NUMERICAL CALCULATION OF RANDOM MATRIX DISTRIBUTIONS AND ORTHOGONAL POLYNOMIALS

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- We are interested in numerically computing eigenvalue statistics of the GUE ensembles, i.e., Hermitian matrices with the distribution (given a particular V)

$$\frac{1}{Z_n} \mathrm{e}^{-n \operatorname{Tr} V(M)} \, \mathrm{d}M$$

- First question: can we automatically calculate the global mean distribution of eigenvalues, i.e., the equilibrium measure?
- Second question: how do statistics which satisfy universality laws differ when n is finite?
- In short, we do the Riemann–Hilbert approach in a numerical way

- Many other physical and mathematical objects have since been found to also be described by random matrix theory, including:
  - Quantum billiards
  - Random Ising model for glass
  - Trees in the Scandinavian forest
  - Resonance frequencies of structural materials
  - Even the nontrivial zeros of the Riemann zeta function!

OUTLINE

1. Relationship of random matrix theory and orthogonal polynomials
2. Equilibrium measures supported on a single interval
    1. Equivalence to a simple Newton iteration
    2. Equilibrium measures supported on multiple intervals
3. Computation of large order orthogonal polynomials, through Riemann–Hilbert problems
4. Calculation of gap eigenvalue statistics

Relationship of random matrix theory with orthogonal polynomials

- For the Gaussian unitary ensemble (i.e., large random Hermitian matrices), gap eigenvalue statistics can be reduced to the Fredholm determinant

$$\det\left[I + \mathcal{K}_n|_\Omega\right]$$

where the kernel $\mathcal{K}_n$ is constructed from p_n and p_{n+1}; the orthogonal polynomials with respect to the weight

$$\mathrm{e}^{-nV(x)}\,\mathrm{d}x$$

- Fredholm determinants can be easily computed numerically (Bornemann 2010), as long as we can evaluate the kernel
- Therefore, computing distributions depends only on evaluating the orthogonal polynomials
  - We will construct a numerical method for computing p_n and p_{n+1} whose computational cost is independent of n, which requires first calculating the equilibrium measure

EQUILIBRIUM MEASURES

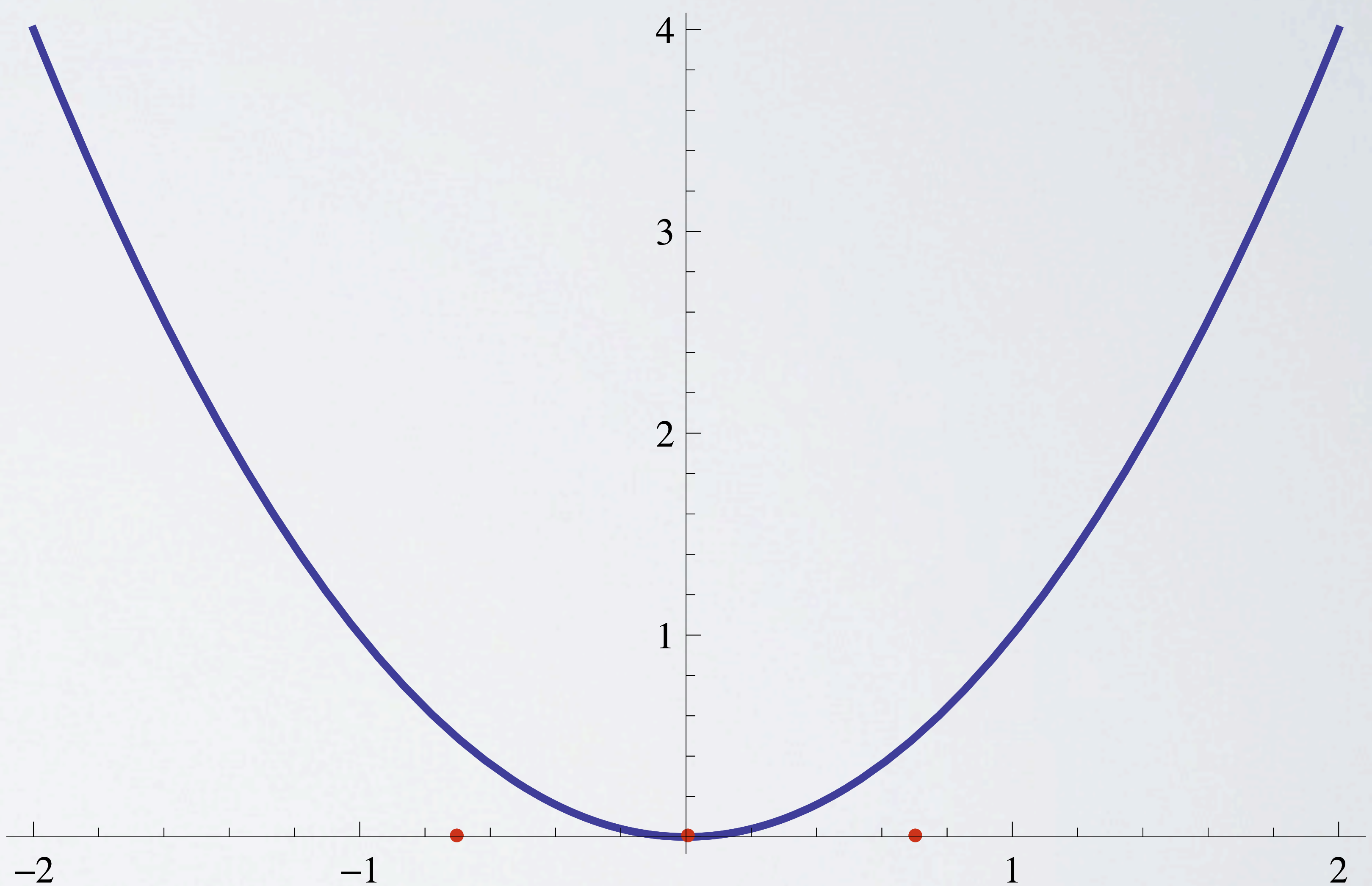
- Suppose the real line is a conductor, on which n discrete charges are placed, with total unit charge
- Suppose further an external field V is present
- The equilibrium measure

$$\mathrm{d}\mu = \psi(x)\,\mathrm{d}x$$

is the limiting distribution (weak* limit) of the charges

- On the right is a sketch for

$$V(x) = x^2$$



(see eg. Saff and Totik 1997)

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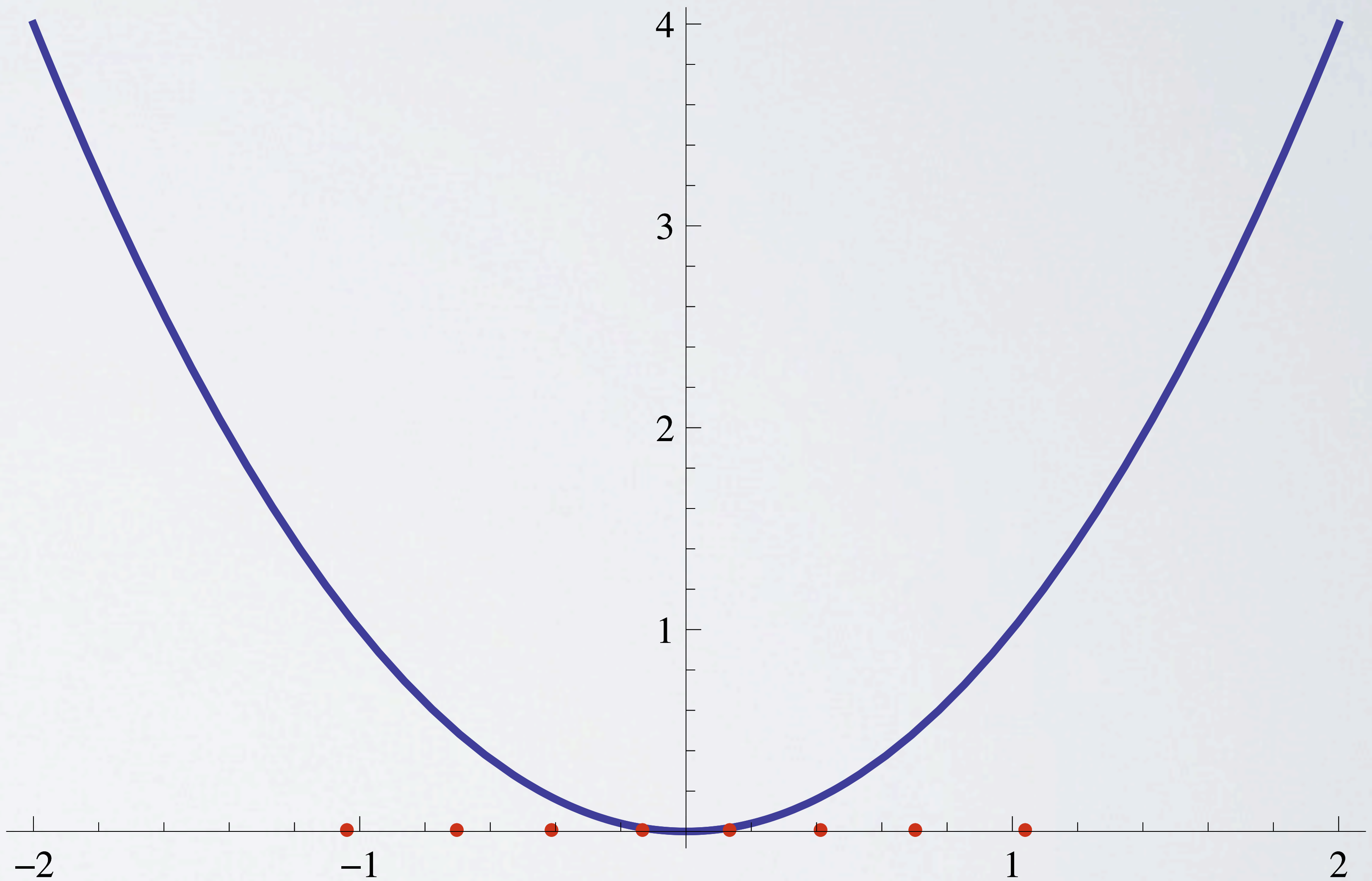

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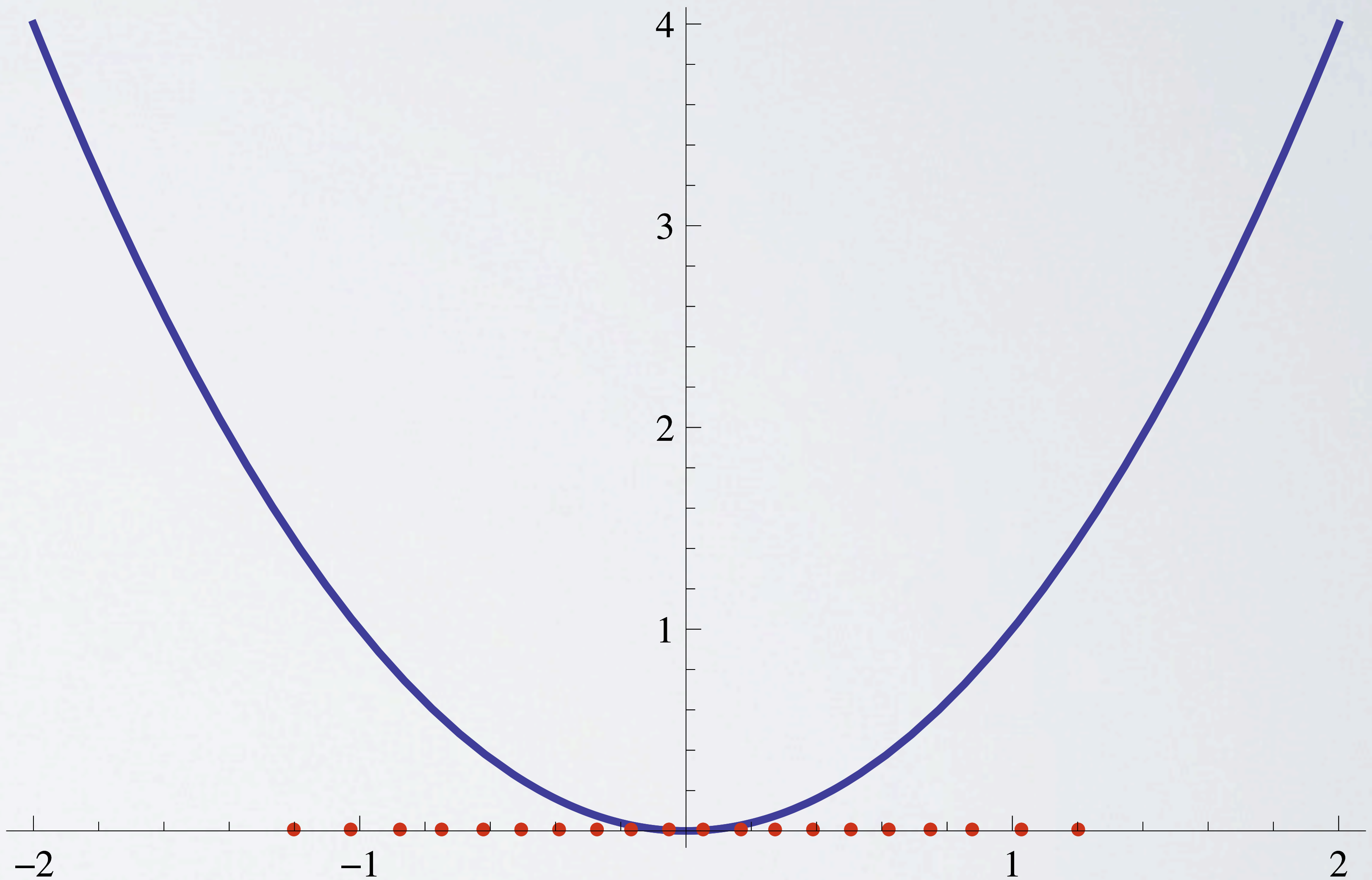

