STAHL'S THEOREM + RANDOM MATRIX THEORY

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arXiv: 2603.04365

SUMMER 2026

QUANTUM STATISTICAL MECHANICS

- **HAMILTONIAN MATRIX:** Self-adjoint $\underline{\underline{H}} \in \mathbb{H}_d$

↳ eigs = energy levels of quantum system

- **PARTITION FUNCTION:** For inverse temp. $\beta > 0$,

$$F_\beta = \operatorname{Tr} e^{-\beta \underline{\underline{H}}}$$

↳ Captures aggregate thermodynamic properties, e.g. entropy, free energy, etc.

<?> How does partition function change when we perturb Hamiltonian: $\underline{\underline{H}} + t\underline{\underline{A}}$?

THE TRACE EXPONENTIAL

RECALL: The matrix exponential is NASTY.

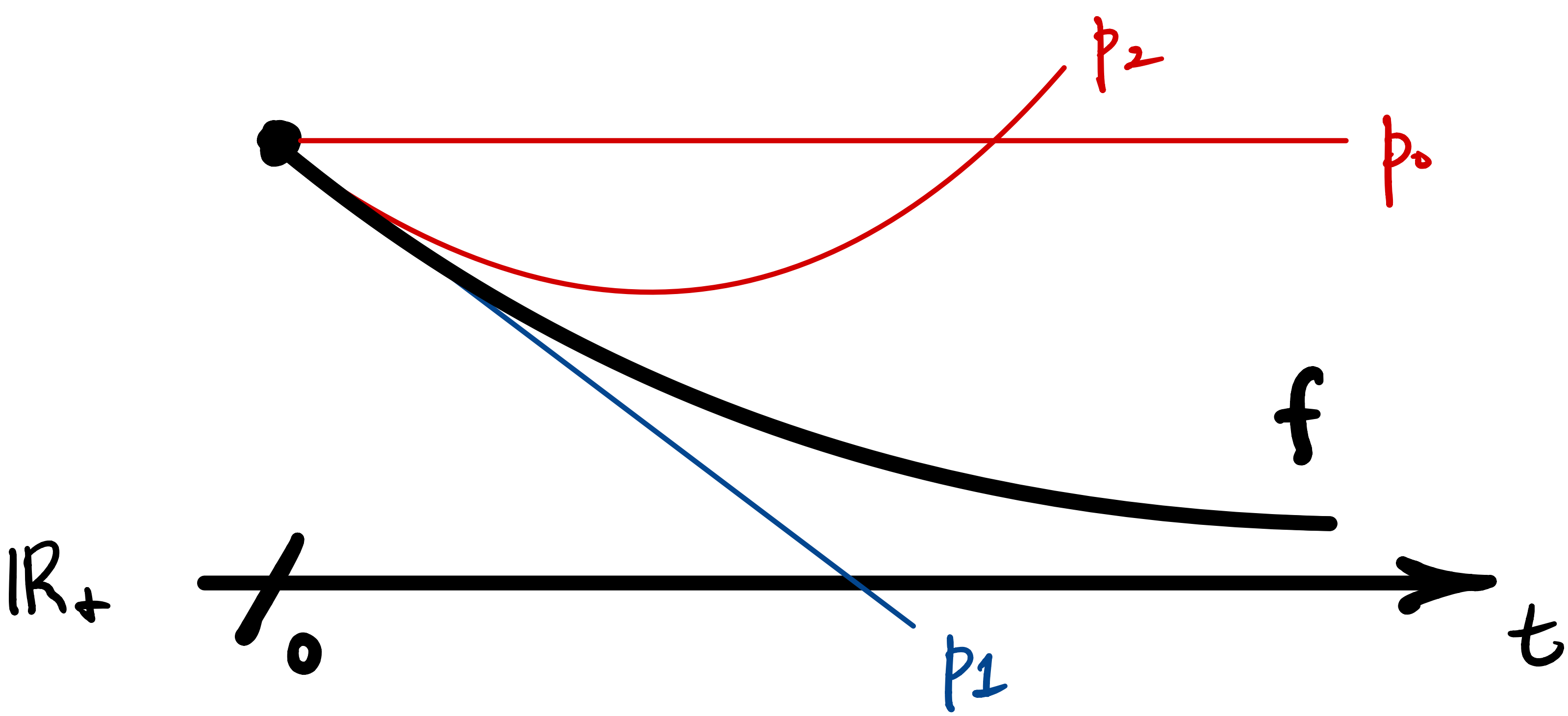
- $e^{\underline{H}+\underline{A}} \neq e^{\underline{H}} e^{\underline{A}}$ unless $\underline{H}, \underline{A}$ commute
- On the positive side...
  - Golden – Thompson (1965):
$$\operatorname{Tr} e^{\underline{H}+\underline{A}} \le \operatorname{Tr}\left[e^{\underline{H}} e^{\underline{A}}\right]$$
  - Lieb concavity (1973):
$$\underline{A} \longmapsto \operatorname{Tr} \exp(\underline{H} + \log \underline{A})$$
is concave on the pd cone

<?> Can we say something more precise?

