# NUMERICAL FREE PROBABILITY

Sheehan Olver
The University of Sydney

Joint work with

Raj Rao Nadakuditi
University of Michigan

# Outline

- Overview of numerical random matrix theory
- Numerical results
- "Generic" edge behaviour
- Algorithm:
  - Computation of inverse Cauchy transforms
  - Recovery of a measure from its inverse Cauchy transforms
- Finite $n$: invariant ensembles + free probability?

# Numerical random matrix theory

Fredholm determinants

[Bornemann 2010]

Fredholm determinants
[Bornemann 2010]

Cauchy transforms
[SO 2011]

Fredholm determinants
[Bornemann 2010]

Cauchy transforms
[SO 2011]

Riemann–Hilbert problems
[SO 2011]

Fredholm determinants
[Bornemann 2010]

Cauchy transforms
[SO 2011]

Riemann–Hilbert problems
[SO 2011]

Equilbrium Measures
[SO 2011]

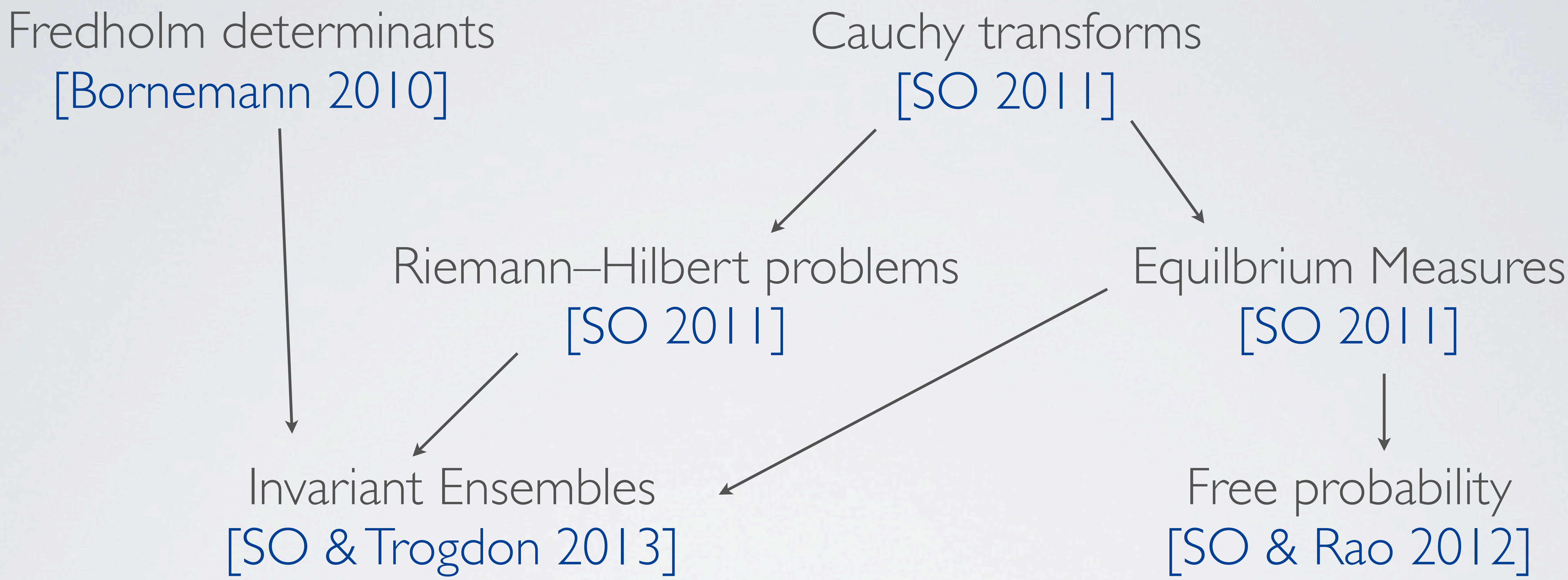
Fredholm determinants
[Bornemann 2010]

Cauchy transforms
[SO 2011]

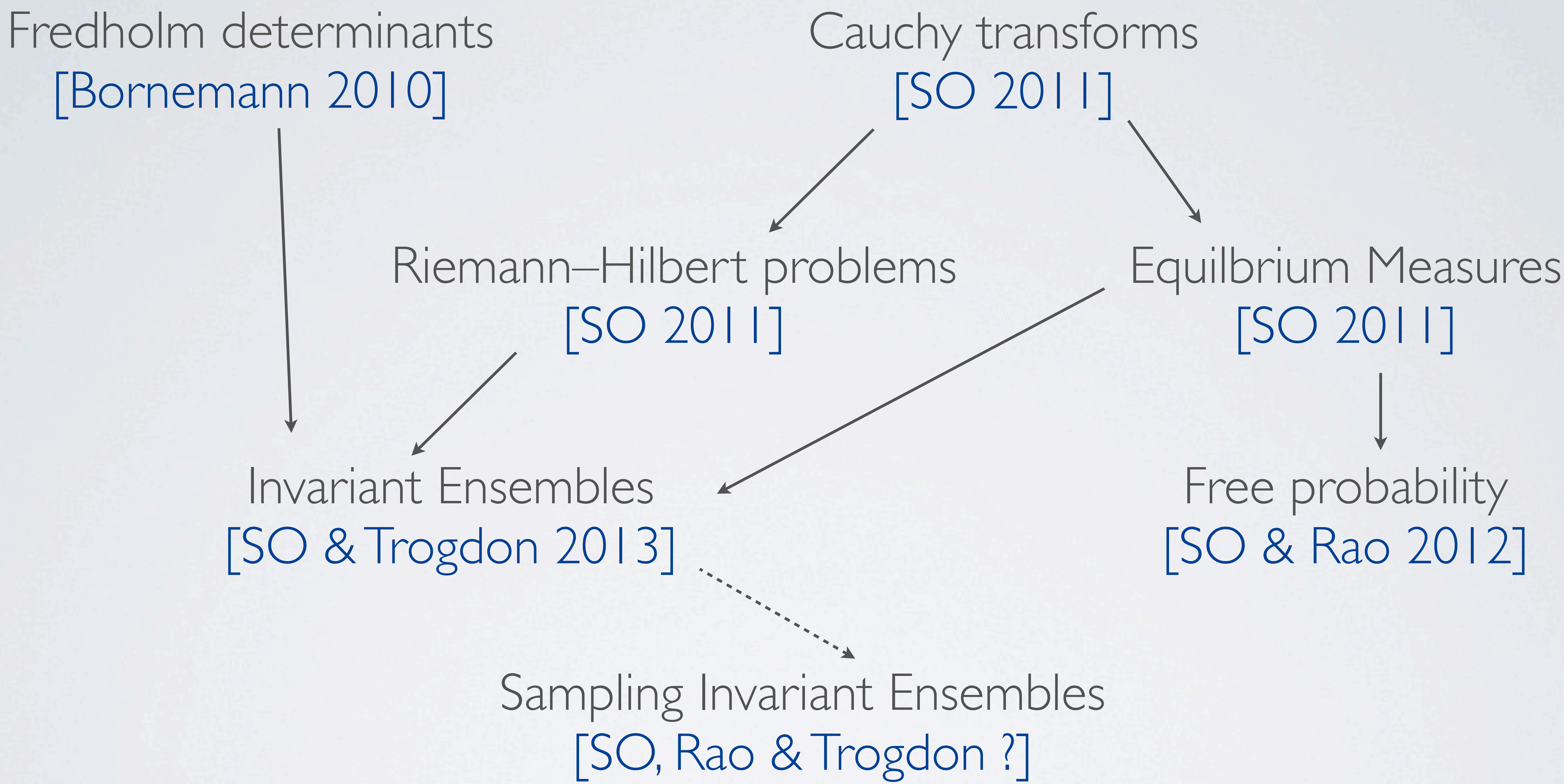
Riemann–Hilbert problems
[SO 2011]

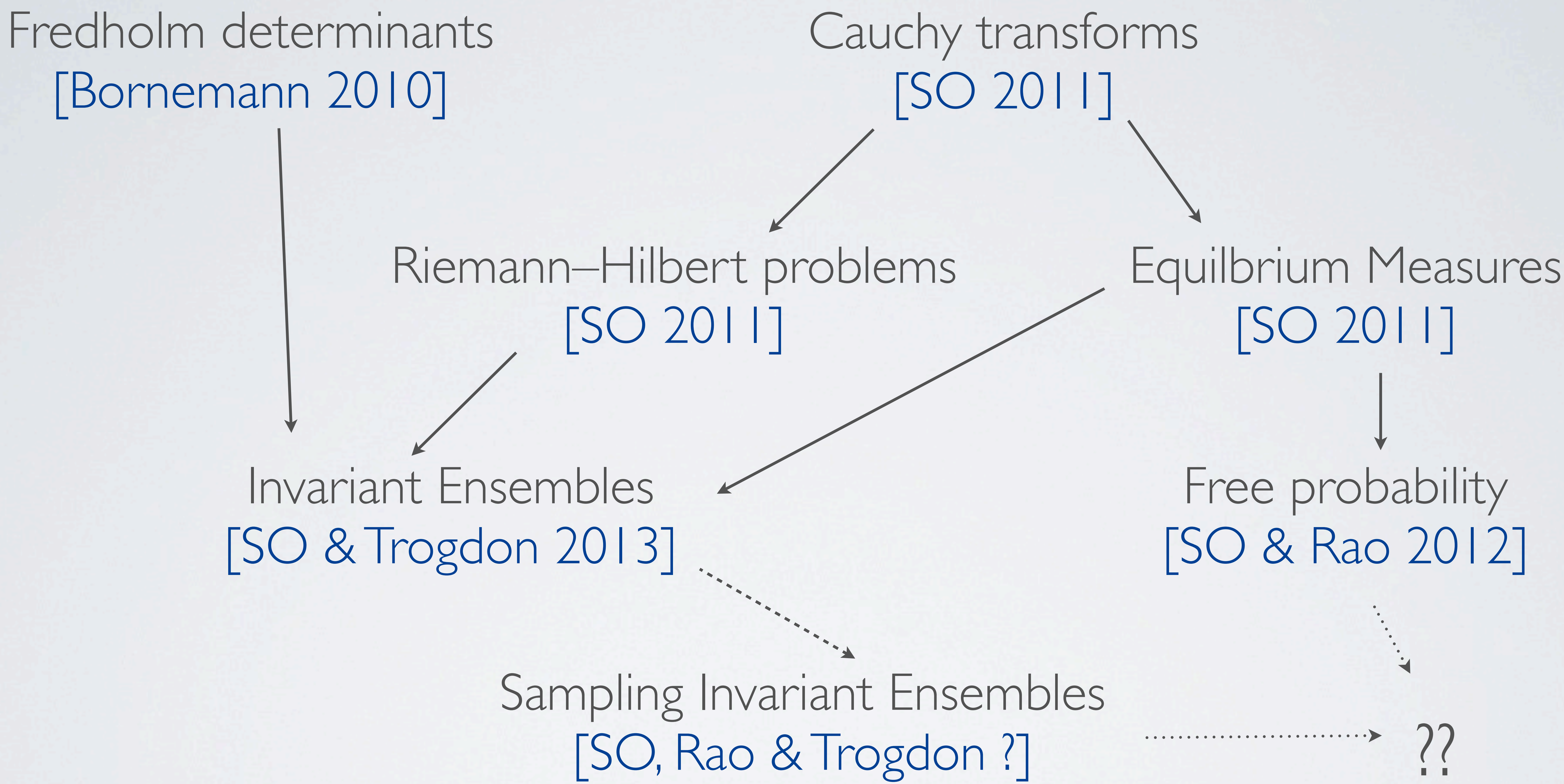
Equilbrium Measures
[SO 2011]

Free probability
[SO & Rao 2012]



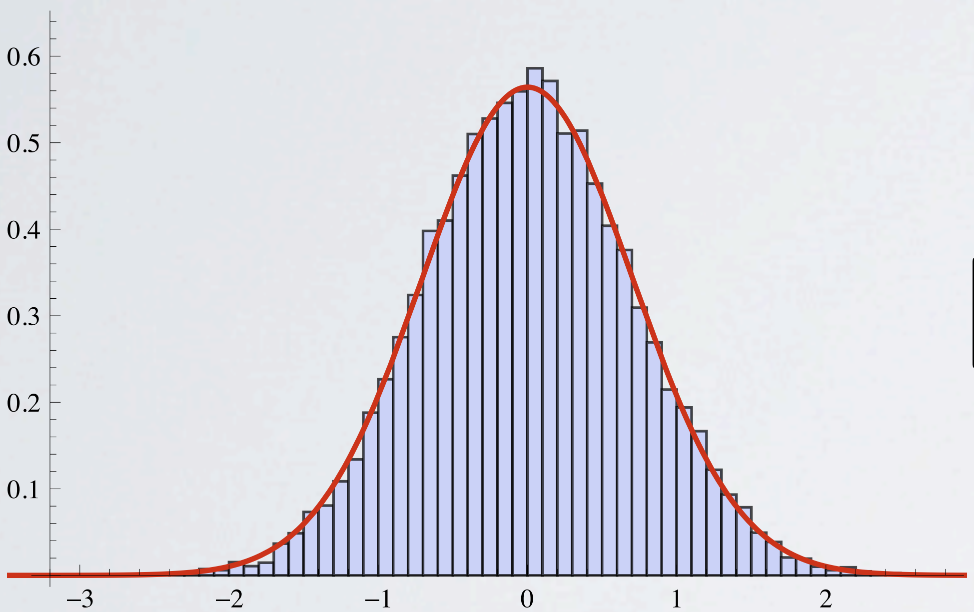
Fredholm determinants
[Bornemann 2010]
Cauchy transforms
[SO 2011]
Riemann–Hilbert problems
[SO 2011]
Equilbrium Measures
[SO 2011]
Invariant Ensembles
[SO & Trogdon 2013]
Free probability
[SO & Rao 2012]


Fredholm determinants
[Bornemann 2010]
Cauchy transforms
[SO 2011]
Riemann–Hilbert problems
[SO 2011]
Equilbrium Measures
[SO 2011]
Invariant Ensembles
[SO & Trogdon 2013]
Free probability
[SO & Rao 2012]
Sampling Invariant Ensembles
[SO, Rao & Trogdon ?]

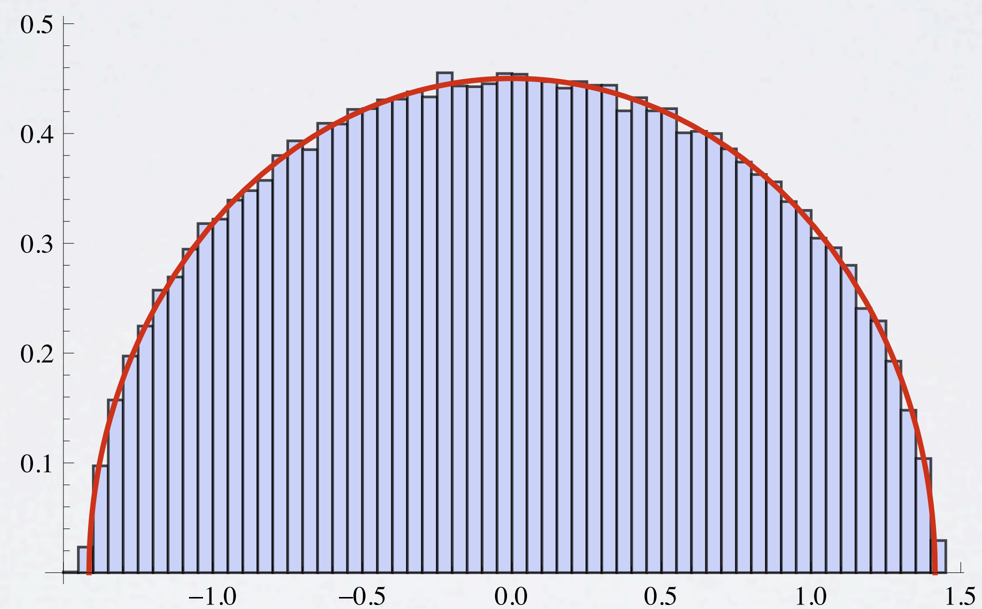

Fredholm determinants
[Bornemann 2010]
Cauchy transforms
[SO 2011]
Riemann–Hilbert problems
[SO 2011]
Equilbrium Measures
[SO 2011]
Invariant Ensembles
[SO & Trogdon 2013]
Free probability
[SO & Rao 2012]
Sampling Invariant Ensembles
[SO, Rao & Trogdon ?]
??

