

#### OPUC

Szegő– Verblunsky Sum Rule

#### OPRL

Killip–Simon Sum Rule

Meromorphi Herglotz

MHT Proc

Mysteries

Large Deviations

 $\mathsf{SNR}\ \mathsf{Strate}_{\mathsf{I}}$ 

**CUE and Szeg** 

GUE and Killip-Simor

### Spectral Theory Sum Rules, Meromorphic Herglotz Functions and Large Deviations

### Barry Simon

IBM Professor of Mathematics and Theoretical Physics, Emeritus California Institute of Technology Pasadena, CA, U.S.A.



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We start with orthogonal polynomials on the unit circle, aka OPUC. Let  $d\mu$  be a probability measure on  $\partial \mathbb{D}$ . Then, there are monic orthogonal polynomials,  $\Phi_n$ , and recursion relations due to Szegő in 1939

$$\Phi_{n+1}(z) = z\Phi_n(z) - \overline{\alpha}_n \Phi_n^*(z)$$

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GUE and Killip–Simon Szegő's Theorem concerns probability measures on  $\partial \mathbb{D}$  of the form

$$d\mu(\theta) = w(\theta)\frac{d\theta}{2\pi} + d\mu_s(\theta)$$

where  $d\mu_s$  is singular w.r.t.  $d\theta$ .



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where  $d\mu_s$  is singular w.r.t.  $d\theta$ . The Toeplitz determinant  $D_n(d\mu)$  is the  $n \times n$  determinant with

$$c_{k\ell} \equiv \int e^{i(k-\ell)\theta} d\mu(\theta) = \langle e^{-ik\cdot}, e^{-i\ell\cdot} \rangle_{L^2(d\mu)}$$



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In 1915, Szegő proved that

$$\lim_{n \to \infty} D_n (d\mu)^{1/n} = \exp \left[ \int \log(w(\theta)) \frac{d\theta}{2\pi} \right]$$

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While this is true in general, Szegő only proved it when  $d\mu_s=0$ .

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### Szegő's Theorem: OPUC version

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so using that  $\|\Phi_j\|$  is monotone decreasing (by a variational argument), one has an equivalent form of his theorem, namely

$$\lim_{n \to \infty} ||\Phi_n||^2 = \exp\left[\int \log(w(\theta)) \frac{d\theta}{2\pi}\right]$$



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$$\lim_{n \to \infty} ||\Phi_n||^2 = \exp\left[\int \log(w(\theta)) \frac{d\theta}{2\pi}\right]$$

But the recursion relation was only published by Szegő in 1939, so he didn't have a form in term's of  $\alpha_n$  and  $\rho_n$ .



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$$\sum_{j=0}^{\infty} \log(1 - |\alpha_j|^2) = \int \log(w(\theta)) \frac{d\theta}{2\pi}$$



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It is critical that this always holds although both sides may be  $-\infty$ .



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It is critical that this always holds although both sides may be  $-\infty$ . This implies what I've called a "spectral theory gem"

$$\sum_{j=0}^{\infty} |\alpha_j|^2 < \infty \iff \int \log(w(\theta)) \frac{d\theta}{2\pi} > -\infty$$



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In particular,  $\sum_{i=0}^{\infty} |\alpha_j|^2 < \infty \Rightarrow \Sigma_{ac} = \partial \mathbb{D}$ .



What makes the gems so interesting is that they allow arbitrary singular parts of the measures so long as the Szegő condition holds, i.e.  $\int \log(w(\theta)) \frac{d\theta}{2\pi} > -\infty$ .

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### Jacobi Parameters

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GUE and Killip–Simon Next orthogonal polynomials on the real line, aka OPRL. One starts with a probability measure,  $\mu$ , of compact support in  $\mathbb R$  and forms the orthonormal polynomials,  $\{p_n(x)\}_{n=0}^\infty$ . They obey recursion relations

$$xp_n(x) = a_{n+1}p_{n+1}(x) + b_{n+1}p_n(x) + a_np_{n-1}(x)$$



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which sets up a one-one correspondence (which we'll call the *Jacobi map*) between such measures (with an infinity of points in their support) and sequences  $\{a_n,b_n\}_{n=1}^{\infty}$  of bounded a's in  $(0,\infty)$  and b's in  $\mathbb R$  (called *Jacobi parameters*).