COMPLETELY MONOTONE FUNCTIONS

DEF. A function $f : \mathbb{R}_+ \to \mathbb{R}_+$ is **completely monotone** when f is continuous at zero and

$$(-1)^k f^{(k)}(t) \geq 0 \quad \text{for all } t > 0, \quad k \in \mathbb{Z}_+$$



upper + lower approx$^{\underline{n}}$ by Taylor polynomials

EXAMPLES? ...

COMPLETELY MONOTONE FUNCTIONS

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EXAMPLE 1: $t \longmapsto \dfrac{1}{\lambda + t}$ for $\lambda > 0$

EXAMPLE 2: $t \longmapsto e^{-\lambda t}$ for $\lambda \geq 0$

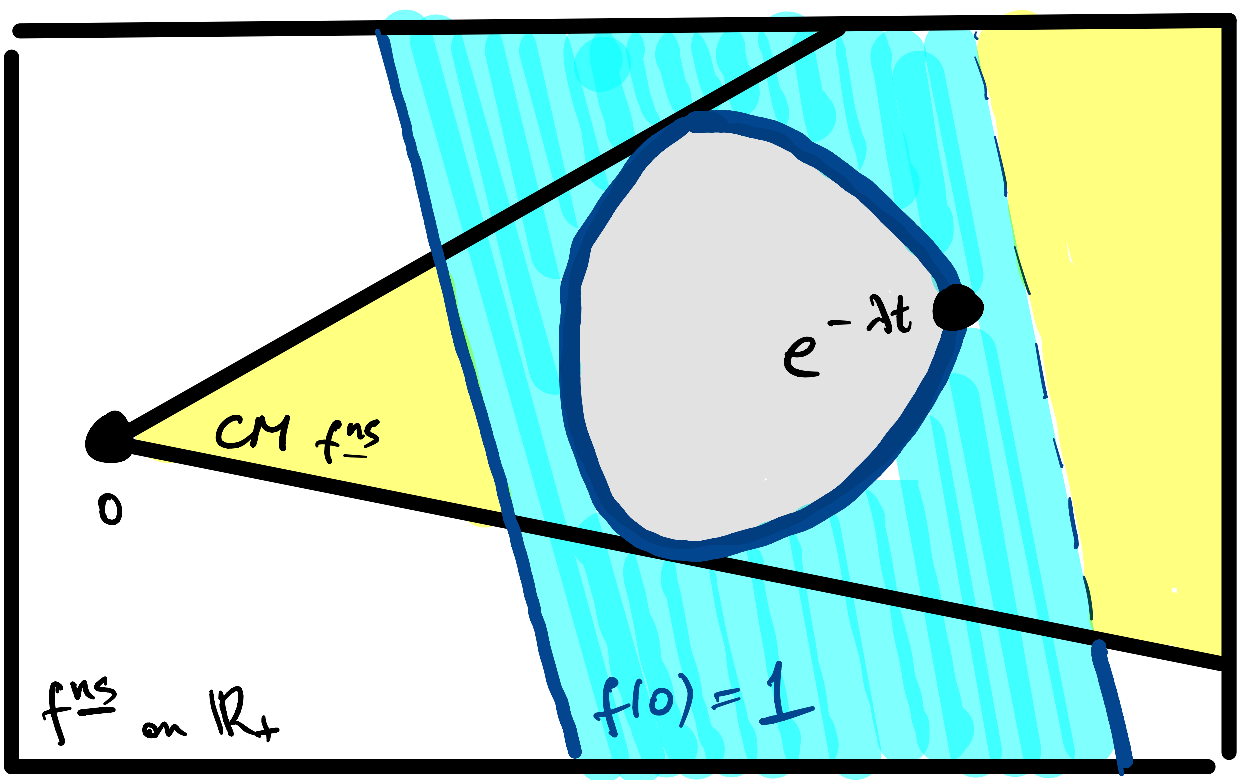
↳ This is the fundamental instance...

