

Perturbation of Wigner matrices and a conjecture ¹

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Abstract Let H_0 be an arbitrary self-adjoint $n \times n$ matrix and $H(n)$ be an $n \times n$ (random) Wigner matrix. We show that $t \mapsto \text{Tr} \exp(H(n) - itH_0)$ is positive definite in the average. This partially answers a long-standing conjecture. On the basis of asymptotic freeness our result implies that $t \mapsto \tau(\exp(a - itb))$ is positive definite whenever the noncommutative random variables a and b are in free relation, with a semicircular.

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Introduction

Let H and H_0 be self-adjoint $n \times n$ matrices. It is a widely known conjecture [1, 6, 9, 10] that the function

$$t \mapsto \text{Tr} e^{H-itH_0} \quad (1)$$

is positive definite on \mathbf{R} . This means that there exists a measure μ on \mathbf{R} whose Fourier transform is the above function:

$$\text{Tr} e^{H-itH_0} = \frac{1}{\sqrt{2\pi}} \int e^{-itx} d\mu(x) \quad (t \in \mathbf{R}),$$

We shall call μ the Bochner measure of the function (1), if it really exists. If this is the case, then μ depends both on the spectra of the two matrices and on the relative position of their eigenvectors. The function (1), and especially its derivatives at $t = 0$, define important quantities in quantum statistical mechanics. Proving positive definiteness would lead to interesting relations among them. The n th derivative at $t = 0$ of (1) is, up to a factor i^n , given by

$$a_n = \int_{\substack{0 \leq t_1, 0 \leq t_2, \dots, 0 \leq t_{n-1} \\ t_1 + t_2 + \dots + t_{n-1} \leq 1}} dt_1 \cdots dt_{n-1} \text{Tr} e^{(1-t_1-\dots-t_{n-1})H} H_0 e^{t_1 H} H_0 \cdots e^{t_{n-1} H} H_0.$$

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Positive definiteness of (1) is then equivalent with

$$\det([a_{i+j}]_{i,j=0,1,\dots,n}) \geq 0 \quad (n \in \mathbf{N}).$$

The aim of this paper is to show that the conjecture holds in the average for some random choices of matrices. More precisely, when the conjecture is true, then for any choice of self-adjoint $n \times n$ random matrix H_n the function

$$F(t) := \frac{1}{n} \mathbb{E}(\mathrm{Tr} e^{H_n - itH_0})$$

is positive definite (for any H_0). We deal with the particular case in which H_n has independent Gaussian entries. We shall give rather explicitly the measure μ whose Fourier transform is $F(t)$. It depends only on the spectrum of the matrix H_0 since the eigenvectors of H_n have a rotationally invariant distribution. It turns out that the support of μ is the convex hull of the spectrum of H_0 .

The result for matrices has a consequence for free random variables a and b when a is semicircular. The pair (a, b) has a random matrix model consisting of a Wigner matrix and a diagonal matrix. From the matrix result we can conclude the positive definiteness of $\tau(e^{a-itb})$ letting the matrix size go to infinity.

$n \times n$ matrices

An $n \times n$ complex self-adjoint random matrix $H(n)$ is called Wigner matrix if

- (i) $\{\mathrm{Re}H_{ij}(n) \mid 1 \leq i \leq j \leq n\} \cup \{\mathrm{Im}H_{ij}(n) \mid 1 \leq i < j \leq n\}$ is an independent family of Gaussian random variables, and
- (ii) $\mathbb{E}(H_{ij}(n)) = 0$ for $1 \leq i \leq j \leq n$, $\mathbb{E}(H_{ii}(n)^2) = 1/n$ for $1 \leq i \leq n$, and $\mathbb{E}((\mathrm{Re}H_{ij}(n))^2) = \mathbb{E}((\mathrm{Im}H_{ij}(n))^2) = 1/2n$ for $1 \leq i < j \leq n$.

The Wigner matrix is standard because $\tau_n(H(n)) = 0$ and $\tau_n(H(n)^2) = 1$, where

$$\tau_n := \frac{1}{n} \mathbb{E} \circ \mathrm{Tr}_n.$$

Our aim is to prove the following:

Theorem. *Let H_0 be a fixed self-adjoint matrix and $H(n)$ a standard Wigner matrix; then the function $t \mapsto \tau_n(\exp(H(n) - itH_0))$ is positive definite. Its corresponding Bochner measure is the sum of an atomic and an absolutely continuous part. The atomic part is concentrated at the eigenvalues of H_0 and the support of the absolutely continuous part coincides with the convex hull of the spectrum of H_0 .*

In the following, we first give the probability density of the $n \times n$ random matrix $H_0 + H(n)$. Then, we assume that H_0 has the eigenvalues $d_1 < d_2 < \dots < d_n$ and compute the above function explicitly in terms of these eigenvalues (cf. [4] or [7]).