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which sets up a one-one correspondence (which we'll call the *Jacobi map*) between such measures (with an infinity of points in their support) and sequences  $\{a_n,b_n\}_{n=1}^{\infty}$  of bounded a's in  $(0,\infty)$  and b's in  $\mathbb R$  (called *Jacobi parameters*). If  $P_n$  are the monic OPs, then one has  $\|P_n\|=a_1\dots a_n$ .



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CUE and Szego

GUE and Killip–Simon There is also a correspondence between point measures with finite support and suitable sets of finitely many Jacobi parameters. If there are n pure points, then  $P_n$  is 0 in  $L^2(d\mu)$  so  $a_n=0$  and again there are 2n-1 Jacobi parameters – n b's and n-1 a's.



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> For later purposes, I need some details on one approach to going from measures to Jacobi parameters. The more usual method than the one I want to discuss just forms the OPs and looks at the recursion parameters. Instead, consider the once stripped Jacobi parameters, i.e.  $\{a_{j+1}, b_{j+1}\}_{i=1}^{\infty}$ obtained by dropping the first row and column of the Jacobi matrix.

#### OPRI



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For later purposes, I need some details on one approach to going from measures to Jacobi parameters. The more usual method than the one I want to discuss just forms the OPs and looks at the recursion parameters. Instead, consider the once stripped Jacobi parameters, i.e.  $\{a_{j+1},b_{j+1}\}_{j=1}^{\infty}$  obtained by dropping the first row and column of the Jacobi matrix. For any non–trivial probability measure of compact support, let  $m(z) = \int d\mu(x)/(x-z)$  and let  $m_1$  be the spectral measure for the once stripped problem.



Then one can prove that

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Then one can prove that

$$m(z) = \frac{1}{b_1 - z - a_1^2 m_1(z)}$$

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Using that  $m_1(z) = -z^{-1} + \mathrm{O}(z^{-2})$ , one sees that one can go from the measure to m



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Using that  $m_1(z)=-z^{-1}+{\rm O}(z^{-2})$ , one sees that one can go from the measure to m to  $a_1,b_1$  and  $m_1$ 



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Then one can prove that

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Using that  $m_1(z) = -z^{-1} + O(z^{-2})$ , one sees that one can go from the measure to m to  $a_1, b_1$  and  $m_1$  (and so inductively all Jacobi parameters) by looking at Taylor coefficients of  $m(z)^{-1}$  near infinity. Conversely, one can go from Jacobi parameters to m (and so  $\mu$ ) by summing a continued fraction expansion (that goes back to Jacobi, Chebyshev and Markov). One can also get the just mentioned Taylor coefficients as polynomials in the Jacobi parameters.

One consequence of this is that the poles of  $m_1$  (i.e. the pure points of  $\mu_1$ ) are precisely the zeros of m.



Here is one version of Szegő's Theorem for OPRL.

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Here is one version of Szegő's Theorem for OPRL. The map  $z\mapsto z+z^{-1}$  maps  $\partial\mathbb{D}$  to [-2,2] (via  $e^{i\theta}\mapsto 2\cos\theta$ )

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$$\liminf_{n \to \infty} \prod_{j=1}^{n} a_j = \sqrt{2} \exp\left(\int_{-2}^{2} \log|\pi s(x)w(x)| s(x) \frac{dx}{4\pi}\right)$$



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The condition for the finiteness of the integral is called the *Szegő condition*:



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$$\int_{-2}^{2} \log|w(x)| (4-x^2)^{-1/2} dx > -\infty$$



This doesn't yield a gem because

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$$\inf_{n} \prod_{j=1}^{n} a_{j} > -\infty \iff \int_{-2}^{2} \log|w(x)| (4 - x^{2})^{-1/2} dx$$



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only holds under the a priori condition that  $\mu$  is supported inside  $\left[-2,2\right]$ 

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only holds under the a priori condition that  $\mu$  is supported inside [-2,2] and this is not simply expressible in terms of the Jacobi parameters; for example, it doesn't only depend on the parameters near  $\infty$  and can be changed by modifying a single a or b.