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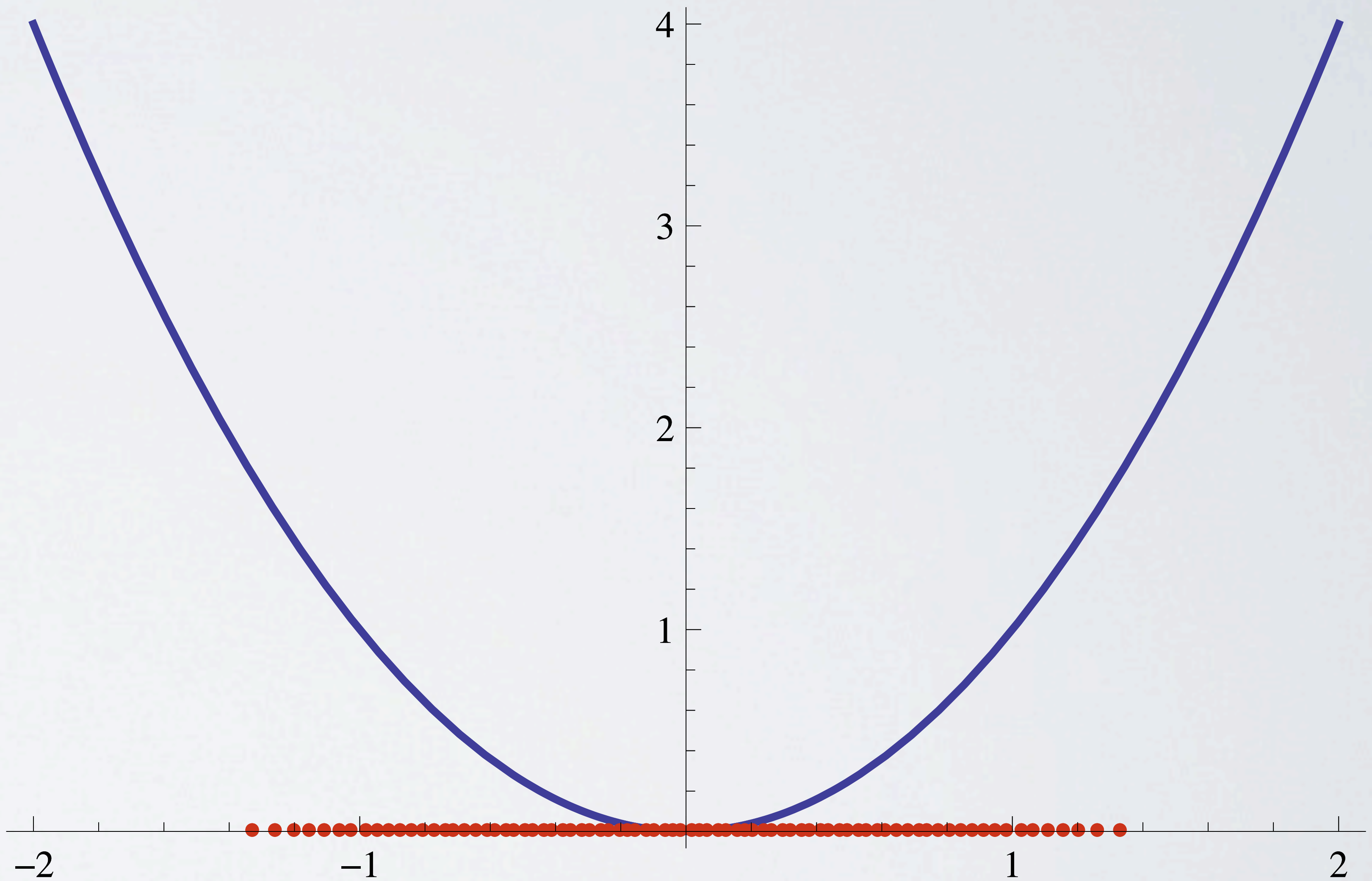

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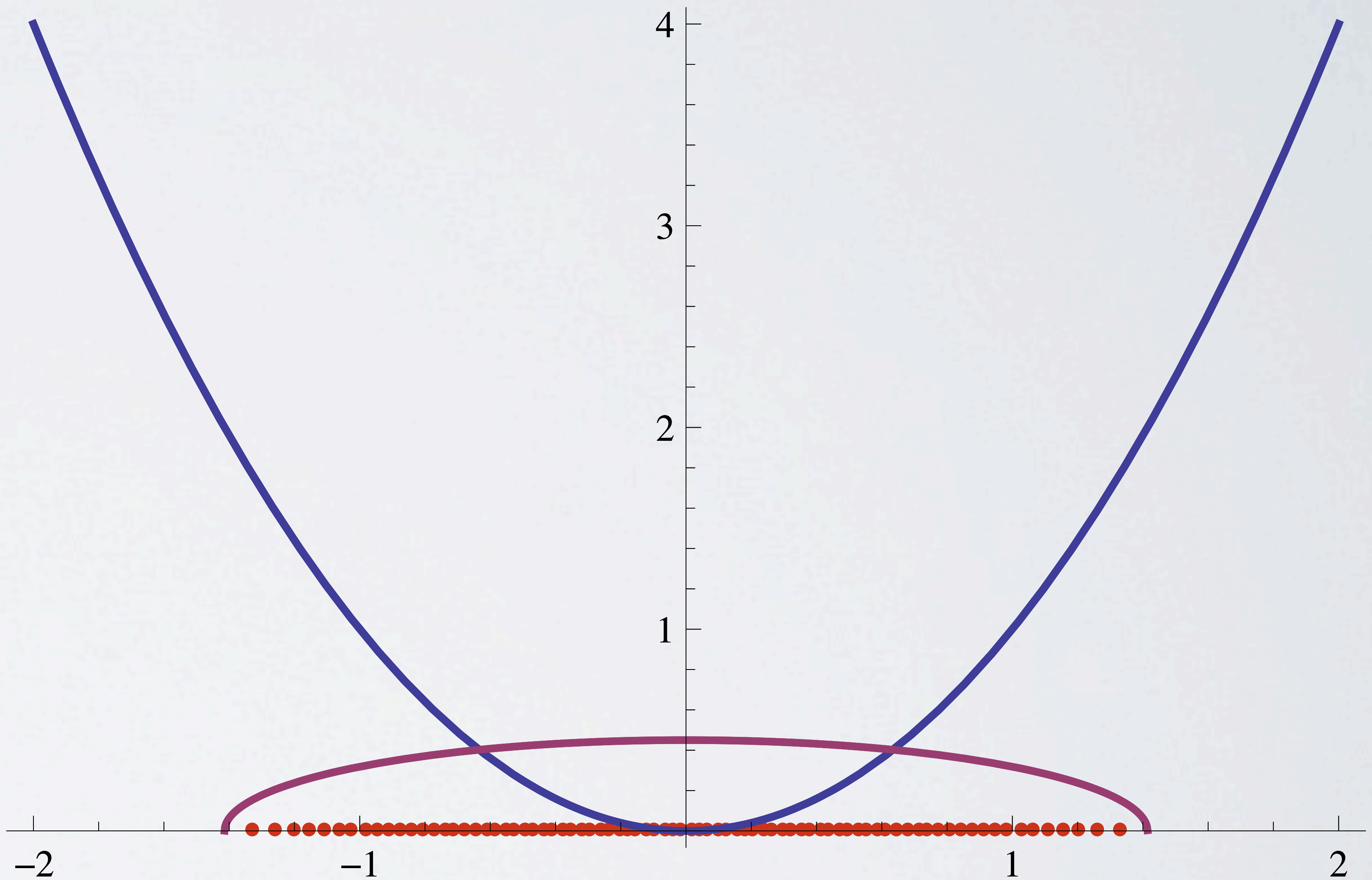

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Applications of the equilibrium measure

- Global mean distribution of the eigenvalues of GUE matrix with distribution

$$\frac{1}{Z_n} \mathrm{e}^{-n \operatorname{Tr} V(M)} \, \mathrm{d}M$$

- Distribution of near optimum interpolation points (*Fekete points*)
- Distribution of zeros of orthogonal polynomials with the weight

$$\mathrm{e}^{-nV(x)} \, \mathrm{d}x$$

  - For $V(x) = x^2$ these are scaled Hermite polynomials
  - In the last slide, I cheated and plotted these roots
- Computing orthogonal polynomials
- Best rational approximation

FORMAL DEFINITION

Given an external field $V : \mathbb{R} \to \mathbb{R}$, the equilibrium measure is the unique Borel measure $\mathrm{d}\mu = \psi(x)\,\mathrm{d}x$ such that

$$\int\int \log \frac{1}{|t-s|}\,\mathrm{d}\mu(t)\,\mathrm{d}\mu(s) + \int V(s)\,\mathrm{d}\mu(s)$$

is minimal.

- This definition can be reduced to the following Euler–Lagrange formulation:

$$2\int \log \frac{1}{|x-z|}\,\mathrm{d}\mu + V(z) = \ell \quad \text{for} \quad z \in \operatorname{supp}\mu$$

$$2\int \log \frac{1}{|x-z|}\,\mathrm{d}\mu + V(z) \geq \ell \quad \text{for all real } z$$

- We let

$$g(z) = \int \log(z-x)\,\mathrm{d}\mu$$

so that (where ± imply limit from the left and right)

$$g^{+} + g^{-} = V - \ell \quad \text{and} \quad g \sim \log z$$

- Differentiating we get

$$\phi^{+} + \phi^{-} = V' \quad \text{and} \quad \phi \sim \frac{1}{z} \quad \text{for} \quad \phi(z) = g'(z) = \int \frac{\mathrm{d}\mu(x)}{z-x}$$

- Now suppose we manage to find an analytic function such that

$$\phi^+ + \phi^- = V' \quad \text{and} \quad \phi \sim \frac{1}{z}$$

on some subset Γ of the real line

- In certain cases (for example, if V is convex), there is only one Γ such that this is possible, hence Γ must be $\mathrm{supp}\ \mu$

- Plemelj's lemma then tells us that we can find $\mathrm{d}\mu = \psi(x)\,\mathrm{d}x$ by:

$$\frac{\mathrm{i}}{2\pi}\left[\phi^+(x) - \phi^-(x)\right] = \psi(x)$$

- For a given Γ, we can find all solutions to

$$\phi^+ + \phi^- = V' \quad \text{and} \quad \phi(z) \sim \frac{c_\Gamma}{z}$$

- The goal, then, is to choose Γ so that:

  - c_Γ is precisely 1

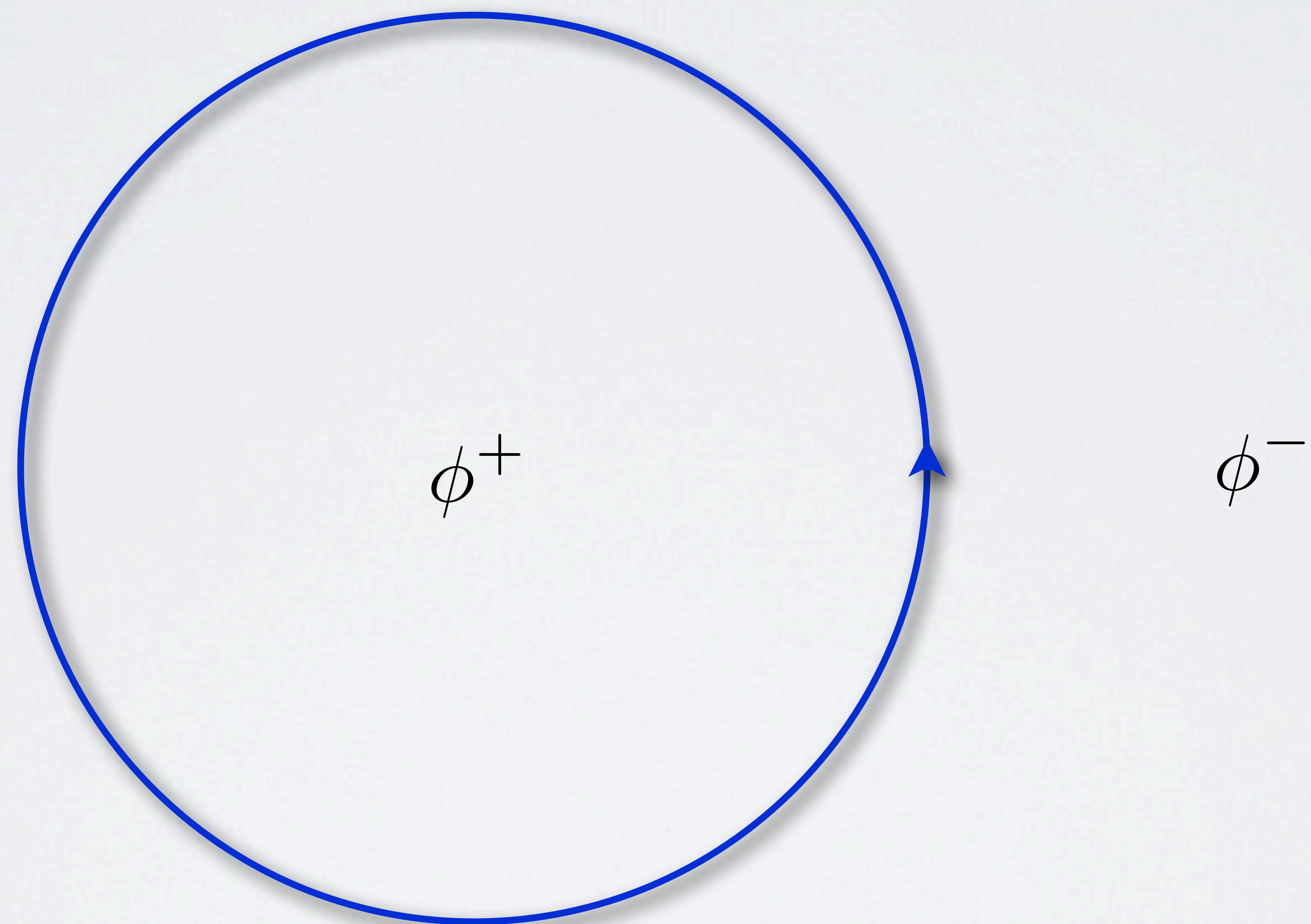
  - ϕ is bounded

- This is the inverse Cauchy transform, which we denote by $\mathcal{P}_\Gamma f$

$$\phi^+(z) + \phi^-(z) = f(z) \qquad \text{and} \qquad \phi(\infty) = 0$$

PROBLEM ON THE CIRCLE

$$f(z) = \sum_{k=-\infty}^{\infty} \hat{f}_k z^k$$



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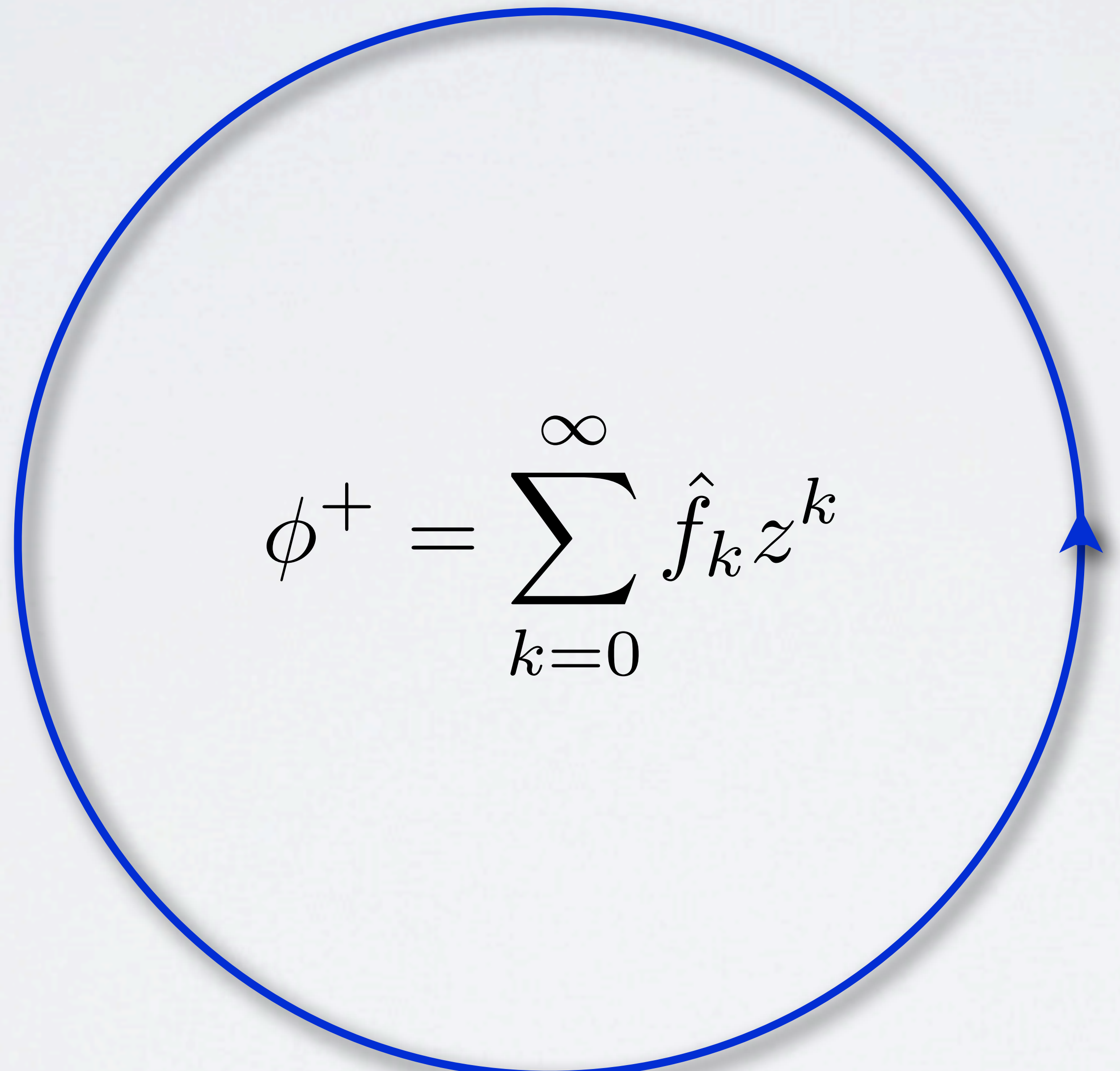


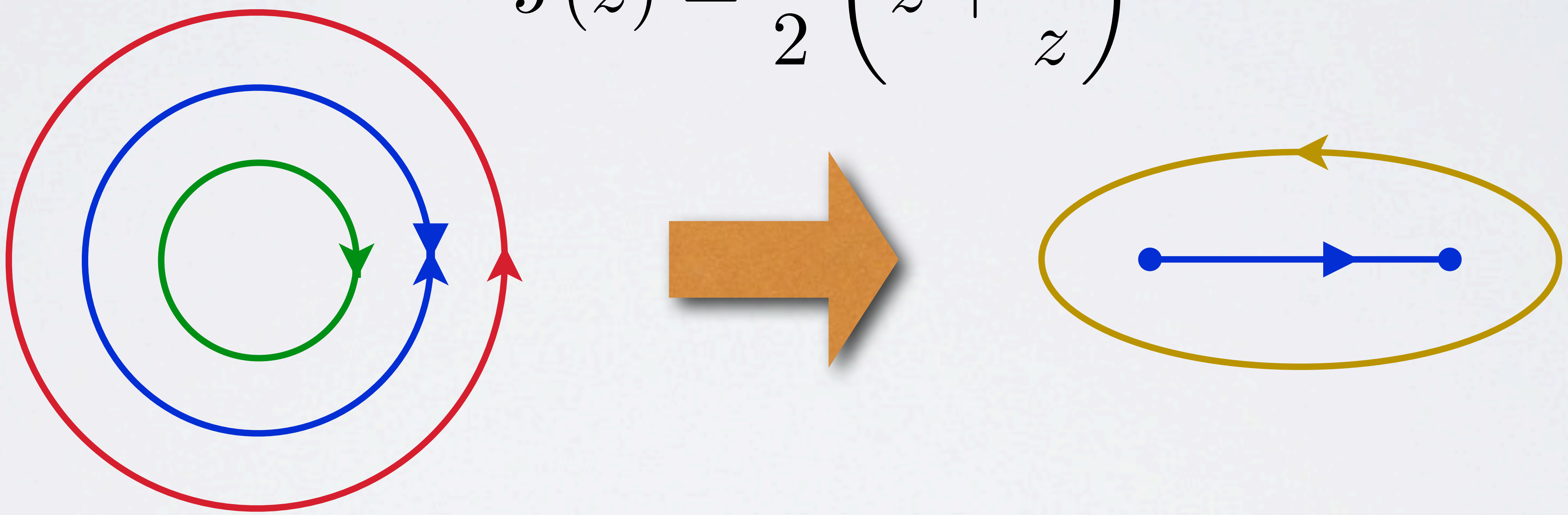
$$\phi^+ = \sum_{k=0}^{\infty} \hat{f}_k z^k$$

$$\phi^- = \sum_{k=-\infty}^{-1} \hat{f}_k z^k$$

PROBLEM ON THE UNIT INTERVAL

Consider the Joukowski map from the unit circle to the unit interval

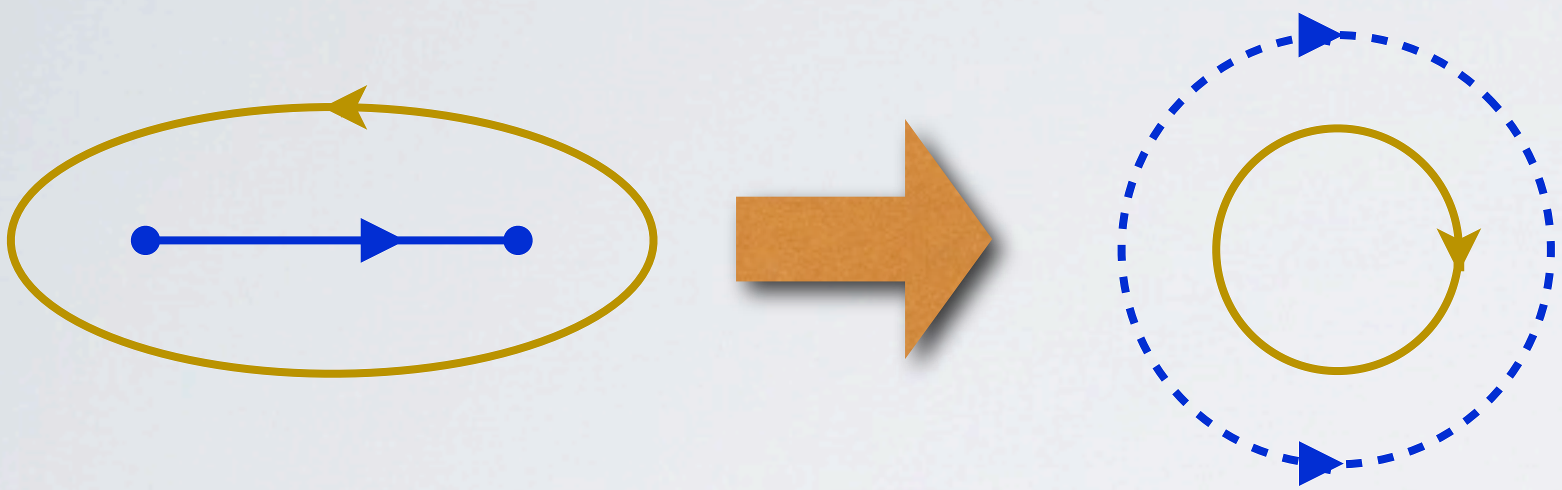
$$J(z) = \frac{1}{2}\left(z + \frac{1}{z}\right)$$