# Numerical results

Gaussian $\boxplus$ Semicircle

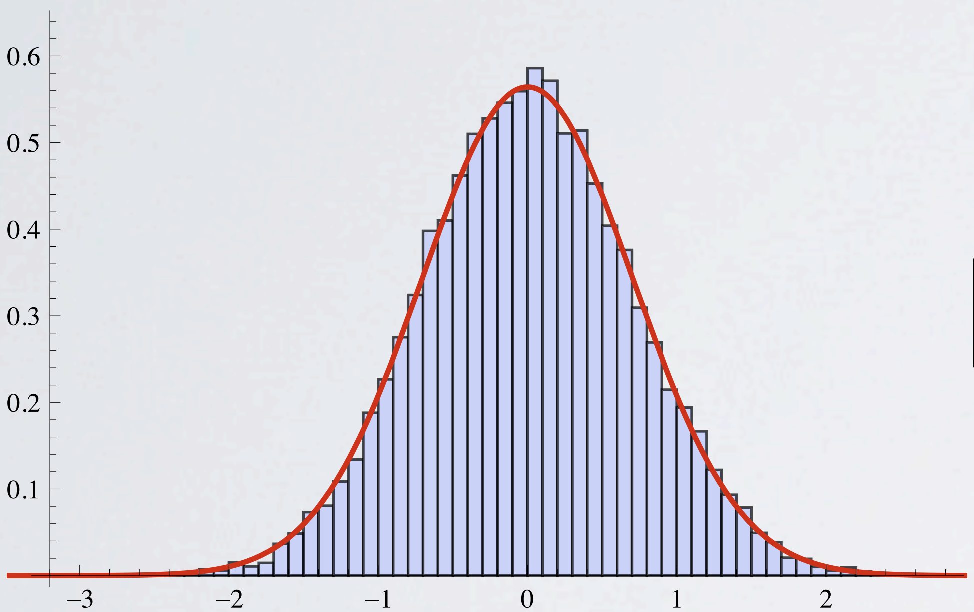



$\boxplus$

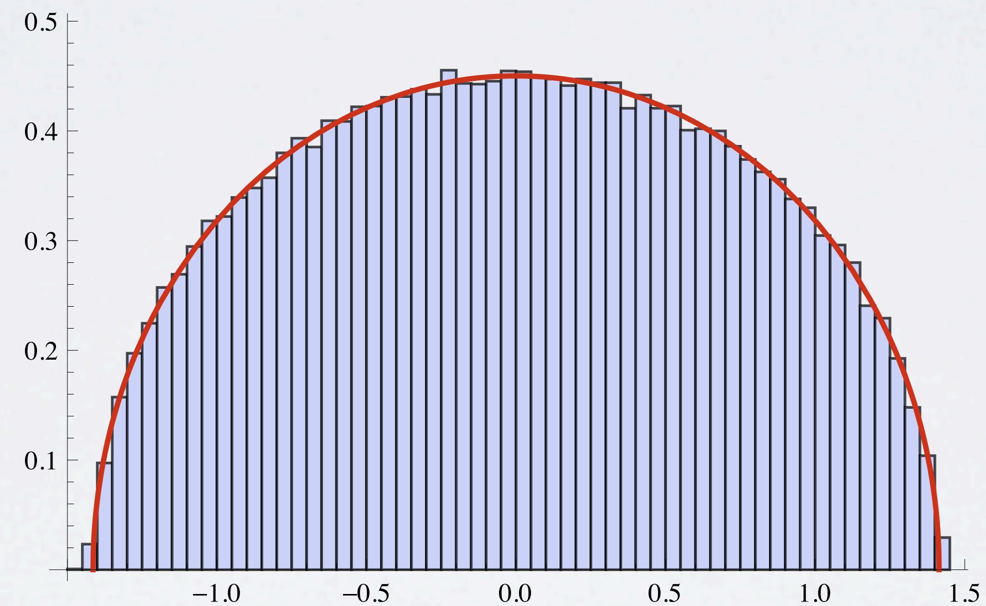



$=$

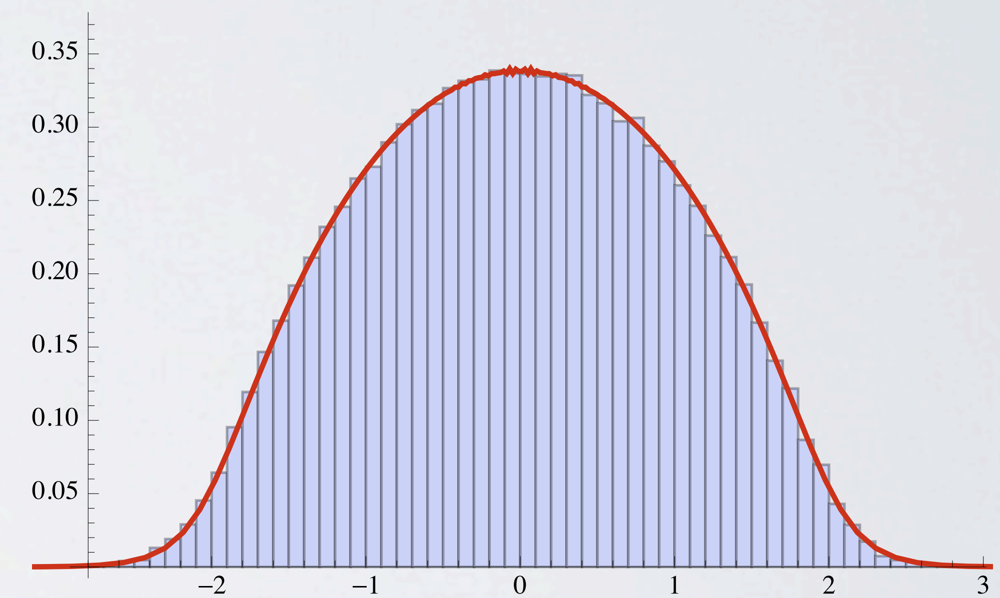
Gaussian $\boxplus$ Semicircle




$\boxplus$

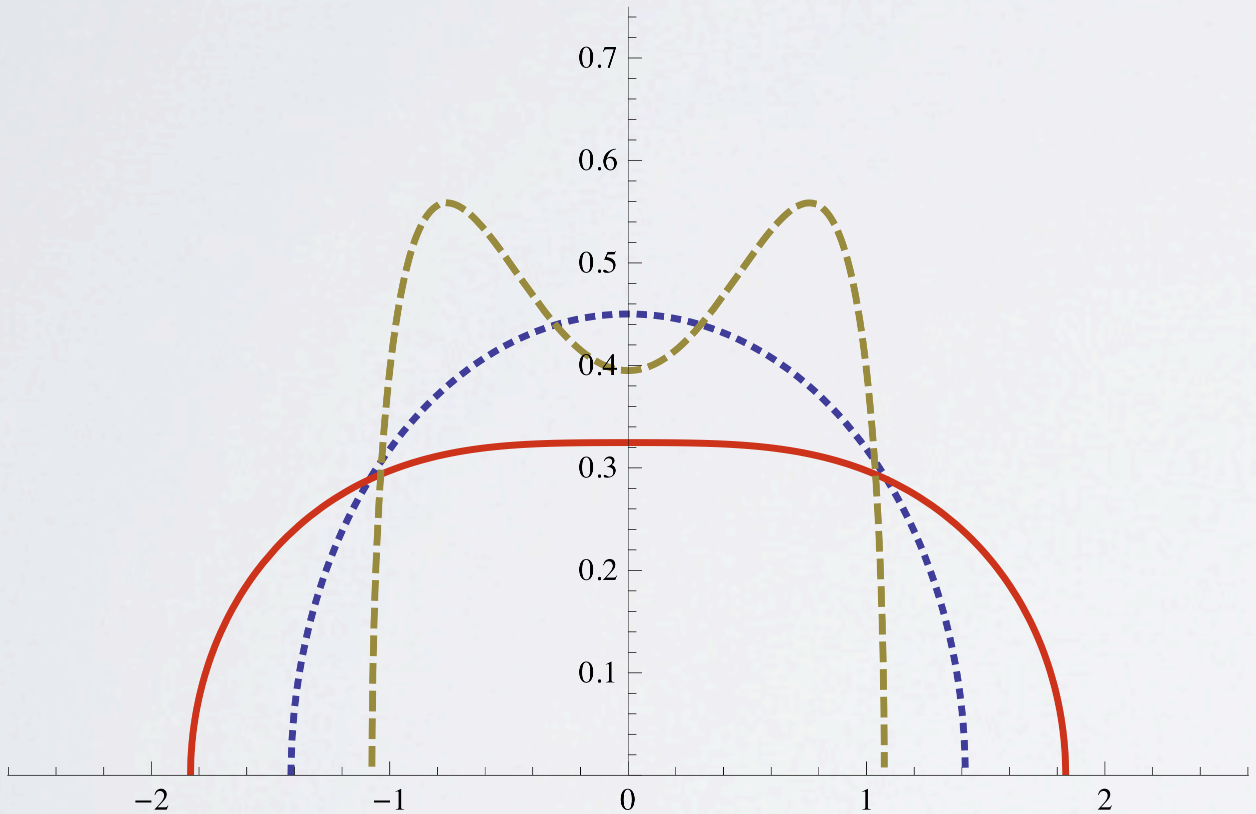



$=$

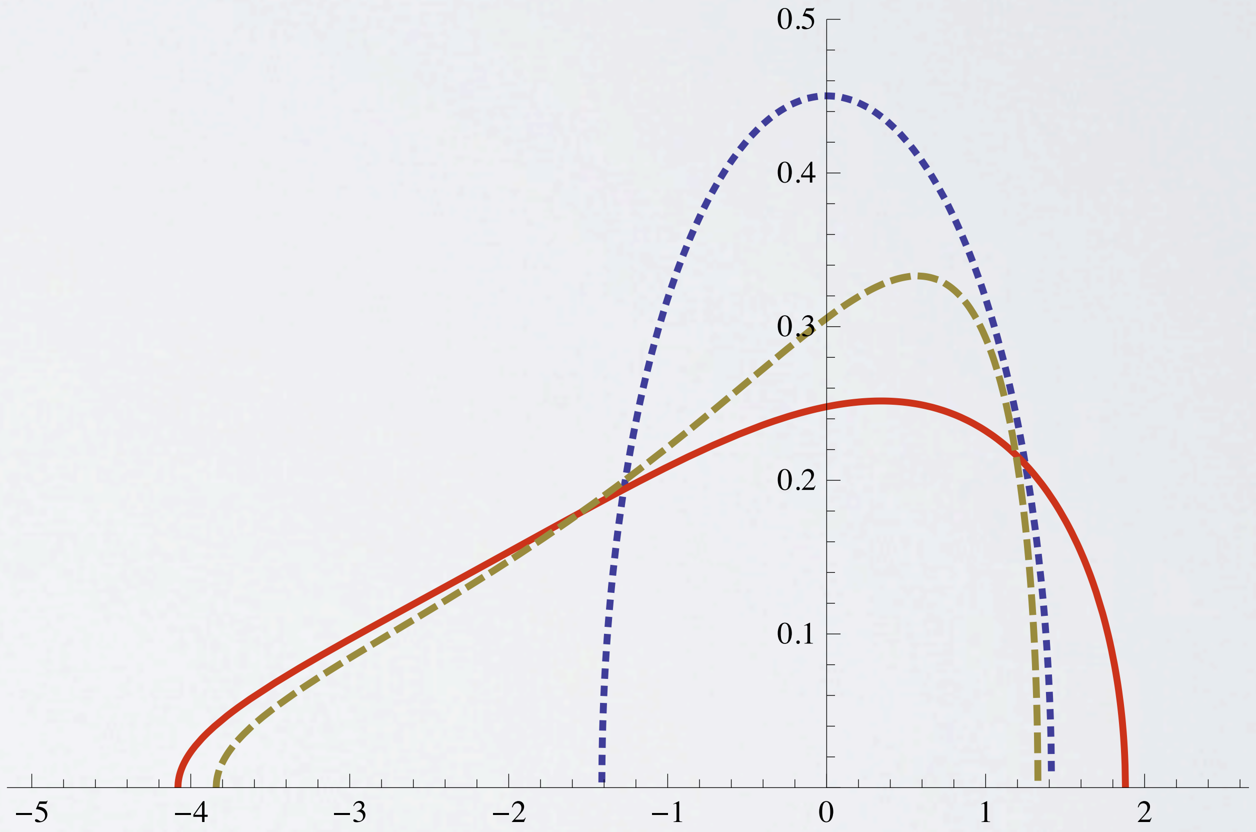


# Examples

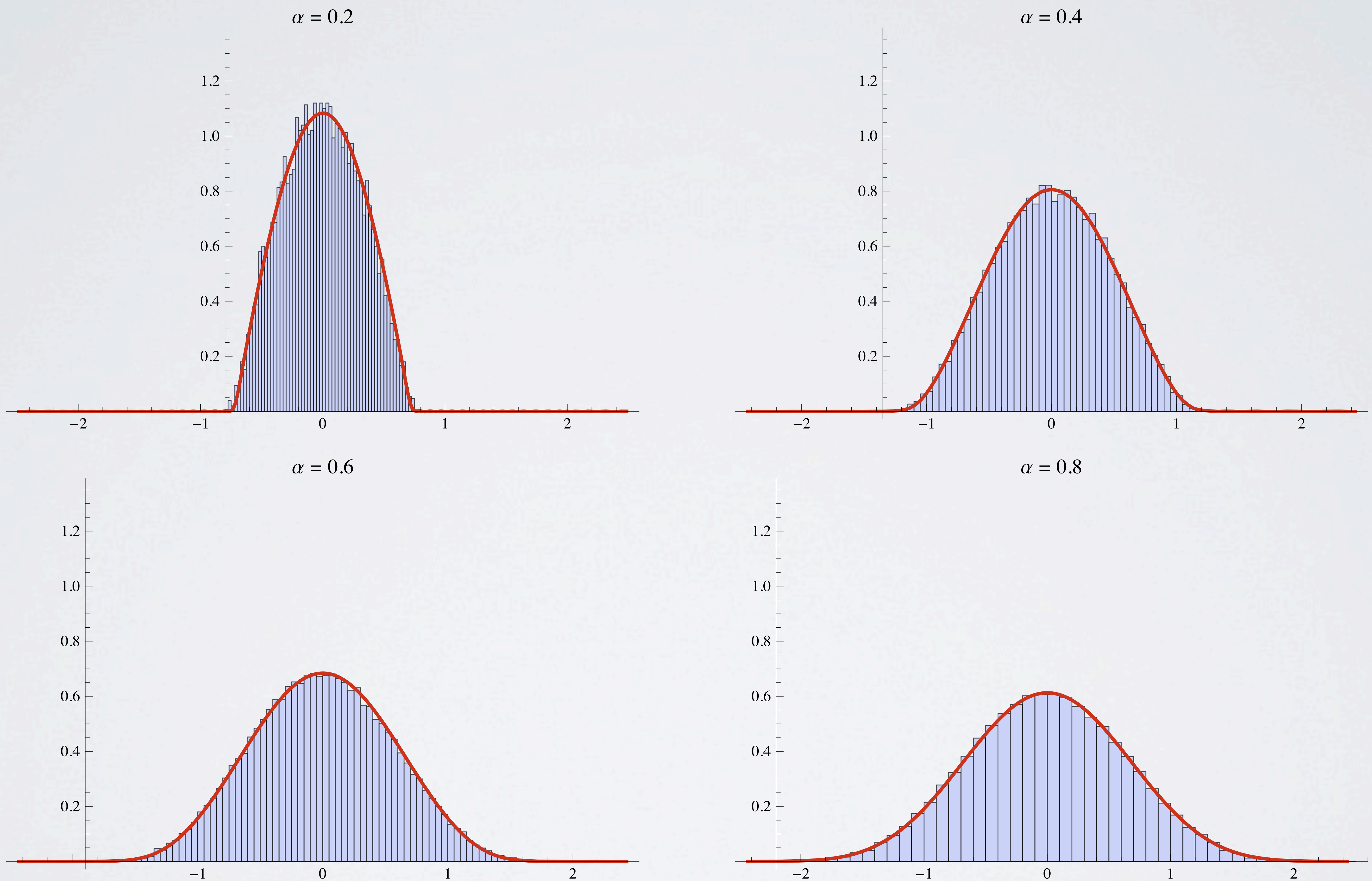
Semicircle + Quartic equilibrium measure