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Killip-Simon Sum Rule

**GNR Strategy** 

In 2001 (published 2003), Killip and I proved the following gem which we regard as an OPRL analog of the Verblunsky–Szegő gem where  $\{E_j^{\pm}\}_{j=1}^{N_{\pm}}$  are the eigenvalues outside [-2,2] (with + above 2 and - below -2):



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Killip-Simon Theorem If  $d\mu=w(x)dx+d\mu_s$  is a measure of compact support on  $\mathbb R$  and  $\{a_n,b_n\}_{n=1}^\infty$  its Jacobi parameters, then

$$\sum_{j=1}^{\infty} |a_j - 1|^2 + b_j^2 < \infty$$



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$$\sum_{j=1}^{\infty} |a_j - 1|^2 + b_j^2 < \infty$$

if and only if the essential support of  $\mu$  is  $\left[-2,2\right]$  and

$$\int_{-2}^{2} \log(w(x)) \sqrt{4 - x^2} \, dx > -\infty \qquad \sum_{j, \pm} (|E_j^{\pm}| - 2)^{3/2} < \infty$$



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GUE and Killip–Simon This result on Jacobi Hilbert-Schmidt perturbations of the free Jacobi matrix should be compared with a celebrated theorem of von-Neumann that any bounded self-adjoint operator has a Hilbert-Schmidt perturbation with only dense point spectrum!



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We called  $\int_{-2}^2 \log(w(x)) \sqrt{4-x^2} \, dx > -\infty$  the quasi-Szegő condition since the square root appeared to the +1/2 power rather than the -1/2 in the Szegő condition.



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$$\sum |E_n|^p \le C \int |V(x)|^{p+d/2} \, dx$$



## Killip-Simon Sum Rule

Killip-Simon Sum Rule

The gem comes from a sum rule. Let

$$Q(\mu) = \frac{1}{2\pi} \int_0^{2\pi} \log \left( \frac{\sin(\theta)}{\operatorname{Im} m(2\cos(\theta))} \right) \sin^2(\theta) d\theta,$$



## Killip-Simon Sum Rule

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$$G(a) = a^2 - 1 - \log(a^2) \text{ and}$$



## Killip-Simon Sum Rule

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$$\begin{split} Q(\mu) &= \tfrac{1}{2\pi} \int_0^{2\pi} \log \left( \tfrac{\sin(\theta)}{\operatorname{Im} m(2\cos(\theta))} \right) \sin^2(\theta) d\theta, \\ G(a) &= a^2 - 1 - \log(a^2) \text{ and} \end{split}$$

$$F(E) \equiv \frac{1}{4} [\beta^2 - \beta^{-2} - \log(\beta^4)]$$
  $E = \beta + \beta^{-1}$   $|\beta| > 1$ 



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$$G(a) = a^2 - 1 - \log(a^2) \text{ and}$$

$$F(E) \equiv \frac{1}{4} [\beta^2 - \beta^{-2} - \log(\beta^4)] \qquad E = \beta + \beta^{-1} \qquad |\beta| > 1$$

Then the Killip-Simon sum rule says

$$Q(\mu) + \sum_{j,\pm} F(E_j^{\pm}) = \sum_{n=1}^{\infty} \frac{1}{4} b_n^2 + \frac{1}{2} G(a_n)$$

As with the Szegő–Verblunsky sum rule, an important point is that it always holds although both sides may be  $+\infty$ .



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GUE and Killip–Simon The gem comes from the fact that  $F \ge 0$ , vanishes exactly at  $E = \pm 2$  and is  $O((|E| - 2)^{3/2})$  there and that  $G \ge 0$ , vanishes exactly at a = 1 and is  $O((a - 1)^2)$  there.



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The positivity of the terms is essential to be sure that there aren't cancelations.



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As in the OPUC case, this sum rule implies the existence of Hilbert–Schmidt perturbations with mixed spectrum.



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$$Q(\mu) - Q(\mu_1) + \sum_{j,\pm} \left[ F(E_j^{\pm}) - F(E_j^{(1)\pm}) \right] = \frac{1}{4}b_1^2 + \frac{1}{2}G(a_1)$$



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Because the eigenvalues  $E_j^\pm$  and  $E_j^{(1)\pm}$  interlace and F is monotone, the sum is of positive terms and always convergent (interlacing sums).