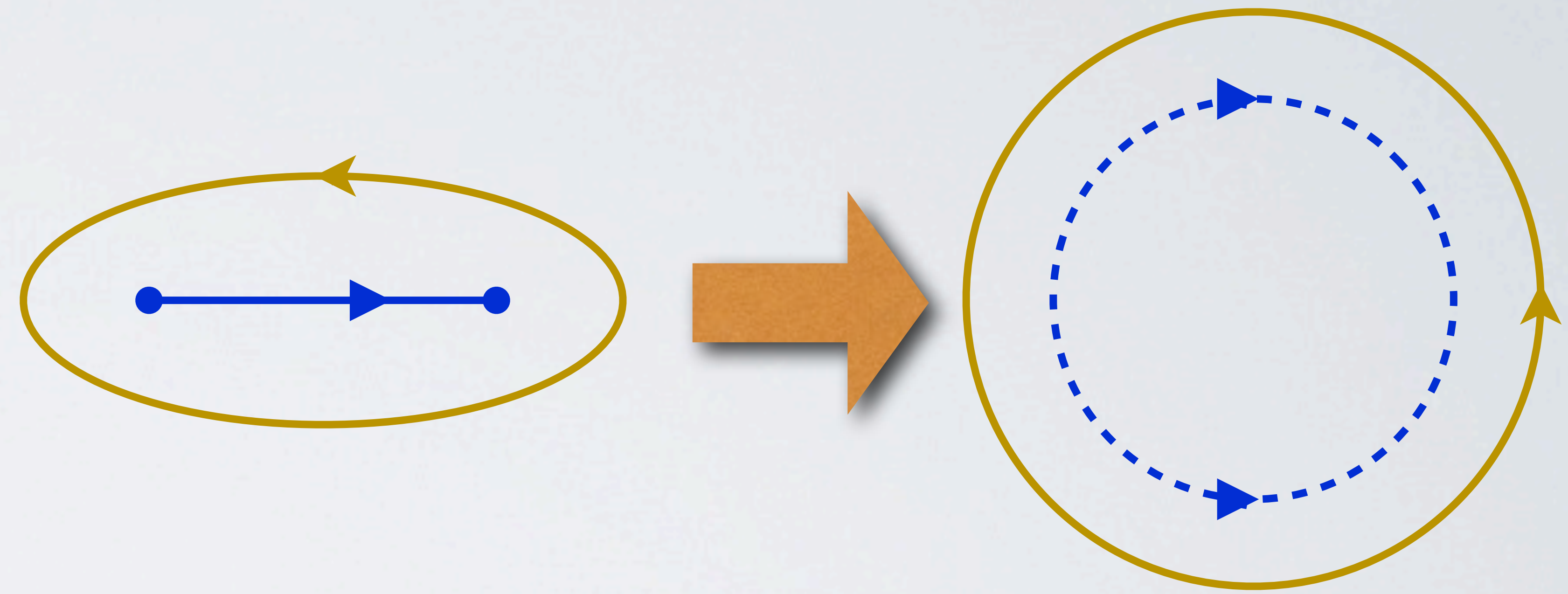
Functions analytic inside and outside the unit circle are mapped to functions analytic off the unit interval.

We define four inverses to the Joukowski map:

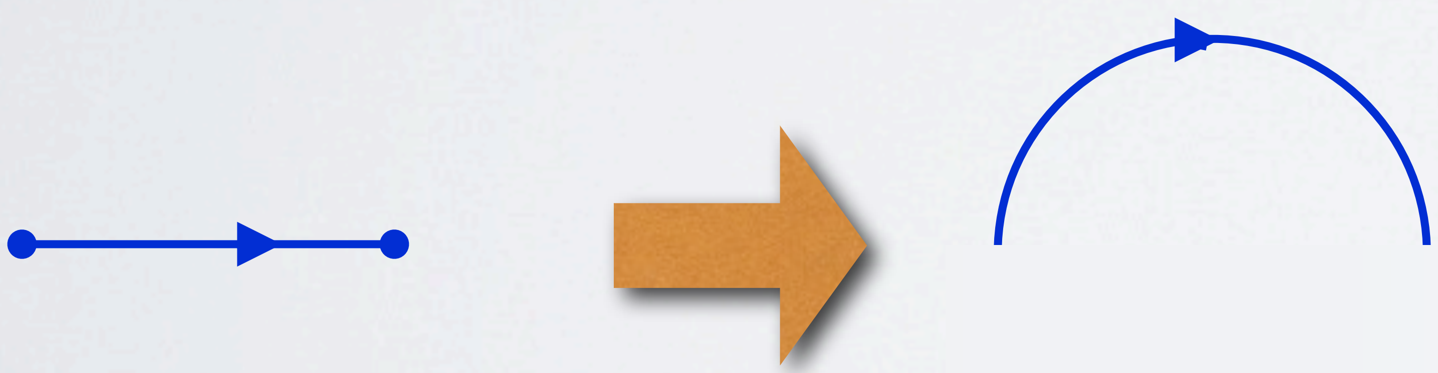
$$J_{+}^{-1}(x) = x - \sqrt{x-1}\sqrt{x+1}$$



$$J_{-}^{-1}(x) = x + \sqrt{x-1}\sqrt{x+1}$$



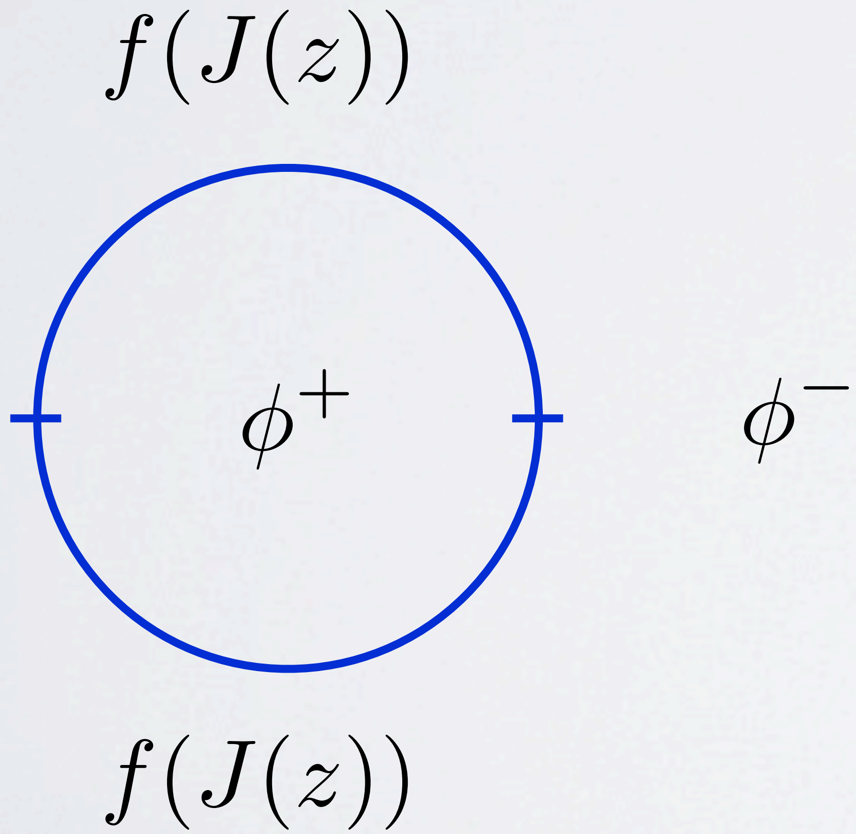
$$J_{\uparrow}^{-1}(x) = x + \mathrm{i}\sqrt{1-x}\sqrt{1+x}$$



$$J_{\downarrow}^{-1}(x) = x - \mathrm{i}\sqrt{1-x}\sqrt{1+x}$$

Suppose we compute the inverse Cauchy transform of the mapped function on the unit circle

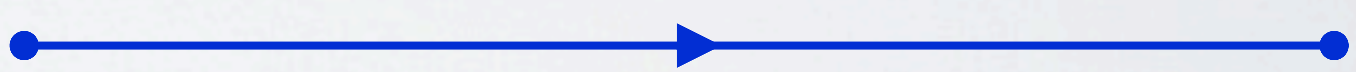
$$\phi = \mathcal{P}_{\circ} f(J(\cdot))$$



Then the following function satisfies the necessary jump

$$\frac{1}{2}\left[\phi(J_{+}^{-1}(x)) + \phi(J_{-}^{-1}(x))\right]$$

$$\frac{1}{2}\left[\phi^{+}(J_{\downarrow}^{-1}(x)) + \phi^{-}(J_{\uparrow}^{-1}(x))\right]$$



$$\frac{1}{2}\left[\phi^{+}(J_{\uparrow}^{-1}(x)) + \phi^{-}(J_{\downarrow}^{-1}(x))\right]$$

- The problem:

$$\frac{1}{2}\left[\phi(J_+^{-1}(\infty)) + \phi(J_-^{-1}(\infty))\right] = \frac{1}{2}\left[\phi(0) + \phi(\infty)\right] = \frac{\hat{f}_0 + 0}{2} = \frac{\hat{f}_0}{2} \neq 0$$

- Fortunately,

$$\kappa(z) = \frac{1}{\sqrt{z+1}\sqrt{z-1}}$$

has no jump on the contour: $\kappa^+ + \kappa^- = 0 \quad \text{and} \quad \kappa(z) \sim \frac{1}{z}$

- Therefore, we find that

$$\mathcal{P}_\xi f = \frac{1}{2}\left[\phi(J_+^{-1}(x)) + \phi(J_-^{-1}(x))\right] - \frac{\hat{f}_0}{2} z\kappa(z) + \xi\kappa(z)$$

where there is now a free parameter

- Now suppose f is sufficiently smooth, so that it can be expanded into Chebyshev series (in $O(n \log n)$ time using the DCT):

$$f(x) = \sum_{k=0}^{\infty} \check{f}_k T_k(x)^k$$

- Then

$$f(J(z)) = \check{f}_0 + \frac{1}{2} \sum_{k=-\infty}^{\infty} \check{f}_k z^k$$

- It follows that (a numerically stable, uniformly convergent expression)

$$\mathcal{P}_\xi f(z) = \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_k J_+^{-1}(z)^k - \frac{\check{f}_0}{2} z\kappa(z) + \xi\kappa(z)$$

OTHER INTERVALS

$$M_{(a,b)}(z) = \frac{2z - a - b}{b - a}$$ maps the interval (a, b) to the unit interval.