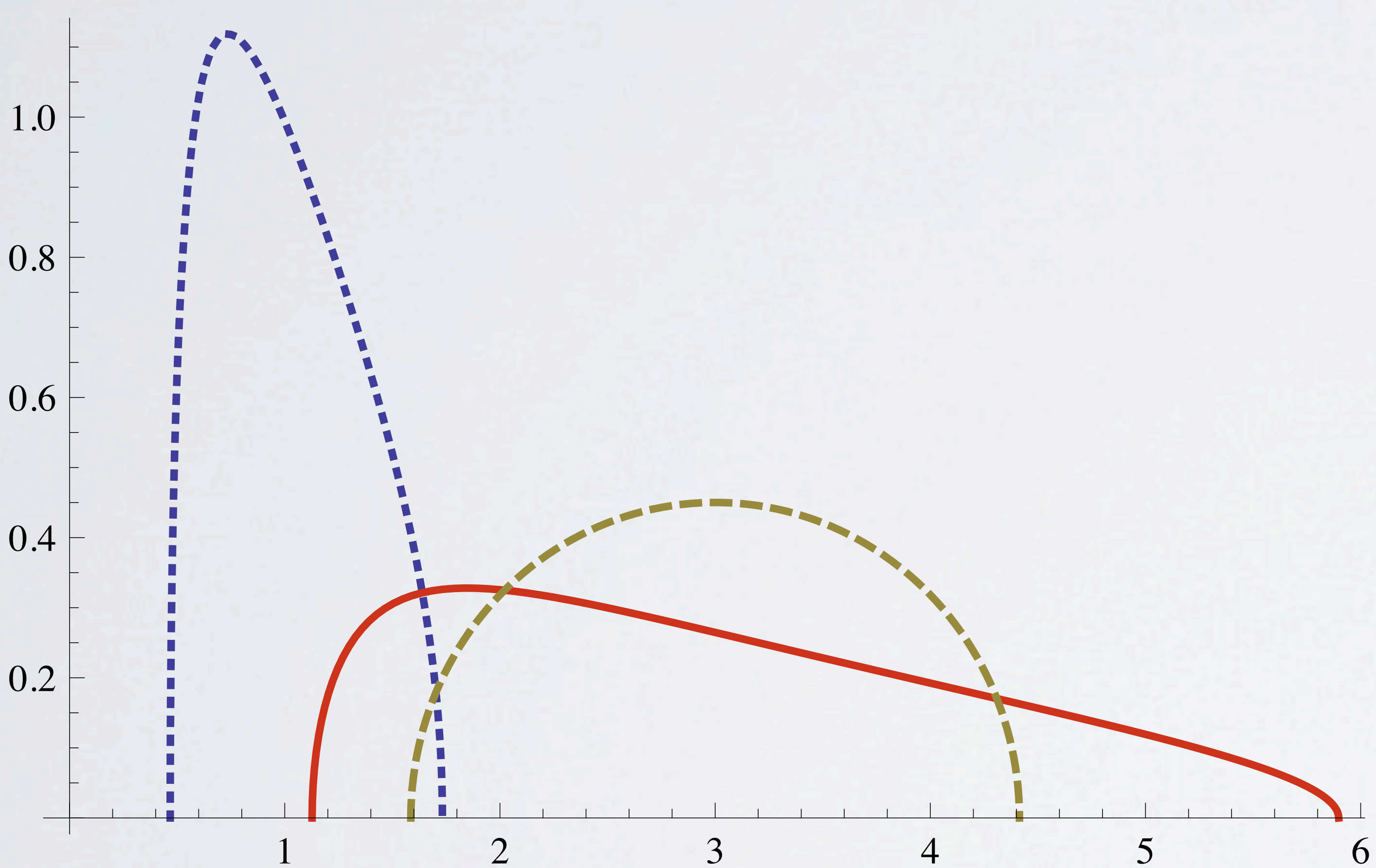

Semicircle + $\exp(x)$ equilibrium measure

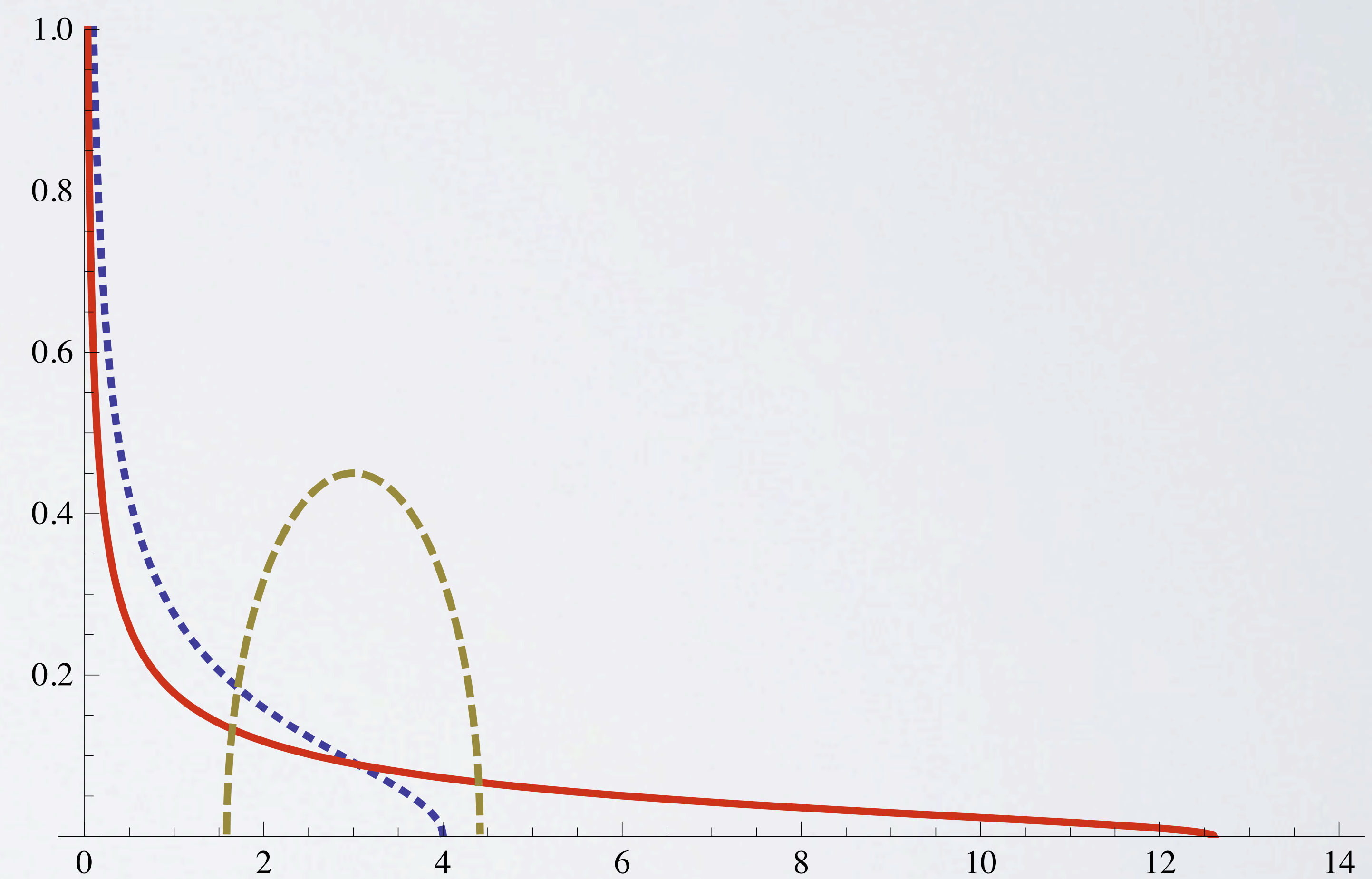


# Compression of a Gaussian

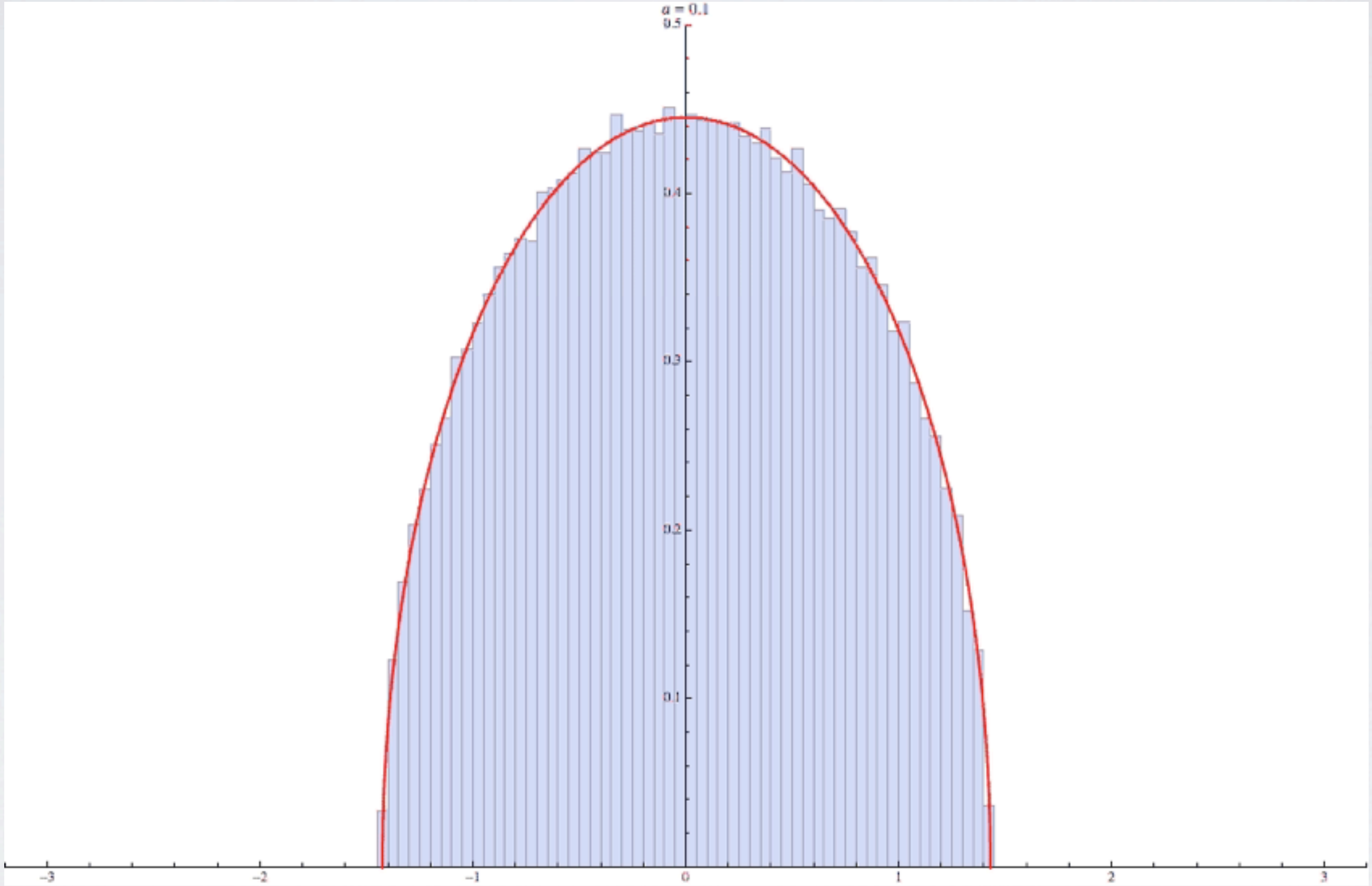


Marchenko–Pastur $\boxtimes$ Shifted semicircle

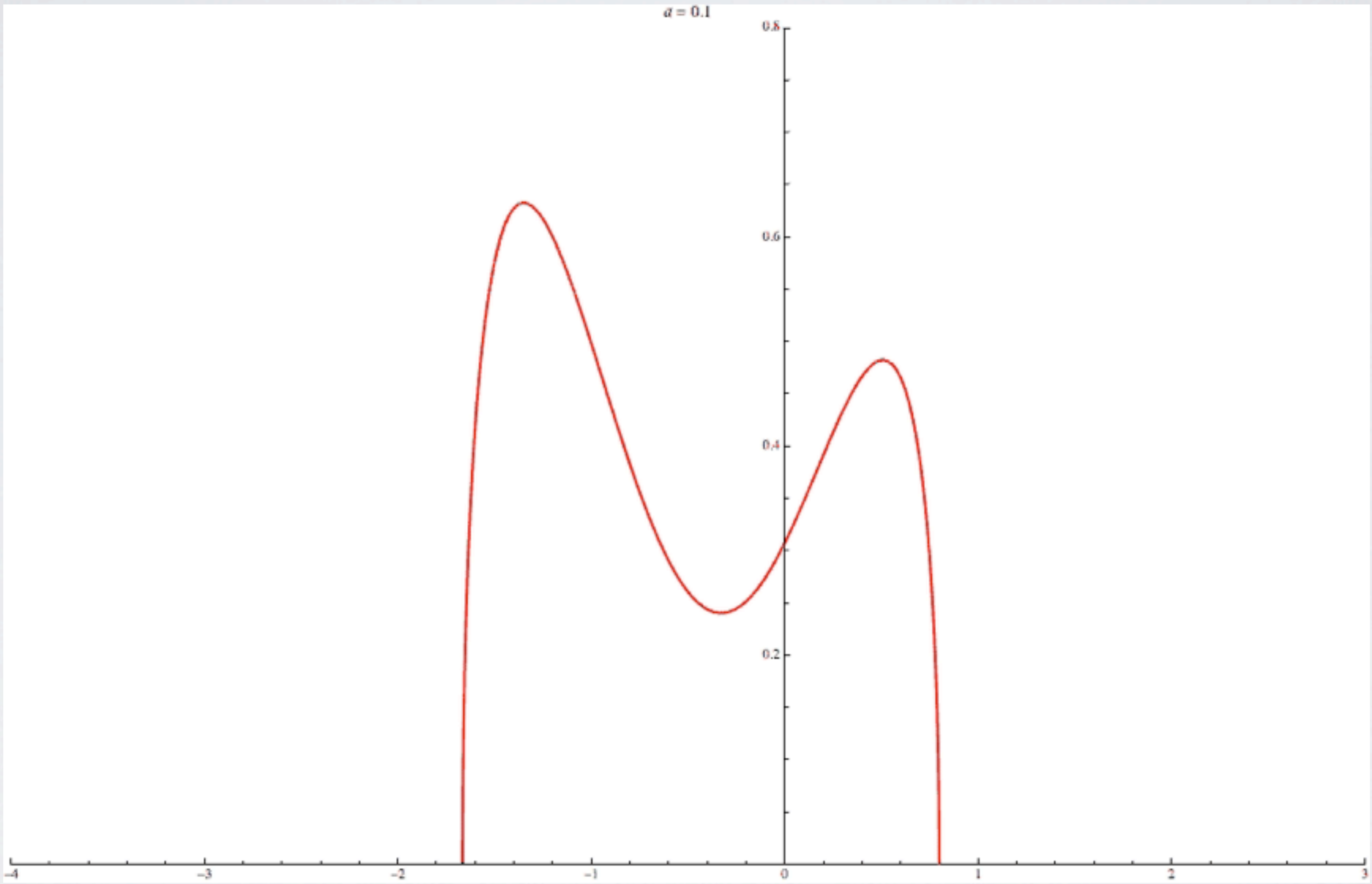


$$\frac{\delta_{-a} + \delta_a}{2} \quad \boxplus \quad \text{Semicircle}$$

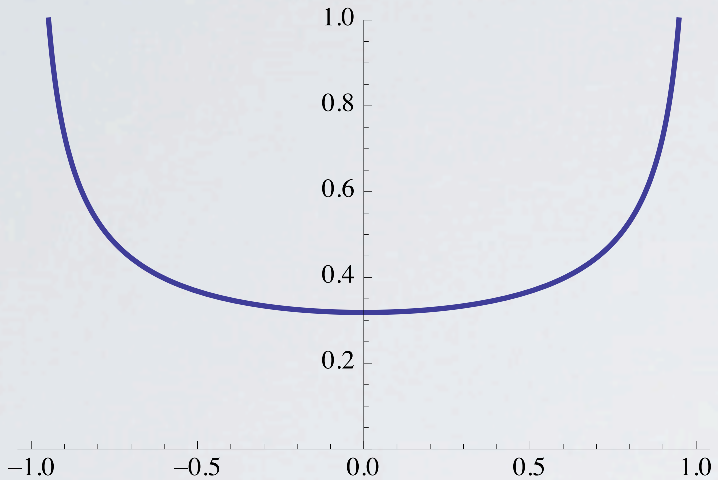


$$\frac{\delta_{-a} + \delta_a}{2} \boxplus$$ Nonsymmetric equilibrium measure



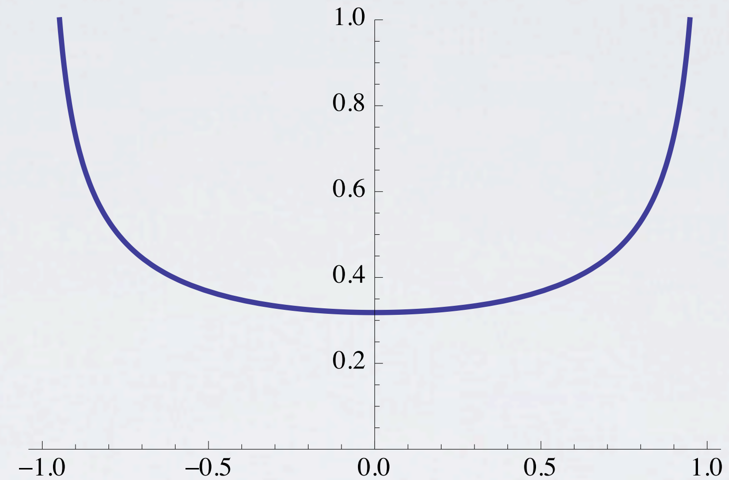
# Numerics can lead to new theorems

Legendre

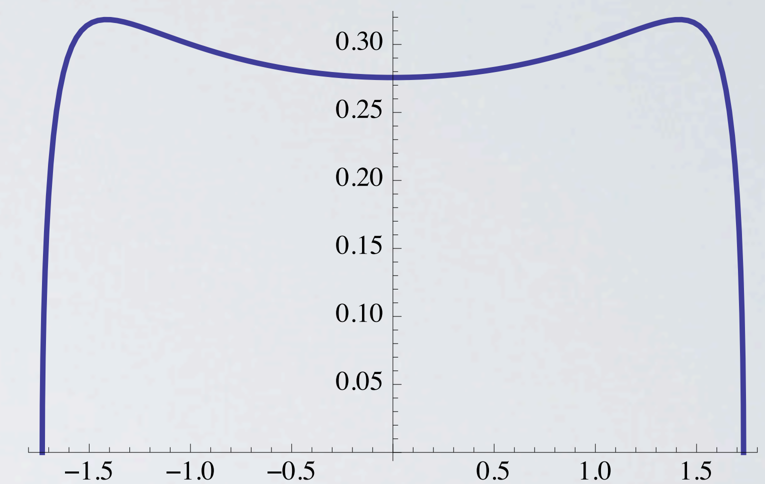



$\boxplus$

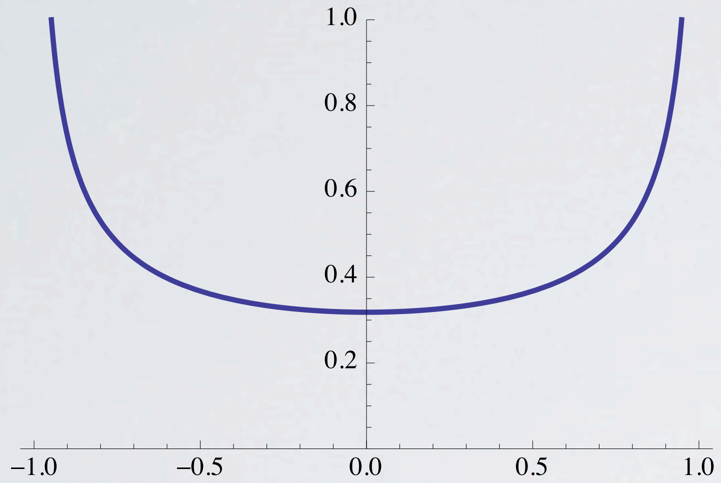
Legendre



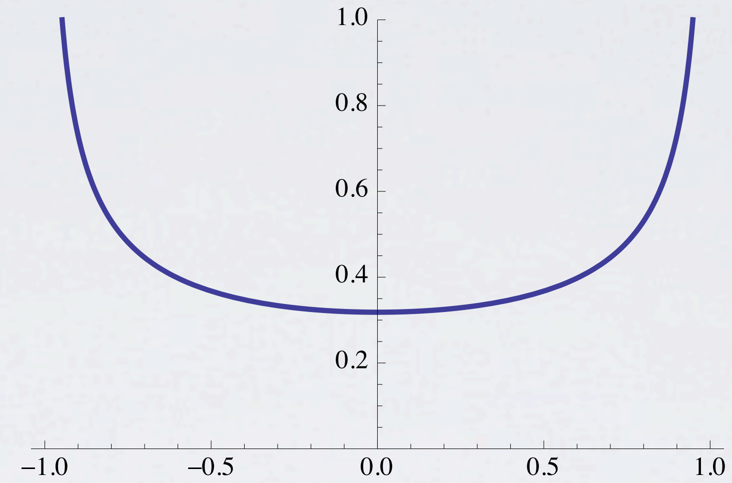

$=$



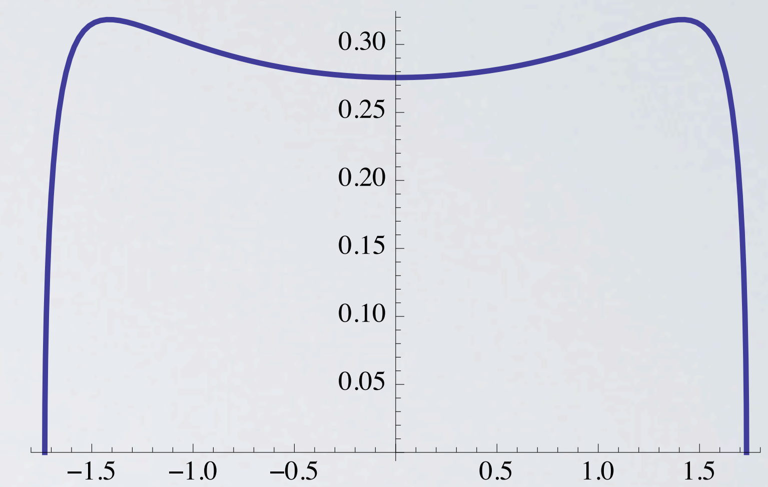
Legendre $\boxplus$ Legendre




$\boxplus$



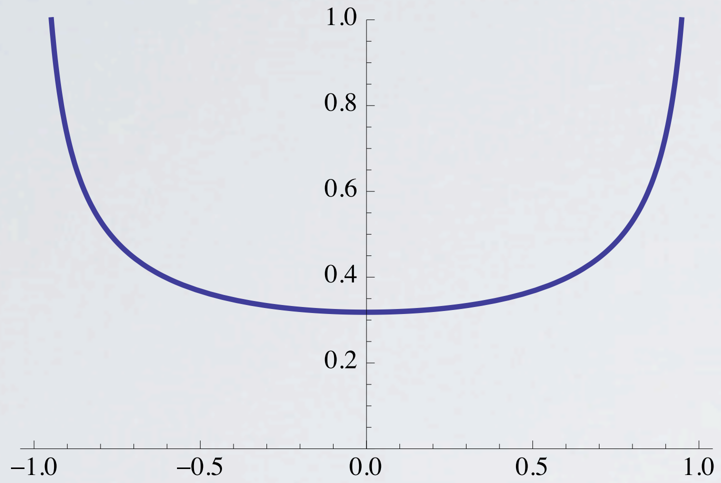

$=$



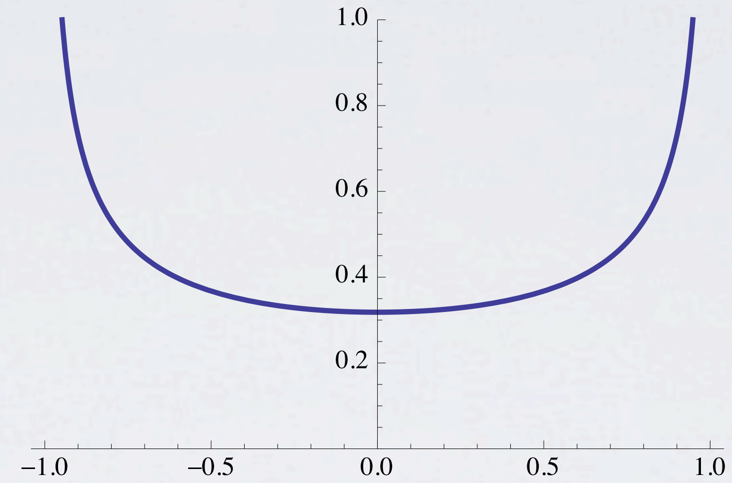

Theorem:

Jacobi measure w/ not too fast decay & univalent Cauchy transform $\boxplus$ Jacobi measure w/ univalent Cauchy transform $=$ Square root measure w/ univalent Cauchy transform

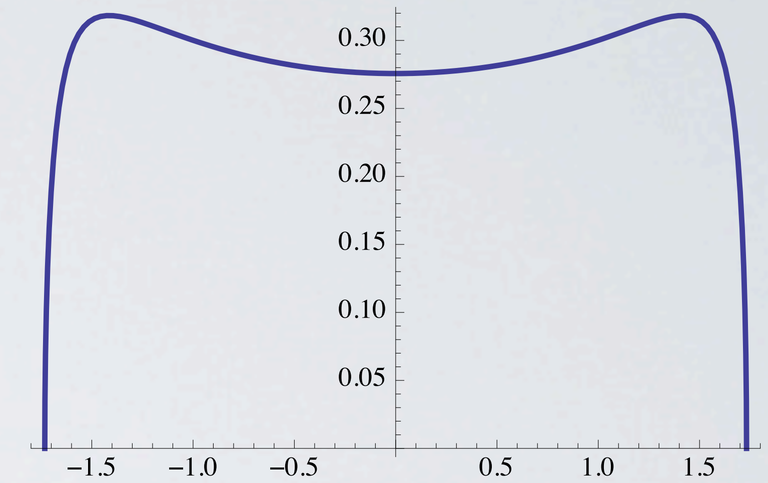
Legendre $\boxplus$ Legendre $=$




$\boxplus$



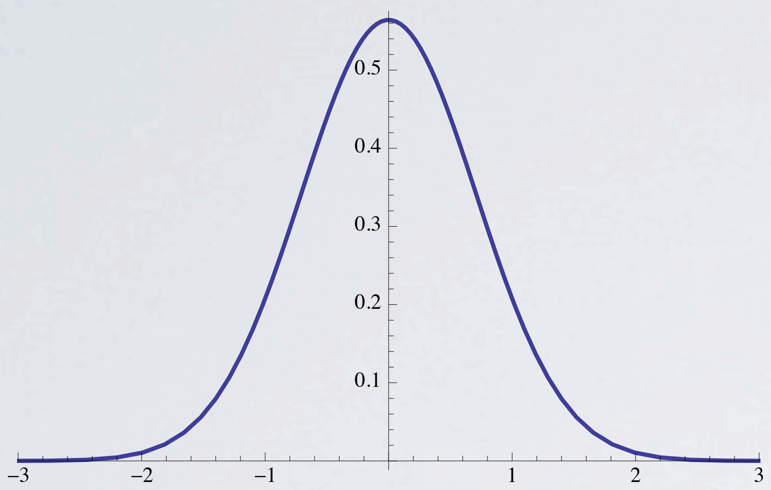

$=$



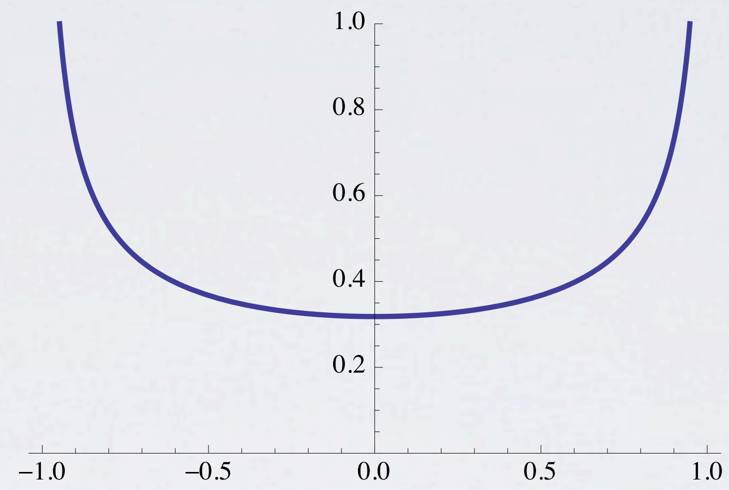

Theorem: Hölder continuous derivative times Jacobi weight $\boxplus$ Analytic times semicircle

Jacobi measure w/ not too fast decay & univalent Cauchy transform $\boxplus$ Jacobi measure w/ univalent Cauchy transform $=$ Square root measure w/ univalent Cauchy transform

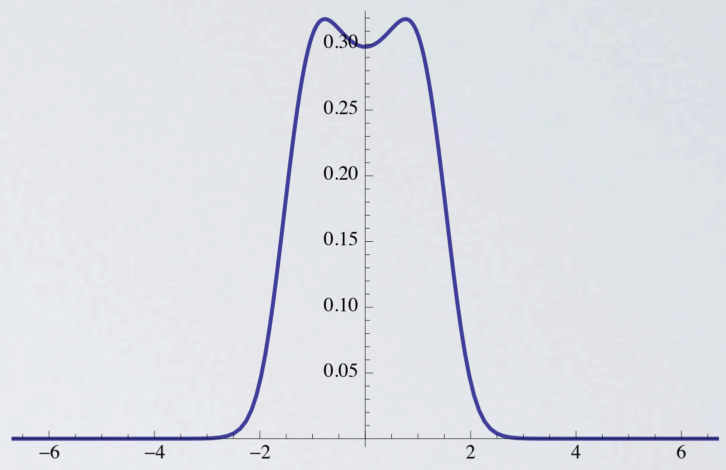
Gaussian Legendre




$\boxplus$

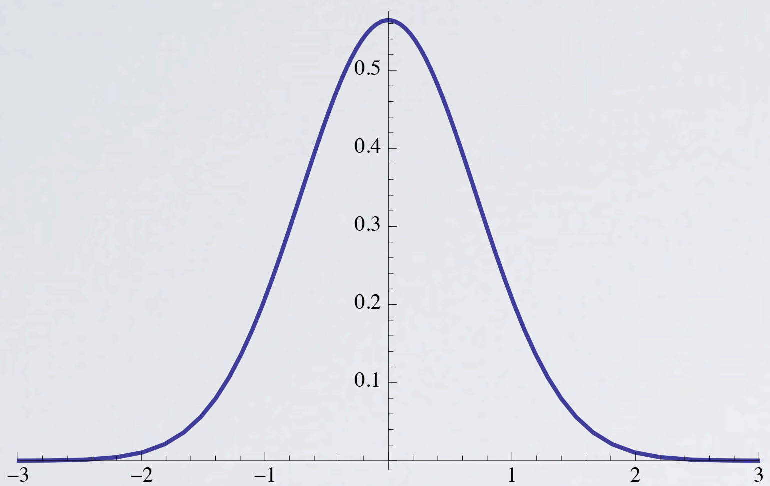



$=$

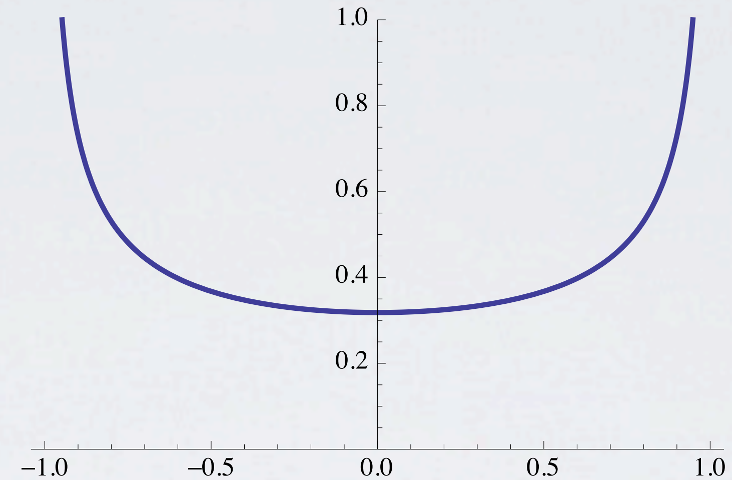


Gaussian

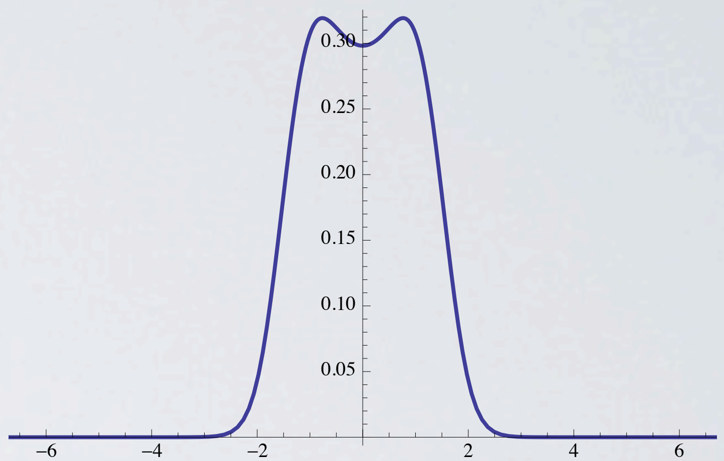
Legendre




$\boxplus$




=




Theorem:

Schwartz w/ univalent Cauchy transform $\boxplus$ Schwartz or compact support w/ univalent Cauchy transform = Schwartz w/ univalent Cauchy transform

# Numerical Free Probability

- The challenge:
  - The measures typically have square root singularities
  - Free probability is a nonlinear operation
  - Representing the measures in a bad basis (like Fourier) will be too computational expensive

