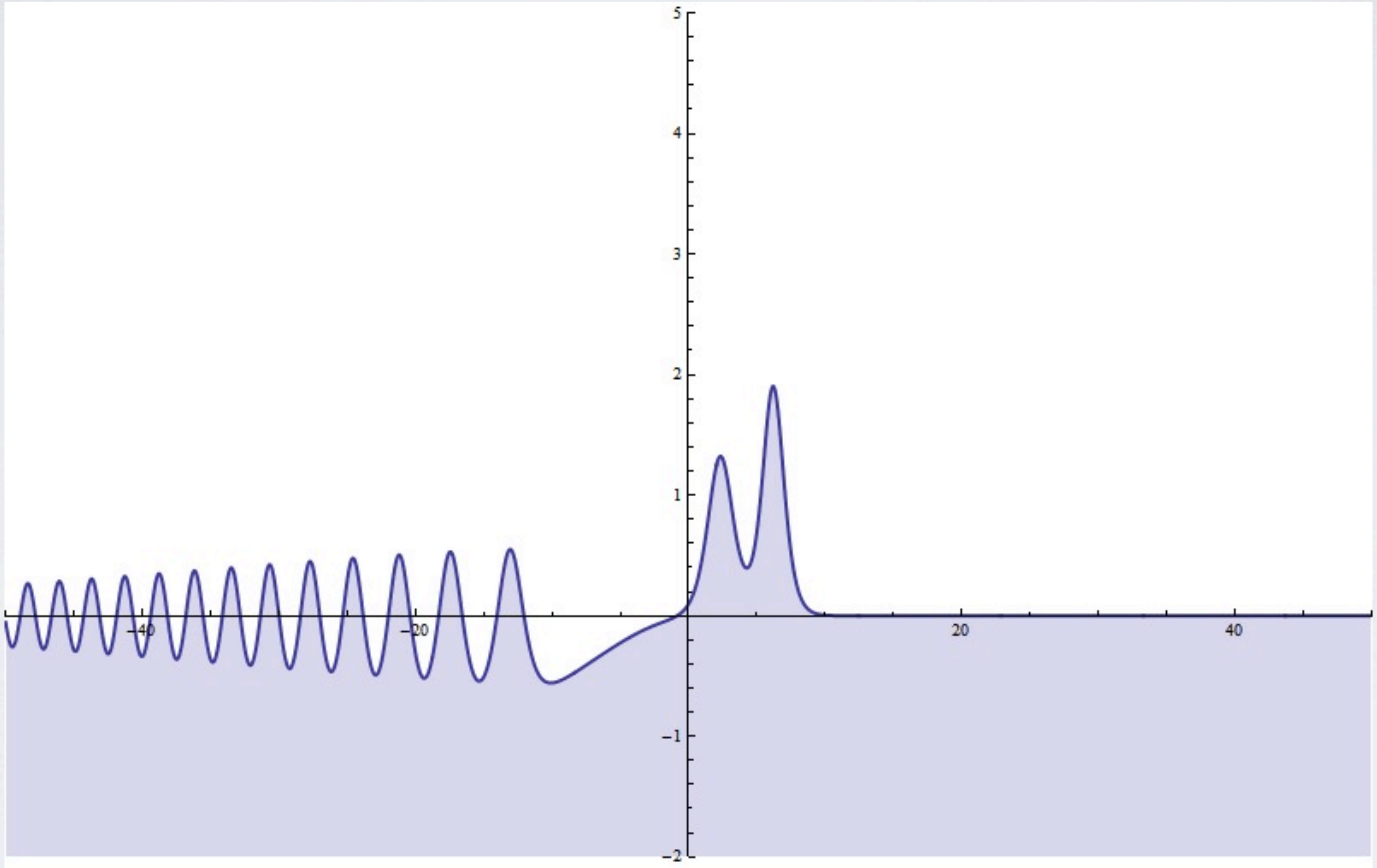
Two solitons



Two solitons

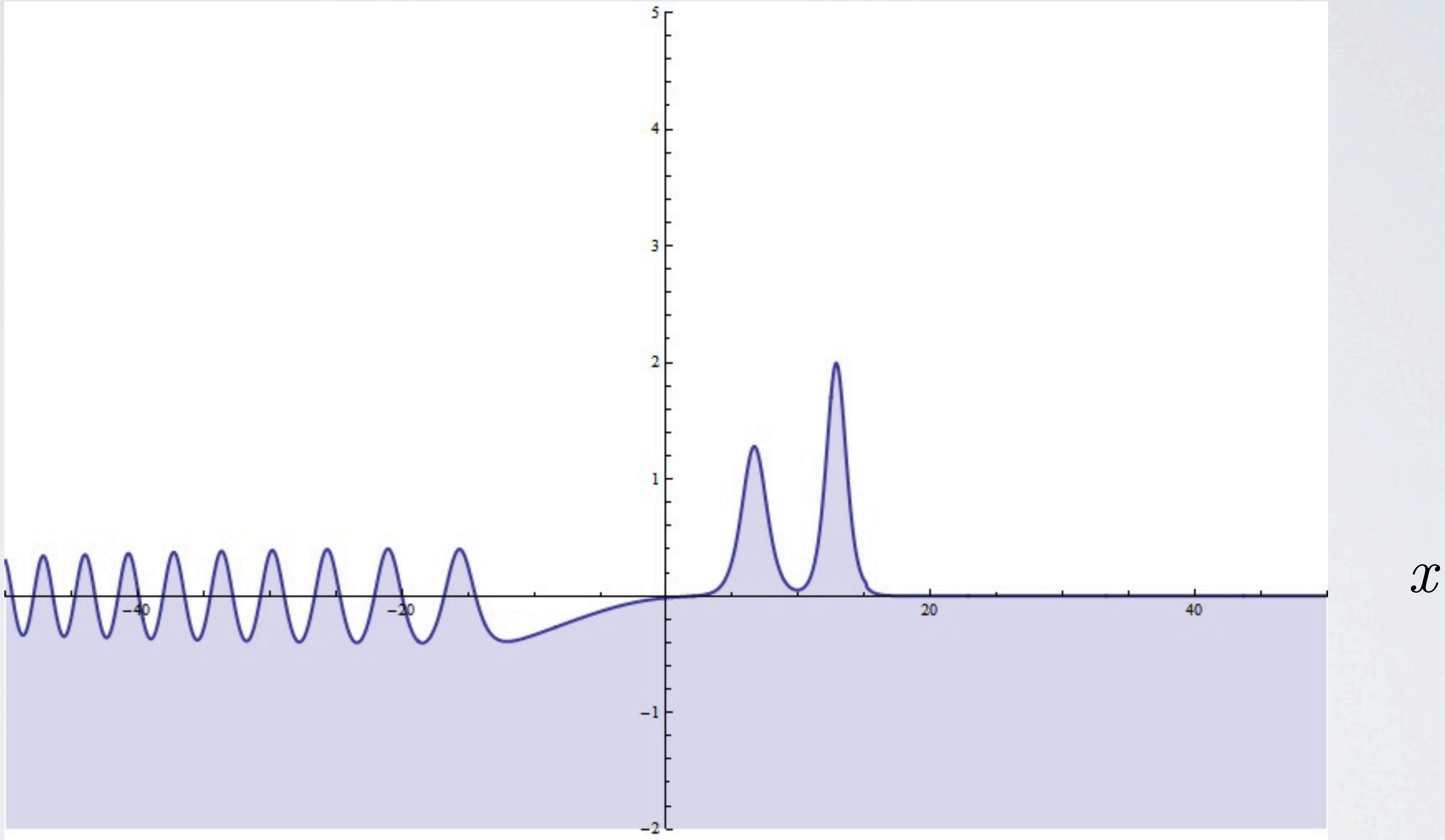


Two solitons



x

Two solitons



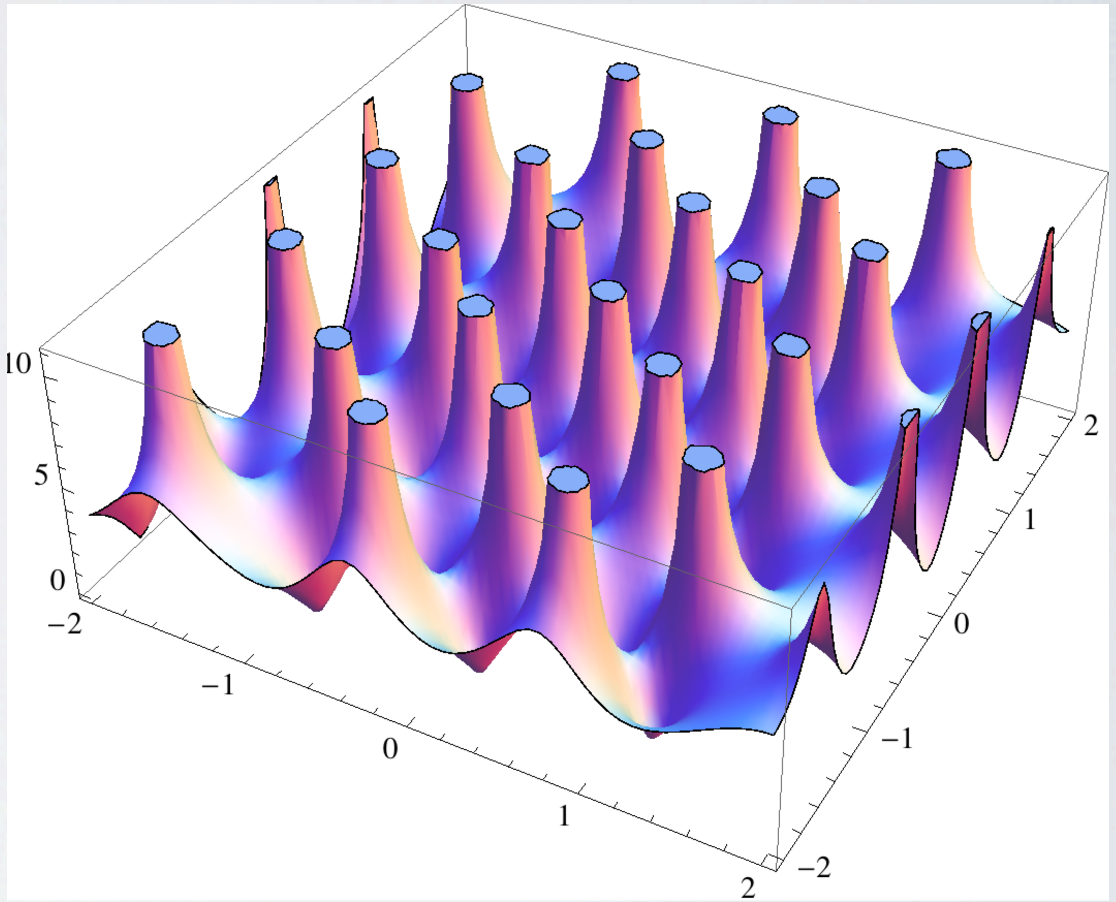
Benefits of an RH numerical approach

- Of course, there are many other numerical methods for such PDEs, however, an approach based on the RH formulation has many benefits, including:
  - x and t are reduced to parameters, therefore we do not need to integrate the solution at a sequence of time steps to compute it for large t
  - Computational cost is bounded for *all* t and x
  - We achieve spectral accuracy and avoid boundary truncation effects
  - The KP and DS equations have two spacial dimensions, making standard numerical methods inefficient
    - y is also simply a parameter in the RH formulation
  - Benjamin–Ono equation has a singular-integral term

Conclusions

- Riemann–Hilbert problems can be numerically solved, efficiently and accurately
- We can now reliably compute solutions to KdV and Painlevé II
    - This could form the building block of a toolbox for computing Painlevé transcendents
    - A first step is the routine `PainleveII[{s1,s2,s3},x]` included in `RHPackage` and reliable for all real x
- Same ideas are applicable to computing other Painlevé transcendents, integrable systems, orthogonal polynomials and random matrix theory distributions