Let $\check{f}_{(a,b),k}$ be the Chebyshev coefficents over (a, b), so that

$$f(z) = \sum_{k=0}^{\infty} \check{f}_{(a,b),k} T_k(M_{(a,b)}(z))^k$$

Then

$$\mathcal{P}_{(a,b),\xi} f(z) = \frac{1}{2} \sum_{k=0}^{\infty} \check{f}_{(a,b),k} J_+^{-1}(M_{(a,b)}(z))^k - \frac{\check{f}_{(a,b),0}}{2} M_{(a,b)}(z) \kappa(M_{(a,b)}(z)) + \xi \kappa(M_{(a,b)}(z))$$

$$\boxed{\mathcal{P}_{(a,b),\xi} f(z) = \frac{1}{2}\sum_{k=0}^{\infty} \check{f}_{(a,b),k} J_+^{-1}(M_{(a,b)}(z))^k - \frac{\check{f}_{(a,b),0}}{2} M_{(a,b)}(z)\kappa(M_{(a,b)}(z)) + \xi\kappa(M_{(a,b)}(z))}$$

- Let $f = V'$. The only way the solution is bounded is if

$$\xi = 0 \qquad \text{and} \qquad \check{f}_{(a,b),0} = 0$$

- Since

$$J_+^{-1}(z) \sim \frac{1}{2z} + \mathcal{O}\big(z^{-2}\big) \quad \text{and} \quad M_{(a,b)}(z) \sim \frac{2z}{b-a} + \mathcal{O}(1)$$

we require

$$\frac{b-a}{8}\check{f}_{(a,b),1} = 1$$

so that

$$\mathcal{P}_{(a,b)} f(z) \sim \frac{1}{z}$$

(equivalent to standard conditions in terms of moments)

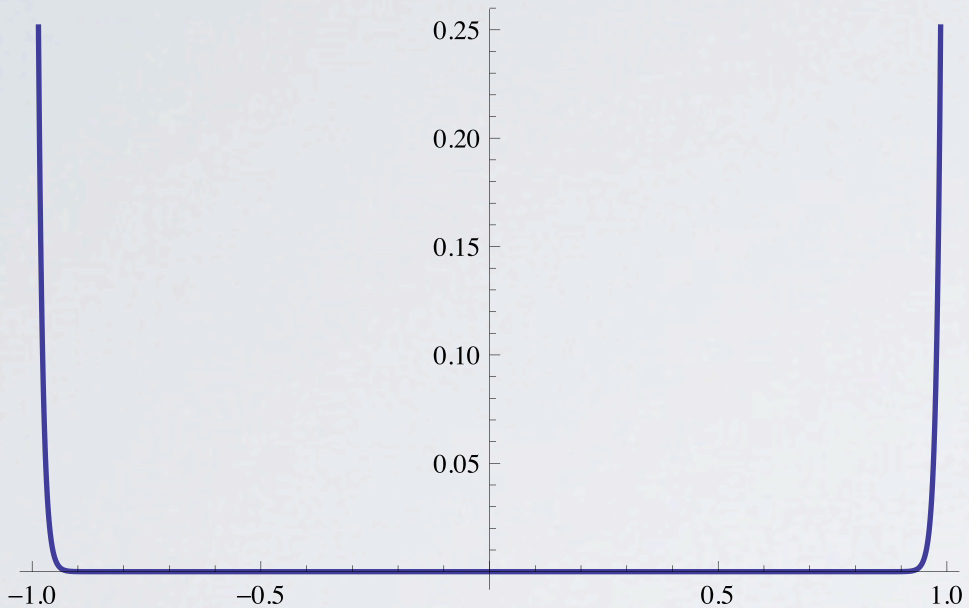
- We thus have two unknowns, a and b, with two conditions:

$$\check{f}_{(a,b),0} = 0 \qquad \text{and} \qquad \frac{b-a}{8}\check{f}_{(a,b),1} = 1$$

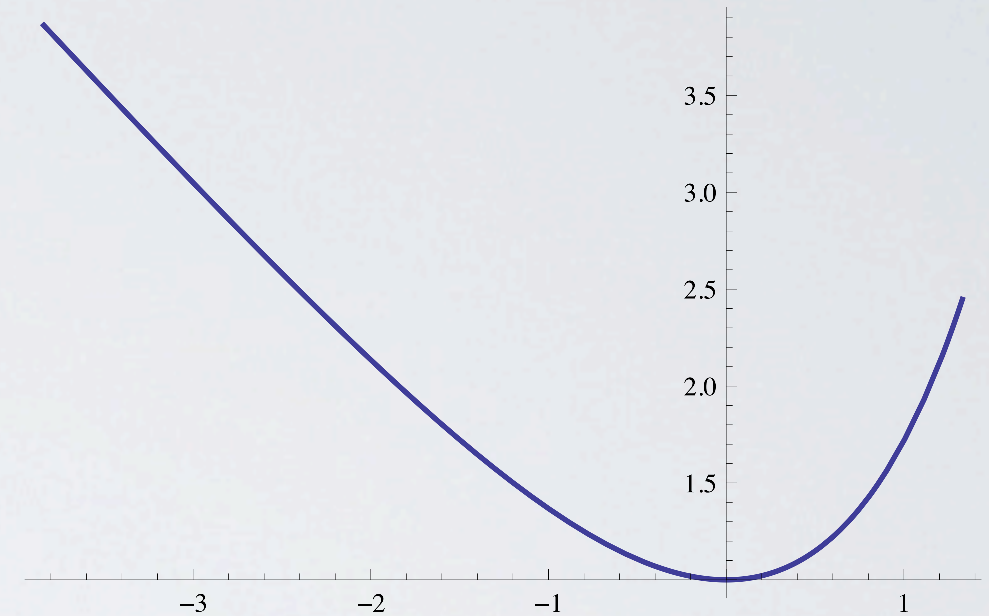
- The Chebyshev coefficients can be computed efficiently using the FFT
- Moreover, each of these equations are differentiable with respect to a and b
- Thus we can setup a trivial Newton iteration to determine a and b
- This iteration is guaranteed to converge to $\operatorname{supp}\,\mu$ whenever V is convex
  - or, if $\operatorname{supp}\,\mu$ is a single interval and the initial guess of a and b are sufficiently accurate
- We then recover the equilibrium measure using the formula

$$\mathrm{d}\mu = \frac{\sqrt{1 - M_{(a,b)}(x)}}{\pi} \sum_{k=1}^{\infty} \check{f}_k U_{k-1}(M_{(a,b)}(x))\,\mathrm{d}x$$

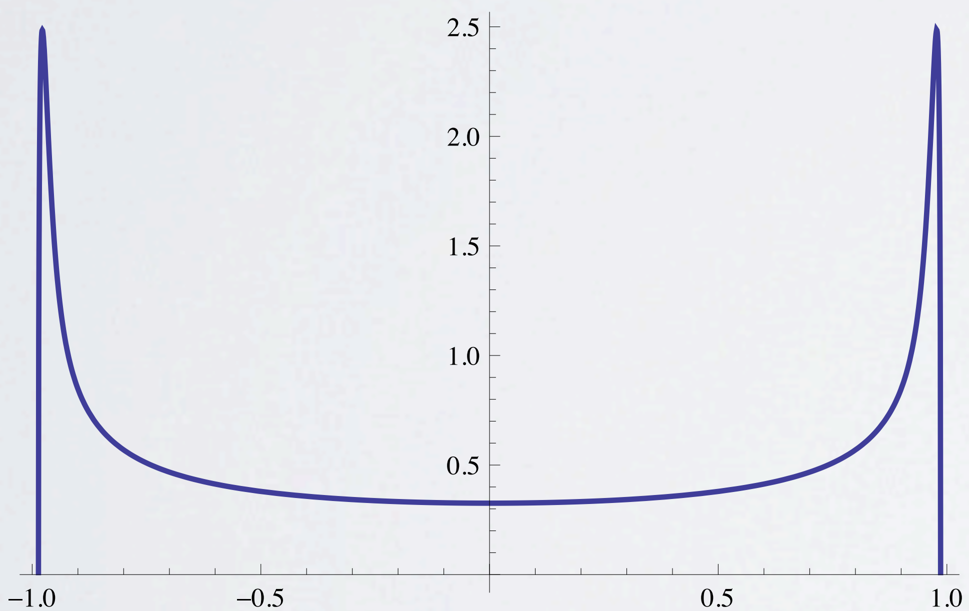
x^{100}



$\mathrm{e}^x - x$



$\mathrm{d}\mu$



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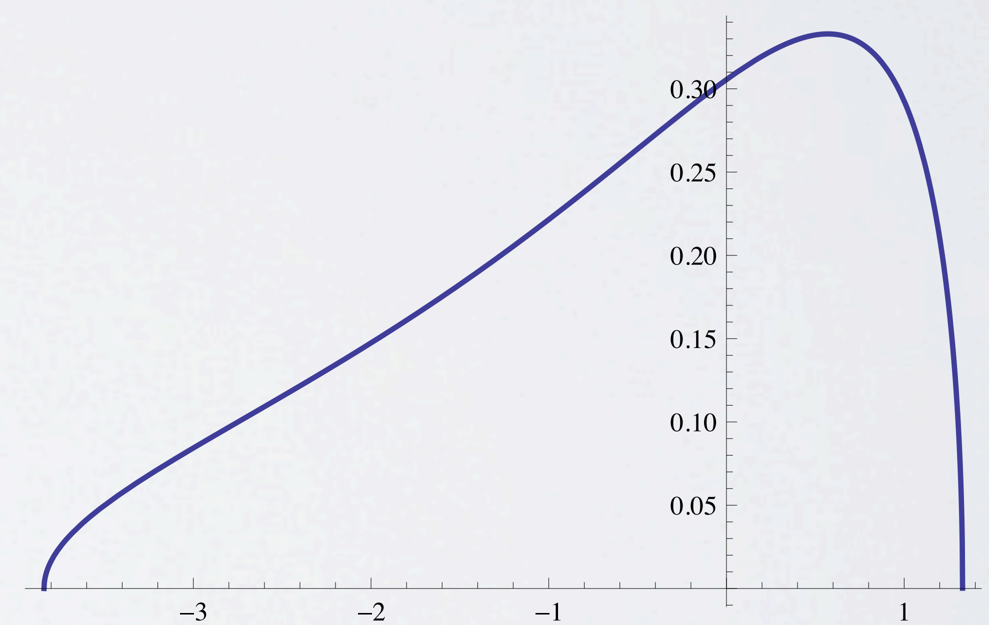
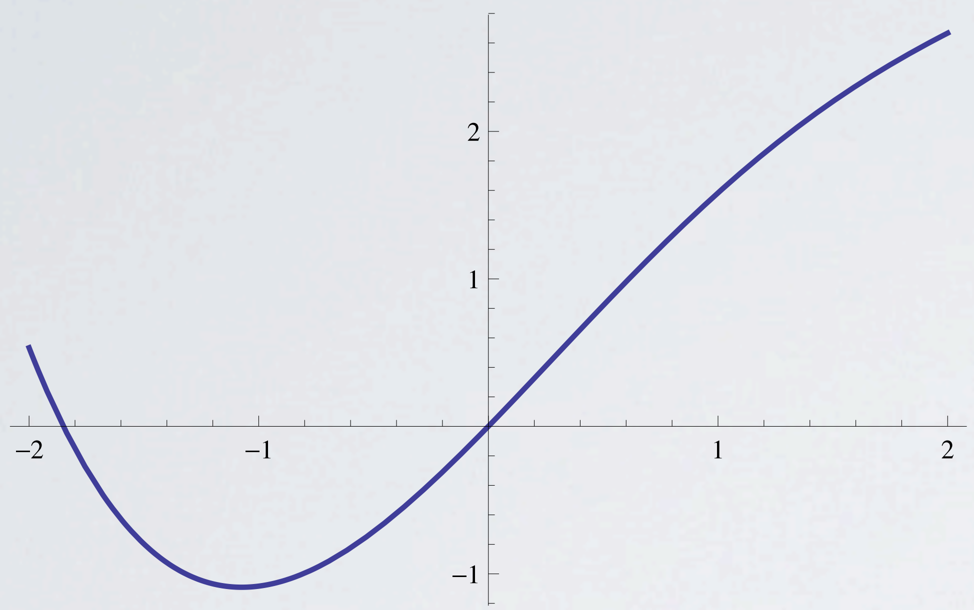
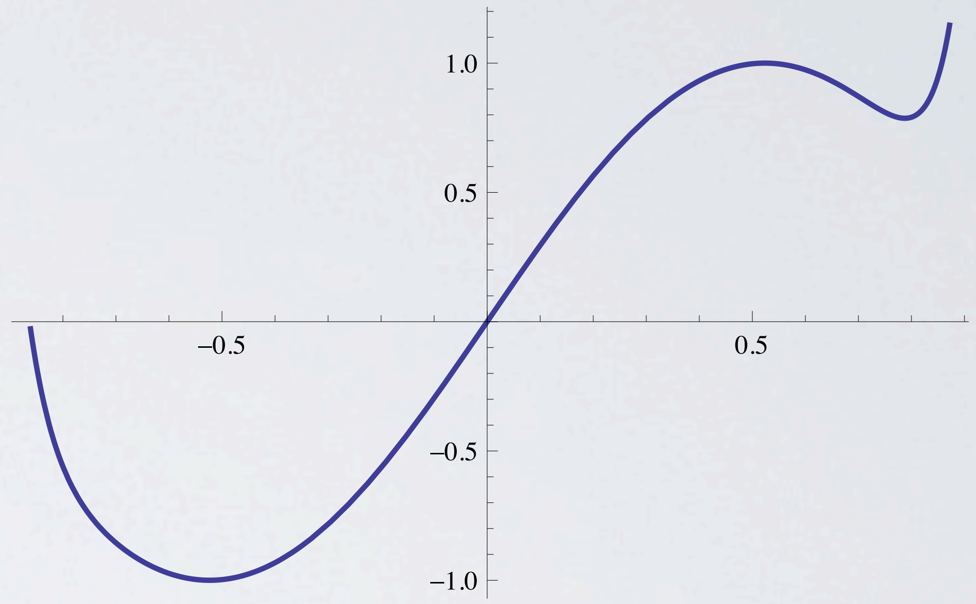