BERNSTEIN'S THEOREM

THM. $f : \mathbb{R}_+ \to \mathbb{R}_+$ is completely monotone iff

$$f(t) = \int_{\mathbb{R}_+} e^{-\lambda t} \, d\mu(\lambda)$$

where μ is a finite, positive Borel measure



Pf. The full set of extreme points of the base $f(0) = 1$ are the $f^{\underline{ns}}$

$$t \mapsto e^{-\lambda t}$$

for $\lambda \geq 0$. ■

THE BMV CONJECTURE

CONJECTURE (Bessis–Moussa–Villani, 1975):

- Let $\underline{\underline{H}}, \underline{\underline{A}} \in \mathbb{H}_d$ be self-adjoint, + $\underline{\underline{A}}$ psd.

$\therefore$
$$t \mapsto \operatorname{Tr} e^{-(\underline{\underline{H}} + tA)}$$
is completely monotone for $t \geq 0$.

APPLICATION: (Rational) approximations bracket the partition function
$$F_\beta(t) = \operatorname{Tr} e^{-\beta(\underline{\underline{H}} + t\underline{\underline{A}})}$$
for fixed inverse temperature $\beta > 0$.

THE BMV CONJECTURE

THEOREM (Stahl, 2013):
~~CONJECTURE~~ (Bessis – Moussa – Villani, 1975):

- Let $\underline{H}, \underline{A} \in \mathbb{H}_d$ be self-adjoint + $\underline{A}$ psd.
- $\therefore$ $$t \mapsto \operatorname{Tr} e^{-(\underline{H} + tA)}$$

  is completely monotone for $t \geq 0$.

Pf. Guess representing measure μ in Bernstein theorem (easy).
Use Riemann surfaces to check positivity (hard).

See also Erëmenko 2015, Clivaz 2017, esp. Heinävaara 2024.

STAHL: CONSEQUENCES

- For $\underline{\underline{H}}, \underline{\underline{A}} \in \mathbb{H}_d$, NOT NEC. PSD, $t \geq 0$

$$F(t) := \operatorname{Tr} e^{\underline{\underline{H}} + t\underline{\underline{A}}} = \int_{\lambda_{\min}(\underline{\underline{A}})}^{\lambda_{\max}(\underline{\underline{A}})} e^{\lambda t} \, d\mu(\lambda)$$

depends on $\underline{\underline{H}}, \underline{\underline{A}}$

- For $k \in \mathbb{N}$,

$$F^{(k)}(t) = \int_{\lambda_{\min}(\underline{\underline{A}})}^{\lambda_{\max}(\underline{\underline{A}})} \lambda^k e^{\lambda t} \, d\mu(\lambda)$$

- Odd derivatives $F^{(2k+1)}$ increase
- Even derivatives have bounded growth:

$$F^{(2k)}(t) \leq e^{t \lambda_{\max}(\underline{\underline{A}})} F^{(2k)}(0)$$

FROM QSM TO RMT...

- **WIGNER'S SURMISE** (1950s): We can model a complicated Hamiltonian by a random matrix with appropriate symmetries.

EXAMPLE:

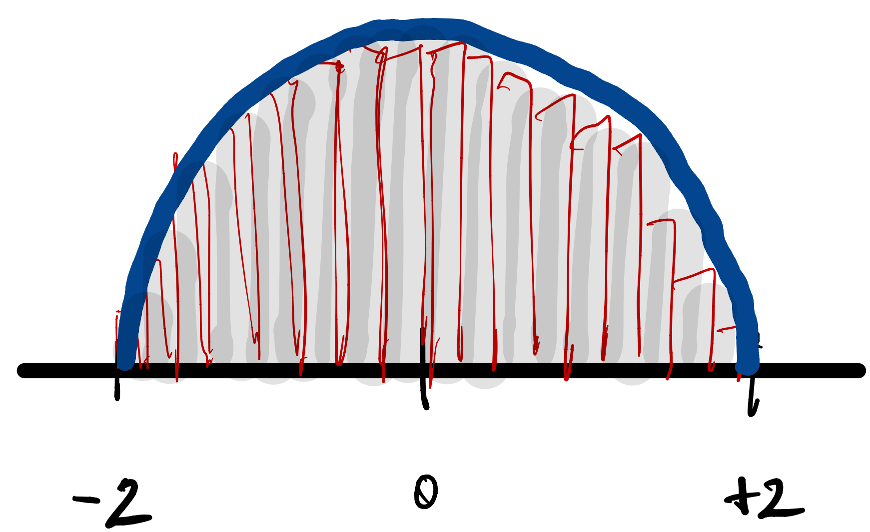
$$GUE_N = \frac{1}{\sqrt{N}} \begin{bmatrix} \gamma_{11} & & \gamma_{ij} \\ & \ddots & \\ * & & \gamma_{NN} \end{bmatrix}$$