The probability density function of $H(n)$ is

$$C_n \exp\left(-\frac{n}{2}\text{Tr} A^2\right) \quad \text{with} \quad C_n = 2^{-n/2} \left(\frac{\pi}{n}\right)^{-n^2/2}$$

with respect to the Lebesgue measure

$$dA := \prod_{i=1}^n dA_{ii} \prod_{i<j} d(\text{Re}A_{ij}) d(\text{Im}A_{ij}) \quad \text{on} \quad M_n(\mathbf{C})^{sa} \cong \mathbf{R}^{n^2}. \quad (2)$$

The density of $H_0 + H(n)$ with respect to the measure (2) is

$$C(H_0) \exp\left(-\frac{n}{2}\text{Tr} A^2 + n\text{Tr} H_0 A\right).$$

We have

$$\begin{aligned} F &:= \tau_n(\exp(H(n) + H_0)) \\ &= \frac{C(H_0)}{n} \int \text{Tr} e^A \exp\left(-\frac{n}{2}\text{Tr} A^2 + n\text{Tr} H_0 A\right) dA. \end{aligned}$$

Since the measure is unitarily invariant, we can first integrate with respect to the Haar probability dU over $\mathcal{U}(n)$:

$$F = \frac{C(H_0)}{n} \int \text{Tr} e^A \exp\left(-\frac{n}{2}\text{Tr} A^2\right) \left(\int \exp(n\text{Tr} U A U^* H_0) dU\right) dA.$$

In this way, we can use the integral formula (see [8], A.5 and also [2], Theorem 7.24 for a more general formula attributed to Harish-Chandra):

$$\int \exp(\text{Tr} U A U^* B) dU = \frac{\det[\exp(\lambda_i \rho_j)]}{\Delta(\lambda)\Delta(\rho)},$$

where A, B are $n \times n$ self-adjoint matrices, the λ_i 's are the eigenvalues of A , the ρ_j 's are those of B , and

$$\Delta(\lambda) \equiv \Delta(\lambda_1, \lambda_2, \dots, \lambda_n) =: \prod_{i<j} (\lambda_i - \lambda_j).$$

Since $dA = C\Delta(\lambda)^2 d\lambda$, we can calculate as follows:

$$\begin{aligned} F &= \frac{C(H_0)}{n} \int \text{Tr} e^A \exp\left(-\frac{n}{2}\text{Tr} A^2\right) \frac{\det[\exp(n\lambda_i d_j)]}{\Delta(\lambda)\Delta(d)} dA \\ &= \frac{C'(H_0)}{n} \int \left(\sum_j e^{\lambda_j}\right) \exp\left(-\frac{n}{2}\sum_i \lambda_i^2\right) \Delta(\lambda)^2 \frac{\det[\exp(n\lambda_i d_j)]}{\Delta(\lambda)\Delta(d)} d\lambda \\ &= \frac{C'(H_0)}{n\Delta(d)} \int \left(\sum_j e^{\lambda_j}\right) \exp\left(-\frac{n}{2}\sum_i \lambda_i^2\right) \Delta(\lambda) \det[\exp(n\lambda_i d_j)] d\lambda, \end{aligned}$$

where the latter integrals are over $\mathbf{R}_{\leq}^n := \{(x_1, x_2, \dots, x_n) \in \mathbf{R}^n \mid x_1 \leq x_2 \leq \dots \leq x_n\}$. Integration over \mathbf{R}^n gives a factor $n!$. We expand the determinant by summing over all permutations σ of $\{1, 2, \dots, n\}$:

$$\frac{C'(H_0)}{n! n\Delta(d)} \sum_{\sigma} \int \left(\sum_j e^{\lambda_j} \right) \exp\left(-\frac{n}{2} \sum_i \lambda_i^2\right) \Delta(\lambda) (-1)^{|\sigma|} \prod_i \exp(n\lambda_i d_{\sigma(i)}) d\lambda,$$

and all summands are the same, due to the fact that Δ changes sign when two of its arguments are exchanged. Hence we arrive at

$$F = \frac{C'(H_0)}{n\Delta(d)} \int \left(\sum_j e^{\lambda_j} \right) \exp\left(-\frac{n}{2} \sum_i \lambda_i^2 + n \sum_i \lambda_i d_i\right) \Delta(\lambda) d\lambda.$$