While the  $\log(w)$  integral might divergence, one can show that a  $\log(w/w_1)$  integral is always convergent.

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If you iterate coefficient striping and assume the boundary term goes away, you get the full sum rule.



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If you iterate coefficient striping and assume the boundary term goes away, you get the full sum rule. What Killip and I found is so long as lots of terms were positive, one could get an always-valid full sum rule from a step-by-step sum rule. The proof is a somewhat subtle. Among other things it used the fact that the function Q is lower semi-continuous in  $\mu$  which we discovered by noting it was a relative entropy. We were proud of this realization although shortly afterwards we discovered Verblubsky's papers and found he also proved and used semicontinuity (although without realizing he had an entropy) - in 1935!



The step-by-step sum rule will involve a Poisson-Jensen formula whose classical form we recall.

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The famous theorem of Smirnov and Beurling says that for some  $\omega \in \partial \mathbb{D}$ , we have that (Poisson–Jensen formula)



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Without the  $L^p$ -condition, there a singular inner part.



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GUE and Killip–Simon By a meromorphic Herglotz function, we mean a function meromorphic on  $\mathbb{D}$ , real on (-1,1) with  $\operatorname{Im} z>0\Rightarrow \operatorname{Im} f(z)>0.$ 



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GUE and Killip–Simor One can prove that in  $\mathbb{D} \cap \mathbb{C}_+$ , one has that  $|\arg zB(z)| \leq 2\pi$  so that  $\arg(f(z)/zB(z))$  is bounded on  $\mathbb{D}$ .



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Taking log's, one gets relations between Taylor coefficients of  $\log(f(z)/z)$ , certain sums involving logs or powers of zeros and poles and integrals  $\cos(n\theta)\log|f(e^{i\theta})|$ .



Recall that  $m(z) = \int d\mu(x)/(x-z)$ . It defines a Herglotz function on  $\mathbb{C}_+$ , real on  $\mathbb{R}$ .

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CUE and Szeg

GUE and Killip–Simor Recall that  $m(z) = \int d\mu(x)/(x-z)$ . It defines a Herglotz function on  $\mathbb{C}_+$ , real on  $\mathbb{R}$ . Thus  $M(z) = -m(z+z^{-1})$  is what we called a meromorphic Herglotz function. Its poles are the eigenvalues of J under the inverse image of the map  $z \mapsto z + z^{-1}$  and its zeros are the same for  $J_1$ .



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The above procedure thus yields a relation between polynomials of Jacobi parameters, the difference of functions of the eigenvalues of J and  $J_1$  and integral of  $\log |M(e^{i\theta})|$ .



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# P<sub>2</sub> Sum Rule

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- Why are there any positive combinations?
- 2 It is easy to understand the  $(4-x^2)^{-1/2}\,dx$  of the Szegő condition. It is  $d\theta$  under  $x=\cos(\theta)$ . Equivalently, it is the potential theoretic equilibrium measure for [-2,2]



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$$F(E) = \tfrac{1}{4} [\beta^2 - \beta^{-2} - \log \beta^4]; \quad E = \beta + \beta^{-1}$$
 mean?



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GUE and Killip-Simon Large deviations go back to Laplace. The modern theory was initiated by Cramér in the 1930's and made into a powerful machine by Donsker–Varadhan and Freidlin–Wentzel and then Varadhan alone (work for which he got the Abel prize).



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We consider a sequence of probability measures,  $\{\mu_n\}_{n=1}^{\infty}$ , on a space, X. Naively, one has a Large Deviation Principle (aka LDP) if the  $\mu_n$ -probability that x is near  $x_0$  is  $O(e^{-nI(x_0)})$ .



