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Integrabilidad, caos y entrelazamiento en sistemas cuánticos

Integrability, chaos and entanglement in quantum systems

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Resumen:

Estudiamos el papel de las matrices aleatorias en la mecánica cuántica. Exploramos en primer lugar cómo el comportamiento del hamiltoniano bajo invariancia temporal determina el tipo de colectividad que lo representa e introducimos las colectividades gaussianas: la ortogonal, la simpléctica y la unitaria. Estudiamos cómo a partir de las transformaciones de simetría características de cada una de estas colectividades se pueden deducir sus distribuciones y propiedades. A continuación, analizamos el espectro (niveles de energía) de estas matrices aleatorias. Calculamos la distribución de los autovalores e introducimos la ley del semicírculo de Wigner, que aproxima asintóticamente esta distribución. Estudiamos también el espaciado entre niveles de energía consecutivos, tras normalizar el espectro mediante el *unfolding*, introduciendo la distribución que deberían seguir estos espaciados en función de la colectividad a la que pertenece la matriz. Comprobamos estos resultados teóricos mediante simulaciones que generan y analizan matrices de estas colectividades. Finalmente, exploramos cómo la distribución de estos espaciados dependen de si el análogo clásico del modelo es integrable o caótico, presentando las conjeturas de Berry-Tabor y Bohigas-Giannoni-Schmit.

Abstract:

We study the role of random matrices in quantum mechanics. We first explore how the behavior of the Hamiltonian under time invariance determines the type of ensemble that represents it and introduce the Gaussian ensembles: the orthogonal, the symplectic and the unitary. We study how from the symmetry transformations characterizing each of these collectivities we can deduce their distributions and properties. We then analyze the spectrum (energy levels) of these random matrices. We calculate the distribution of the eigenvalues and introduce Wigner's semicircle law, which asymptotically approximates this distribution. We also study the spacing between consecutive energy levels, after normalizing the spectrum by *unfolding* it, introducing the distribution that these spacings should follow depending on the ensemble to which the matrix belongs. We verify these theoretical results through simulations that generate and analyze matrices of these ensembles. Finally, we explore how the distribution of these spacings depends on whether the classical analogue of the model is integrable or chaotic, presenting the Berry-Tabor and Bohigas-Giannoni-Schmit conjectures.

Contents

1 Introduction

In general, in the study of a physical process the first thing one needs to model is the form of the interactions between particles, which rule the evolution of the system. In mathematical terms, these interactions are described by the Hamiltonian. However, when dealing with especially complex systems, such as those in nuclear processes involving heavy nuclei, it is impossible to explicitly know or compute the interactions between particles, and hence the particular Hamiltonian of the system remains unknown. Nevertheless, when dealing with a large number of this kind of systems, instead of trying to deal with the impossible task of analyzing the interaction of each of them one might use statistical analysis and draw qualitative conclusions from a probability distribution associated with the system.

Following this probabilistic approach using Hamiltonians that act on an infinite-dimensional space (which is the usual space where the states of a quantum system live) would be impossible. Hence, the correct way to proceed is to truncate the Hamiltonian, keeping only N degrees of freedom (choosing N to be a large integer), and treat the Hamiltonian as an $N \times N$ matrix. Then, one can observe that the qualitative behavior of a series of magnitudes of the system (e.g., the spacing between two consecutive energy levels) matches the results we would obtain from a random matrix of a certain ensemble. However, the way we choose these random matrices in order to match the behavior of our

system is a subtle matter. Namely, we should ask ourselves questions like what is the "average look" of a Hamiltonian for a specific system of particles? Are there any symmetries that must be always included in the resulting Hamiltonian? How do these properties affect the distribution of the random matrix elements? The theory of random matrices applied to quantum physics aims to answer these types of questions.

2 Time reversal invariance

The first thing one needs to understand to model the probability distribution of the Hamiltonian is the fact that the general structure of the matrix H is heavily influenced by the symmetries of the system. Recall that a quantum system described by H is said to have a symmetry A if

$$[H, A] = 0,$$

where $[\cdot, \cdot]$ denotes the commutator and A is the operator implementing this symmetry. Indeed, due to a well-known theorem by Wigner, we know that in Quantum Mechanics any symmetry must be implemented by a unitary or antiunitary operator.

2.1 Time reversal symmetry

One of the most important symmetries that a general quantum system has is time reversal, which will be implemented by the operator T. In a system of N spin $\frac{1}{2}$ particles it is clear that this operator must satisfy the following relations:

$$T\mathbf{r}_j T^{-1} = \mathbf{r}_j, \quad T\mathbf{p}_j T^{-1} = -\mathbf{p}_j, \quad T\mathbf{s}_j T^{-1} = -\mathbf{s}_j, \tag{1}$$

with $j = 1, \ldots, N$ and

$$\mathbf{s}_j = \frac{\hbar}{2}\boldsymbol{\sigma}_j \coloneqq \frac{\hbar}{2}(\sigma_j^x, \sigma_j^y, \sigma_j^z)$$

the spin operator of the j-th particle, where σ_j^α denotes the Pauli matrix σ^α acting on the j-th particle.

Using these relations one can prove the following:

Proposition 1. *Any time reversal operator (in the sense that it satisfies* (1)*) must be antiunitary.*

Proof. Recall that the commutator of the position and momentum operators is given by

$$[\mathbf{r}, \mathbf{p}] = \mathbf{rp} - \mathbf{pr} = i\hbar\mathbb{1}.$$

Now, let T be an operator satisfying (1). Then, if we multiply the last expression by this operator and use (1) we obtain:

$$T(i\hbar\mathbb{1}) = T(\mathbf{rp} - \mathbf{pr}) = -\mathbf{rp}T + \mathbf{pr}T = -i\hbar\mathbb{1}T.$$

Hence,

$$Ti = -Ti.$$

This means that this operator can never be unitary. As it implements a symmetry, we can then conclude that it can only be antiunitary. □

Once we know that T is antiunitary, we can write it as $T = KC$, where K is unitary and C is the complex conjugation.

These commutation relations not only allow us to deduce this property of the time reversal operator, but they also determine it:

Proposition 2. *Equation* (1) *is enough to unambiguously determine the operator* T *(up to a unitary transformation).*

Proof. In order to prove this statement, let us take $\tilde{T}$ to be another antiunitary operator satisfying (1). Then, applying such relations we get that

$$\tilde{T}T^{-1}\mathbf{r}_j = \tilde{T}\mathbf{r}_jT^{-1} = \mathbf{r}_j\tilde{T}T^{-1}, \tilde{T}T^{-1}\mathbf{p}_j = -\tilde{T}\mathbf{p}_jT^{-1} = \mathbf{p}_j\tilde{T}T^{-1}, \tilde{T}T^{-1}\mathbf{s}_j = -\tilde{T}\mathbf{s}_jT^{-1} = \mathbf{s}_j\tilde{T}T^{-1}.$$

This means that the operator $\tilde{T}T^{-1}$ commutes with $\mathbf{r}_j, \mathbf{p}_j$ and $\mathbf{s}_j$, which is a complete set of observables for our system. Hence, we must have

$$\tilde{T}T^{-1} = \lambda\mathbb{1},$$

where $\mathbb{1}$ is the identity operator and $\lambda \in \mathbb{C}$. Moreover, as both $\tilde{T}$ and T^{-1} are antiunitary, their product is unitary, and hence $\lambda = e^{2i\alpha}$ with α real, i.e., we have that

$$\tilde{T} = e^{2i\alpha}T.$$

We know that a global phase change has no physical relevance. Therefore, we can conclude that T and $\tilde{T}$ are essentially the same. □

2.2 Construction of the operator K

To study the effect of time reversal symmetry in the Hamiltonian, we are going to focus on the properties of the operator K. In order to do so, notice that if we apply the operator $C\mathbf{r}_j$ to a state ψ we get

$$C\mathbf{r}_j\psi = \mathbf{r}_j\overline{\psi} = \mathbf{r}_j(C\psi).$$

Hence, we can conclude that C commutes with $\mathbf{r}_j$.