# Cauchy–Stieltjes transform

- Associated with a measure is its Cauchy–Stieltjes transform:

$$G_\mu(z) = \int \frac{1}{z-x}\,\mathrm{d}\mu(x)$$

- This is analytic off the support of the measure
- Because we are working with probability measures, we have

$$G_\mu(z) = \frac{1}{z}\int \frac{z}{z-x}\,\mathrm{d}\mu(x) \sim \frac{1}{z}\int \mathrm{d}\mu = \frac{1}{z}$$

- Therefore, the Cauchy–Stieltjes transform is invertible near $\infty$

# Free probability algorithm

- Input: measures $\mu_A$ and $\mu_B$ in expansion form
- Output: $\mu_A \boxplus \mu_B$ in expansion form
  1. Construct scheme to evaluate $G_{\mu_A}^{-1}(y)$ and $G_{\mu_B}^{-1}(y)$ pointwise
  2. Recover $\mu_A \boxplus \mu_B$ from pointwise knowledge of

$$G_{\mu_A \boxplus \mu_B}^{-1}(y) = G_{\mu_A}^{-1}(y) + G_{\mu_B}^{-1}(y) - \frac{1}{y}$$

# Free probability algorithm

- Input: measures $\mu_A$ and $\mu_B$ in expansion form
- Output: $\mu_A \boxplus \mu_B$ in expansion form
    1. Construct scheme to evaluate $G_{\mu_A}^{-1}(y)$ and $G_{\mu_B}^{-1}(y)$ pointwise
    2. Recover $\mu_A \boxplus \mu_B$ from pointwise knowledge of

$$G_{\mu_A \boxplus \mu_B}^{-1}(y) = G_{\mu_A}^{-1}(y) + G_{\mu_B}^{-1}(y) - \frac{1}{y}$$

# Numerical Cauchy transforms and their inverse

- We will consider the following three types of measures:
  - Point measures

$$\mathrm{d}\mu = \delta(x - x_0)\,\mathrm{d}x$$

  - Measures with square root singularities (such as semicircle)

$$\mathrm{d}\mu = \psi(x)\sqrt{x-a}\sqrt{b-x}\,\mathrm{d}x$$

  - Smoothly decaying measures (such as Gaussian)

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

# Numerical Cauchy transforms and their inverse

- We will consider the following three types of measures:
  - Point measures

$$\mathrm{d}\mu = \delta(x - x_0)\,\mathrm{d}x$$

  - Measures with square root singularities (such as semicircle)

$$\mathrm{d}\mu = \psi(x)\sqrt{x-a}\sqrt{b-x}\,\mathrm{d}x$$

  - Smoothly decaying measures (such as Gaussian)

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

Assume Hölder–continuous derivative

# Point measures

- Trivial:

$$G_\mu(z) = \int \frac{\delta(x - x_0)}{z - x}\,\mathrm{d}x = \frac{1}{z - x_0}$$

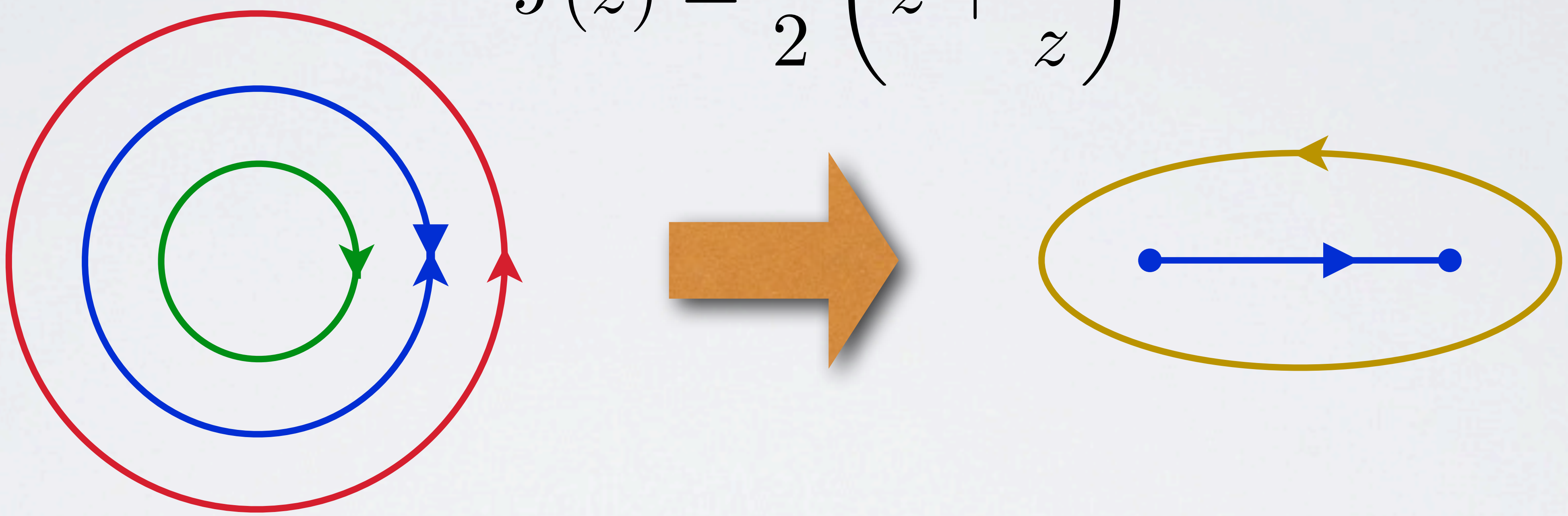
- Thus the inverse is:

$$G_\mu^{-1}(w) = \frac{1}{w} + x_0$$

# Chebyshev series and function approximation

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

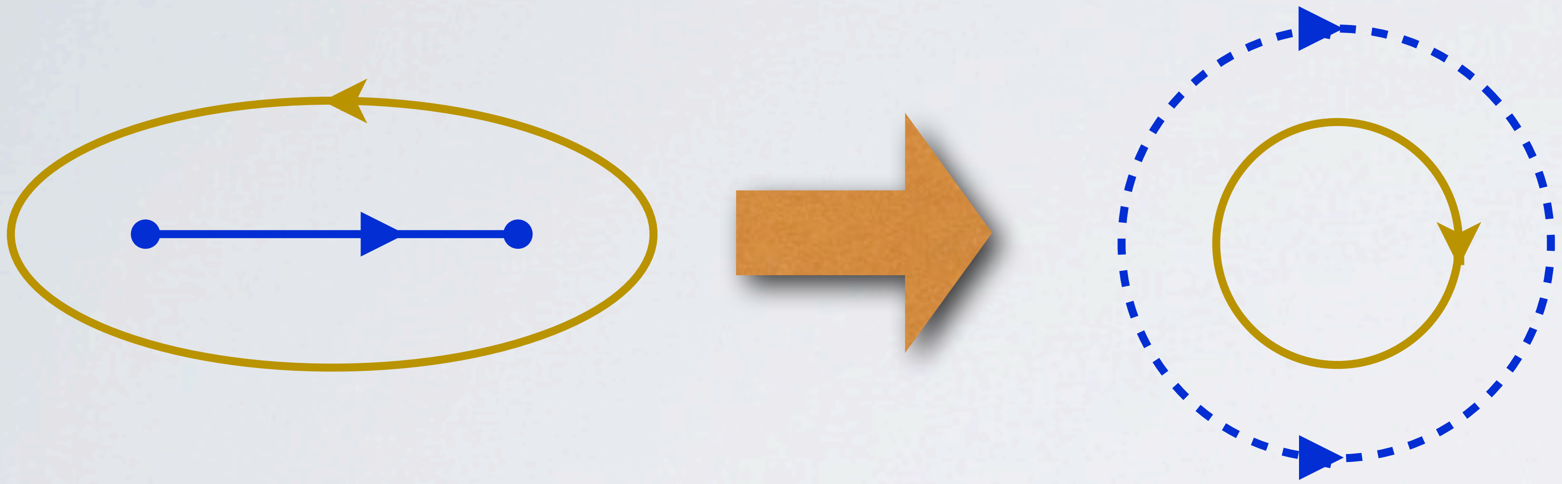
$$J(z) = \frac{1}{2}\left(z + \frac{1}{z}\right)$$



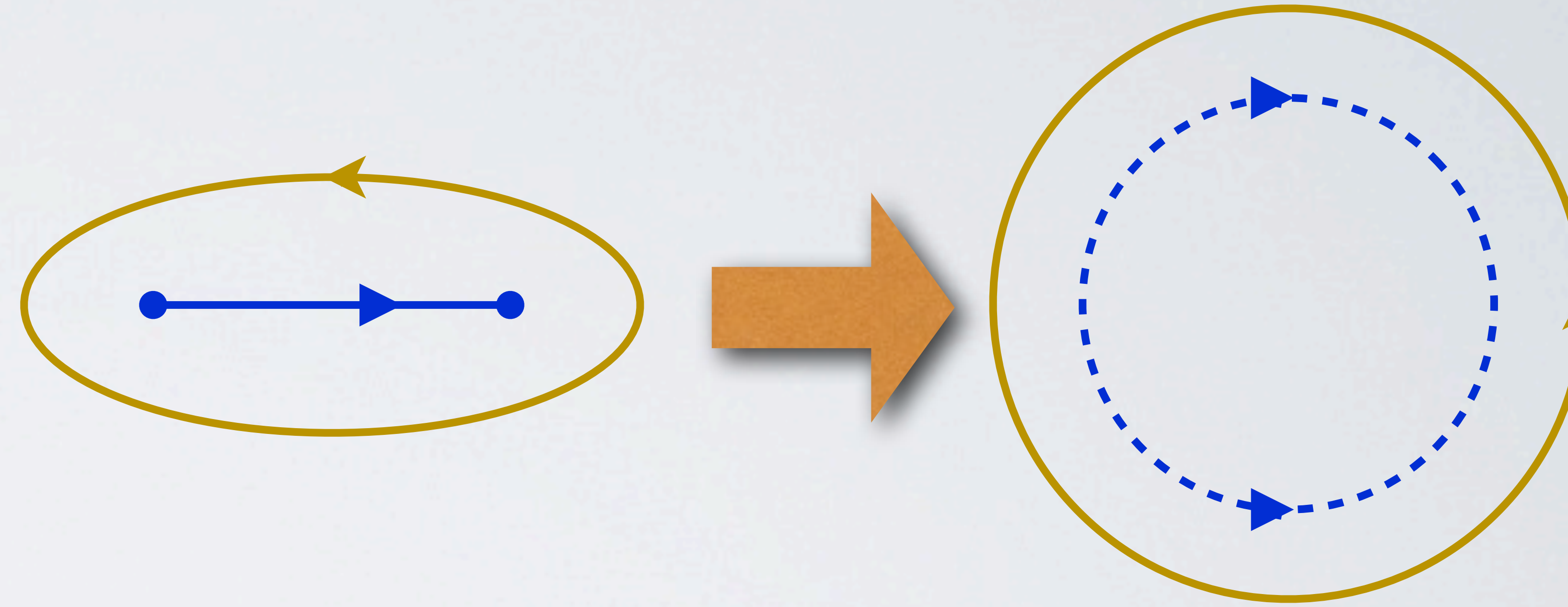
Functions analytic inside and outside the unit circle are mapped to functions analytic off the unit interval

# We define four inverses to the Joukowski map:

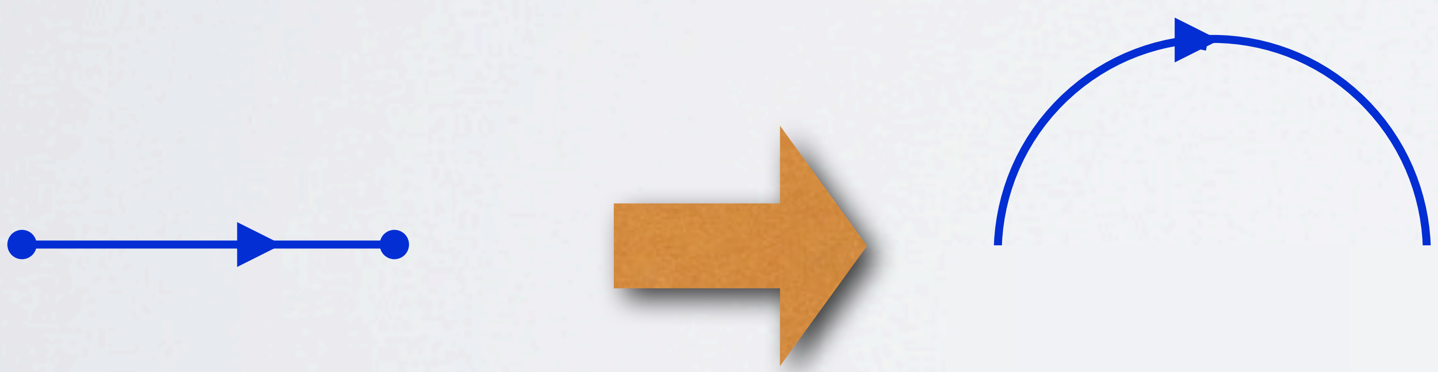
$$J_+^{-1}(x) = x - \sqrt{x-1}\sqrt{x+1}$$



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



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



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

- For smooth $\psi$ in

$$\mathrm{d}\mu = \psi(x)\sqrt{x-1}\sqrt{1-x}\,\mathrm{d}x$$

we want to find a representation that converges rapidly

- We can map to the unit circle and in expand in Laurent series:

$$\psi(J(\zeta)) = \psi\left(\frac{1}{2}\left(\zeta + \frac{1}{\zeta}\right)\right) = \sum_{k=-\infty}^{\infty} \psi_k \zeta^k$$

- $\psi(J(\zeta))$ is smooth (so $\psi_k$ decays fast) and symmetric (so $\psi_k = \psi_{-k}$)
- Thus we get the representation:

$$\begin{aligned}\psi(x) &= \psi(J(J_{\downarrow}^{-1}(x))) = \sum_{k=-\infty}^{\infty} \psi_k J_{\downarrow}^{-1}(x)^k \\ &= \psi_0 + \sum_{k=1}^{\infty} \psi_k \left[J_{\downarrow}^{-1}(x)^k + J_{\uparrow}^{-1}(x)^k\right] \\ &= \psi_0 + \sum_{k=1}^{\infty} \psi_k T_k(x)\end{aligned}$$

where $T_k(x) = \cos k \arccos x$ is the *Chebyshev T polynomial*

- We also need the *Chebyshev U series*
- Define $U_k(x)$ by

$$U_k(x) = \frac{T'_{k+1}(x)}{k+1}$$

- When mapped to the unit circle this gives

$$U_k(J(\zeta)) = \frac{1}{J'(\zeta)} \frac{(T_{k+1}(J(\zeta)))'}{k+1} = \frac{\zeta^k - \zeta^{-k-2}}{1 - \frac{1}{\zeta^2}}$$

- Going between Chebyshev T and U expansions is fast due to:

$$\begin{aligned} T_0(x) &= U_0(x) \\ T_1(x) &= \frac{U_1(x)}{2} \\ T_k(x) &= \frac{U_k(x) - U_{k-2}(x)}{2} \end{aligned}$$

# Plemelj's lemma and square root decaying measures

- We want to calculate $G_\mu(z)$ for

$$\mathrm{d}\mu = \psi(x)\sqrt{x-1}\sqrt{1-x}\,\mathrm{d}x$$

Recall that $\phi(z) = -\frac{1}{2\pi \mathrm{i}} G_\mu(z)$ is analytic off $(-1,1)$, vanishes at $\infty$ and satisfies the jump:

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

- We have expanded in Chebyshev U series $\psi(x) = \sum_{k=0}^{\infty} \psi_k U_k(x)$

- A simple calculation shows that

$$\left[J_+^{-1}(x)^{k+1}\right]^+ - \left[J_+^{-1}(x)^{k+1}\right]^- = J_\downarrow^{-1}(x)^{k+1} - J_\uparrow^{-1}(x)^{k+1}$$
$$= -2\mathrm{i}U_k(x)\sqrt{1-x^2}$$

- So

$$G_\mu(z) = \pi \sum_{k=0}^{\infty} \psi_k J_+^{-1}(z)^{k+1}$$

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

- We have expanded in Chebyshev U series $\psi(x) = \sum_{k=0}^{\infty} \psi_k U_k(x)$

- A simple calculation shows that

$$\left[J_+^{-1}(x)^{k+1}\right]^+ - \left[J_+^{-1}(x)^{k+1}\right]^- = J_\downarrow^{-1}(x)^{k+1} - J_\uparrow^{-1}(x)^{k+1}$$
$$= -2\mathrm{i}U_k(x)\sqrt{1-x^2}$$

Smoothness implies absolute convergence

- So

$$G_\mu(z) = \pi \sum_{k=0}^{\infty} \psi_k J_+^{-1}(z)^{k+1}$$

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

# Inverting the Cauchy transform

- We want to solve

$$G_\mu(z) = \pi \sum_{k=0}^{\infty} \psi_k J_+^{-1}(z)^{k+1} = w$$

- We make the transformation back to the unit circle

$$z = J(\zeta) = \frac{1}{2}\left(\zeta + \frac{1}{\zeta}\right) \qquad \text{so that} \qquad \sum_{k=0}^{\infty} \psi_k \zeta^{k+1} = w$$

- This is again a polynomial, and reliably solvable using eigenvalues of companion matrices!

# Free probability algorithm

- Input: measures $\mu_A$ and $\mu_B$ in expansion form
- Output: $\mu_A \boxplus \mu_B$ in expansion form

1. Construct scheme to evaluate $G_{\mu_A}^{-1}(y)$ and $G_{\mu_B}^{-1}(y)$ pointwise
2. Recover $\mu_A \boxplus \mu_B$ from pointwise knowledge of

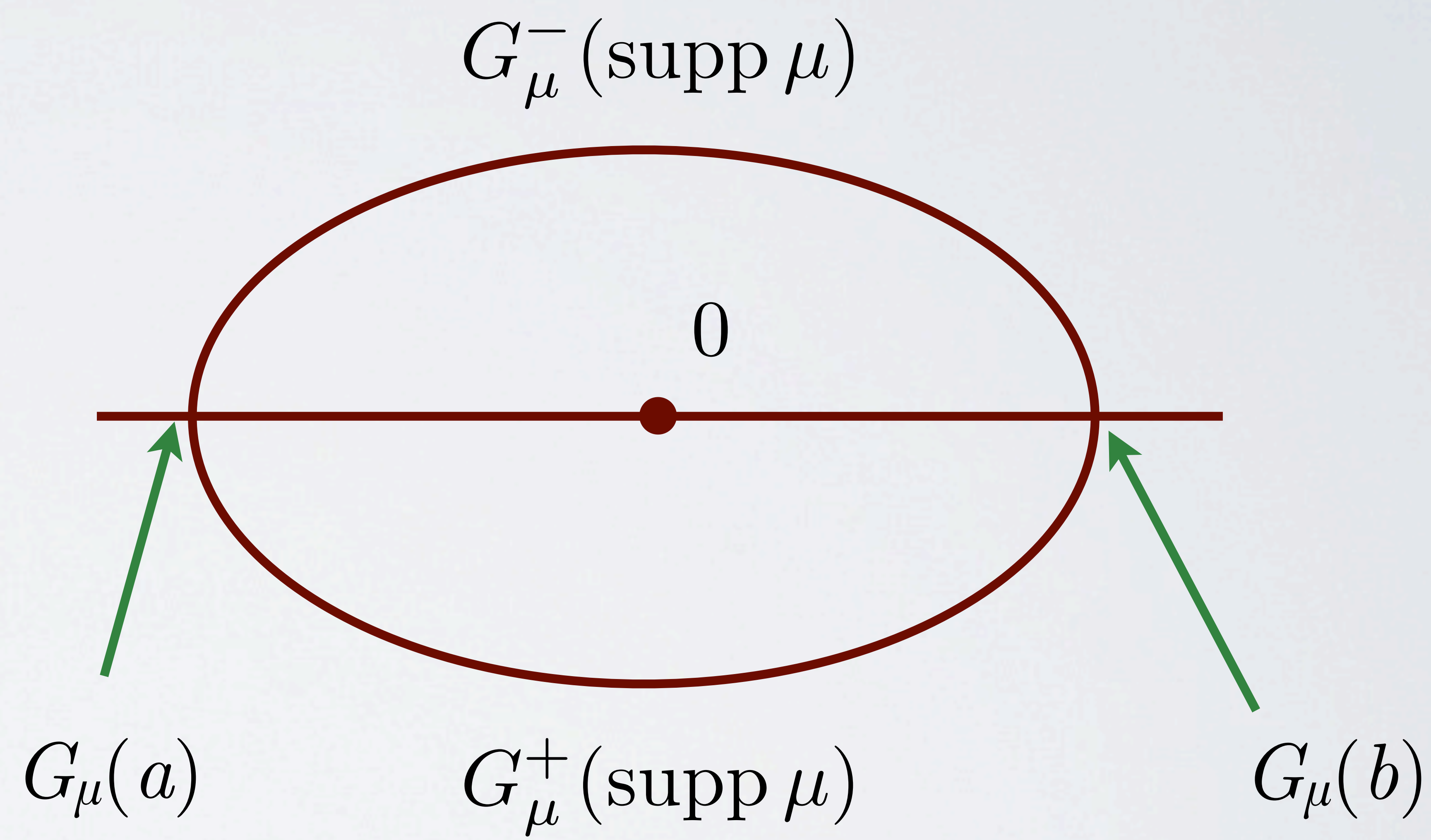
$$G_{\mu_A \boxplus \mu_B}^{-1}(y) = G_{\mu_A}^{-1}(y) + G_{\mu_B}^{-1}(y) - \frac{1}{y}$$

# Recovering endpoints of a square root measure

- Along $(b,\infty)$ and $(a,\infty)$, $G_\mu$ is real and tends to zero
- For $x$ in $(a,b)$,

$$G_\mu(x+\epsilon \mathrm{i}) = \overline{G_\mu(x-\epsilon \mathrm{i})}$$

- Because it is real in two different directions, $G_\mu^{-1}$ has a stationary point at $G_\mu(a)$ and $G_\mu(b)$
- Thus we can compute them using bisection