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 $oldsymbol{0}$  I is lower semicontinuous

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- I is lower semicontinuous
- ② For all closed sets  $F \subset X$   $\limsup_{n \to \infty} \frac{1}{a_n} \log \mu_n(F) \le -\inf_{x \in F} I(x)$



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$$I(x) = \sup_{\theta} \left[ \theta x - \log \left( \mathbb{E}(e^{\theta X}) \right) \right]$$



Let X be an exponential random variable, i.e. with density  $\chi_{[0,\infty)}(x)e^{-x}\,dx.$  Then

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$$\log\left(\mathbb{E}(e^{\theta X})\right) = \begin{cases} -\log(1-\theta), & \text{if } \theta < 1\\ \infty, & \text{if } \theta \ge 1 \end{cases}$$

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# Cramér Example

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Notice that  $G(a) = I(a^2)$ ,



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For  $x \leq 0$ , taking  $\theta \to -\infty$  in  $\theta x - \log\left(\mathbb{E}(e^{\theta X})\right)$ , we see that  $I(x) = \infty$ . If x > 0, the  $\theta$  derivative of  $\theta x - \log\left(\mathbb{E}(e^{\theta X})\right)$  vanishes at  $\theta = 1 - x^{-1}$  at which point  $\theta x - \log\left(\mathbb{E}(e^{\theta X})\right)$  has the value  $x - 1 - \log(x)$ . Thus

$$I(x) = \begin{cases} x - 1 - \log(x), & \text{if } x > 0\\ \infty, & \text{if } x \le 0 \end{cases}$$

Notice that  $G(a) = I(a^2)$ , which we'll see is no coincidence!!!



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> As is well-known, the  $\lambda$ 's and w's are independent of each other, the w's are uniformly distributed on the simplex  $\{\mathbf{w}|\sum_{i=1}^n w_i=1\}$  and by the Weyl integration formula, the  $\theta$ 's have distribution

$$\frac{1}{n!} \prod_{1 \le j < k \le n} |e^{i\theta_j} - e^{i\theta_k}|^2 \prod_{j=1}^n \frac{d\theta_j}{2\pi}$$

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GUE and Killip–Simon The first step in the analysis of the measure side is to analyze what probabilists call the *empirical measure* and physicists the density of states, namely the random measure  $\frac{1}{n}\sum_{j=1}^{n} \delta_{\theta_{j}}$ .



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This is easy to understand. The Weyl distribution can be viewed as a discrete two dimensional Coulomb gas in the canonical ensemble (2D because  $|x-y|^{-2}$  is the exponential of  $-2\log|x-y|$ ). The  $n\to\infty$  limit is a high density limit and due to repulsion, there is a strong tendency towards equal spacing.



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GUE and Killip–Simon To get a significant difference from equal spacing, one has  $\mathrm{O}(n^2)$  smaller distances and so the speed is  $n^2$ . The optimal spacing will still be locally equal and the discrete Coulomb energy will converge to the continuum.



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The weights are close to independent (except for the normalization they are) – a slick way to see this is to note if  $Y_j$  are positive exponentially distributed iidrv, then  $w_j = Y_j / \sum_{j=1}^n Y_j$ . This allows one (using Cramér's theorem on small blocks) to prove an LDP for the spectral measure with speed n and rate function the Szegő integral  $-\int \log(w(\theta)) \frac{d\theta}{2\pi}$ .



In 2004, Killip and Nenciu wrote down the distribution of  $\{\alpha_j\}_{j=0}^{n-1}$  induced by restricting Haar measure as we are.

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$$\frac{n-j-1}{\pi}(1-|z|^2)^{n-j-2}d^2z$$



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 $\prod \rho_j^2$  appears to the nth power so the rate function is  $-\sum_{j=1}^\infty \log(1-|\alpha_j|^2).$ 



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CUE and Szegő

GUE and Killip–Simon In 2004, Killip and Nenciu wrote down the distribution of  $\{\alpha_j\}_{j=0}^{n-1}$  induced by restricting Haar measure as we are. The  $\alpha$ 's are independent with  $\alpha_{n-1}$  (which lies on  $\partial\mathbb{D}$ ) uniformly distributed on  $\partial\mathbb{D}$  and for  $j=0\dots n-2$ ,  $\alpha_j$  has density on  $\mathbb{D}$ 

$$\frac{n-j-1}{\pi}(1-|z|^2)^{n-j-2}d^2z$$

which says that  $\alpha_j$  is distributed as the first complex component of a unit vector in  $\mathbb{C}^{n-j}$ .