On the other hand, we have

$$C\mathbf{p}_j|\psi\rangle = C(-i\hbar\nabla_j|\psi\rangle = i\hbar\nabla_j\overline{|\psi\rangle} = -\mathbf{p}_jC|\psi\rangle,$$

which means that $C\mathbf{p}_jC^{-1} = -\mathbf{p}_j$.

Therefore, by taking into account that $T = KC$ satisfies (1), these relations between C and the position and momentum operators clearly imply

$$K\mathbf{r}_jK^{-1} = \mathbf{r}_j, \quad K\mathbf{p_j}K^{-1} = \mathbf{p}_j.$$

Hence, K commutes with $\mathbf{r}_j$ and $\mathbf{p}_j$ for all $j = 1, \ldots, N$. If we are dealing with zero spin particles, this means that K commutes with a complete set of observables, which means that it can be taken as $K = \mathbb{1}$. In this scalar case we will have that T is the complex conjugation, and hence $[H, T] = 0$ implies that H must be real.

If we are dealing with spin $\frac{1}{2}$ particles, although the operator K cannot be taken to be the identity, it can only act non-trivially on the spin part of the state. This means that if our state is of the form $|\psi\rangle = \varphi|s\rangle$, where φ is a scalar function and $|s\rangle \in \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$, it must be

$$K(\varphi|s\rangle) = \varphi K|s\rangle.$$

Therefore, we can conclude that we are dealing with a unitary operator $K : \mathbb{C}^{2^N} \to \mathbb{C}^{2^N}$.

Now, in order to further determine the properties of K we need to use again the expressions in (1), taking into account that $T = KC$. We can repeat the same strategy as before and compute the commutator of the operator C with the $\mathbf{s}_j$. In order to do so, recall that in the usual representation

of the Pauli matrices both σ_j^x and σ_j^z are real, while σ_j^y is pure imaginary. Therefore, since the spin operators are a (real) multiple of these matrices, it follows that

$$Cs_j^{x,z}C = s_j^{x,z}, \quad Cs_j^yC = -s_j^y.$$

Hence, in order for $T = KC$ to anticommute with $\mathbf{s}_j$, K must satisfy the opposite relations, i.e.,

$$Ks_j^{x,z}K^{-1} = -s_j^{x,z}, \quad Ks_j^yK^{-1} = s_j^y. \tag{2}$$

Since the Pauli matrices anticommute with each other, this last relation suggests that we try

$$K = \prod_{k=1}^{N} \sigma_k^y.$$

Notice that the order of this product does not matter since the spin operators of different particles commute with each other. We can apply this, together with the fact σ_j^y is an involutory matrix, to deduce that $K^2 = \mathbb{1}$. In addition, since K is the product of self-adjoint matrices that commute with each other, it must be self-adjoint itself. Therefore, $KK^\dagger = K^2 = \mathbb{1}$, which means that K is unitary, as it should.

Now, let us check that it actually satisfies (2). The fact that it commutes with the operators s_j^y is trivial by its definition. Moreover, we can apply again that spin operators acting on different particles commute to get

$$K\sigma_j^{x,z} = \prod_{k=1,k\neq j}^{N} \sigma_k^y \cdot \left(\sigma_j^y\sigma_j^{x,z}\right) \prod_{k=1,k\neq j}^{N} \sigma_k^y \cdot \left(-\sigma_j^{x,z}\sigma_j^y\right) = -\sigma_j^{x,z}K.$$

Here we have used that different components of the spin operator acting on the same particle anticommute. We have thus finally arrived at an operator K that satisfies equation (2), and hence $T = KC$ satisfies the corresponding equation (1).

Finally, it is customary to redefine the operator K as

$$K = \prod_{j=1}^{N} (i\sigma_j^y).$$

This extra phase i^N has no physical meaning, but it allows us to rewrite K more compactly in terms of the total spin operator $S_y = \sum_{j=1}^{N} s_j^y$ as

$$K = e^{\frac{i\pi}{\hbar}S_y}.$$

This equality is a direct consequence of the following more general result:

Proposition 3. *For any $\theta \in \mathbb{R}$, we have*

$$e^{i\theta\sigma_j^y} = \cos\theta\mathbb{1} + i\sin\theta\sigma_j^y.$$

Proof. By definition of the exponential of an operator,

$$\exp(i\theta\sigma_j^y) = \sum_{n=0}^{\infty} \frac{(i\theta\sigma_j^y)^n}{n!}.$$

We can use that $(\sigma_j^y)^2 = \mathbb{1}$ and get

$$\exp(i\theta\sigma_j^y) = \mathbb{1}\sum_{n=0}^{\infty} \frac{(i\theta)^{2n}}{(2n)!} + \sigma_j^y \sum_{n=0}^{\infty} \frac{(i\theta)^{2n+1}}{(2n+1)!} = \cos\theta\mathbb{1} + i\sin\theta\sigma_j^y.$$

□

Using the result from this proposition we get

$$K = \prod_{j=1}^{N} (i\sigma_j^y) = \prod_{j=1}^{N} e^{\frac{i\pi}{2}\sigma_j^y} = e^{\frac{i\pi}{2}\sum_{j=1}^{N}\sigma_j^y} = e^{\frac{i\pi}{\hbar}S_y}. \tag{3}$$

2.3 Consequences of the structure of the time reversal operator

First of all, notice that since σ_j^y is pure imaginary and self-adjoint we have

$$(\sigma_j^y)^T = \overline{\sigma_j^y} = -\sigma_j^y,$$

and hence $K^T = (-1)^N K$. In particular, if N is even, $K = K^T$, which means that K is real. Therefore, the condition H commutes with T implies that the Hamiltonian commutes with the complex conjugation, which can only happen if H is real.

On the other hand, if N is odd we need to add the extra condition that H is invariant under rotations around some axis. Then, we can take as such axis the y direction which implies $[H, S_y] = 0$, which in particular means that H commutes with $K = e^{\frac{i\pi}{\hbar}S_y}$. We then have

$$H = THT^{-1} = K\overline{H}K^{-1} = KH^TK^{-1} = H^T = \overline{H},$$

and thus we can conclude that H is also represented by a real matrix in this case.