# Recovering coefficients of a square root decaying measure

- We have

$$G_\mu(G_\mu^{-1}(w)) = w$$

Whenever $w$ is in the range of $G_\mu$

- Thus given a sequence of points $w_1, \ldots, w_m$ in the range of $G_\mu$, we can treat the problem as a linear least squares problem:

$$\frac{1}{2}\sum_{k=1}^{n} u_k J_+^{-1}(M(G_\mu^{-1}(w_j)))^k \approx w_j$$

# Choosing $w_j$

- We need to choose points that like in the image of $G_\mu$
- Suppose we have a distribution of points $y_1,\ldots,y_M$ which cover (as $M$ tends to ∞) a domain which contains the image of $G_\mu$ as a subset
- Note that

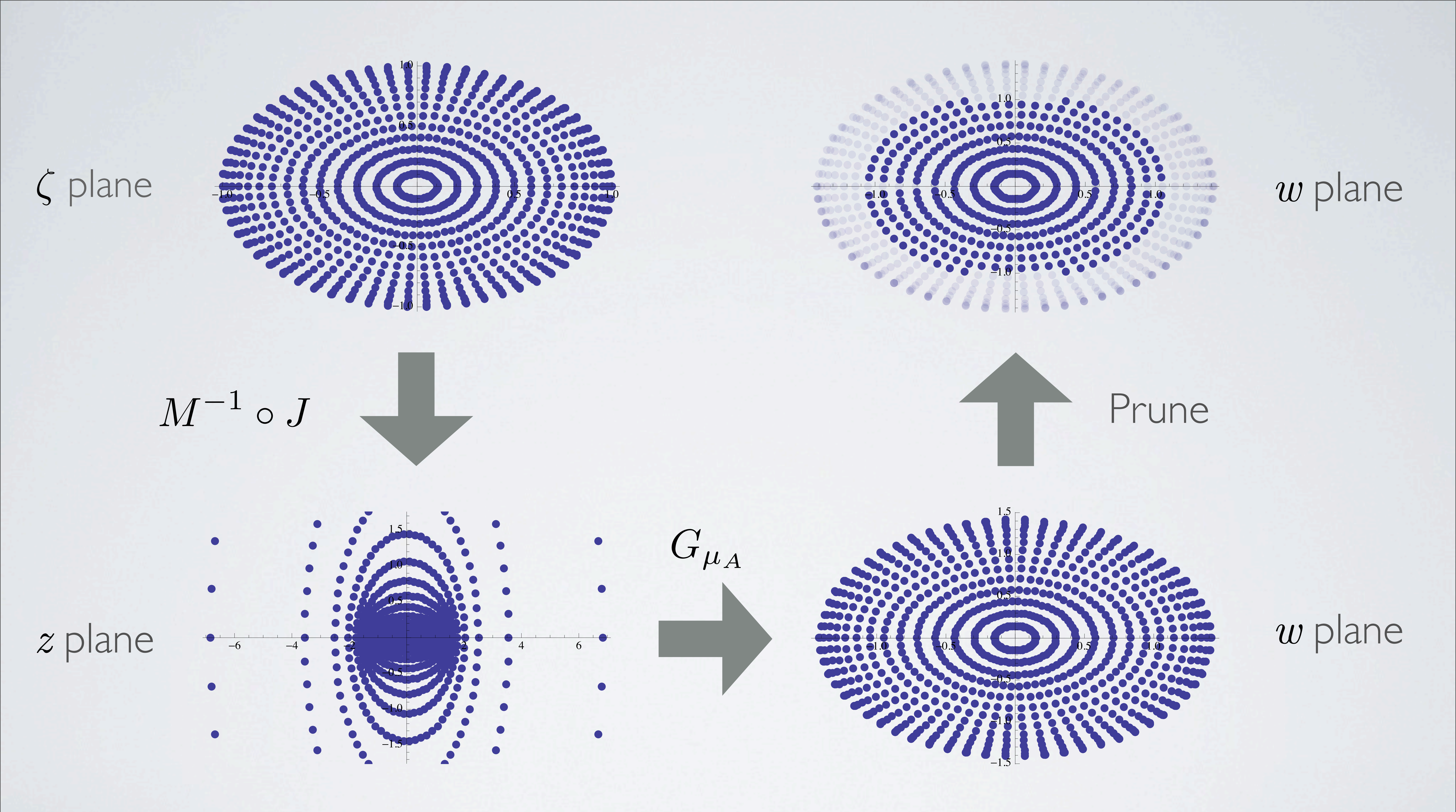
$$G_\mu(u + \mathrm{i}v) = \int \frac{1}{u - x + \mathrm{i}v} \, \mathrm{d}\mu$$

Since $u - x + \mathrm{i}v$ is in the upper half plane for $v$ positive,

$$\Im \frac{1}{u - x + \mathrm{i}v} < 0 \Rightarrow \Im G_\mu(u + \mathrm{i}v) < 0$$

- Thus we choose $w_j$ as the $y_j$ such that

$$\operatorname{sgn} \Im w_j \neq \operatorname{sgn} \Im G_\mu^{-1}(w_j)$$


ζ plane
w plane
$M^{-1} \circ J$
Prune
z plane
$G_{\mu_A}$
w plane

# Finite $n$:

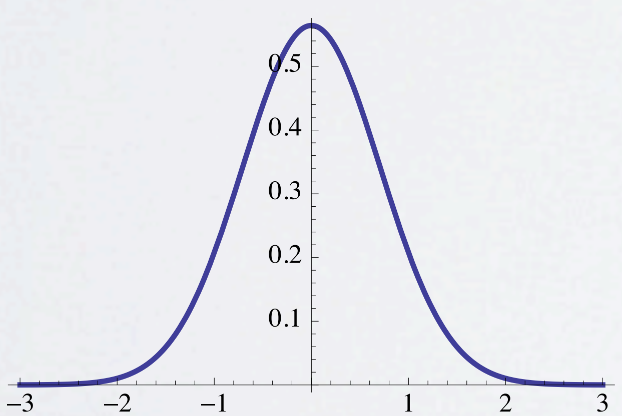
# Free Probability & Invariant Ensembles?