 $\prod \rho_j^2$  appears to the nth power so the rate function is  $-\sum_{j=1}^\infty \log(1-|\alpha_j|^2).$  In this calculation, one makes use of the theory of LDP projective limits to handle the technicalities of going from finite to infinite support.



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GUE and Killip-Simon The Gaussian Unitary Ensemble, aka GUE, is the probability measure on  $n \times n$  self adjoint matrices so that  $\{a_{ii}\}_{i=1,\dots,n}, \{\operatorname{Re}(a_{ij})\}_{1 \leq i < j \leq n}$  and  $\{\operatorname{Im}(a_{ij})\}_{1 \leq i < j \leq n}$  are independent identically distributed Gaussian random variables of mean zero and suitable, n-dependent variance.



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The argument for GUE, normalized so the limiting density is the semicircle law on [-2,2], is similar to that for CUE.



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What results is a new proof of the Killip-Simon sum rule.



We can now solve the mysteries:

**1** Why are there any positive combinations?

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We can now solve the mysteries:

**1** Why are there any positive combinations? This is the basic GNR theory of positive sum rules.

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- Why are there any positive combinations? This is the basic GNR theory of positive sum rules.
- ② It is easy to understand the  $(4-x^2)^{-1/2}\,dx$  of the Szegő condition but where the heck does the  $(4-x^2)^{1/2}\,dx$  come from?



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- **3** What does the function

$$G(a) = a^2 - 1 - \log(a^2)$$

mean?



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*mean?* As we've seen, this is the rate function for square roots of sums of exponential RVs.



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- **6** What does the function

$$G(a) = a^2 - 1 - \log(a^2)$$
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4 What does the function

$$F(E) = \frac{1}{4} [\beta^2 - \beta^{-2} - \log \beta^4]; \quad E = \beta + \beta^{-1}$$
 mean?



GUF and Killip-Simon We can now solve the mysteries:

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- 2 It is easy to understand the  $(4-x^2)^{-1/2} dx$  of the Szegő condition but where the heck does the  $(4-x^2)^{1/2} dx$  come from? This is the Wigner semi-circle law; essentially the measure is the potential theory equilibrium measure in quadratic external field.
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mean? As we've seen, this is the rate function for square roots of sums of exponential RVs.

What does the function

$$F(E) = \frac{1}{4}[\beta^2 - \beta^{-2} - \log \beta^4]; \quad E = \beta + \beta^{-1}$$
 mean? This is the Coulomb potential of the Wigner semi-circle distribution plus a quadratic external field.



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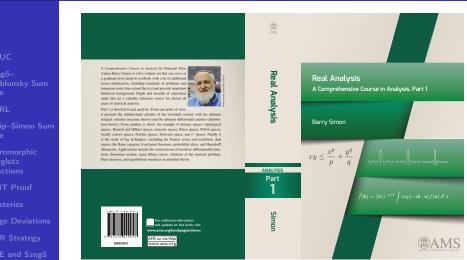
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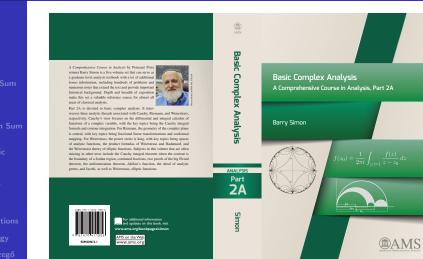
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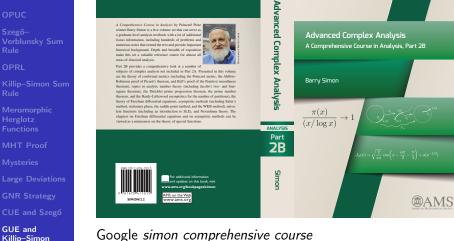
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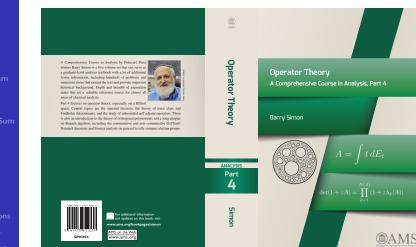
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