Summarizing, the Hamiltonian of a system of N particles can be represented by a real symmetric matrix (in a suitable basis) if any of the following conditions is satisfied:

(i) The particles are scalar (i.e., spinless).

(ii) The particles have spin $\frac{1}{2}$ and N is even.

(iii) The particles have spin $\frac{1}{2}$ and H is invariant under rotations around some axis.

3 Gaussian orthogonal ensemble

Let us suppose then that our Hamiltonian satisfies one of the previous conditions, and hence it is represented by a real matrix. We should determine the appropriate distribution for this real matrix. The simplest distribution one might consider is to assign to each matrix element an independent Gaussian distribution [1]. Then, we could take as our $N \times N$ random matrix X, the one whose elements are independent standard Gaussians $N[0, 1]$. However, this would not be a valid Hamiltonian, as the matrix H must be Hermitian. When H is real this simply means that $H = H^T$, so we symmetrize X and take

$$H = \frac{1}{2}(X + X^T),$$

and let this be our definition for a random matrix belonging to the Gaussian orthogonal ensemble. Using the properties of the Gaussian distribution[2], it is clear that an equivalent definition of GOE matrices is given by:

[1] Recall that the probability distribution function of a Gaussian of mean μ and deviation σ, denoted by $N[\mu, \sigma]$, is given by $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$.

[2] In particular, we will use that if $X_i \sim N[\mu_i, \sigma_i]$ with $i = 1, 2$, and $a \in \mathbb{R}$, then $aX_1 \sim N[a\mu_1, a\sigma_1]$ and $X_1 + X_2 \sim N[\mu_1 + \mu_2, \sqrt{\sigma_1^2 + \sigma_2^2}]$.

Definition 1. *A random real symmetric $N \times N$ matrix H is said to belong to the Gaussian orthogonal ensemble (GOE) if the diagonal and upper triangular elements are independently chosen with probability distribution functions (p.d.f.'s)*

$$\frac{1}{\sqrt{2\pi}} e^{-h_{jj}^2/2} \quad \textit{and} \quad \frac{1}{\sqrt{\pi}} e^{-h_{jk}^2},$$

respectively.

The joint p.d.f. of all the independent elements is

$$\begin{aligned} P(H) &= \prod_{j=1}^{N} \frac{1}{\sqrt{2\pi}} e^{-h_{jj}^2/2} \prod_{1 \leqslant j < k \leqslant N} \frac{1}{\sqrt{\pi}} e^{-h_{jk}^2} = A_N \prod_{j,k=1}^{N} e^{-h_{jk}^2/2} \\ &= A_N e^{-\sum_{j,k=1}^{N} h_{jk}^2/2} = A_N e^{-\frac{1}{2}\operatorname{tr} H^2}, \end{aligned} \tag{4}$$

where A_N is the normalization constant and tr denotes the trace.

We have chosen this distribution not only due to its simplicity, but also because it satisfies certain important properties. Indeed, as we will discuss later, these properties uniquely characterizes this distribution.

The first and most important property of any matrix H of the GOE is that given any orthogonal matrix $X \in O(N)$, we have $P(X^T H X) = P(H)$. Physically, we require this condition to hold because we want that our results do not depend on the specific (inertial) frame of reference we choose. In Quantum Mechanics, we know that a change of frame of reference is given by a unitary operator U, transforming the Hamiltonian as $H \to U^\dagger H U$. However, as we need the Hamiltonian to remain a symmetric real matrix, we are forced to take U an orthogonal matrix[3]. Thus, for any $X \in O(n)$, $X^T H X$ is a matrix as equally valid to represent the Hamiltonian operator as H. Hence, their joint probability distributions should agree. If we look at (4), we can see that any GOE matrix does satisfy this condition, as its joint p.d.f. only depends on its eigenvalues[4], which are invariant under orthogonal transformations.

The second property we ask for is the factorization of the joint p.d.f. This means that $P(H) = \prod_{j,k=1}^{N} f_{jk}(h_{jk})$, where f_{jk} are differentiable functions.

Imposing these two requirements leads to the following result:

Proposition 4. *Let H be a real symmetric random matrix satisfying that for any $X \in O(N)$, $P(X^T H X) = P(H)$. Then, the most general p.d.f. satisfying the factorization property $P(H) = \prod_{1 \leqslant j \leqslant k \leqslant N} f_{jk}(h_{jk})$ for f_{jk} differentiable is*

$$P(H) = C e^{-a \operatorname{tr}(H^2) + b \operatorname{tr}(H)}.$$

The proof of this proposition can be found in the Appendix. Its general idea is to use the symmetries of the matrix to deduce some differential equations the functions f_{jk} must satisfy, which one can solve in order to obtain $P(H)$.

Finally, in order to get the specific joint p.d.f. for the GOE, which takes $a = \frac{1}{2}$ and $b = 0$, we need one final constraint, which is given in terms of the entropy. We will define this entropy S of a joint p.d.f. P as

$$S[P] := -\langle \log P \rangle_P.$$

This entropy will be a measure of uncertainty. Then, taking into account that we know nothing about our system apart from the symmetries we already implemented, we will seek to maximize S. Indeed, one can show the following:

[3]Actually, it can be shown that both $U = X$ and $U = iX$, with $X \in O(N)$, are the only valid options, but we can obviously disregard the latter.

[4]Recall that if a matrix H has eigenvalues $\{\lambda_j\}$, then $\operatorname{tr} H^k = \sum \lambda_j^k$

Proposition 5. *The joint p.d.f. P given in* (4) *maximizes $S[P] = -\langle \log P \rangle_P$ subject to the constraint $\langle \operatorname{tr} H^2 \rangle_P = N^2$.*

Proof. We are dealing with a constrained optimization problem, and hence we can use Lagrange multipliers. Notice that apart from the constraint $\langle \operatorname{tr} H^2 \rangle_P = N^2$ we also have the normalization constraint $\langle 1 \rangle_P = 1$. Then, if λ_1 and λ_2 are our Lagrange multipliers, the optimization condition reads

$$-\log P - \lambda_1 \operatorname{tr} H^2 + \lambda_2 = 0.$$

This means that $P = e_2^{\lambda} e^{-\lambda_1 \operatorname{tr} H^2}$. Now, if we impose the normalization condition (and define $A_N := e^{\lambda_2}$ as the normalization constant) and the constraint $\langle \operatorname{tr} H^2 \rangle_P = N^2$, we can deduce that $\lambda_1 = \frac{1}{2}$. Hence, $P(H)$ must be given by (4). □

This allows us to conclude that our definition of GOE is the one we should use when dealing with real symmetric matrices.

4 Gaussian symplectic ensemble

Our next step will be to consider systems with an odd number of spin $\frac{1}{2}$ particles which are invariant under time reversal but not under rotations around some axis. As we have discussed before, this is not enough to force our Hamiltonian to be a real symmetric matrix. However, time reversal invariance alone still enforces some conditions that our Hamiltonian must meet.