where $\gamma_{ii} \sim N_{\mathbb{R}}(0,1)$ iid

$\gamma_{ij} \sim N_{\mathbb{C}}(0,1)$ iid

$\gamma_{ij} = \bar{\gamma}_{ji}$

SEMICIRCLE DISTRIBUTION



HISTOGRAM of EIGENVALUES (N large)

THE INDEPENDENT SUM MODEL

- **CLASSICAL RMT:**
  - INSPIRED BY MATHEMATICAL PHYSICS
  - HIGHLY SYMMETRIC MODELS (eg. INDEPENDENT ENTRIES)
  - SPECIAL DISTRIBUTIONS (eg. JOINTLY GAUSSIAN)

  ↳ VERY WELL UNDERSTOOD

- **CONTEMPORARY RMT:**
  - INSPIRED BY COMPUTATIONAL MATH;
  - WIDE RANGE OF APPLICATIONS
  - NEED MORE FLEXIBLE MODELS

STILL <u>EVOLVING</u>

<u>KEY EXAMPLE</u>: INDEP SUM MODEL

$$\underline{\underline{Y}} = \sum_{i=1}^{n} \underline{\underline{X}}_i \quad \text{where } \underline{X}_i \text{ s.a., independent}$$

THE MATRIX LAPLACE TRANSFORM

⟨?⟩ Bound extreme eigenvalues of a s.a. random matrix?

DEF. For a random s.a. matrix $\underline{\underline{Y}} \in \mathbb{H}_d$, define mgf

$$\theta \mapsto \mathbb{E}\operatorname{Tr} e^{\theta \underline{\underline{Y}}} \quad \text{for } \theta \in \mathbb{R}$$

PROP.

$$\mathbb{P}\{\lambda_{\max}(\underline{\underline{Y}}) \geq t\} \leq \inf_{\theta > 0} e^{-\theta t}\, \mathbb{E}\operatorname{Tr} e^{\theta \underline{\underline{Y}}}$$

$$\mathbb{P}\{\lambda_{\min}(\underline{\underline{Y}}) \leq t\} \leq \inf_{\theta < 0} e^{-\theta t}\, \mathbb{E}\operatorname{Tr} e^{\theta \underline{\underline{Y}}}$$

Pf. EXERCISE; Extension to expect$^{\underline{n}}$ bounds.

⟨?⟩ Bound matrix LT? Use QSM tools... How?

MATRIX BENNETT INEQUALITY

PROP (T10). Fix an s.a. matrix $\underline{H} \in \mathbb{H}_d$.

- Let $\underline{X} \in \mathbb{H}_d$ rdm s.a.; $\mathbb{E}\underline{X} = \underline{0}$, $\lambda_{max}(\underline{X}) \le 1$
- Define $\underline{V} = \mathbb{E}\underline{X}^2$. "matrix variance"

$$\therefore \quad \mathbb{E}\,\mathrm{Tr}\, e^{\underline{H} + \theta \underline{X}} \le \mathrm{Tr}\, e^{\underline{H} + g_\theta^2 \underline{V}}, \qquad \theta \ge 0$$

where $g_\theta^2 = e^\theta - \theta - 1$. In particular,

$$\mathbb{E}\,\lambda_{max}(\underline{X}) \le \sqrt{2\lambda_{max}(\underline{V}) \log d} + \tfrac{1}{3}\log d$$

Pf. Lieb concavity, mgf estimates sim. to Bennett ineq.

↳ Extends to indep sums. ISSUE: logs

GAUSSIAN COMPARISON METHOD

IDEA: Compare a random matrix with matching Gaussian

PROP (T26). Fix a s.a. matrix $\underline{\underline{H}} \in \mathbb{H}_d$.