Now we proceed by means of the integral

$$\int \exp\left(-\frac{n}{2} \sum_i (\lambda_i - a_i)^2\right) \Delta(\lambda) d\lambda = C(n)\Delta(a)$$

and conclude that

$$\begin{aligned} F &= \frac{C''(H_0)}{n} \exp\left(\frac{n}{2} \sum_i d_i^2\right) \\ &\quad \times \sum_j e^{d_j} \frac{\Delta(d_1, \dots, d_{j-1}, d_j + 1/n, d_{j+1}, \dots, d_n)}{\Delta(d_1, d_2, \dots, d_n)} \\ &= \frac{1}{n} \exp\left(\frac{1}{2n}\right) \sum_j e^{d_j} \prod_{i \neq j} \frac{d_i - d_j - 1/n}{d_i - d_j} \\ &= \frac{1}{n} \exp\left(\frac{1}{2n}\right) \sum_j e^{d_j} \prod_{i \neq j} \left(1 - \frac{1}{n(d_i - d_j)}\right). \end{aligned}$$

Using analytic continuation, we replace d_j by $-itd_j$ and obtain

$$\tau_n(\exp(H(n) - itH_0)) = \frac{1}{n} \exp\left(\frac{1}{2n}\right) \sum_j e^{-id_j t} \prod_{i \neq j} \left(1 + \frac{1}{int(d_i - d_j)}\right).$$

Our theorem states that this is a positive definite function of t . We shall explicitly obtain the inverse Fourier transform of $\tau_n(\exp(H(n) - itH_0))$ and show that it is a positive measure supported on $[d_1, d_n]$. So, we compute, given an n -tuple $\mathbf{d} = \{d_1, d_2, \dots, d_n\}$ with $d_1 < d_2 < \dots < d_n$, the inverse Fourier transform of the function

$$F(\mathbf{d}; t) := \sum_{j=1}^n e^{-id_j t} \prod_{\substack{k=1 \\ k \neq j}}^n \left(1 + \frac{1}{itn(d_k - d_j)}\right). \quad (3)$$

The computation is rather direct, expanding the product in (3) in inverse powers of t

$$F(\mathbf{d}; t) = \sum_{m=0}^n \left(\frac{i}{nt}\right)^m \sum_{j=1}^n \sum_{\substack{k_1, k_2, \dots, k_m \\ k_1 < k_2 < \dots < k_m \\ k_\ell \neq j}} \frac{e^{-id_j t}}{(d_j - d_{k_1}) \cdots (d_j - d_{k_m})}. \quad (4)$$

The singularity at $t = 0$ in (4) is only apparent and we shall first remove it by using for each m -term the Taylor expansion of the function $d \mapsto \exp(-idt)$ around the point d_1 up to order m

$$\begin{aligned} e^{-idt} &= e^{-id_1 t} + (-it)(d - d_1)e^{-id_1 t} + \dots + \frac{1}{(m-1)!}(-it)^{m-1}(d - d_1)^{m-1}e^{-id_1 t} \\ &+ (-it)^m \frac{1}{(m-1)!} \int_{d_1}^d (d-s)^{m-1} e^{-ist} ds. \end{aligned} \quad (5)$$

The expression

$$t \mapsto \sum_{j=1}^n d_j^\ell \prod_{\substack{k=1 \\ k \neq j}}^n \left(1 + \frac{t}{(d_j - d_k)}\right) \quad (6)$$

is a polynomial in t of degree not larger than ℓ . Indeed, it is obviously permutation symmetric in the d_j and jointly homogeneous of degree ℓ in t and the d_j . Replacing all the d_j by $d_j + \alpha$, we obtain a polynomial in α of degree less or equal to ℓ . We then differentiate (6) m times with respect to t and put $t = 0$. For $\ell < m$ we obtain

$$\sum_{j=1}^n d_j^\ell \sum_{\substack{k_1, k_2, \dots, k_m \\ k_1 < k_2 < \dots < k_m \\ k_\ell \neq j}} \frac{1}{(d_j - d_{k_1}) \cdots (d_j - d_{k_m})} = 0$$

and therefore also

$$\sum_{j=1}^n (d_j - d_1)^\ell \sum_{\substack{k_1, k_2, \dots, k_m \\ k_1 < k_2 < \dots < k_m \\ k_\ell \neq j}} \frac{1}{(d_j - d_{k_1}) \cdots (d_j - d_{k_m})} = 0. \quad (7)$$