Let us come back to the expression for K in (3). We know that the Pauli matrix in the y direction is given by $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Thus, it must be

$$K = \prod_{j=1}^{n} e^{\frac{i\pi}{2}\sigma_j^y} = \prod_{j=1}^{n} \exp\left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes \cdots \otimes \underset{j}{\begin{pmatrix} 0 & \frac{\pi}{2} \\ -\frac{\pi}{2} & 0 \end{pmatrix}} \cdots \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right)$$
$$= \prod_{j=1}^{n} \left(\mathbb{1} \otimes \cdots \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \cdots \otimes \mathbb{1} \right) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \cdots \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

where n is the number of particles. Once we have expressed the operator K in this form we claim the following:

Proposition 6. *If n is odd, then by a suitable unitary transformation (change of basis), we can write K as*

$$K = \mathbb{1}_N \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} =: Z_{2N},$$

with $N = 2^{n-1}$. On the other hand, if n is even, we have

$$K = \begin{pmatrix} 0 & Z_{2N} \\ Z_{2N} & 0 \end{pmatrix},$$

with $N = 2^{n-2}$.

Proof. We can prove this result using induction on n. The case $n = 1$ is trivial, since $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = Z_2$. Let us show then that if the result is true for n assuming that the case $n - 1$ holds.

First, if n is even, we know that

$$K = \bigotimes_{j=1}^{n} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \left(\bigotimes_{j=1}^{n-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes Z_{2^{n-1}} = \begin{pmatrix} 0 & Z_{2N} \\ Z_{2N} & 0 \end{pmatrix},$$

with $N = 2^{n-2}$.

On the other hand, if n is odd, we get

$$K = \bigotimes_{j=1}^{n} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 0 & Z_{2^{n-2}} \\ Z_{2^{n-2}} & 0 \end{pmatrix} = \begin{pmatrix} & & & Z_{2^{n-2}} \\ & & -Z_{2^{n-2}} & \\ & -Z_{2^{n-2}} & & \\ Z_{2^{n-2}} & & & \end{pmatrix}.$$

One can check that performing a change of basis by permuting basis vectors, we get

$$K = Z_{2N}, \quad \text{with } N = 2^{n-1}.$$

□

Actually, this result can be extended as one can show that every unitary antisymmetric operator can be reduced to the form $K = Z_{2N}$ (see [4]).

As a corollary of this result one obtains that $K^T = K$ if n is even, while $K^T = -K$ for n odd, as we argued in previous sections.

For this section, we will consider n to be odd, and hence the time reversal operator is given by $T = Z_{2N}C$, which means that if our system has time reversal symmetry, its Hamiltonian H must satisfy

$$H = THT^{-1} = Z_{2N}CHC^{-1}Z_{2N}^{-1} = Z_{2N}CHCZ_{2N}^{-1} = Z_{2N}\overline{H}Z_{2N}^{-1}. \tag{5}$$

4.1 Quaternionic matrices

Notice that since Z_{2N} is block diagonal with blocks $\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, we can treat H as a $N \times N$ matrix whose elements are 2×2 blocks. In this context, it will be useful to introduce the language of *quaternions*.

Abstractly speaking, the algebra of quaternions consists of elements of the form

$$q = a_0 + a_1\mathbf{i} + a_2\mathbf{j} + a_3\mathbf{k},$$

where $a_0, \ldots, a_3 \in \mathbb{C}$ and

$$\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1, \quad \mathbf{ijk} = -1,$$

(do not confuse $\mathbf{i}$ with the imaginary unit i).

The basis elements can be represented by the following 2×2 matrices with complex elements:

$$\mathbb{1}_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad e_1 := i\sigma_z = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad e_2 := i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad e_3 := i\sigma_x = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}.$$

These matrices form a complete set, and any 2×2 complex matrix can be expressed by a complex linear combination of them :

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \frac{1}{2}(a+d)\mathbb{1}_2 - \frac{i}{2}(a-d)e_1 + \frac{1}{2}(b-c)e_2 - \frac{i}{2}(b+c)e_3.$$

Using this language, we can show the following:

Proposition 7. *A $N \times N$ quaternionic matrix H satisfies*

$$H = Z_{2N}\overline{H}Z_{2N}^{-1},$$

if, and only if, the elements of H are real quaternions (quaternions whose coefficients are real).

Proof. First of all, notice that Z_{2N} can be expressed as a diagonal quaternionic matrix $Z_{2N} = e_2 \mathbb{1}_N$. Therefore, $H = Z_{2N}\overline{H}Z_{2N}^{-1}$ is equivalent to require that every (quaternionic) element$q$ of H satisfies

$$q = e_2 \overline{q} e_2^{-1}. \tag{6}$$

In this representation $\mathbb{1}_2$ and e_2 are real while e_1 and e_3 are purely imaginary. Therefore, if

$$q = c_0\mathbb{1}_2 + c_1e_1 + c_2e_2 + c_3e_3,$$

we have

$$\overline{q} = \overline{c_0}\mathbb{1}_2 - \overline{c_1}e_1 + \overline{c_2}e_2 - \overline{c_3}e_3.$$

Clearly, $\mathbb{1}_2$ and e_2 commute with e_2, while $e_2e_i = -e_ie_2$ for $i = 1, 3$. Then, condition (6) is equivalent to

$$c_0\mathbb{1}_2 + c_1e_1 + c_2e_2 + c_3e_3 = e_2(\overline{c_0}\mathbb{1}_2 - \overline{c_1}e_1 + \overline{c_2}e_2 - \overline{c_3}e_3)e_2^{-1} = \overline{c_0}\mathbb{1}_2 + \overline{c_1}e_1 + \overline{c_2}e_2 + \overline{c_3}e_3.$$

Since $\{\mathbb{1}_2, e_1, e_2, e_3\}$ are linearly independent, this is equivalent to require

$$c_i = \overline{c_i}$$

for $i = 0, \ldots, 3$. In other words, the matrix H satisfies the condition if, and only if, its elements are real quaternions. □

If we have a quaternion $q = c_0\mathbb{1}_2 + \sum_j c_je_j$ in this representation, its Hermitian conjugate is given by

$$q^\dagger = \overline{c_0}\mathbb{1}_2^\dagger + \overline{c_1}e_1^\dagger + \overline{c_2}e_2^\dagger + \overline{c_3}e_3^\dagger = \overline{c_0}\mathbb{1}_2 - \overline{c_1}e_1 - \overline{c_2}e_2 - \overline{c_3}e_3.$$

Then, if $H_{kj} = q_{kj}$ is a quaternionic matrix we have that

$$(H)_{kj}^\dagger = q_{jk}^\dagger.$$

In the case of our Hamiltonian H, we want it to be Hermitian apart from having real quaternionic elements. Therefore, its elements must satisfy:

$$q_{jj} = q_{jj}^\dagger \Rightarrow q_{jj} \text{ is a multiple of } \mathbb{1}_2, q_{jk} = q_{kj}^\dagger \Rightarrow q_{kj} \text{ is determined by } q_{jk},$$

for every $1 \leqslant j, k \leqslant N$.