$$\frac{1}{5}x^2 - \frac{4}{15}x^3 + \frac{1}{20}x^4 + \frac{8}{5}x$$

$$\sin 3x + 10x^{20}$$





$$\mathrm{d}\mu$$

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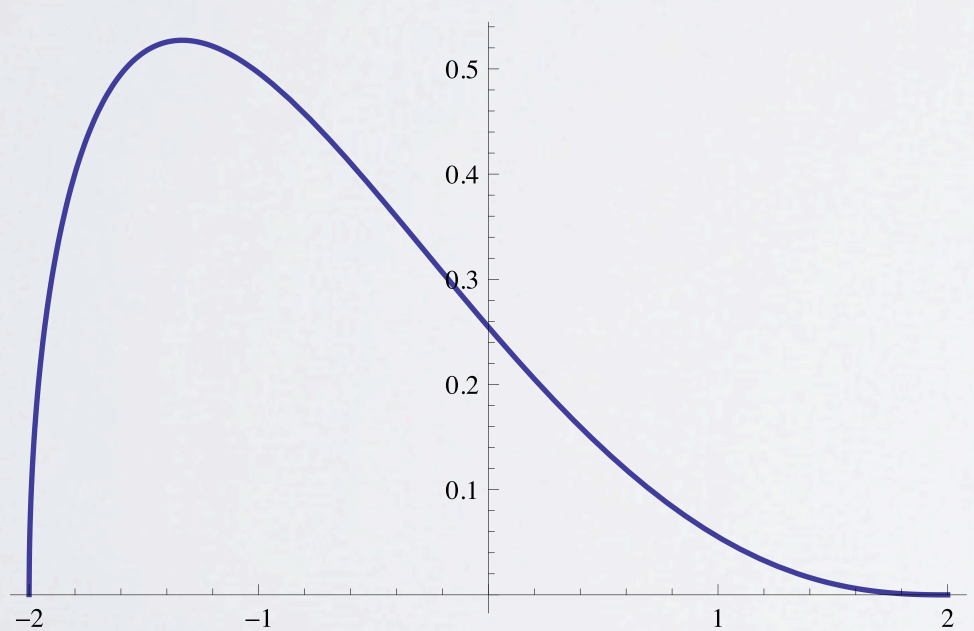
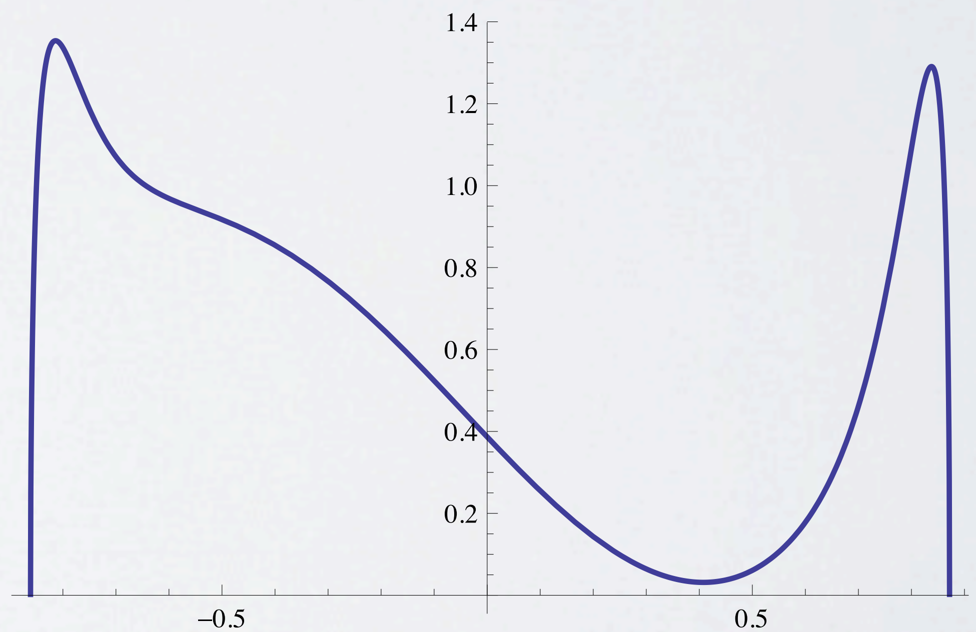




- In the last two examples, the potential was not convex
- Therefore, we have no guarantee that these are indeed the equilibrium measures
- However, we can verify that they are, by testing the conditions that

$$g^+ + g^- = V - \ell \text{ on supp } d\mu$$

$$\text{and} \quad g^+ + g^- \leq V - \ell \text{ on the real line,}$$

where $g = \int \mathcal{P} f$ and ℓ is some constant

- We must therefore calculate the indefinite integral of $\mathcal{P} f$
- This will be needed for the multiple interval case as well

- It is straightforward to find the following formulæ:

$$\begin{aligned}
\int \kappa_\Sigma(z)\,\mathrm{d}z &= \frac{a-b}{2}\log J_+^{-1}(M_\Sigma(z)),\\
\int M_\Sigma(z)\kappa_\Sigma(z)\,\mathrm{d}z &= \frac{b-a}{2}\left[M_\Sigma(z) - J_+^{-1}(M_\Sigma(z))\right],\\
\int J_+^{-1}(M_\Sigma(z))\,\mathrm{d}z &= \frac{b-a}{4}\left[\frac{1}{2}J_+^{-1}(M_\Sigma(z))^2 - \log J_+^{-1}(M_\Sigma(z))\right],\\
\int J_+^{-1}(M_\Sigma(z))^k\,\mathrm{d}z &= \frac{b-a}{4}\left[\frac{1}{k+1}J_+^{-1}(M_\Sigma(z))^{k+1} - \frac{1}{k-1}J_+^{-1}(M_\Sigma(z))^{k-1}\right].
\end{aligned}$$

- The first three have a branch cut along $(-\infty, b)$, the rest only along (a, b)

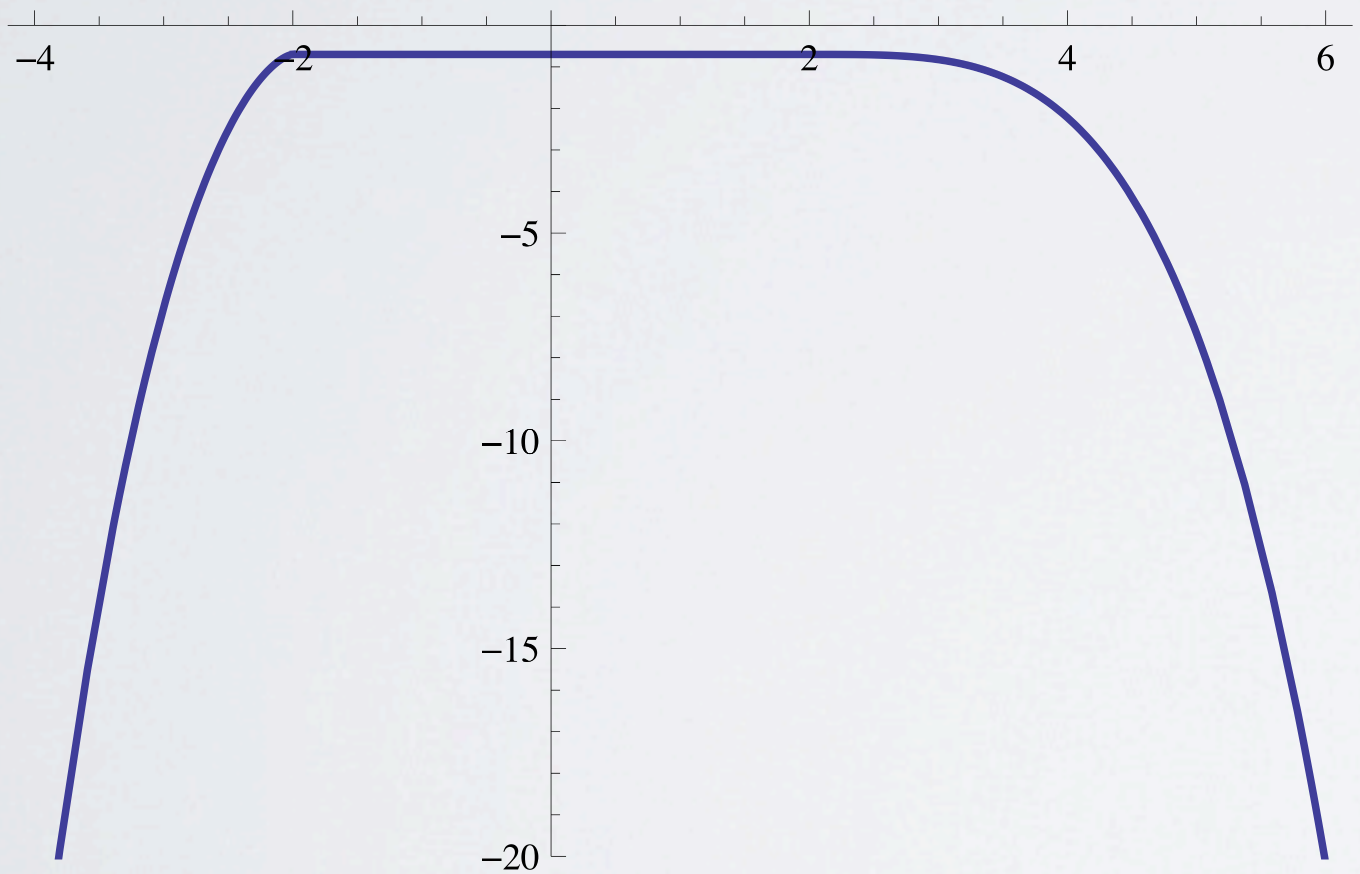
- By using $J_\uparrow^{-1}(M_\Sigma(x))$ and $J_\downarrow^{-1}(M_\Sigma(x))$ we can reliably evaluate these along the branch cut

- The constant of integration is a free parameter, chosen so that

$$g(z) - \log z = \mathcal{O}\left(\frac{1}{z}\right)$$

$$g^{+} + g^{-} - V$$

$$\frac{1}{5}x^2 - \frac{4}{15}x^3 + \frac{1}{20}x^4 + \frac{8}{5}x$$



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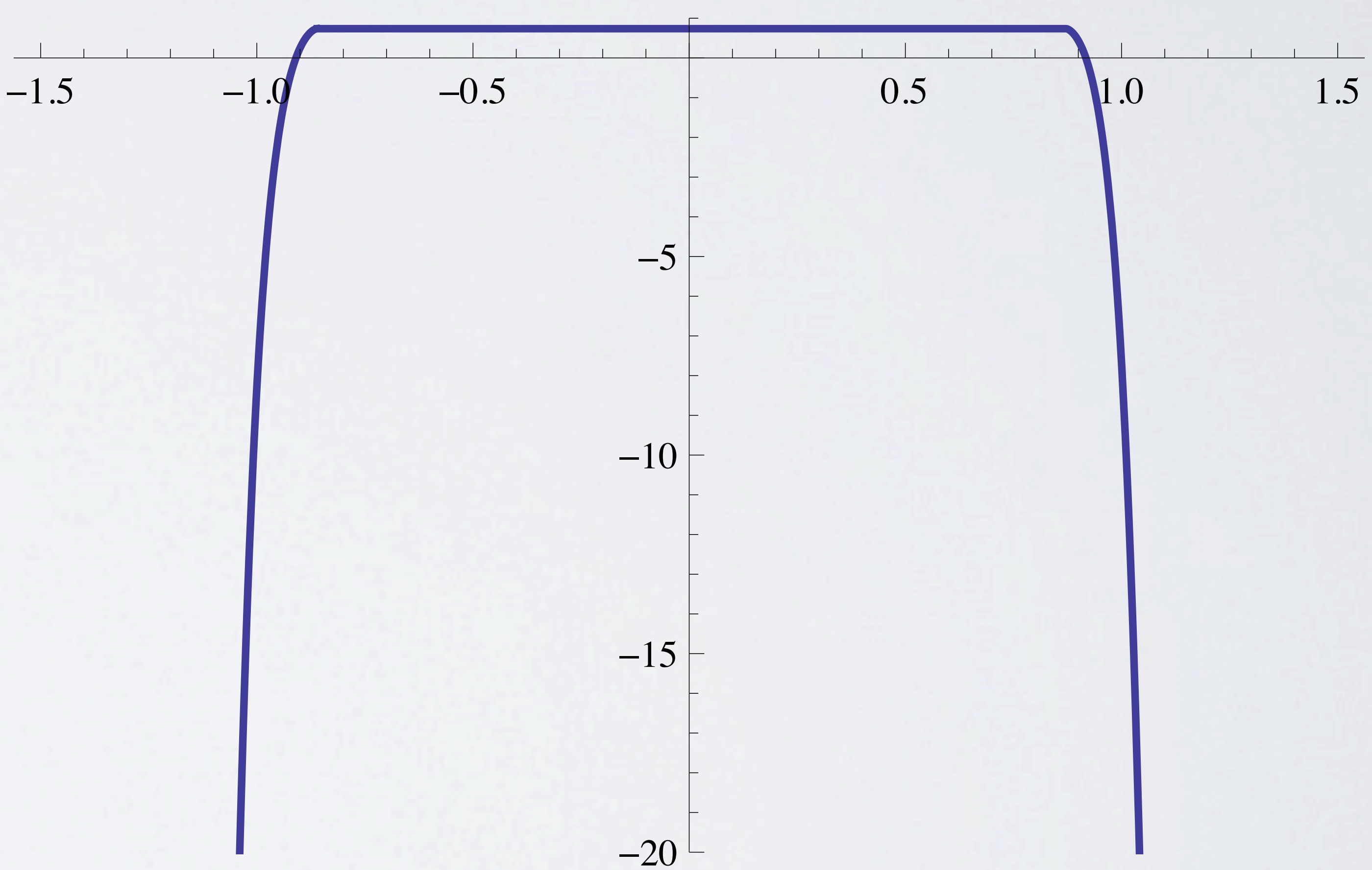