We plug the Taylor expansion (5) in (4) and observe that, by (7), the coefficients of negative powers of t all vanish. Thus, we obtain

$$\begin{aligned} F(\mathbf{d}; t) &= \sum_{k=1}^n e^{-id_k t} + \sum_{m=1}^n \frac{1}{n^m} \sum_{j=1}^n \sum_{\substack{k_1, k_2, \dots, k_m \\ k_1 < k_2 < \dots < k_m \\ k_\ell \neq j}} \frac{1}{(m-1)!} \times \\ &\int_{d_1}^{d_j} e^{-ist} \frac{(d_j - s)^{m-1}}{(d_j - d_{k_1}) \cdots (d_j - d_{k_m})} ds. \end{aligned}$$

We shall now rewrite this formula as

$$F(\mathbf{d}; t) = \sum_{k=1}^n e^{-id_k t} + \sum_{m=1}^{n-1} \frac{1}{n^m (m-1)!} \int_{d_1}^{d_n} e^{-ist} G_m(\mathbf{d}; s) ds. \quad (8)$$

The first term corresponds to an atomic measure attributing an equal weight to each of the eigenvalues of H_0 , while the m -terms are the m -point contributions to the absolutely

continuous part of the inverse Fourier transform of F . More precisely,

$$G_m(\mathbf{d}; s) = \sum_{\substack{\tilde{\mathbf{d}} \subset \mathbf{d} \\ \#(\tilde{\mathbf{d}})=m+1}} S_m(\tilde{\mathbf{d}}; s),$$

where for any ordered $(m+1)$ -tuple $\tilde{\mathbf{d}} = \{\tilde{d}_1, \tilde{d}_2, \dots, \tilde{d}_{m+1}\}$

$$S_m(\tilde{\mathbf{d}}; s) := \begin{cases} 0 & \text{if } x \leq \tilde{d}_1, \\ \sum_{j=\ell+1}^{m+1} \frac{(\tilde{d}_j - s)^{m-1}}{(\tilde{d}_j - \tilde{d}_1) \cdots (\tilde{d}_j - \tilde{d}_{m+1})} & \text{if } x \in [\tilde{d}_\ell, \tilde{d}_{\ell+1}], \\ 0 & \text{if } x \geq \tilde{d}_{m+1}. \end{cases}$$

On $(\tilde{d}_1, \tilde{d}_{m+1})$, S_m consists piecewise of polynomials of degree $m-1$ and it is $(m-2)$ times continuously differentiable. The function S_m lands like $(\tilde{d}_{m+1} - \cdot)^{m-1}$ at \tilde{d}_{m+1} and, by reflection symmetry, one shows that S_m has the simple expression

$$S_m(\tilde{\mathbf{d}}; s) = \frac{(s - \tilde{d}_1)^{m-1}}{(\tilde{d}_2 - \tilde{d}_1)(\tilde{d}_3 - \tilde{d}_1) \cdots (\tilde{d}_{m+1} - \tilde{d}_1)}$$

on $[d_1, d_2]$. Therefore, S_m starts off like $(\cdot - \tilde{d}_1)^{m-1}$ at \tilde{d}_1 . Hence, S_m is $(m-2)$ times continuously differentiable on the real line. As

$$\int_{\tilde{d}_1}^{\tilde{d}_{m+1}} S_m(\tilde{\mathbf{d}}; s) ds = \frac{1}{m}, \quad (9)$$

the $S_m(\tilde{\mathbf{d}}; \cdot)$ are precisely the well-known B-splines from approximation theory [3]. Each $\tilde{\mathbf{d}}$, together with the normalization condition (9), uniquely determines a spline S_m of order $(m-1)$ and $S_m > 0$ on $(\tilde{d}_1, \tilde{d}_{m+1})$. If this were not true, then S'_m should have at least three roots in $(\tilde{d}_1, \tilde{d}_{m+1})$ and the piecewise linear $(m-2)$ th derivative should have $m+1$ roots, which is impossible.