- Let $\underline{\underline{X}} \in \mathbb{H}_d$ rdm s.a., $\mathbb{E}\,\underline{\underline{X}} = \underline{\underline{0}}$; $\lambda_{\max}(\underline{\underline{X}}) \leq 1$
- Let $\underline{\underline{Z}} \in \mathbb{H}_d$ have jointly Gaussian entries,

$$\mathbb{E}\,\underline{\underline{Z}} = \mathbb{E}\,\underline{\underline{X}} = \underline{\underline{0}} \quad ; \quad \operatorname{Var}[\underline{\underline{Z}}] = \operatorname{Var}[\underline{\underline{X}}].$$

$$\therefore \quad \mathbb{E}\operatorname{Tr} e^{\underline{\underline{H}} + \theta \underline{\underline{X}}} \leq \mathbb{E}\operatorname{Tr} e^{\underline{\underline{H}} + g_\theta \underline{\underline{Z}}} \qquad \theta \geq 0$$

where $g_\theta^2 = e^\theta - \theta - 1.$

(cf. Bennett's inequality

COMPARISON: PROOF SKETCH

STRATEGY: Taylor expansion + Stahl's theorem

Let $\theta = 1$. Define $f(t; \underline{\omega}) = \mathbb{E} \operatorname{Tr} e^{\underline{H} + t \underline{\omega}}$

Expand $f(1; X)$ to 2° order at $t = 0$ + integral remain.
$f(1; gZ)$ to 3° order

Notice
$$f(0; X) = f(0; Z)$$
$$f'(0; X) = f'(0; Z) = 0 \quad \text{ZERO MEAN}$$
$$f''(0; X) = f''(0; Z) \quad \text{SAME VARIANCE}$$

$$f''(t; X) \leq e^t f''(0; X) \quad \text{STAHL, } \lambda_{\max}(X) \leq 1$$
$$f'''(t; Z) \geq f'''(0; Z) = 0 \quad \text{STAHL, } Z \sim -Z.$$

BACK TO INDEPENDENT SUMS

THM (T26).

- Let $\underline{Y} = \sum_{i=1}^{n} \underline{X}_i$ where $\underline{X}_i \in \mathbb{H}_d$ independent, $\mathbb{E}\underline{X}_i = \underline{0}$ and $\lambda_{max}(\underline{X}_i) \le 1$
- Let $\underline{Z} \sim \text{NORMAL}(\underline{0}, \text{Var}[\underline{Y}])$.

$$\therefore \quad \mathbb{E}\,\mathrm{Tr}\, e^{\theta \underline{Y}} \le \mathbb{E}\,\mathrm{Tr}\, e^{g_\theta \underline{Z}} \qquad (\theta \ge 0)$$

where $g_\theta^2 = e^\theta - \theta - 1$.

In particular,

$$\mathbb{E}\,\lambda_{max}(\underline{Y}) \le \mathbb{E}\,\lambda_{max}(\underline{Z}) + (\text{error})$$

NO LOG!

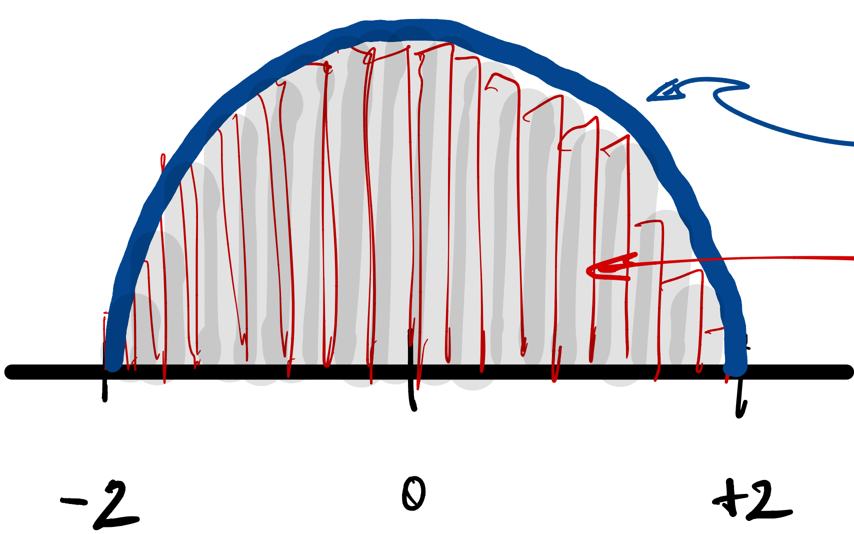
Proof. Iterate proposition, Gauss. concentr^n, LT method.