$$V_A(x) = x^2 \qquad\qquad V_B(x) = x^4$$

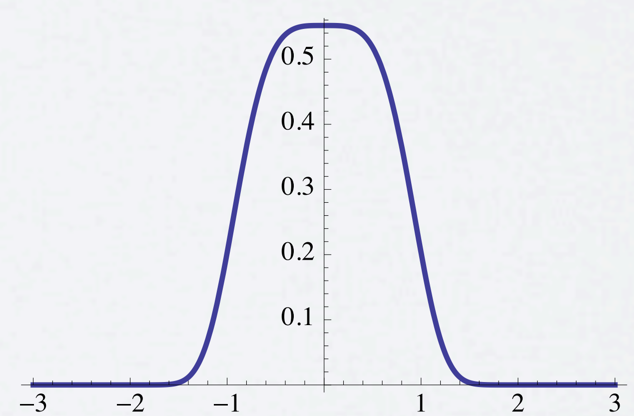
$n = \infty$

$n = 5$

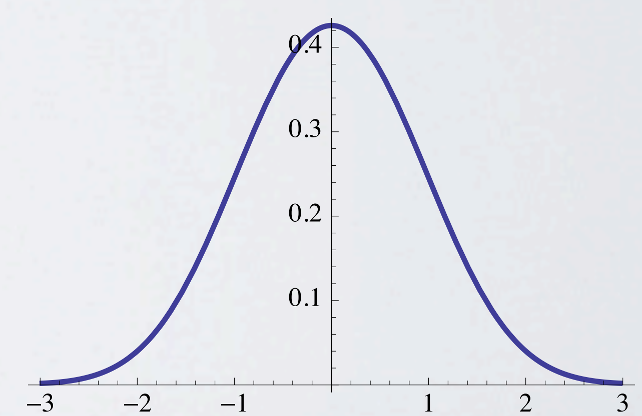
$n = 1$




$\star$

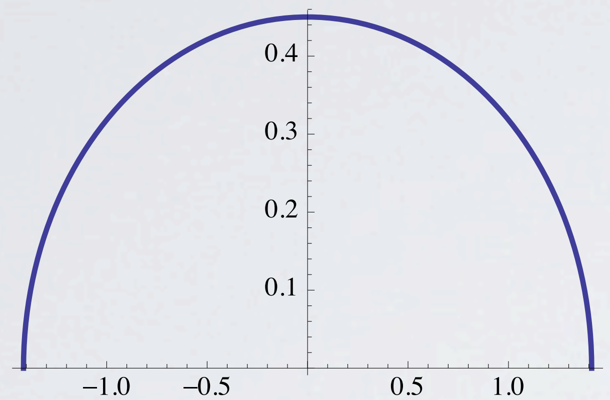



$=$

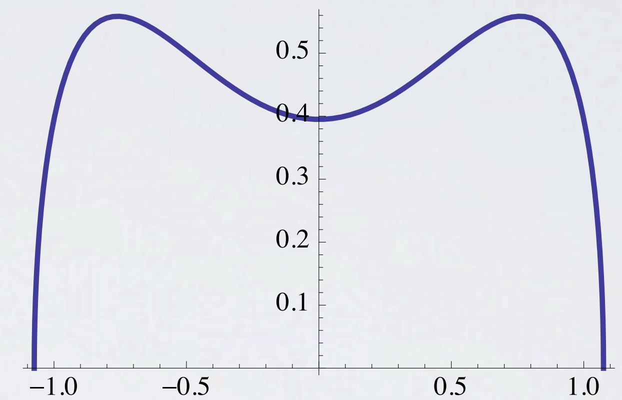


$V_A(x) = x^2$ $\qquad$ $V_B(x) = x^4$

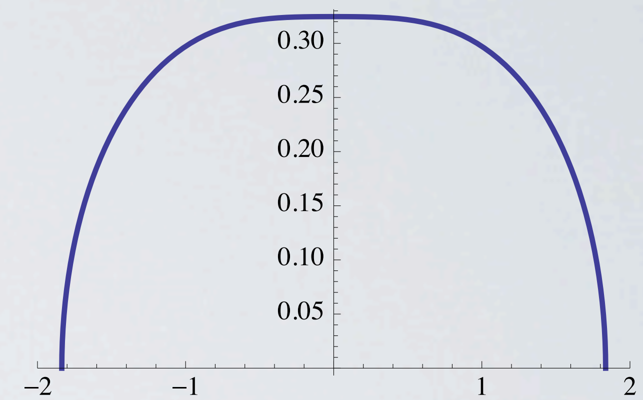
$n = \infty$




$\boxplus$

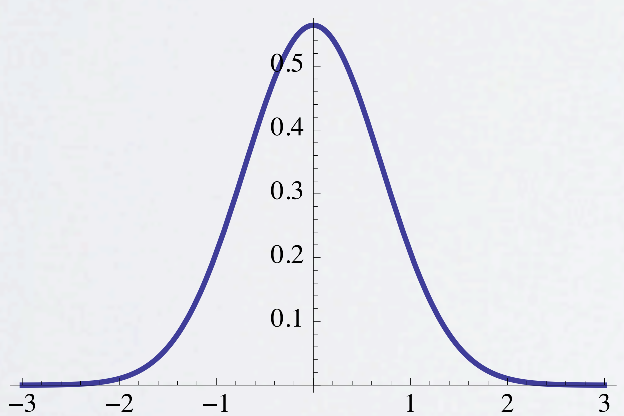



$=$

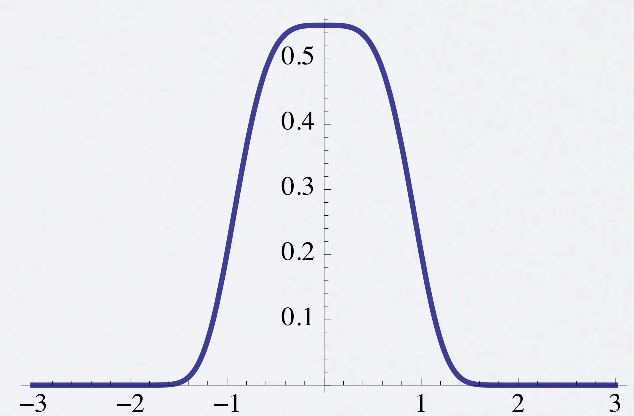



$n = 5$

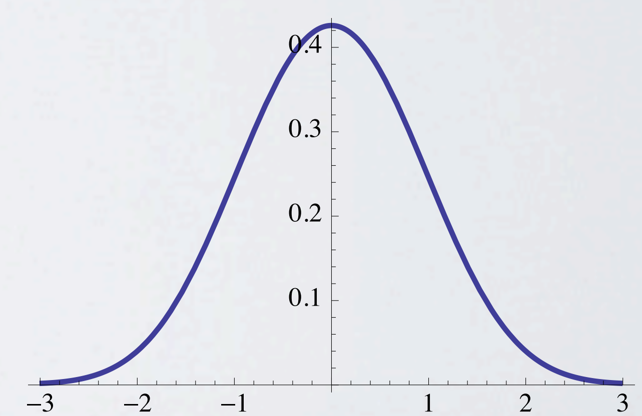
$n = 1$




$\star$

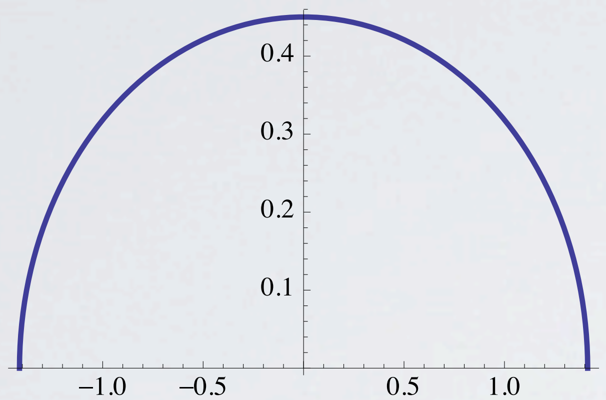



$=$

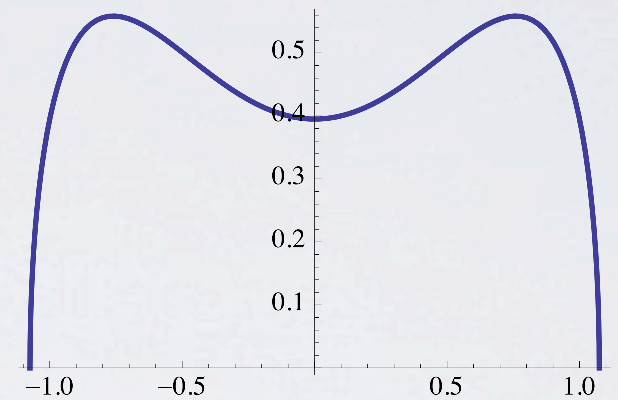


$V_A(x) = x^2$ $\qquad$ $V_B(x) = x^4$

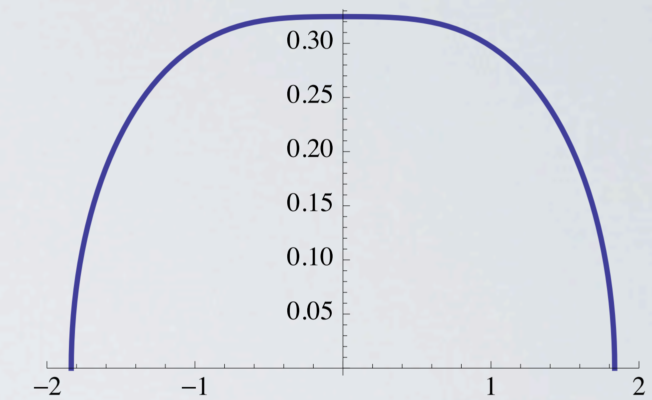
$n = \infty$



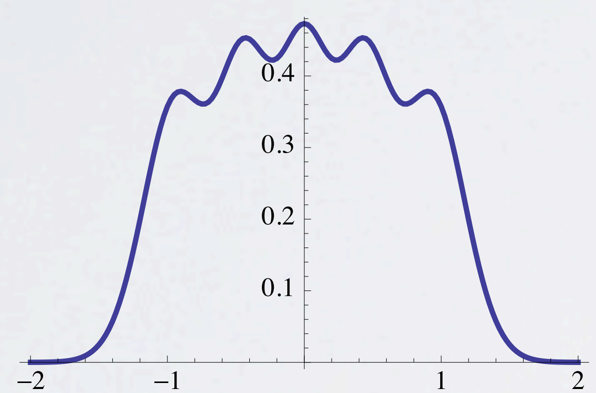

$\boxplus$



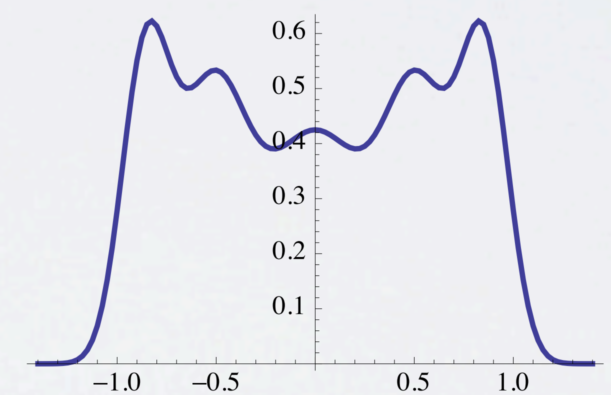

$=$




$n = 5$

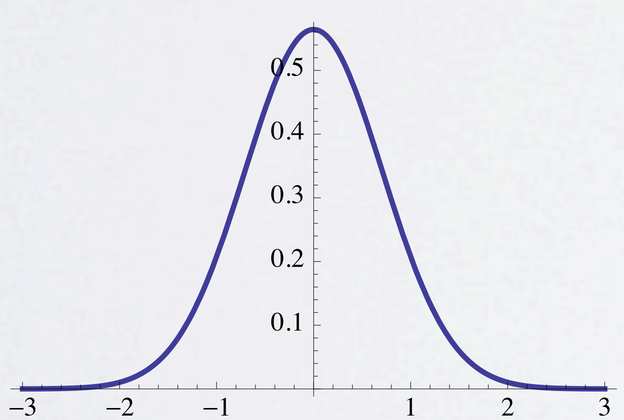



$\boxplus_n$

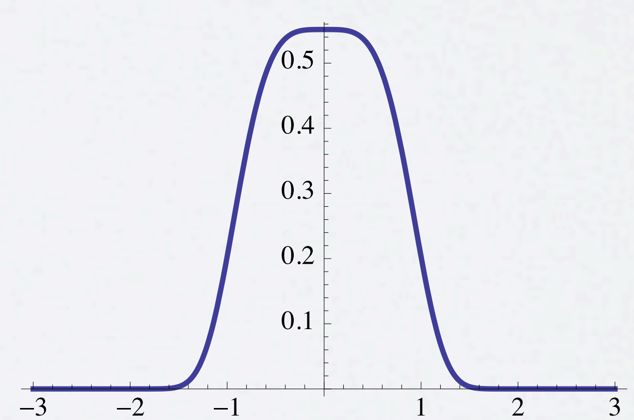



$=$

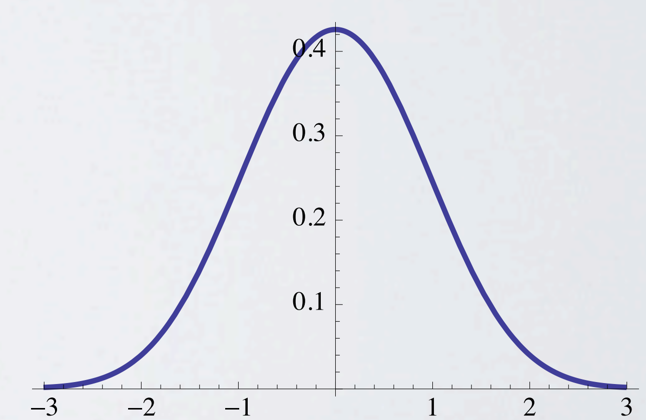
$n = 1$




$\star$

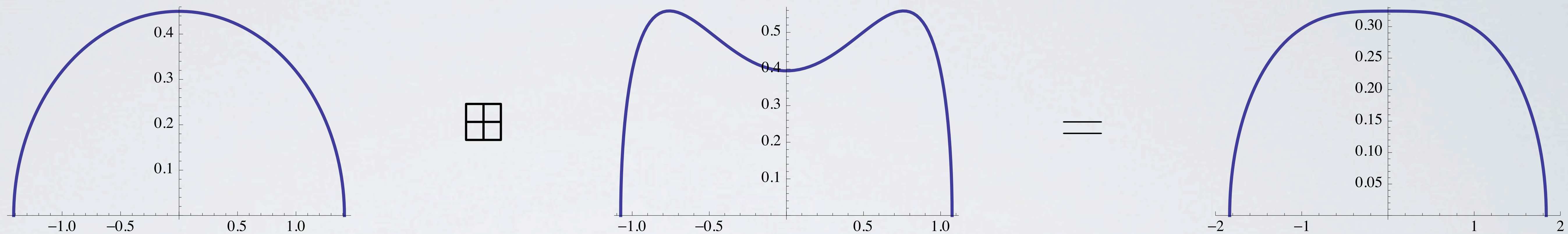



$=$

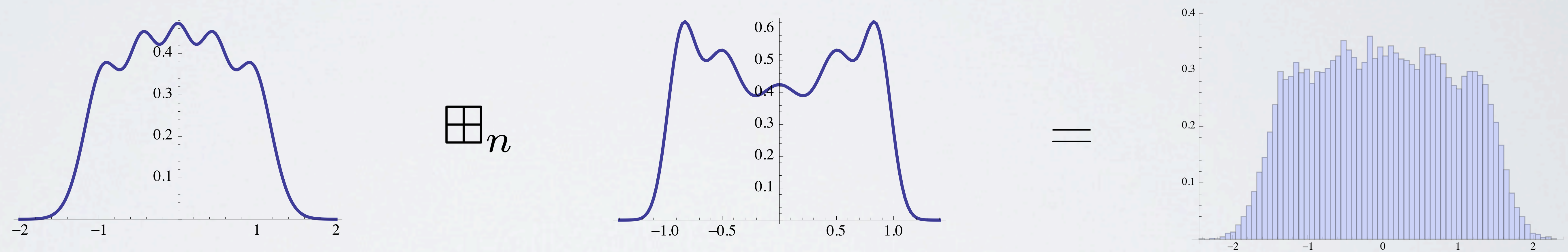


$$V_A(x) = x^2 \qquad\qquad V_B(x) = x^4$$

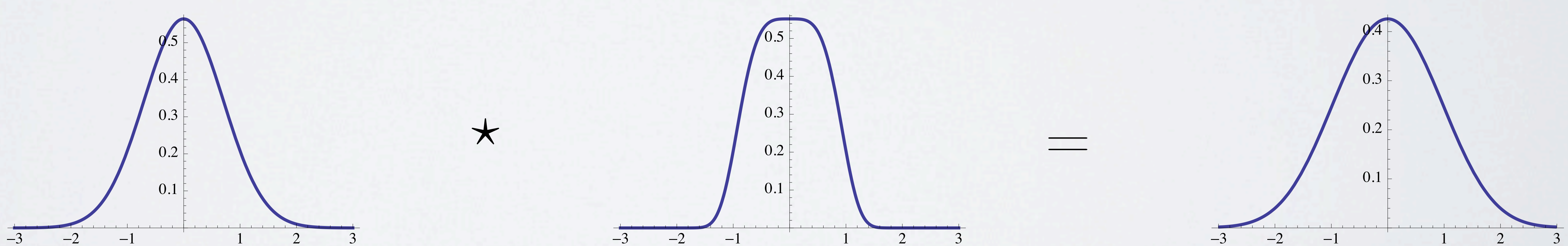
$n = \infty$




$n = 5$

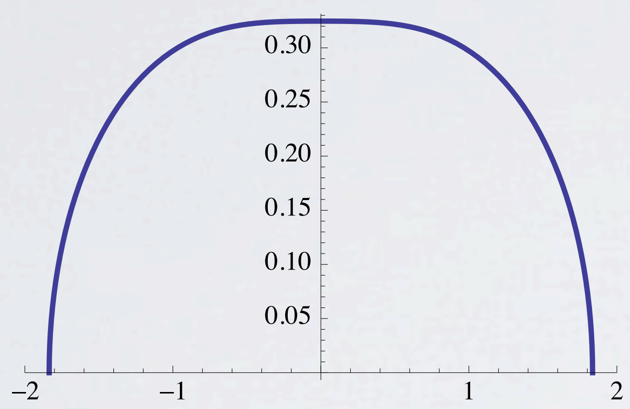



$n = 1$

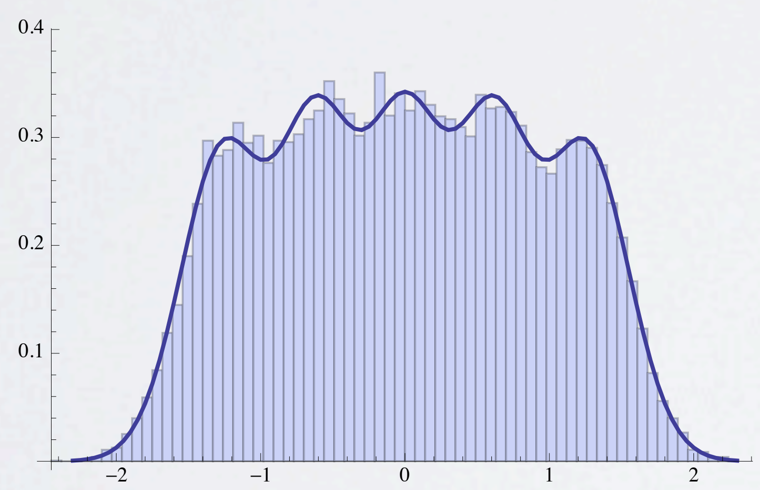


# Finite $n$ is close to invariant ensemble

$n = \infty$

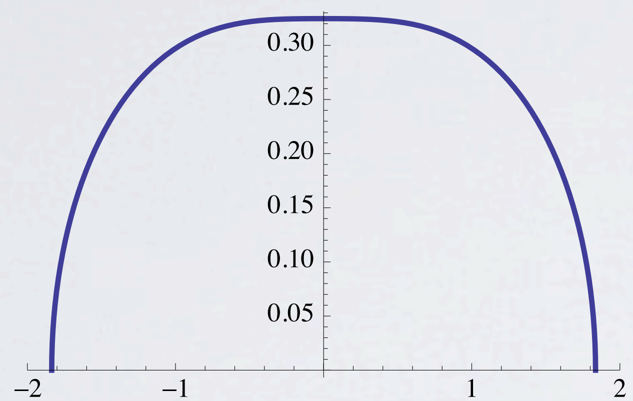



$n = 5$



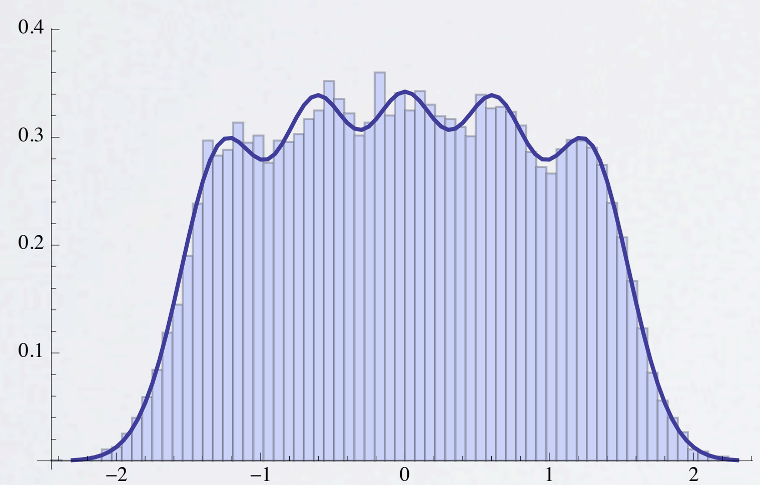
# Finite $n$ is close to invariant ensemble

$n = \infty$



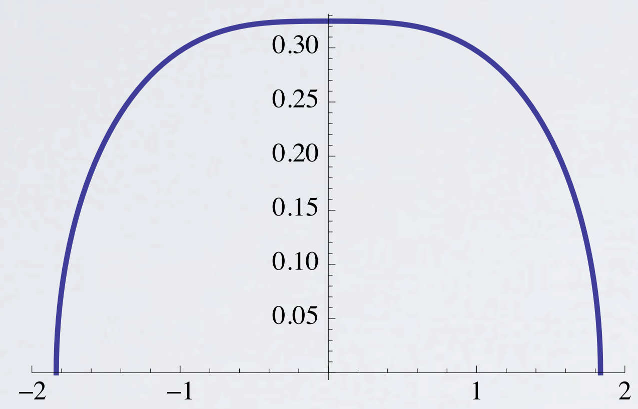

Take as equilibrium measure for new invariant ensemble $C_n$

$n = 5$



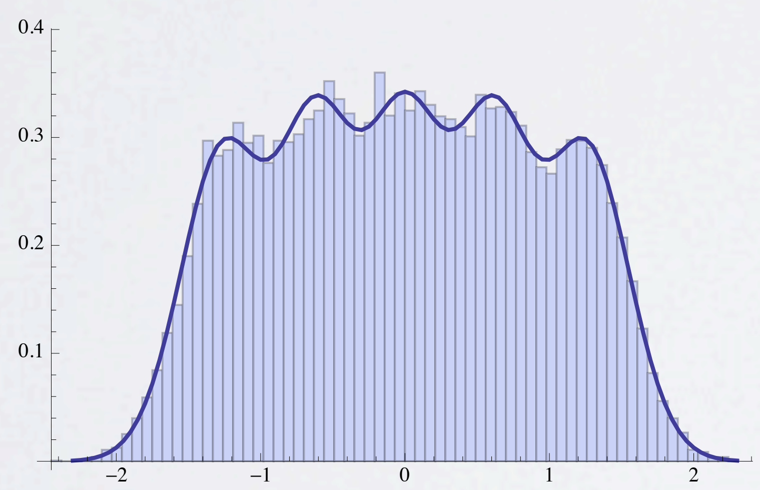
# Finite $n$ is close to invariant ensemble

$n = \infty$




Take as equilibrium measure for new invariant ensemble $C_n$

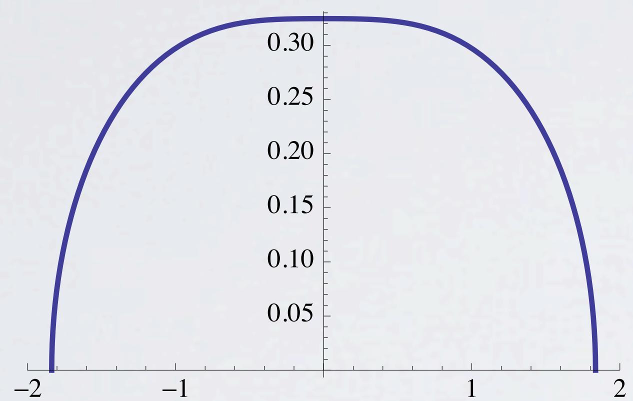
$n = 5$




Calculate spectral density of $C_5$

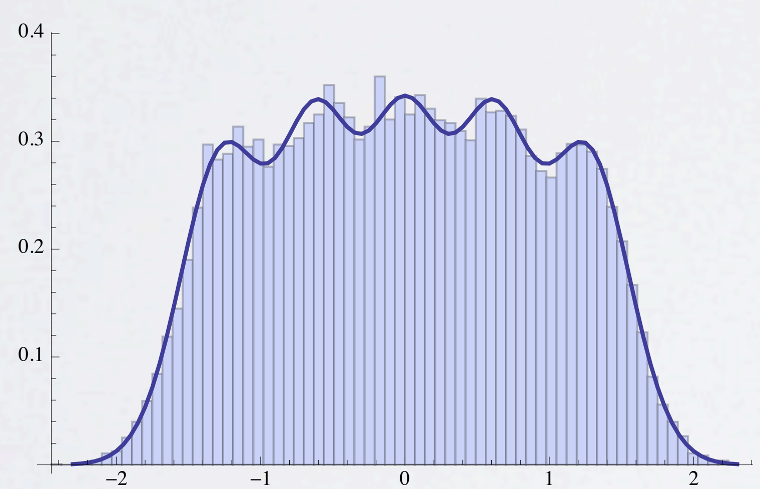
# Finite $n$ is close to invariant ensemble

$n = \infty$



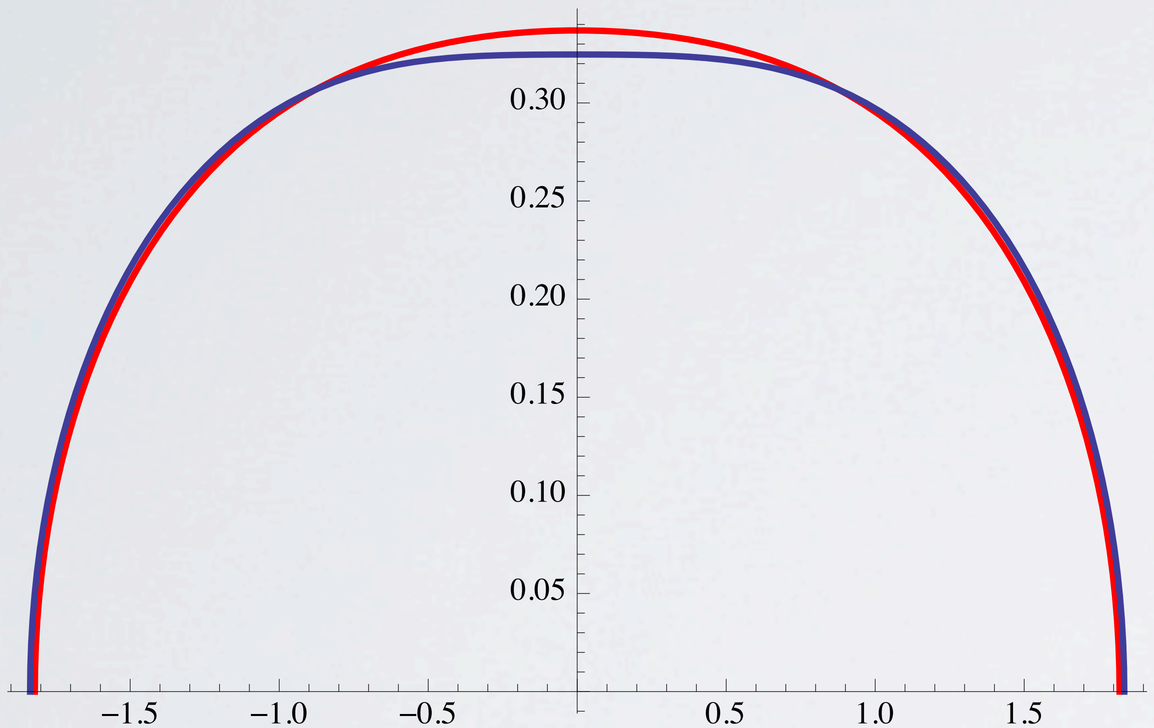

Take as equilibrium measure for new invariant ensemble $C_n$

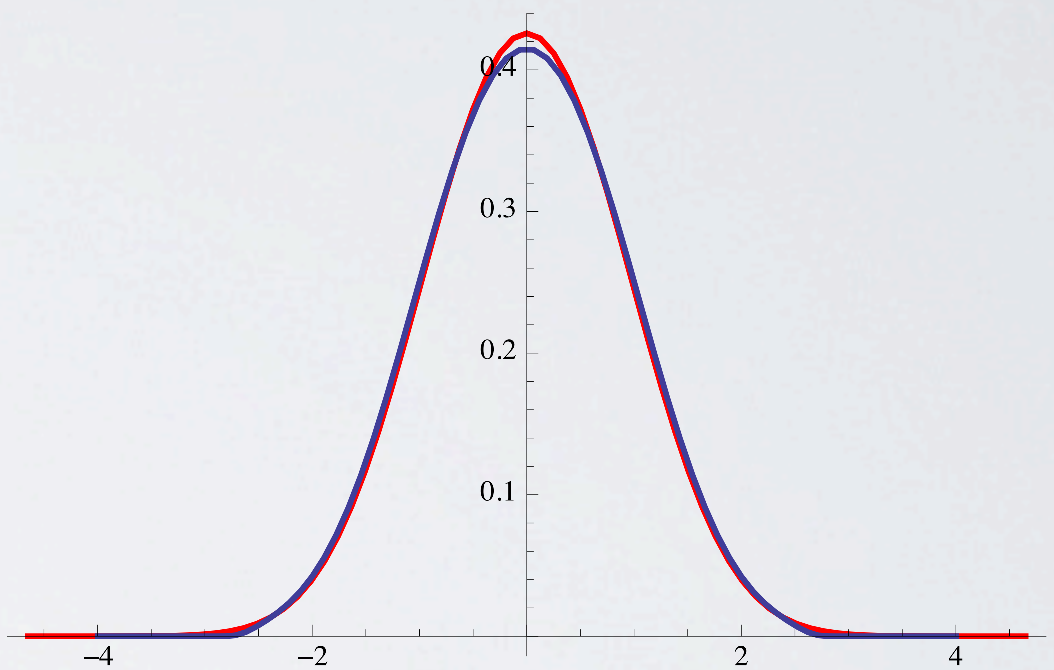
$n = 5$




Calculate spectral density of $C_5$

# Observation: $1 \approx \infty$



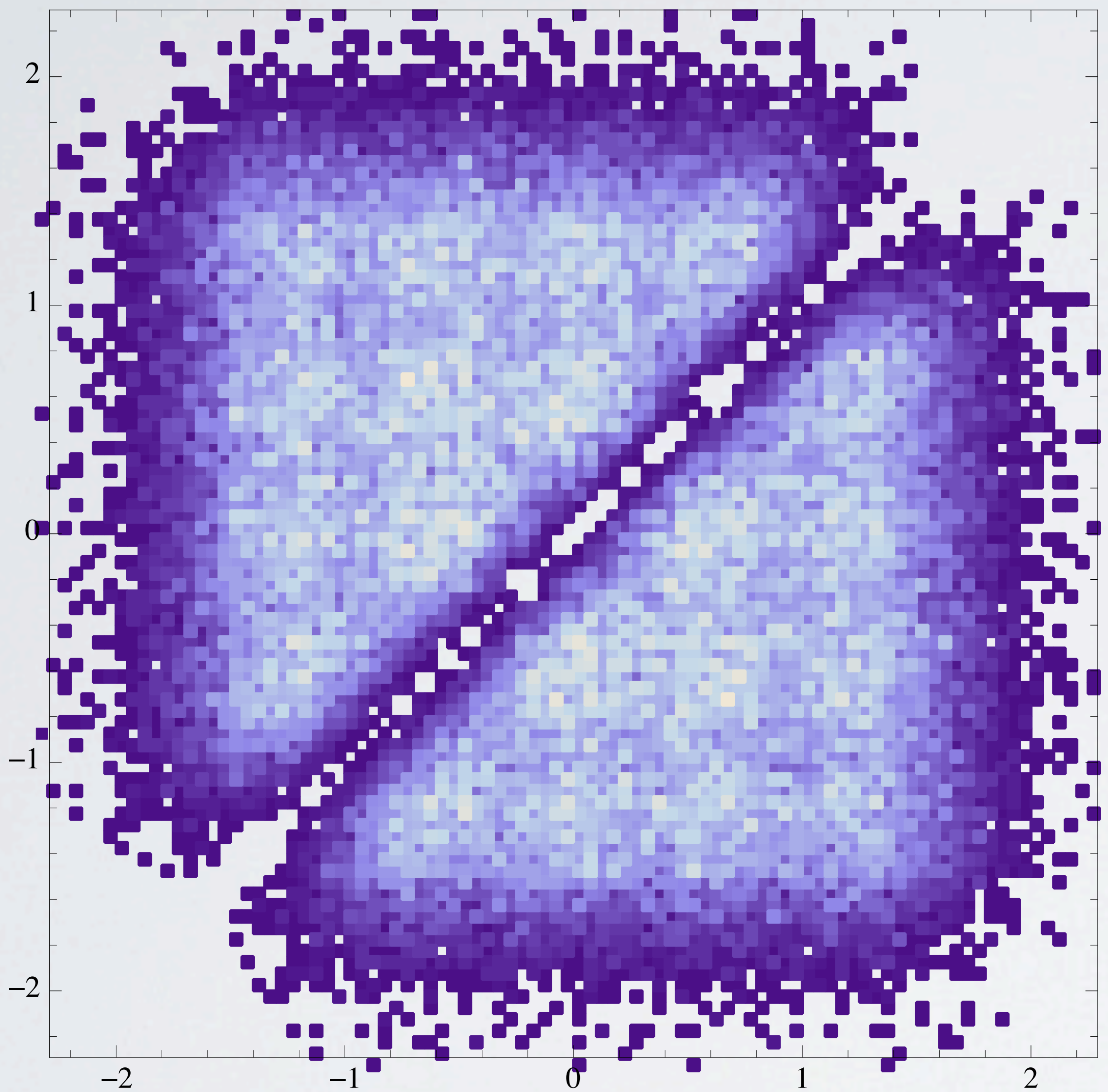

$n = \infty$: Free convolution $\mu_A \boxplus \mu_B$

$n = 1$: Equilibrium measure of $\mathrm{e}^{-x^2} \star \mathrm{e}^{-x^4}$

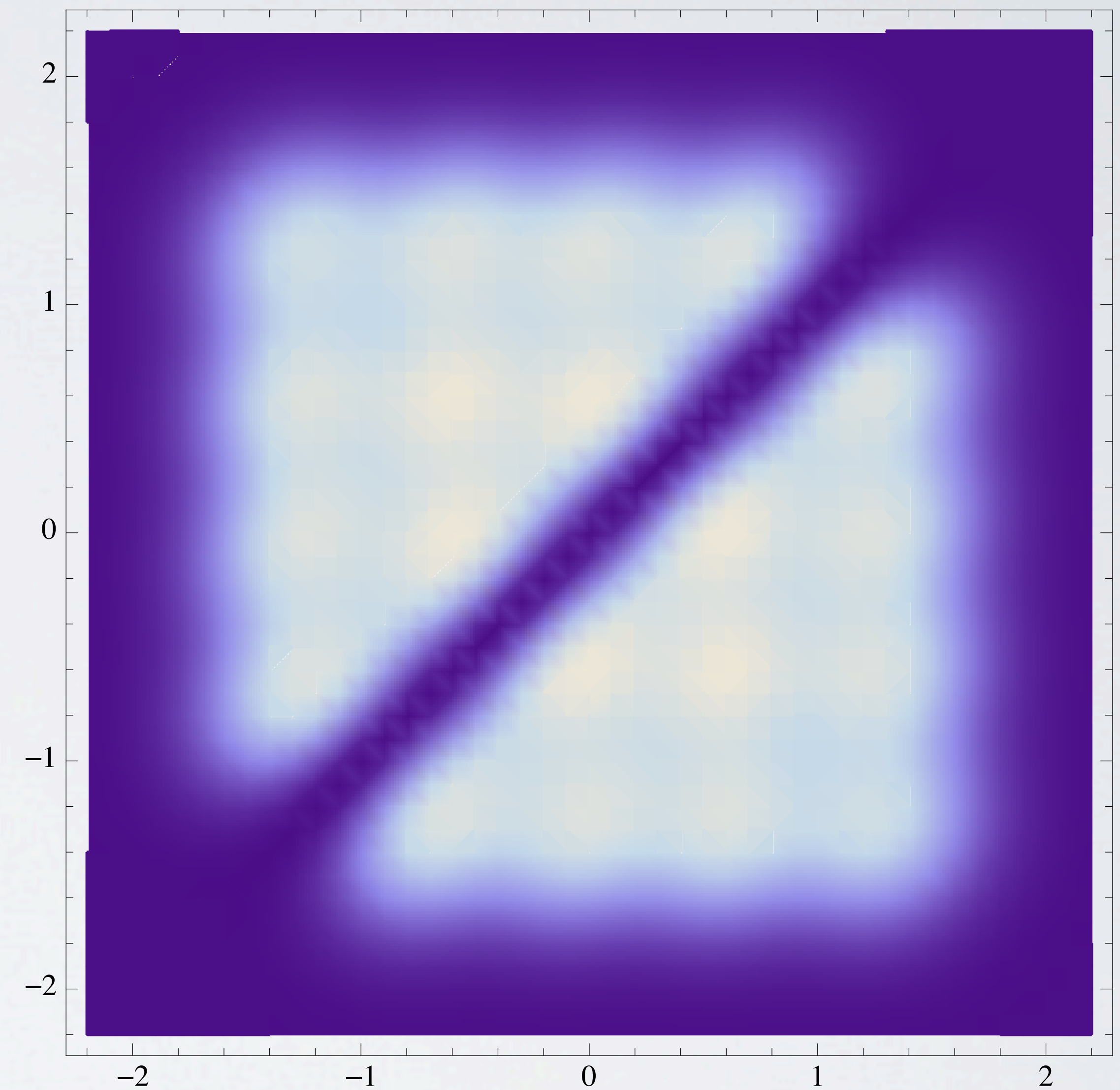
Weight with equilibrium measure $\mu_A \boxplus \mu_B$