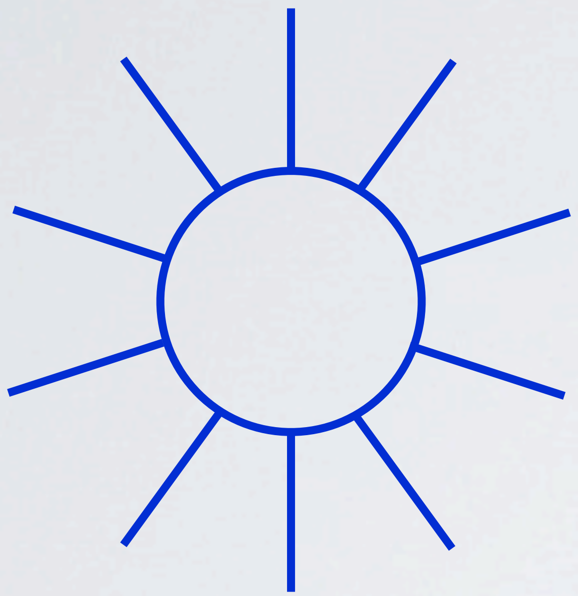
A solution to Painlevé IV



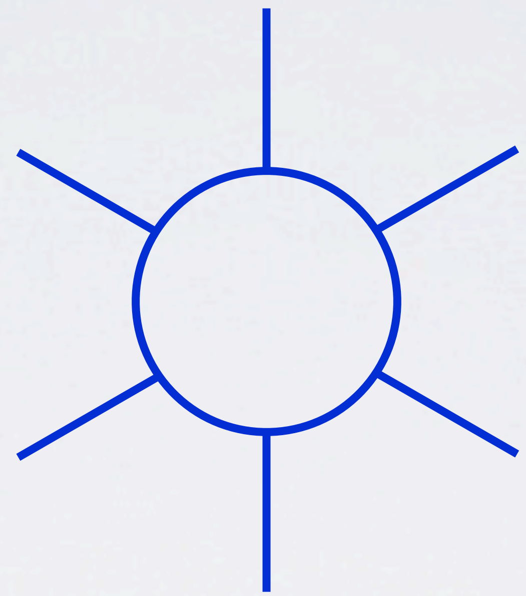
(Mathematica package RHPackage available on my website)

OTHER PAINLEVÉ RH PROBLEMS

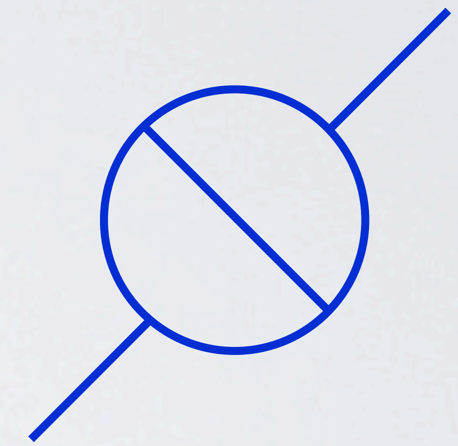
I



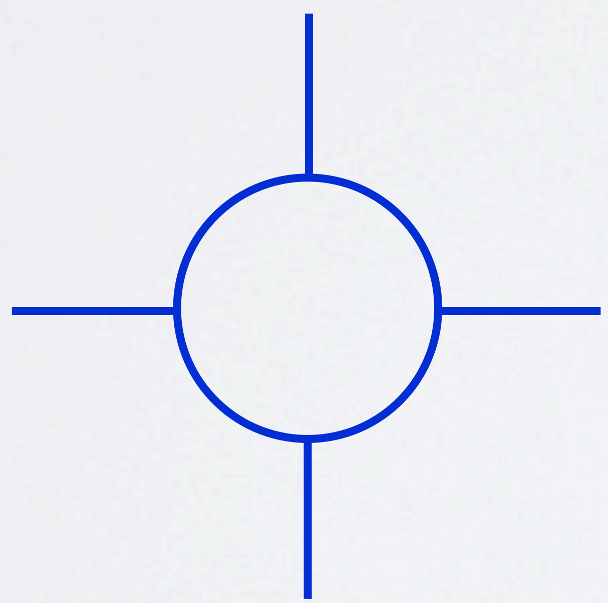
II



III



IV



V