4.2 Definition of GSE and its properties

Once we know the structure of the Hamiltonian of our system, it makes sense to define the following ensemble of Gaussian symplectic random matrices:

Definition 2. *A random Hermitian $N \times N$ matrix H with real quaternions elements is said to belong to the Gaussian symplectic ensemble (GSE) if the elements $q_{jj} = a_{jj}\mathbb{1}_2$ of each diagonal are independently chosen with p.d.f.*

$$\frac{2}{\pi}e^{-2a_{jj}^2}$$

(or equivalently, have distribution $N[0, 1/2]$), while the upper triangular off-diagonal elements $q_{jk} = a_{jk}\mathbb{1}_2 + bjke_1 + c_{jk}e_2 + d_{jk}e_3$ are independently chosen with p.d.f.

$$\frac{4}{\pi}e^{-4(a_{jk}^2+b_{jk}^2+c_{jk}^2+d_{jk}^2)}$$

(or equivalently have distribution $N[0, 1/(2\sqrt{2})]\mathbb{1}_{2N} + N[0, 1/(2\sqrt{2})]e_1 + N[0, 1/(2\sqrt{2})]e_2 + N[0, 1/(2\sqrt{2})]e_3$).

Thus, $H = (X + X^\dagger)^2$, where X is an $N \times N$ random matrix of independent real quaternions having a distribution

$$N[0, 1/2]\mathbb{1}_{2N} + N[0, 1/2]e_1 + N[0, 1/2]e_2 + N[0, 1/2]e_3.$$

From this definition, it follows that the joint p.d.f. of all independent elements of GSE is given by

$$P(H) = A_N e^{-2\,\mathrm{tr}(H^2)},$$

where A_N is a normalization constant. In particular, this implies that this probability distribution is invariant under similarity transformations of the right unitary matrices. In this case, we are interested in the subgroup of the unitary matrices that do not only conserve the property of being Hermitian, but that it also maps quaternion real Hermitian matrices into themselves. We can identify this subgroup using the following result:

Proposition 8. *(a) Let H be an arbitrary $N \times N$ quaternion real Hermitian matrix, which means that the only symmetry of H is the time reversal operator $T = Z_{2N}C$. Then, any unitary matrix U which under a similarity transformation maps H to another matrix with this symmetry must commute or anticommute with T.*
(b) A unitary matrix U which commutes with $T = Z_{2N}C$ has the property

$$UZ_{2N}U^T = Z_{2N},$$

which implies that U is equivalent to a symplectic matrix, while unitary matrix U which anticommutes with T has the property $-UZ_{2N}U^T = Z_{2N}$.

Proof. (a) Let $H' = U^{-1}HU$. Since both H and H' commute with T, we have that

$$HTUT^{-1} = TUT^{-1}H'.$$

If we substitute $H' = U^{-1}HU$ in this expression and multiply on the right by U^{-1}, we get

$$HTUT^{-1}U^{-1} = TUT^{-1}U^{-1}H,$$

which means that $TUT^{-1}U^{-1}$ commutes with H. Since the only non-trivial symmetry of H is T, $TUT^{-1}U^{-1}$ must be a multiple of T or the identity. If $TUT^{-1}U^{-1} = \lambda T$ (with $\lambda \neq 0$), we can multiply by T^{-1} on the left, get that $UT^{-1}U^{-1} = \lambda\mathbb{1}$ and conclude that $T = \lambda^{-1}\mathbb{1}$, which is clearly a contradiction.

Therefore, it must be $TUT^{-1}U^{-1} = \lambda\mathbb{1}$, and hence

$$TU = \lambda UT.$$

We know that for systems with an odd number of spin $\frac{1}{2}$ particles, $T^2 = -\mathbb{1}$. This implies that if we multiply the previous expression by T on the left and the right, we get

$$-UT = -\lambda TU = -\lambda(\lambda UT) = -\lambda^2 UT,$$

thus letting us deduce that $\lambda = \pm 1$, concluding that $TU = \pm UT$.

(b) We know, as noted at the beginning of this section, that any matrix U which commutes with T has the property $U = Z_{2N}\overline{U}Z_{2N}^{-1}$. Then, as $\overline{U} = (U^{-1})^T$ because U is unitary, we can deduce from the previous expression that

$$U = Z_{2N}(U^{-1})^T Z_{2N}^{-1} \Rightarrow UZ_{2N}U^T = Z_{2N}.$$

Recall that a matrix is symplectic if

$$X^T J_{2N} X = J_{2N}, \quad J_{2N} := \begin{pmatrix} \mathbf{0}_N & \mathbb{1}_N \\ \mathbb{1}_N & \mathbf{0}_N \end{pmatrix}.$$

It is clear that J_{2N} is related to Z_{2N} by a similarity transformation (it is a matter of rearranging the columns and rows). Therefore, it is straightforward to check that this same similarity transformation changes U into a symplectic matrix.

The anticommuting case is obtained similarly by adding a minus sign. □

After this result, we can see how the Gaussian symplectic ensemble is precisely characterized by being invariant under similarity transformation by symplectic matrices.

5 Gaussian unitary ensemble

Finally, let us consider a quantum system without time reversal symmetry. In this situation the Hamiltonian of our system can be any Hermitian complex matrix. Then, the only constraint for the distribution of these matrices is to be invariant under a similarity transformation of unitary matrices. In other words, the probability of obtaining a certain Hamiltonian should not depend on the basis we choose. This condition is satisfied by the following ensemble.

Definition 3. *A random Hermitian $N \times N$ matrix H is said to belong to the Gaussian unitary ensemble (GUE) if the (real) diagonal elements h_{jj} are independently chosen with p.d.f.*

$$\frac{1}{\sqrt{\pi}} e^{-h_{jj}^2},$$

while the upper triangular off-diagonal elements $h_{jk} = a_{jk} + ib_{jk}$ are independently chosen with p.d.f.

$$\frac{2}{\pi} e^{-2(a_{jk}^2 + b_{jk}^2)} = \frac{2}{\pi} e^{-2|h_{jk}|^2}.$$

Equivalently, the diagonal entries have distribution $N[0, 1/\sqrt{2}]$, while the upper triangular elements have distribution $N[0, 1/2] + iN[0, 1/2]$.

Indeed, $H = (X + X^\dagger)/2$ where X is a complex random matrix with entries independently chosen from $N[0, 1/\sqrt{2}] + iN[0, 1/\sqrt{2}]$.

It follows directly from the definition that the joint p.d.f. of all the independent elements is

$$P(H) = \prod_{j=1}^{N} \frac{1}{\sqrt{\pi}} e^{-h_{jj}^2} \prod_{i \leqslant j < k \leqslant N} \frac{2}{\pi} e^{-2|h_{jk}|^2} = A_n e^{-\operatorname{tr}(H^2)}.$$

Therefore, as the trace of a matrix is invariant under similarity transformation of unitary matrices, we can conclude that the joint probability of obtaining a specific Hamiltonian does not depend on the basis we choose to represent it.

6 Joint probability density function for eigenvalues

We know that given a random matrix its eigenvalues represent the energy levels of the system. It will therefore be interesting to ask about the distribution of the eigenvalues and try to relate it to some physical properties.