MULTIPLE INTERVALS

- We first compute $\mathcal{P}_\Gamma$ where Γ consists of two, disjoint intervals $\Gamma = \Gamma_1 \cup \Gamma_2$
- We represent the solution as a sum over each interval:

$$\mathcal{P}_\Gamma f = \mathcal{P}_{\Gamma_1} r_1 + \mathcal{P}_{\Gamma_2} r_2$$

- We need to determine r_1 and r_2

- We represent r_1 and r_2 as Chebyshev series
- From the one interval case, we can compute

$$\mathcal{P}_{\Gamma_\lambda} r_\kappa(z) = \sum \check{r}_{\lambda,k} \mathcal{P}_{\Gamma_\lambda} T_k(M_{\Gamma_\lambda}(z))$$

- Thus, at mapped Chebyshev points $x_1^{\Gamma_\lambda}, \ldots, x_N^{\Gamma_\lambda}$ we determine $r_{\lambda,k}$ by solving the linear system

$$r_1(x_j^{\Gamma_1}) + [\mathcal{P}_{\Gamma_2}^+ + \mathcal{P}_{\Gamma_2}^-] r_2(x_j^{\Gamma_1}) = f(x_j^{\Gamma_1})$$
$$\left[\mathcal{P}_{\Gamma_1}^+ + \mathcal{P}_{\Gamma_1}^-\right] r_1(x_j^{\Gamma_2}) + r_2(x_j^{\Gamma_2}) = f(x_j^{\Gamma_2})$$

- In coefficient space, this linear system can be written as the identity matrix plus a sparse, compact matrix, whose nonzero entry count only depends on Γ_1 and Γ_2, not on the length of the Chebyshev series of f
- Thus it is still an $\mathcal{O}(n \log n)$ algorithm

- We can now setup the Newton iteration
- The solution must be bounded, so we have two conditions

$$\check{r}_{1,0} = \check{r}_{2,0} = 0$$

- The solution must be asymptotic to $\frac{1}{z}$, so (for $\Gamma_1 = (a_1, b_1)$ and $\Gamma_2 = (a_2, b_2)$)

$$\frac{b_1 - a_1}{8}\check{r}_{1,1} + \frac{b_2 - a_2}{8}\check{r}_{2,1}$$

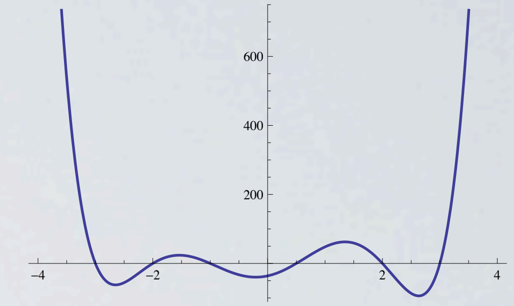
- We need one more condition. Recall that $g = \int \mathcal{P} f$ satisfies

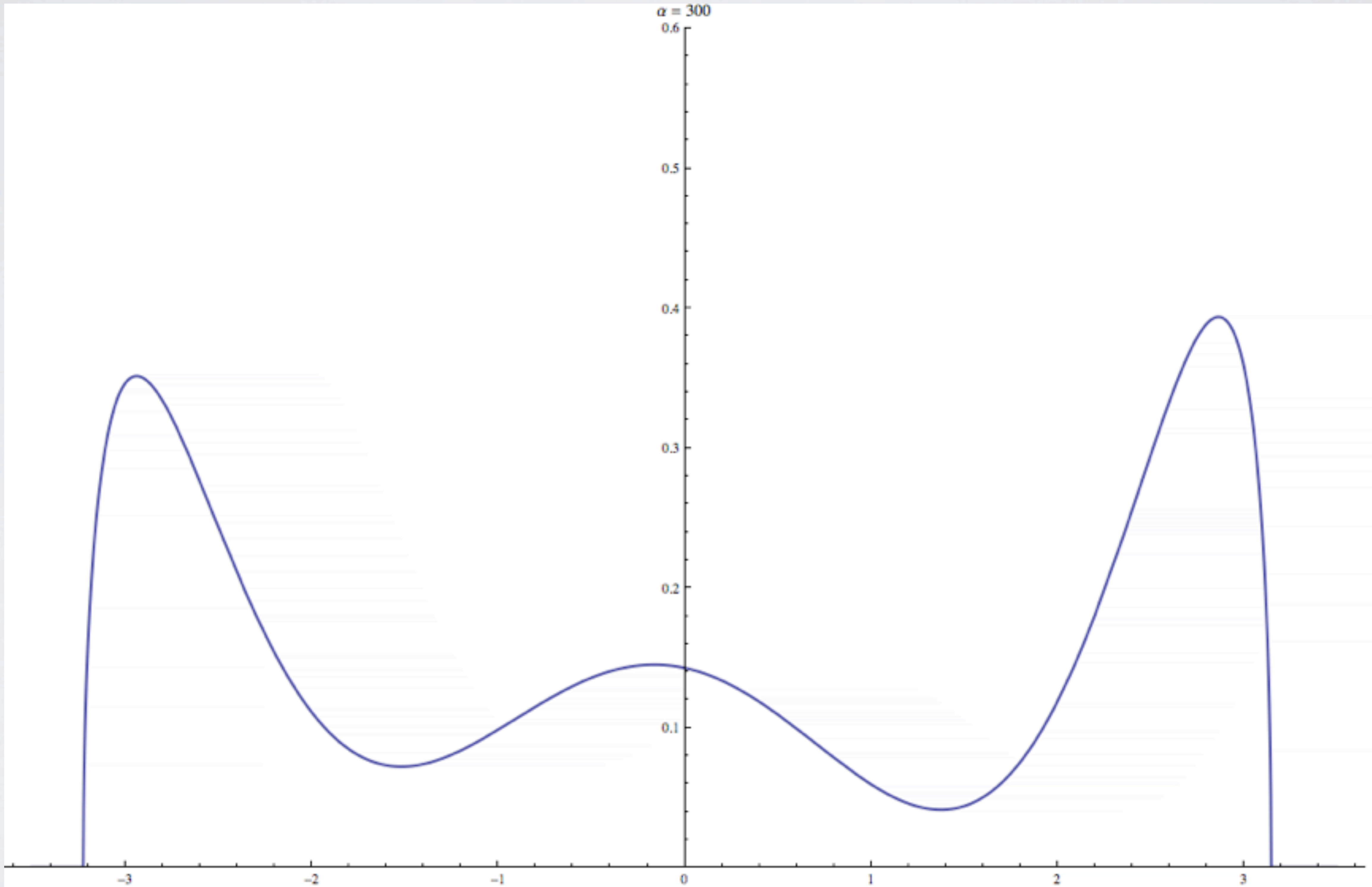
$$g^+ + g^- = V - \ell \text{ on } \Gamma_1 \text{ and } \Gamma_2$$

The key is the constant of integration is the same on both intervals, i.e.,

$$g^+(b_1) + g^-(b_1) - V(b_1) = g^+(a_2) + g^-(a_2) - V(a_2)$$

$$V(x) = \frac{(-3+x)(-2+x)(1+x)(2+x)(3+x)(-1+2x)}{\alpha} = \frac{1}{\alpha}$$





ORTHOGONAL POLYNOMIALS

- Once we have computed the equilibrium measure, we can set up the Riemann–Hilbert problem for the orthogonal polynomials
  - RH problems can be computed numerically (as described last week)
  - We need to write the RH problem so that the solution is smooth (no singularities) along each contour, and localized around stationary points
  - This will be accurate in the asymptotic regime: arbitrarily large n
- The key result: we can systematically compute arbitrarily large order orthogonal polynomials with respect to general weights
  - We could also use this to compute the nodes and weights of Gaussian quadrature rules with respect to general weights in $O(n)$ time

- The unaltered Riemann–Hilbert problem for orthogonal polynomials is

$$\Phi^+ = \Phi^- \begin{pmatrix} 1 & e^{-nV} \\ & 1 \end{pmatrix} \qquad \text{and} \qquad \Phi \sim \begin{pmatrix} z^n & \mathcal{O}(z^{-n-1}) \\ \mathcal{O}(z^{n-1}) & z^{-n} \end{pmatrix}$$

- We know how to compute g such that $g(z) \sim \log z$ and $g^+ + g^- = V - \ell$ on supp $\mathrm{d}\mu$

- We thus let

$$\Phi = \Psi \begin{pmatrix} e^{ng} & \\ & e^{-ng} \end{pmatrix}$$

where $\Psi \sim I$ and

$$\Psi^+ = \Psi^- \begin{pmatrix} e^{ng^-} & \\ & e^{-ng^-} \end{pmatrix} \begin{pmatrix} 1 & e^{-nV} \\ & 1 \end{pmatrix} \begin{pmatrix} e^{-ng^+} & \\ & e^{ng^+} \end{pmatrix}$$
$$= \Psi^- \begin{pmatrix} e^{n(g^- - g^+)} & e^{n(g^+ + g^- - V)} \\ & e^{n(g^+ - g^-)} \end{pmatrix}$$

(based on Deift 1999)

From the construction of g, the matrix

$$\begin{pmatrix} e^{n(g^- - g^+)} & e^{n(g^+ + g^- - V)} \\ & e^{n(g^+ - g^-)} \end{pmatrix}$$

has the following nice properties:

- Off of supp μ, it has the form

$$\begin{pmatrix} 1 & e^{n(g^+ + g^- - V)} \\ & 1 \end{pmatrix}$$

  which decays exponentially (g decays at infinity, so V dominates)