Convolution $\mathrm{e}^{-x^2} \star \mathrm{e}^{-x^4}$

# GUE + Quartic 2 point correlation

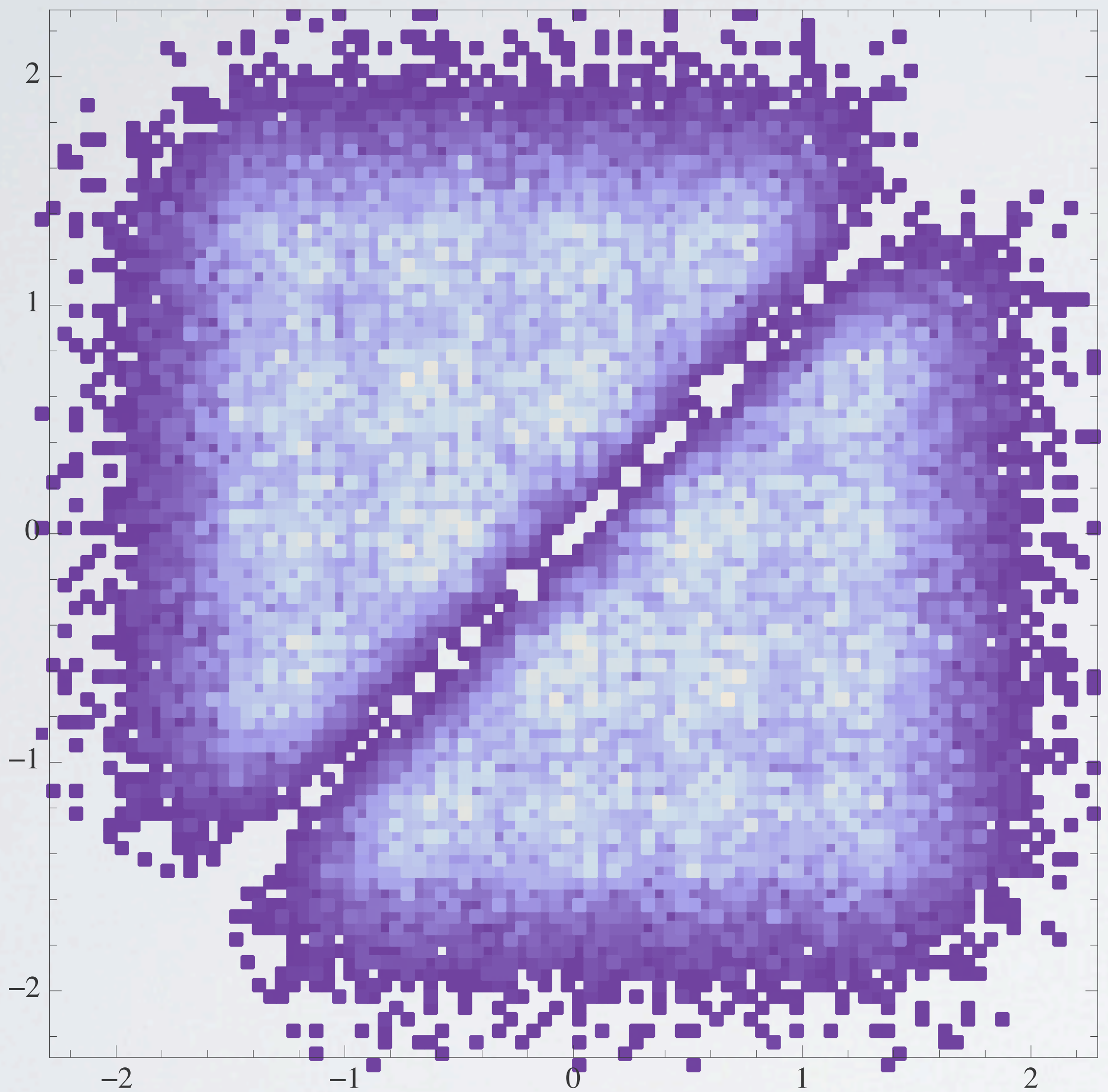



Monte Carlo

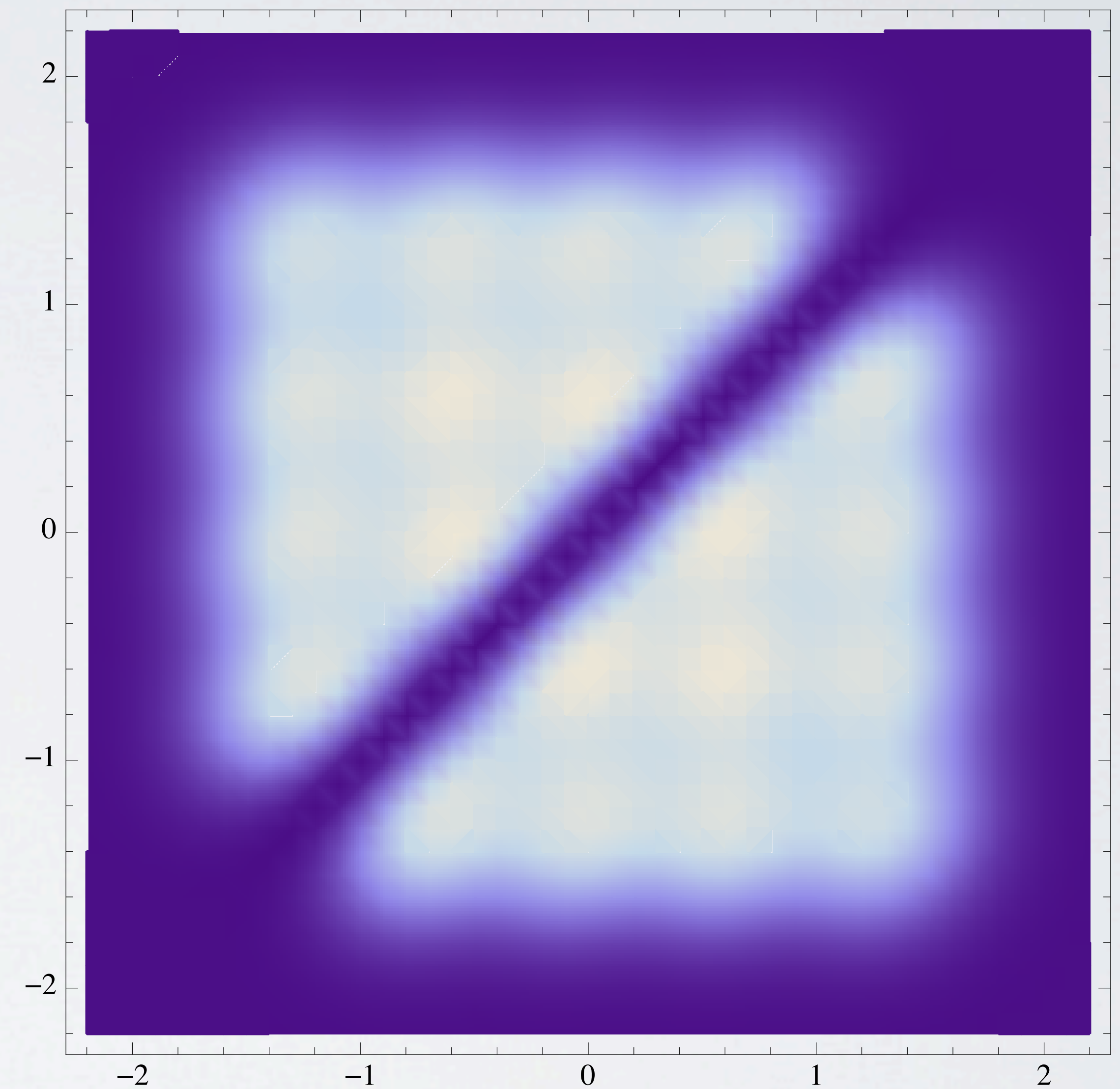



Invariant ensemble

# GUE + Quartic 2 point correlation

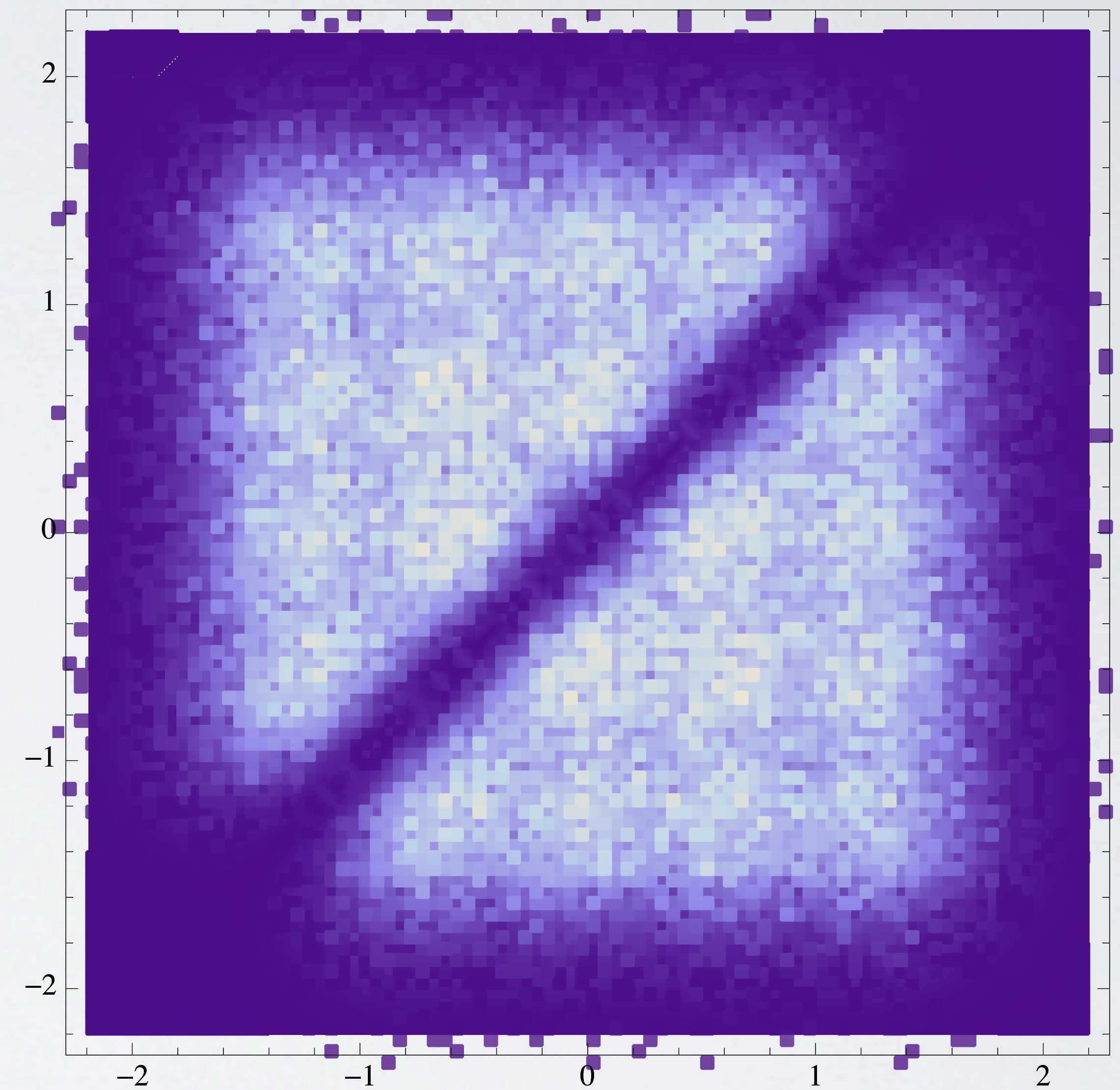



Monte Carlo




Invariant ensemble

# GUE + Quartic 2 point correlation

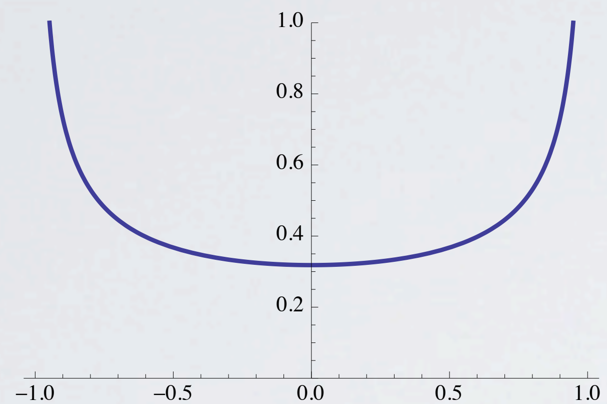



Monte Carlo

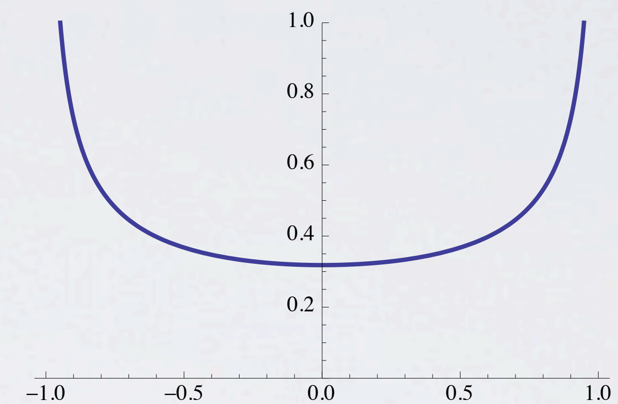
Invariant ensemble

## Legendre ⊞ Legendre

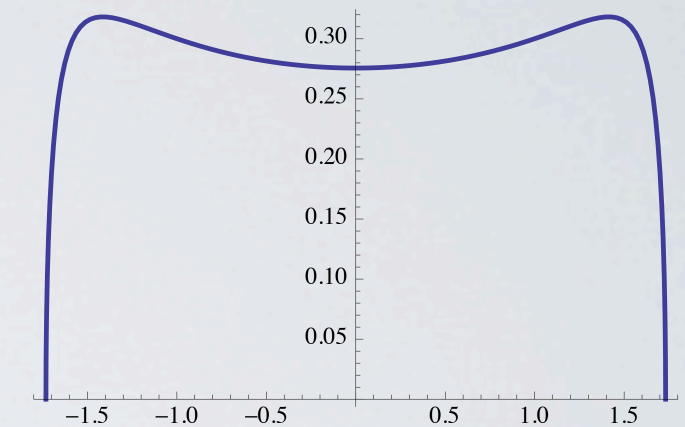
$n = \infty$




$\boxplus$

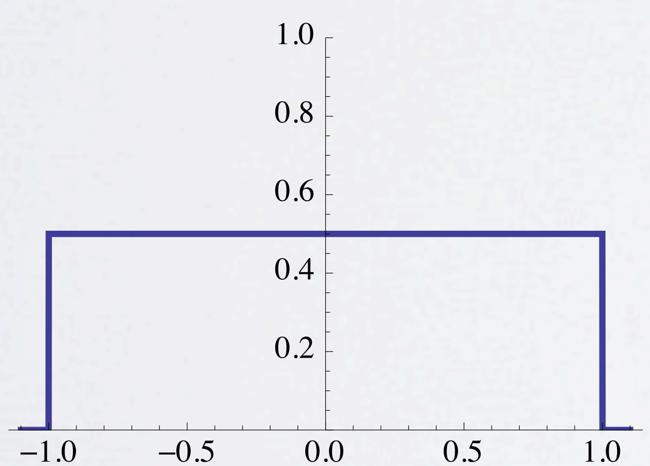



$=$

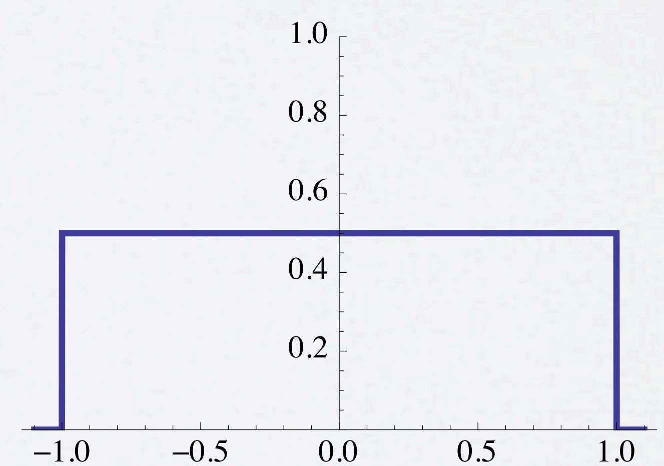



$n = 5$

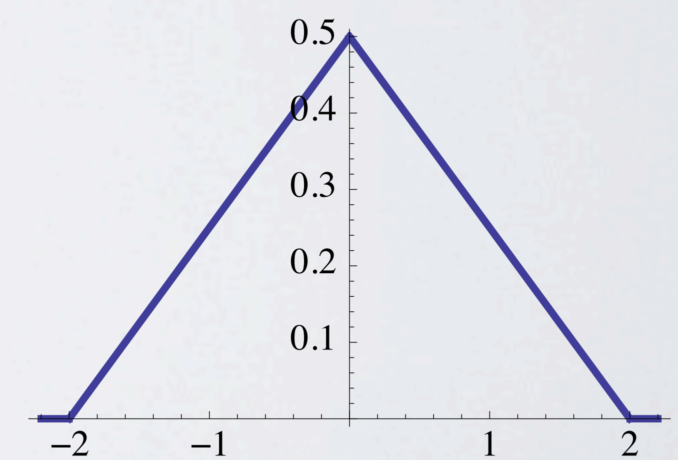
$n = 1$




$\star$

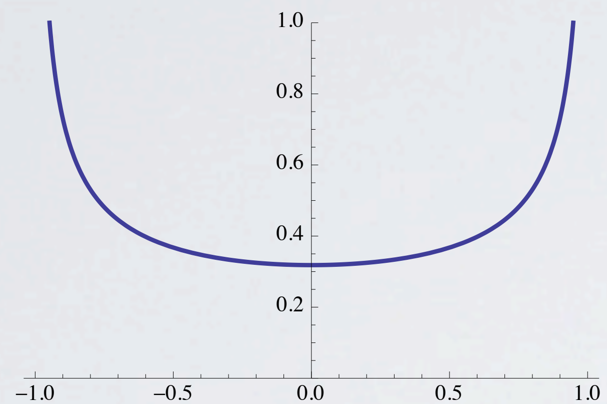



$=$

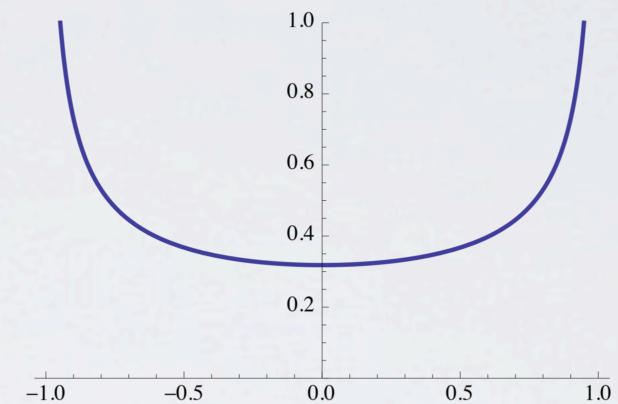


Legendre Legendre

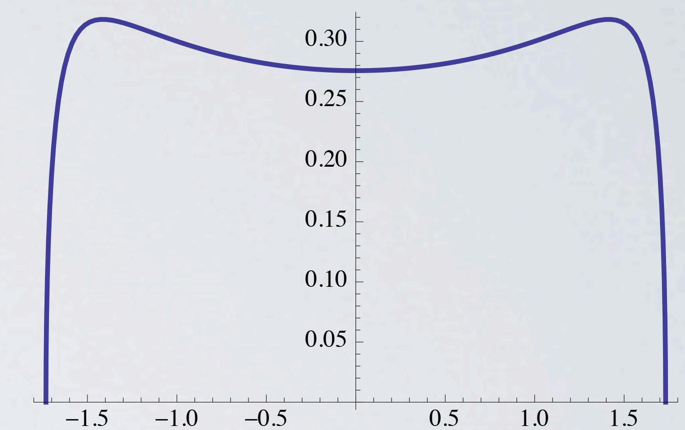
$n = \infty$