First of all, using the joint p.d.f. of the elements of a random Gaussian matrix, we can compute the joint probability distribution function of its eigenvalues. Let us first consider a matrix H belonging to the GOE and let $\lambda_1, \ldots, \lambda_N$ denote its eigenvalues. We can determine H using these eigenvalues together with other mutually independent variables, which we shall call p_μ. Since H is a real symmetric matrix of order N, it is described by $\frac{1}{2}N(N+1)$ independent real parameters (it suffices to fix H_{jk} with $k \leqslant j$). Hence, the number of parameters p_μ needed is

$$l = \frac{1}{2}N(N+1) - N = \frac{1}{2}N(N-1).$$

We know that the joint p.d.f. of the matrix H is given by (4), i.e.,

$$P(H) = P(H_{11}, H_{12}, \ldots, H_{NN}) = A_N e^{-\frac{1}{2}\operatorname{tr} H^2} = A_N e^{-\frac{1}{2}\sum_{j=1}^{N} \lambda_j^2}.$$

Therefore, if we change variables by expressing H_{jk} in terms of $\lambda_1, \dots, \lambda_N$ and $p_1, \dots, p_l$, we get that the joint probability density function in terms of these new variables is given by

$$P(\lambda_1, \dots, \lambda_N; p_1, \dots, p_l) = A_N e^{-\frac{1}{2}\sum_j \lambda_j^2} |J(\boldsymbol{\lambda}, \mathbf{p})|, \tag{7}$$

where $|J|$ is the Jacobian of this change of variables:

$$|J(\boldsymbol{\lambda}, \mathbf{p})| = \left| \frac{\partial(H_{11}, \dots, H_{NN})}{\partial(\lambda_1, \dots, \lambda_N, p_1, \dots, p_l)} \right|.$$

We can obtain the j.p.d.f. of the eigenvalues as the marginal of the previous distribution. In other words, we just need to integrate (7) over the parameters $p_1, \dots, p_l$.

In order to perform this integration, we first need to compute the Jacobian corresponding to the change of variables. This task becomes much easier if we carefully define the parameters p_μ. In order to do so, first recall that any real symmetric matrix H can be diagonalized by a real orthogonal matrix. In other words, we can find a matrix $U \in O(N)$ satisfying

$$H = U\Lambda U^{-1} = U\Lambda U^T,$$

where Λ is the diagonal matrix with elements $\lambda_1, \dots, \lambda_N$ (we can assume that they are arranged following the order $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_N$). If we assume that the eigenvalues of H are distinct[5] we can choose Λ and U uniquely. Namely, we know that the columns of U are the normalized eigenvectors of H. In order to fix which of the two possible normalizations we pick for each of them, we can ask, for example, for the first nonvanishing coordinate to be positive.

Once we know that we can determine U from H, recall that $O(N)$ is a Lie group of dimension $\frac{1}{2}N(N-1)$. Hence, we can describe any matrix $U \in O(N)$ by $\frac{1}{2}N(N-1)$ coordinates, which will be our parameters p_μ. In other words, in terms of these new parameters we have that

$$H(\boldsymbol{\lambda}, \mathbf{p}) = U(\mathbf{p})\Lambda(\boldsymbol{\lambda})U(\mathbf{p})^T. \tag{8}$$

If we differentiate the equation $U^T U = \mathbb{1}$, we get

$$\frac{\partial U^T}{\partial p_\mu} U + U^T \frac{\partial U}{\partial p_\mu} = 0,$$

which means that the matrix

$$S^\mu = U^T \frac{\partial U}{\partial p_\mu}$$

is antisymmetric for each $\mu = 1, \dots, l$.

Differentiating (8) with respect to p_μ, we get:

$$\frac{\partial H}{\partial p_\mu} = \frac{\partial U}{\partial p_\mu}\Lambda U^T + U\Lambda \frac{\partial U^T}{\partial p_\mu}.$$

Multiplying by U^T on the left and by U on the right, we get

$$U^T \frac{\partial H}{\partial p_\mu} U = S^\mu \Lambda - \Lambda S^\mu.$$

[5]The subset where at least one of the eigenvalues is degenerate has measure zero, and hence it is not relevant for our discussion.

In terms of its component, this equation reads

$$\sum_{j,k} \frac{\partial H_{jk}}{\partial p_\mu} U_{j\alpha} U_{k\beta} = S^\mu_{\alpha\beta}(\lambda_\beta - \lambda_\alpha). \tag{9}$$

We can proceed in a similar way, this time differentiating with respect to λ_γ, and get

$$\sum_{j,k} \frac{\partial H_{jk}}{\partial \lambda_\gamma} U_{j\alpha} U_{k\beta} = \frac{\partial \Lambda_{\alpha\beta}}{\partial \lambda_\gamma} = \delta_{\alpha\gamma}\delta_{\beta\gamma}. \tag{10}$$

As we said, we can describe H by the N parameters H_{jj} with $j = 1, \ldots, N$ and the $\frac{1}{2}N(N-1)$ parameters H_{jk} with $1 \leqslant j < k \leqslant N$. This means that the Jacobian matrix can be partitioned into the following blocks

$$J(\boldsymbol{\lambda}, \mathbf{p}) = \begin{pmatrix} \dfrac{\partial H_{jj}}{\partial \lambda_\gamma} & \dfrac{\partial H_{jk}}{\partial \lambda_\gamma} \\ \\ \dfrac{\partial H_{jj}}{\partial p_\mu} & \dfrac{\partial H_{jk}}{\partial p_\mu} \end{pmatrix}.$$

Now, let us multiply this matrix by

$$V(\mathbf{p}) = \begin{pmatrix} U_{j\alpha} U_{j\beta} \\ U_{j\alpha} U_{k\beta} \end{pmatrix}.$$

Using (9) and (10), this gives

$$J \cdot V = \begin{pmatrix} \delta_{\alpha\gamma}\delta_{\beta\gamma} \\ S^\mu_{\alpha\beta}(\lambda_\beta - \lambda_\alpha) \end{pmatrix}.$$

Taking the determinant, we get

$$|J(\boldsymbol{\lambda}, \mathbf{p})| \cdot |V(\mathbf{p})| = \prod_{\alpha<\beta} (\lambda_\beta - \lambda_\alpha) \begin{vmatrix} \delta_{\alpha\gamma}\delta_{\beta\gamma} \\ S^\mu_{\alpha\beta} \end{vmatrix},$$

and hence

$$|J(\boldsymbol{\lambda}, \mathbf{p})| = \prod_{\alpha<\beta} (\lambda_\beta - \lambda_\alpha) f(\mathbf{p}),$$

with $f(\mathbf{p})$ a function independent of λ_j.

By inserting this result into (8) and integrating over $\mathbf{p}$, we get that the j.p.d.f. for the eigenvalues of matrices from the GOE is

$$P_{N1}(\lambda_1, \ldots, \lambda_N) = C_{N1} e^{-\frac{1}{2}\sum_j \lambda_j^2} \prod_{j<k} |\lambda_j - \lambda_k|,$$

where C_{N1} is a constant.