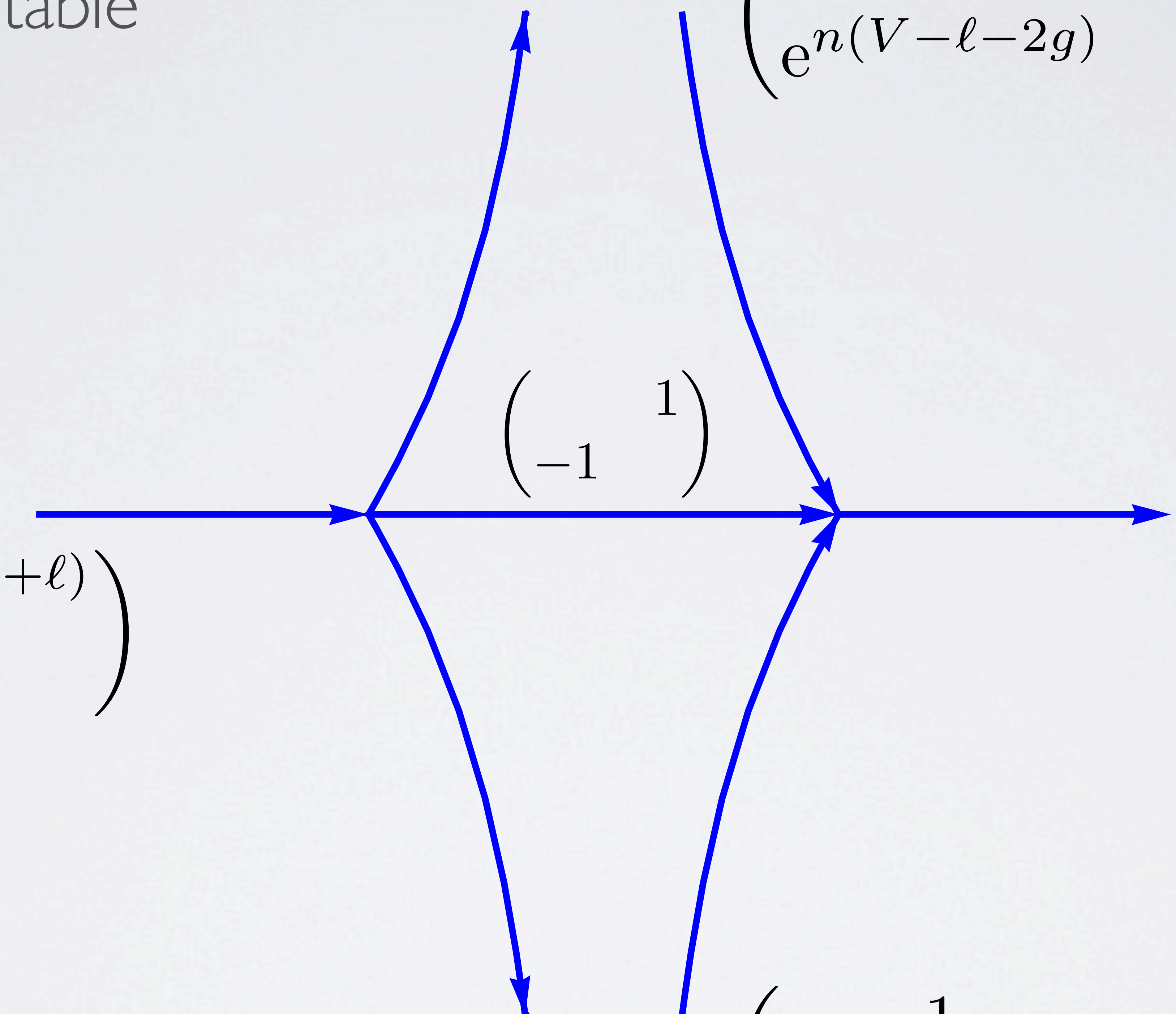
- On supp μ, it has the form

$$\begin{pmatrix} e^{n(g^- - g^+)} & e^{-\ell n} \\ & e^{n(g^+ - g^-)} \end{pmatrix} = L \begin{pmatrix} 1 & \\ e^{n(V - \ell - 2g^-)} & 1 \end{pmatrix} \begin{pmatrix} & 1 \\ -1 & \end{pmatrix} \begin{pmatrix} 1 & \\ e^{n(V - \ell - 2g^+)} & 1 \end{pmatrix} L^{-1}$$

  for $L = \begin{pmatrix} e^{-n\ell/2} & \\ & e^{n\ell/2} \end{pmatrix}$

(based on Deift 1999)

We thus want to solve the RH problem (where all the jumps are computable numerically!)

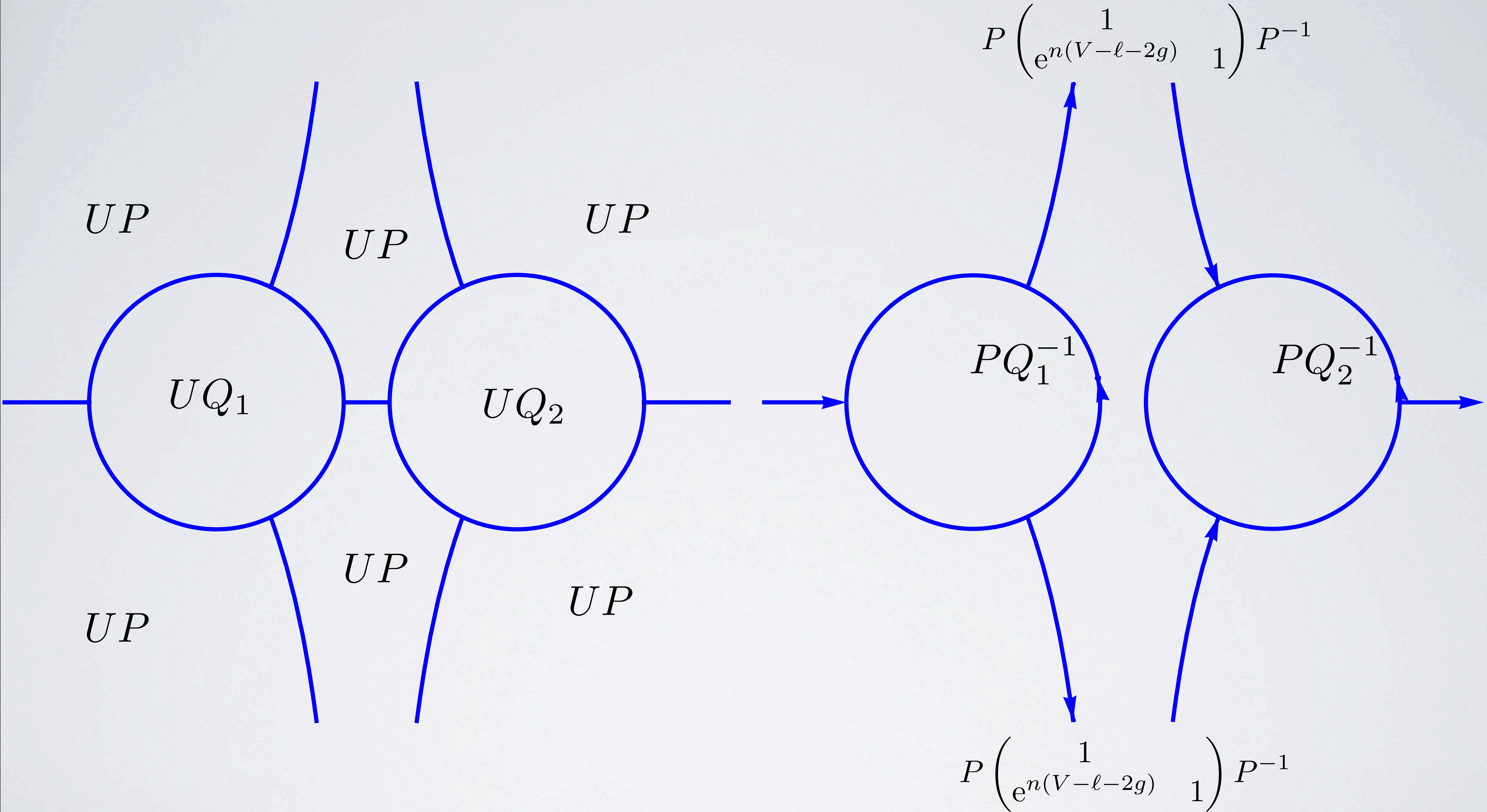


(based on Deift 1999)

- We can find a parametrix $P(z)$ in closed form that satisfies

$$P^+ = P^- \begin{pmatrix} & 1 \\ -1 & \end{pmatrix} \quad \text{and} \quad P(z) \sim I$$

- We can also construct parametrices Q_1 and Q_2 around each stationary point, by using the jump curves


$P\begin{pmatrix}1 & \\ \mathrm{e}^{n(V-\ell-2g)} & 1\end{pmatrix}P^{-1}$
UP
UP
UP
UQ_1
UQ_2
PQ_1^{-1}
PQ_2^{-1}
UP
UP
UP
$P\begin{pmatrix}1 & \\ \mathrm{e}^{n(V-\ell-2g)} & 1\end{pmatrix}P^{-1}$

RANDOM MATRIX DISTRIBUTIONS

- We want to compute gap probabilities

- These are expressible as

$$\det \left[I + \mathcal{K}_n|_\Omega\right]$$

for (where Φ is still the solution the RH problem)

$$\mathcal{K}_n(x,y) = \frac{1}{2\pi \mathrm{i}} \mathrm{e}^{-n/2[V(x)+V(y)]} \frac{\Phi_{11}(x)\Phi_{21}(y) - \Phi_{11}(y)\Phi_{21}(x)}{x-y}$$

ALGORITHM

- Input: potential V, dimension of random matrix n, gap interval Ω
- Output: probability that there are no eigenvalues in Ω
  - Step 1: Compute the equilibrium measure using Newton iteration
  - Step 2: Construct and solve the orthogonal polynomial RH problem numerically
  - Step 3: Use Bornemann's Fredholm determinant solver

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- Let

$$\Omega = a + \frac{1}{\mathcal{K}_n(a,a)}(-s,s)$$

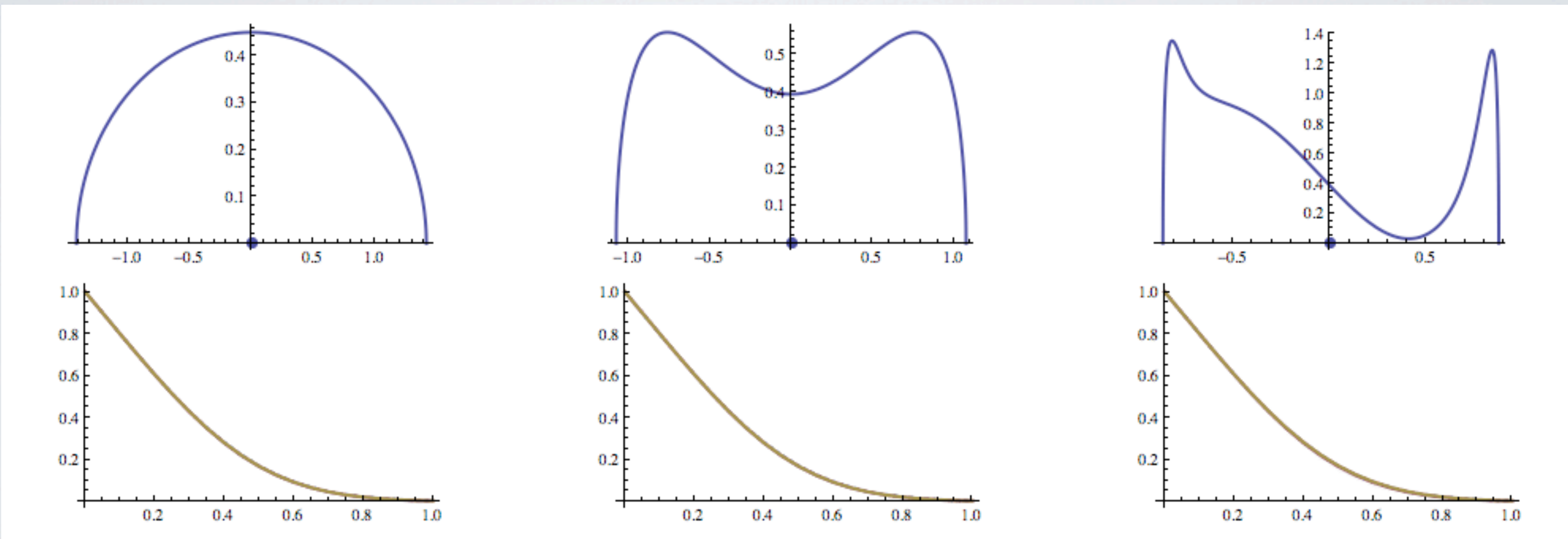
- Then it is known that, for a inside the support of the equilibrium measure and any polynomial potential, the Fredholm determinant converges to the Fredholm determinant over $(-s,s)$ with the sine kernel

$$\mathcal{K}_\infty(x,y) = \frac{\sin \pi(x-y)}{x-y}$$

- However, for finite n, the distributions vary

$$n = 30,\ 50,\ \infty$$

x^2 $\quad$ x^4 $\quad$ $\sin 3x + 10x^{20}$



Potential of numerical RH approach for random matrix theory

- Discovery of unknown universality laws?
- Inverse problem: determining information about the potential V from observed data?
  - Can we determine which random matrix ensemble generates the zeros of the Riemann–Zeta function?
- Modelling physical systems?