The simplest non-trivial case is the roof function $S_2(\{d_1, d_2, d_3\}; \cdot)$ which is continuous and piecewise linear with nodes at $\{d_1, d_2, d_3\}$. Its explicit form is given by

$$S_2(\{d_1, d_2, d_3\}; s) = \begin{cases} 0 & \text{if } s \leq d_1, \\ \frac{s - d_1}{(d_2 - d_1)(d_3 - d_1)} & \text{if } d_1 \leq s \leq d_2, \\ \frac{d_3 - s}{(d_3 - d_1)(d_3 - d_2)} & \text{if } d_2 \leq s \leq d_3, \\ 0 & \text{if } d_3 \leq s. \end{cases}$$

Free non-commutative random variables

Let \mathcal{M} be a type II_1 von Neumann algebra with faithful normal tracial state τ . Self-adjoint elements of \mathcal{M} are called non-commutative random variables. Random variables $a = a^*, b = b^* \in \mathcal{M}$ are said to be in free relation if

$$\tau(p_1(a)q_1(b)p_2(a)q_2(b) \dots p_n(a)q_n(b)) = 0$$

whenever $p_1, p_2, \dots, p_n, q_1, q_2, \dots, q_n$ are polynomials such that $\tau(p_i(a)) = \tau(q_i(b)) = 0$ ($1 \leq i \leq n$). Non-commutative random variables in free relation arise from random matrix models. (For an introduction to free random variables and their random matrix model, see the book [7].) Let H_n and K_n be $n \times n$ random matrices for every $n \in \mathbf{N}$. They form a random matrix model for the pair $a = a^*, b = b^* \in \mathcal{M}$ if

$$\tau_n(P(H_n, K_n)) \rightarrow \tau(P(a, b))$$

for any polynomial P of two non-commuting indeterminates. A very remarkable result, due to Voiculescu, tells us that if (a, b) has a random matrix model such that H_n is a Wigner matrix and K_n is independent of H_n , then a and b are in free relation. This fact is a manifestation of asymptotic freeness, see [11, 12] or [7]. It is a much easier fact (called Wigner theorem) that under the above conditions a is a standard semicircular element, that is,

$$\tau(a^n) = \frac{1}{2\pi} \int_{-2}^2 x^n \sqrt{4-x^2} dx \quad (n \in \mathbf{N}).$$

Theorem. *Let a and b be self-adjoint operators in a von Neumann algebra with faithful normal trace τ . Assume that a and b are in free relation with respect to τ and that a is standard semicircular. Then $t \mapsto \tau(\exp(a - itb))$ is a positive definite function: there exists a unique measure μ such that*

$$\tau(\exp(a - itb)) = \frac{1}{\sqrt{2\pi}} \int e^{-itx} d\mu(x) \quad (t \in \mathbf{R}).$$

The support of μ is contained in the convex hull of the spectrum of b .

Since a pair (a, b) in the theorem admits a random matrix model with Wigner matrices H_n and nonrandom diagonal matrices K_n (see [11] or Cor. 4.3.6 in [7]), the result follows from our first theorem for finite matrices.

It was computed in [5] that in the case when both a and b are standard semicircular, we have

$$\tau(e^{a+itb}) = \frac{1}{2\pi} \int_{-2}^2 e^{iut} \sinh(\sqrt{4-u^2}) du.$$

In this example the Bochner measure is explicit, however this situation is rather exceptional. We consider the example in which the spectrum of b is $\{\alpha, \beta\}$ and the distribution gives equal weights $1/2$ at the points $\alpha < \beta$. A matrix model for this situation is obtained by choosing, for even n , H_0 diagonal with $n/2$ eigenvalues close to α and the others close to β . In this case, we may take the limit $n \rightarrow \infty$ in (8) term by term. The limit of a spline function $G_m(\tilde{\mathbf{d}}; s)$ when $\tilde{d}_1, \tilde{d}_2, \dots, \tilde{d}_k$ tend to α and $\tilde{d}_{k+1}, \tilde{d}_{k+2}, \dots, \tilde{d}_{m+1}$ to β is easily seen to be

$$\binom{m-1}{k-1} \frac{(s-\alpha)^{m-k}(\beta-s)^{k-1}}{(\beta-\alpha)^m} \quad (\alpha \leq s \leq \beta)$$

and 0 elsewhere. The limit $n \rightarrow \infty$ is now straightforward:

$$\tau(\exp(a - itb)) = \frac{1}{2} \left(e^{-i\alpha t} + e^{-i\beta t} \right) + \int_{\alpha}^{\beta} e^{-ist} f(s) ds,$$

where $f(s)$ is explicitly given by

$$\sum_{m=0}^{\infty} \frac{1}{2^{m+2} ((m+1)!)^2 (\beta - \alpha)^{m+1}} \sum_{k=0}^m \binom{m+1}{k} \binom{m+1}{k+1} (s - \alpha)^{m-k} (\beta - s)^k.$$

The Bochner measure of $t \mapsto \tau(\exp(a - itb))$ is therefore a sum of an atomic part giving equal weight to the points which support the Bernoulli variable and an absolutely continuous part with support $[\alpha, \beta]$.

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