APPLICATION: QUANTUM SUPREMACY

<?> Find computational problems that are easy for quantum computers, hard for classical computers.

CANDIDATE: Estimating minimum eigenvector of a (large) structured Hamiltonian

STRATEGY: Construct "simple" rdm $\underline{\underline{Y}} \in \mathbb{H}_N$ for $N = 2^n$ whose spectrum aligns with the GUE_N spectrum



spectrum of GUE

histogram of eigenvalues of target Hamiltonian

EXAMPLE: RANDOM PAULI MODEL

DEF (PAULI MATRICES).

$$H_0 = I_2, \quad H_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad H_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad H_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

↳ orthogonal basis for $\mathbb{H}_2(\mathbb{C})$.

- RANDOM PAULI STRING: For $n \in \mathbb{N}$, $N = 2^n$,

$$\underline{S} \sim \text{UNIF}\{\underline{H}_{i_1} \otimes \cdots \otimes \underline{H}_{i_n}\} \in \mathbb{H}_N \quad (n \text{ qubits})$$

- RANDOM "SPARSE" PAULI HAMILTONIAN: For $K \in \mathbb{N}$,

$$\underline{Y} = \frac{1}{\sqrt{K}} \sum_{k=1}^{K} \varepsilon_k \underline{S}_k \quad \text{where } \underline{S}_k \sim \underline{S} \text{ iid}$$
$$\varepsilon_k \sim \text{UNIF}\{\pm 1\} \text{ iid}$$

- Just $K \cdot (2n+1)$ random bits! (cf. $N^2 = 4^n$ entries

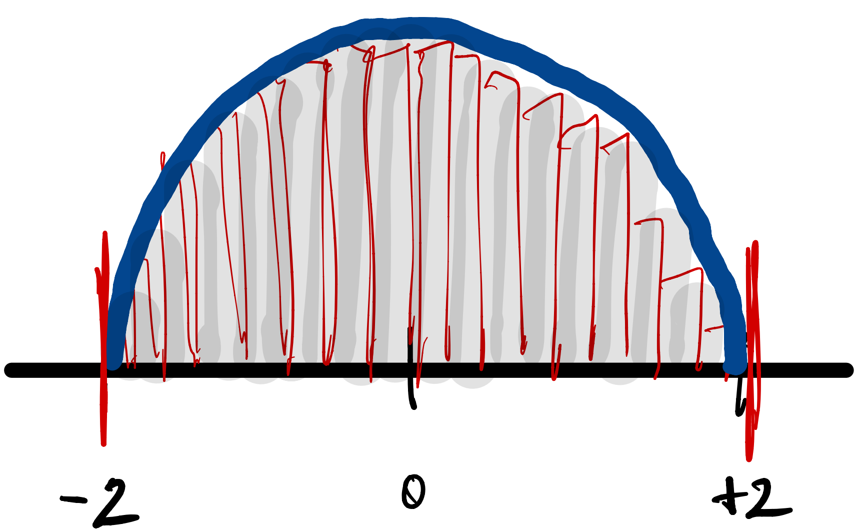
EXAMPLE: RANDOM PAULI MODEL

- $\underline{\underline{Y}} = \frac{1}{\sqrt{K}} \sum_{k=1}^{K} \varepsilon_k \underline{\underline{S}}_k$ $\qquad S_k \sim \text{UNIF}\{H_{i_1} \otimes \cdots \otimes H_{i_n}\}$
  $\varepsilon_k \sim \text{UNIF}\{\pm 1\}$.
- Comparison model: GUE_N where $N = 2^n$.

<?> How many terms to match GUE spectral edge?

Thm (T26). If $K \gtrsim n^2$, then (optimal???)

$$-2 \lesssim \lambda_{\min}(\underline{\underline{Y}}) \quad ; \quad \lambda_{\max}(\underline{\underline{Y}}) \lesssim +2.$$



Semicircle = limiting GUE eigs

histogram of eigs from random Pauli model.

(MSD requires separate study)

SUMMARY

QSM $\longleftrightarrow$ RMT

- QSM provides theorems + conjectures about matrix $f^{\underline{ns}}$
  eg. Golden-Thompson, Lieb concavity, BMV, ...
- QSM motivated field of RMT (Wigner)
- Modern RMT leads to challenging new models
  eg. Indep. sums, matrix martingales, etc.
- QSM tools provide novel methods for RMT
- New RMT results have implications for QSM
  eg. quantum supremacy ... More?

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