Using this same strategy one can prove the following general result:

Theorem 1. *The joint probability density function for the eigenvalues of matrices from a Gaussian ensemble is given by*

$$P_{N\beta}(\lambda_1, \ldots, \lambda_N) = C_{N\beta} e^{-\frac{1}{2}\beta\sum_{j=1}^N \lambda_j^2} \prod_{j<k} |\lambda_j - \lambda_k|^\beta,$$

where $\beta = 1$ if the ensemble is orthogonal, $\beta = 4$ if it is symplectic, and $\beta = 2$ if it is unitary, while $C_{N\beta}$ is a normalization constant.

The proof of this general result can be found in [4].

7 Wigner's semicircle law

In the previous section, we computed the joint probability density function for the eigenvalues, i.e., how likely it is to obtain a certain spectrum $\{\lambda_1, \ldots, \lambda_n\}$ in a random Gaussian matrix. From this result we can already observe some qualitative behaviors, such as *repulsion* through the factor $\prod_{j<k} |\lambda_j - \lambda_k|^\beta$, which increases the further apart the eigenvalues are. However, due to the Gaussian decay, given by $\exp\left(-\frac{1}{2}\beta\lambda_j^2\right)$, these eigenvalues also tend to cluster around zero. One might then ask what is the overall shape of the spectrum as these two opposing tendencies interact with each other. In other words, we are interested in the probability distribution of a single eigenvalue from a Gaussian matrix.

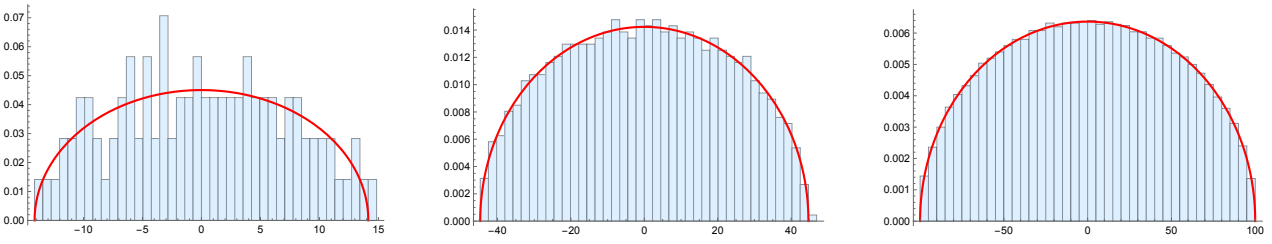
The distribution of the eigenvalues can be indeed computed exactly (as shown in [4]), however, it is more interesting for us to analyze what happens in the limit $N \to \infty$. In addition, remember that the main motivation of random matrix theory in physics was studying highly complex systems with a large number of particles and degrees of freedom (for example, nuclear decays in heavy nuclei). Thus, taking this limit is physically well-justified.

In this asymptotic regime, one obtains the following result:

Theorem 2 (Wigner's semicircle law)**.** *Let H be a Gaussian matrix of order N as previously described above (a real, quaternionic or complex matrix depending on whether H belongs to the GOE, GSE or GUE, respectively). Then, the probability distribution function of the eigenvalues of H converges when $N \to \infty$ to the semicircle distribution:*

$$\rho_N(x) = \frac{\sqrt{2N}}{\pi}\sqrt{1 - \frac{x^2}{2N}}, \quad \text{with } |x| \leqslant \sqrt{2N}.$$

A proof of this result can be found in [3]. This theorem shows us that in many-particle systems, the repulsion phenomenon between energy levels and the tendency to have an energy as close to 0 as possible are balanced, resulting in a distribution centered at 0 that has the shape of a semicircle and whose radius grows as $\sqrt{N}$.



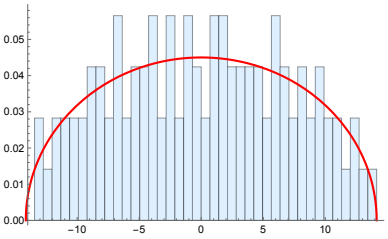
GOE with $N = 100$ GOE with $N = 1000$ GOE with $N = 5000$

Figure 1: Histograms with the empirical eigenvalues distribution of GOE matrices for increasing matrix sizes. As N increases, the distribution approaches the semicircle law (in red).

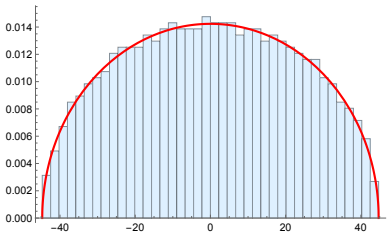
7.1 Empirical eigenvalues distribution

Once we have introduced the concept of Wigner's Semicircle Law, we can test it and check how accurate this approximation is for different values of N. In order to do so, we have created a *Mathematica* notebook which generates random matrices from the GOE, GSE and GUE, computes their eigenvalues and then plots the results as histograms together with the expected probability density function coming from Wigner's semicircle law. The results of these computations are displayed in Figures 1, 2 and 3 for the GOE, GUE and GSE, respectively.

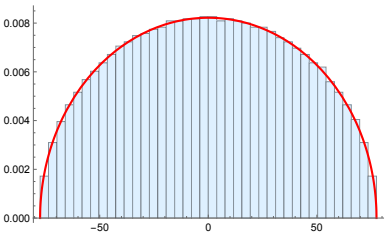
We can see that for the three ensembles the distribution of the eigenvalues for an $N = 100$ matrix vaguely looks like a semicircle, while in the case of $N = 1000$, and especially for $N = 3000$ or 5000, the empirical eigenvalue distribution and the semicircle distribution are almost identical.



GSE with $N = 100$

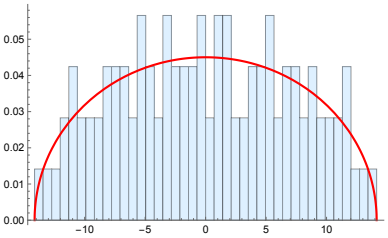


GSE with $N = 1000$

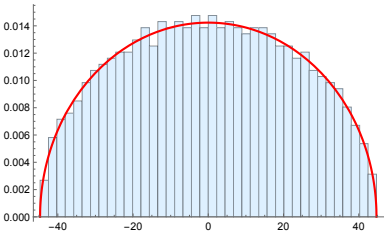


GSE with $N = 3000$

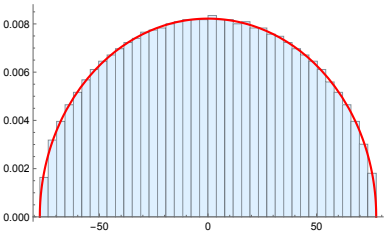
Figure 2: Histograms with the empirical eigenvalues distribution of GSE matrices for increasing matrix sizes. As N increases, the distribution approaches the semicircle law (in red).



GUE with $N = 100$



GUE with $N = 1000$



GUE with $N = 3000$

Figure 3: Histograms with the empirical eigenvalues distribution of GUE matrices for increasing matrix sizes. As N increases, the distribution approaches the semicircle law (in red).