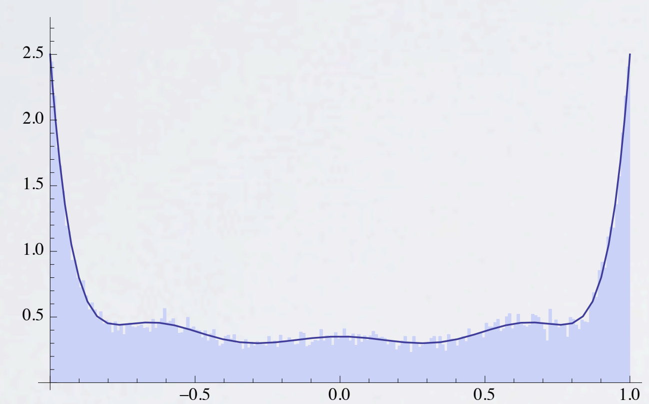

$\boxplus$



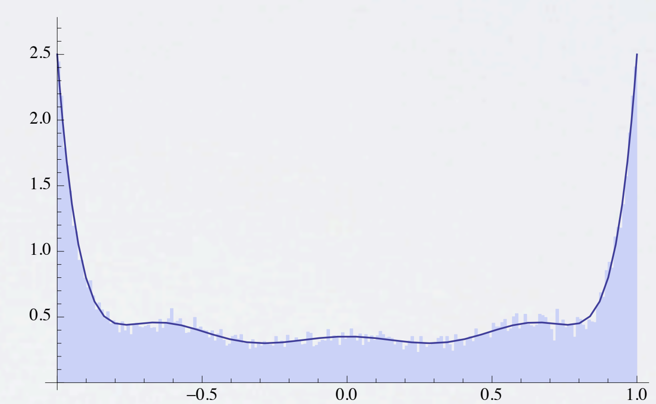

$=$




$n = 5$

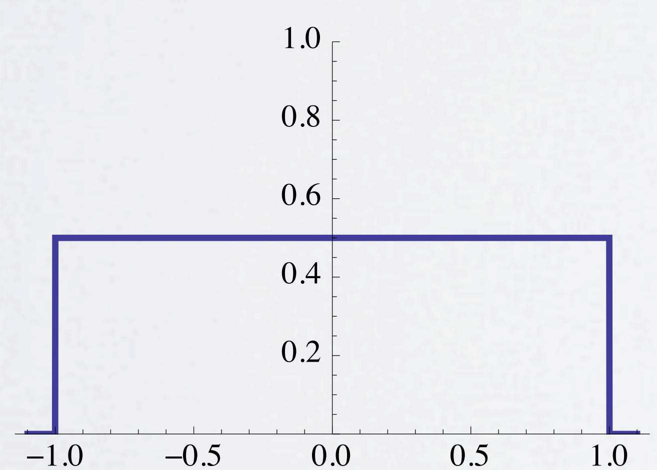



$\boxplus_n$

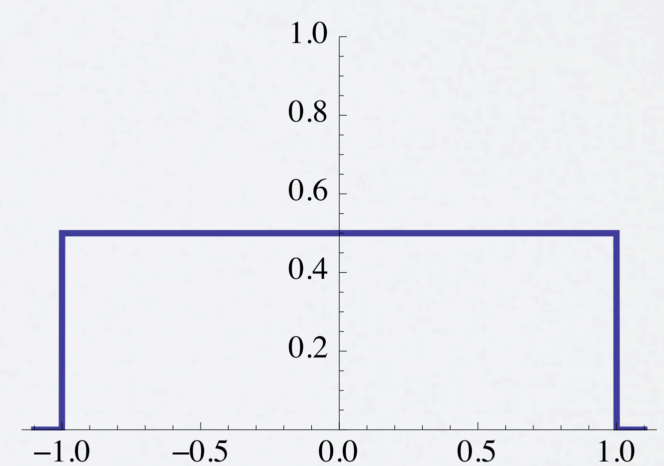



$=$

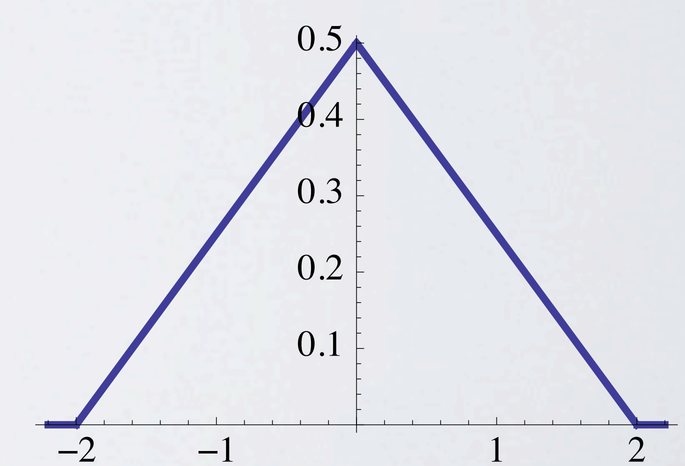
$n = 1$

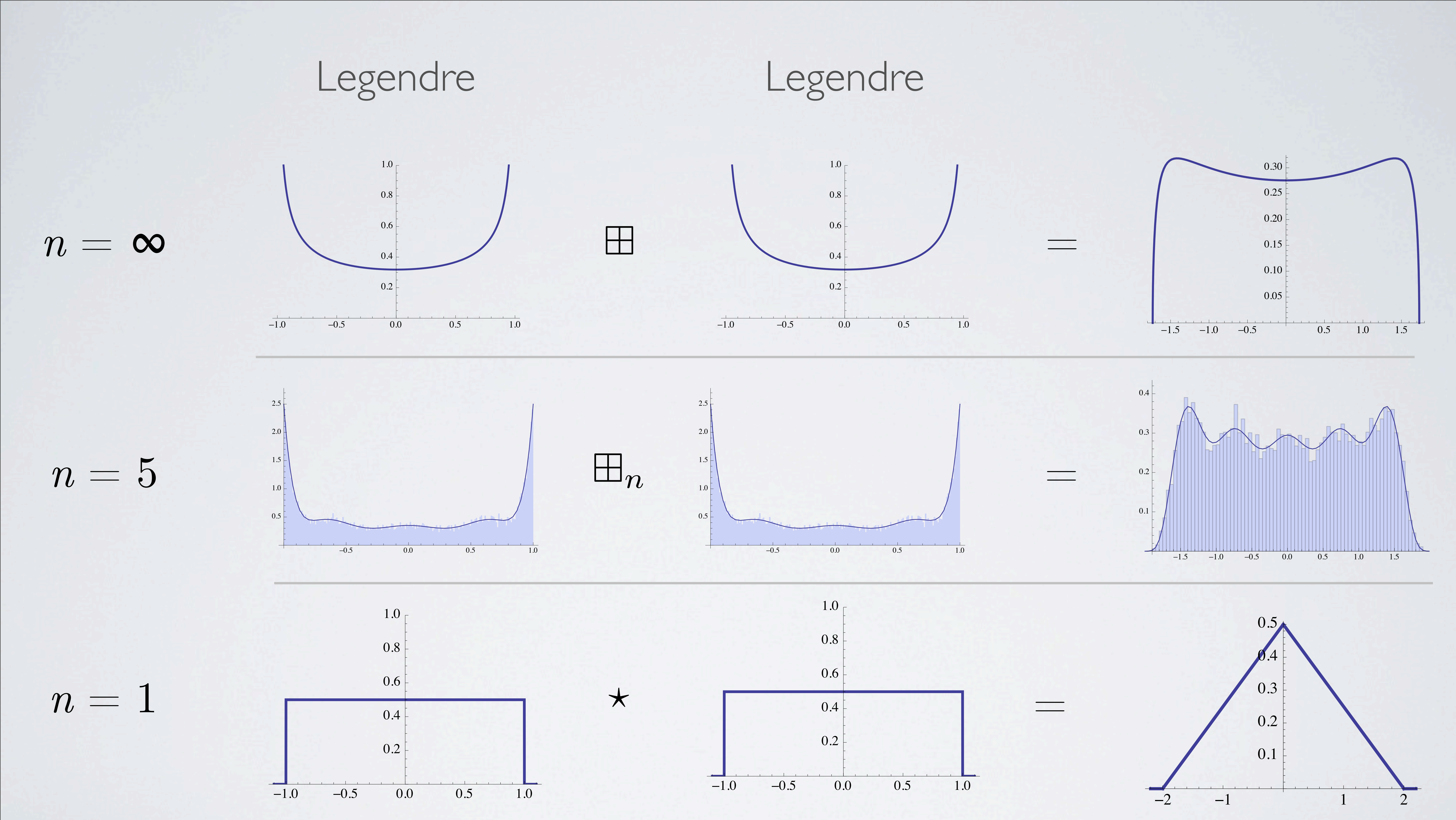



$\star$

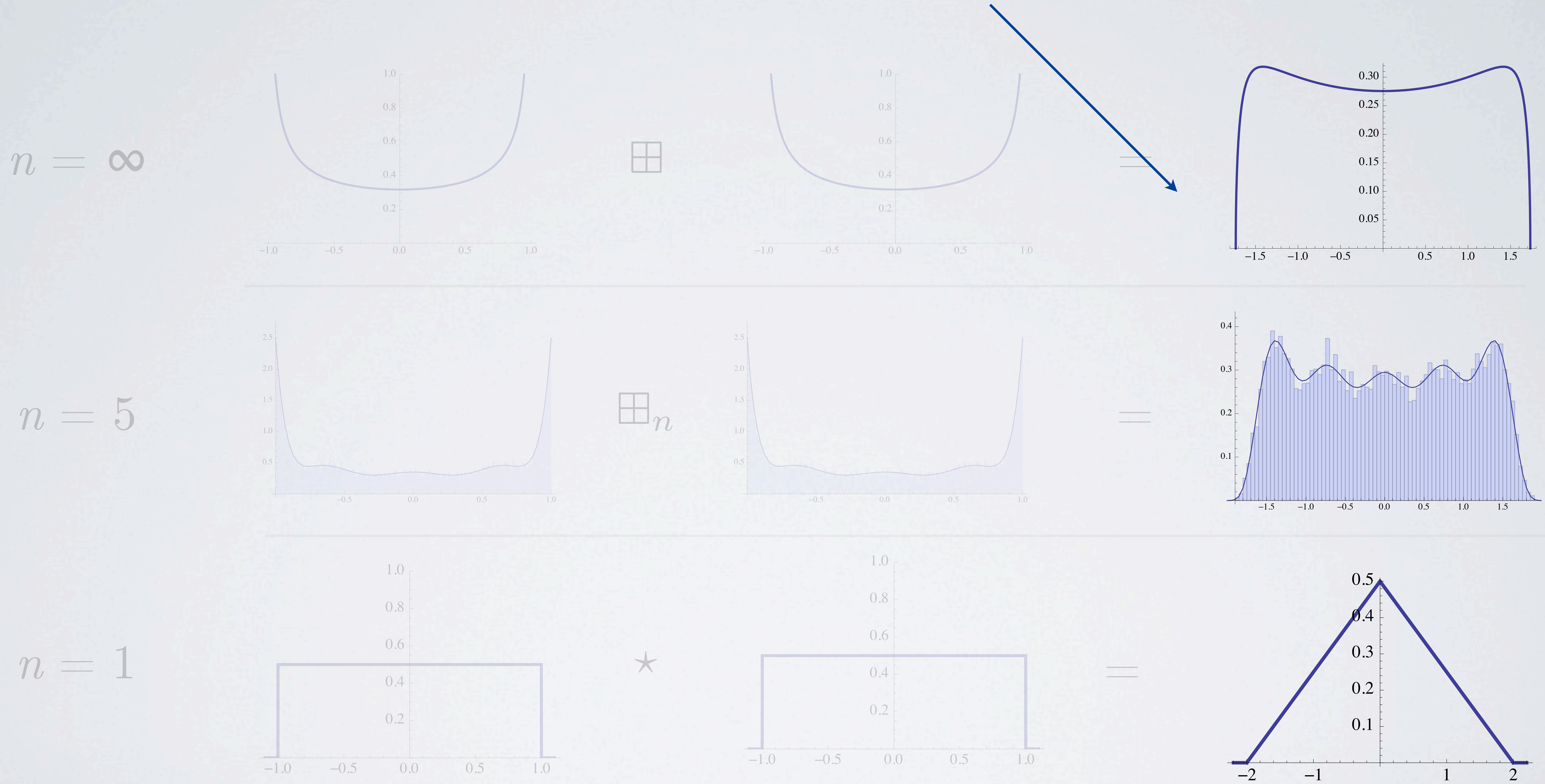



$=$

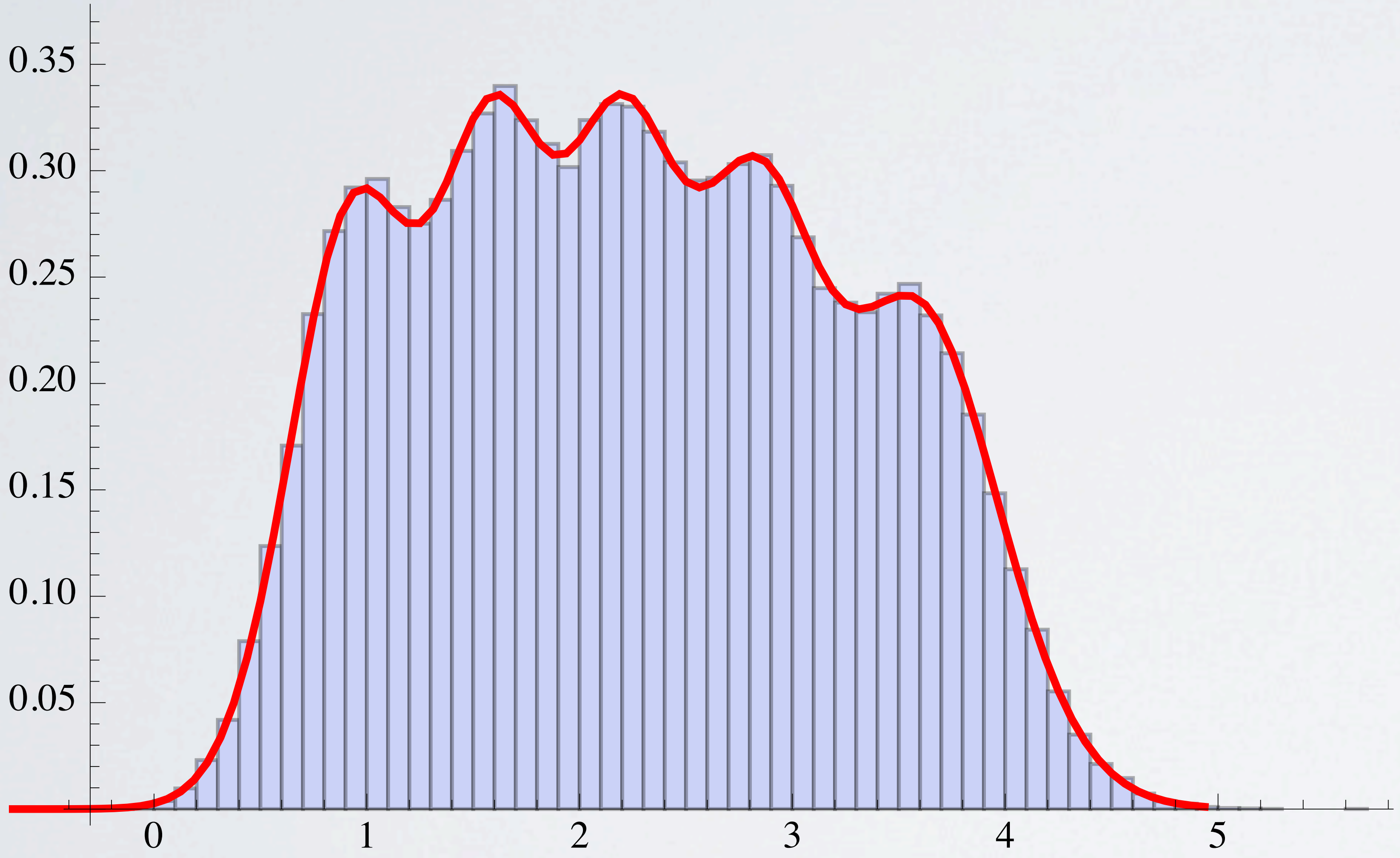



Legendre
Legendre
$n = \infty$
$\boxplus$
=
$n = 5$
$\boxplus_n$
=
$n = 1$
$\star$
=

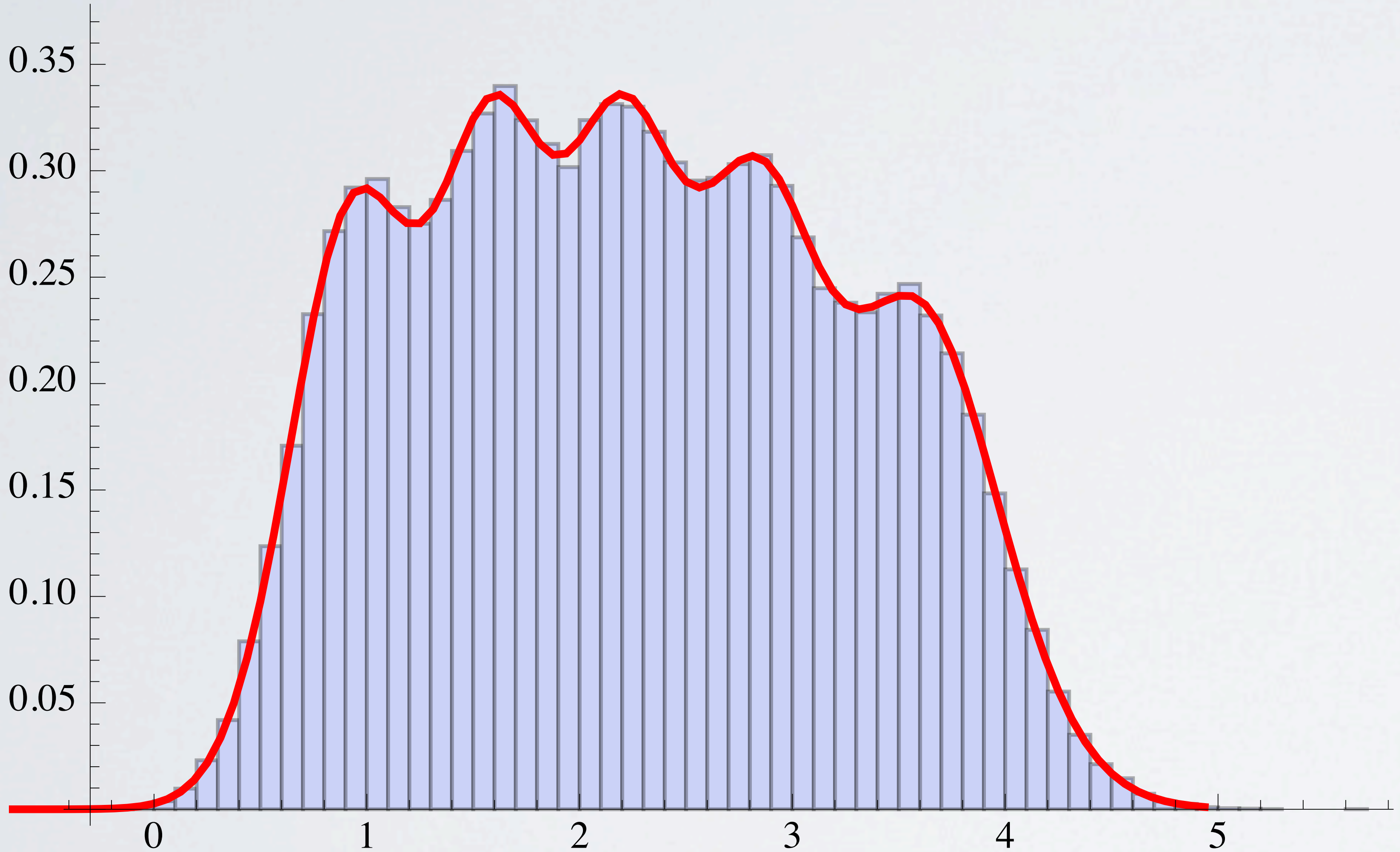
# Satisfies Tracy–Widom!



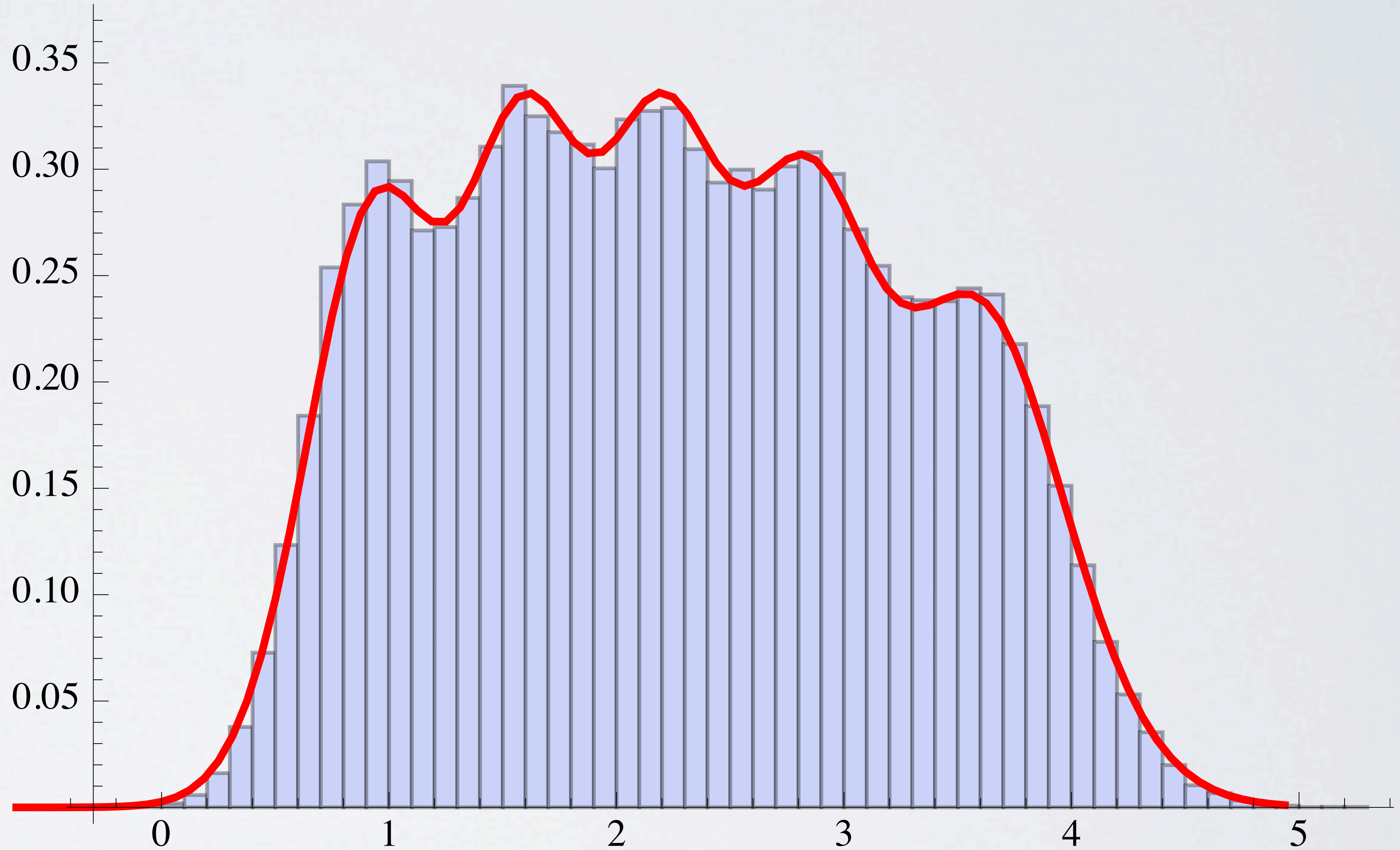
# GUE + LUE



GUE + LUE




Bernoulli Wigner + LUE



# Conclusions

- Free probability operations can be accomplished numerically
- This can lead to a better understanding of free probability
- The approach can be generalized to multiple support intervals
    - Not clear how to invert Cauchy transforms for multiple support intervals