8 Unfolding and consecutive levels spacings

Another property of the spectrum of the Hamiltonian that we can analyze is the spacing (separation) between two consecutive energy levels, and see how this value changes depending on the random matrix distribution we are working with. However, in order to properly analyze the spacing between consecutive levels in a random matrix and consistently compare it with other matrices, we first need to *unfold* its spectrum. This unfolding process will let us normalize the spectrum. The new unfolded spectrum will follow a level density distribution which is approximately uniform in $[0, 1]$. It will be precisely the small fluctuations from that uniform distribution what we will analyze.

8.1 Unfolding the spectrum

Let us describe how to unfold an spectrum. We start with the energy levels of the matrix H, $E_1, \ldots, E_n$, which satisfy $E_1 < \cdots < E_n$. Then, the cumulative distribution function (CDF) of these levels is given by a staircase function:

$$F(E) = \sum_{E_i \leqslant E} \frac{d_i}{D}, \tag{11}$$

where d_i is the degeneracy of level E_i and $D = \sum_i d_i$ the dimension of the Hilbert space of the system.

We want to decompose F into

$$F(E) = \xi(E) + \tilde{F}(E),$$

where ξ is smooth and monotone increasing with $0 \leqslant \xi(E) \leqslant 1$, and $|\tilde{F}(E)| \ll 1$. The idea is that ξ smoothly approximates the CDF while $\tilde{F}$ measures the small fluctuations around ξ. We should choose ξ so it is smooth enough not to include the fluctuations of our data, while fitting well enough the original CDF of the raw spectrum $\{E_i\}$.

Once we have chosen the function ξ, we can define the unfolded spectrum as

$$\varepsilon_i = \xi(E_i), \quad 1 \leqslant i \leqslant n.$$

Since ξ is monotone increasing, they will satisfy $\varepsilon_1 < \cdots < \varepsilon_n$, and each of the unfolded energy levels will have the same degeneracy as the corresponding raw level. In addition, due to this monotone increasing property as well, we have

$$\varepsilon_i \leqslant \varepsilon \iff E_i \leqslant \xi^{-1}(\varepsilon),$$

Thus, the CDF of the unfolded levels is given by

$$\hat{F}(\varepsilon) = \sum_{\varepsilon_i \leqslant \varepsilon} \frac{d_i}{D} = \sum_{E_i \leqslant \xi^{-1}(\varepsilon)} \frac{d_i}{D} = F(\xi^{-1}(\varepsilon)) = \xi(\xi^{-1}(\varepsilon)) + \tilde{F}(\xi^{-1}(\varepsilon)) = \varepsilon + \tilde{F}(\xi^{-1}(\varepsilon)).$$

Therefore,

$$\hat{F}(\varepsilon) = \varepsilon + \tilde{\hat{F}}(\varepsilon),$$

with $\tilde{\hat{F}}(\varepsilon) = \tilde{F}(\xi^{-1}(\varepsilon))$, and hence $|\tilde{\hat{F}}| \ll 1$. This implies

$$\varepsilon_1 \gtrsim 0, \quad \varepsilon_n \lesssim 1,$$

which means that $\varepsilon_i \in [0, 1]$ for all i.

Notice that the smooth part of $\hat{F}$ is simply the identity function $\varepsilon \mapsto \varepsilon$, independently of the initial distribution of E_i. Indeed, this smooth part of the CDF of the unfolded spectrum corresponds to a uniform distribution in $[0, 1]$. Therefore, the unfolded spectrum $\varepsilon_1, \ldots, \varepsilon_n$ is always approximately distributed following a uniform distribution in $[0, 1]$. The fluctuations around this uniform distribution are carried inside of $\tilde{\hat{F}}$, which does depend on the initial distribution of the raw spectrum.

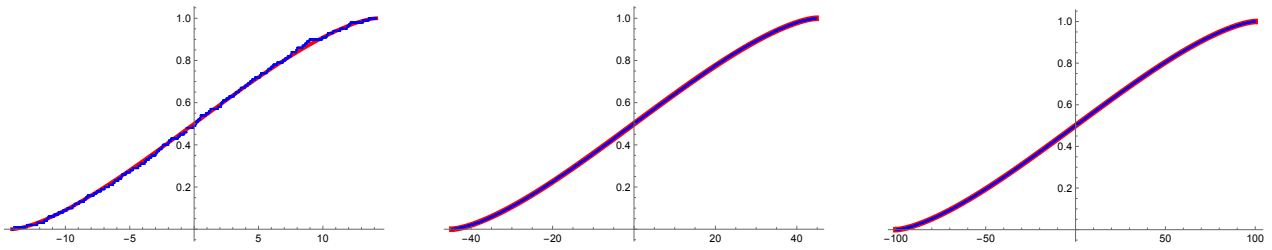
8.2 Cumulative distribution functions of the Gaussian ensembles

In the case of the unfolding of a Gaussian matrix spectrum, we could try to approximate $F(E)$ by any smooth and monotone increasing function that takes values in $[0, 1]$ (for example, we could fit F by a polynomial). However, we know that the distribution of the eigenvalues is approximately given by Wigner's semicircle law. Therefore, using this extra information, it is better to use as ξ the function defined by integrating the semicircle density:

$$\xi_N(x) := \int_{-\sqrt{2N}}^{x} \rho_N(t)\, dt = \int_{-\sqrt{2N}}^{x} \frac{\sqrt{2N}}{\pi} \sqrt{1 - \frac{t^2}{2N}}\, dt, \quad \text{for } |x| \leqslant \sqrt{2N}.$$

This integral can be computed explicitly taking $t = \sqrt{2N} \sin\theta$. As the final result we obtain:

$$\xi_N(x) = \frac{1}{2} + \frac{1}{\pi} \left[\frac{1}{2} \arcsin\left(\frac{x}{\sqrt{2N}} \right) + \frac{1}{2} \cdot \frac{x}{\sqrt{2N}} \cdot \sqrt{1 - \frac{x^2}{2N}} \right], \quad |x| \leqslant \sqrt{2N}.$$

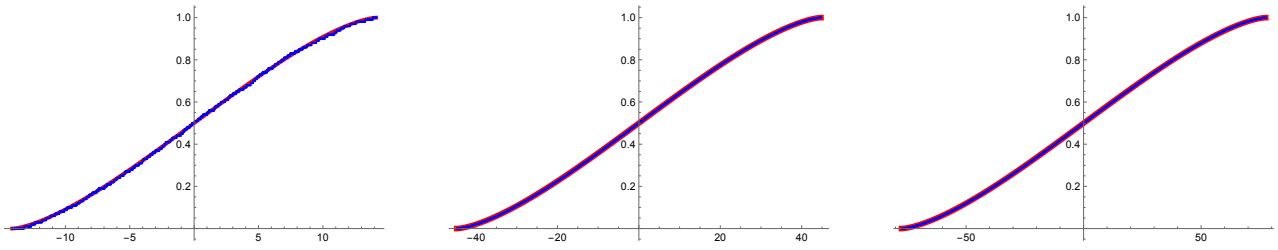


GOE with $N = 100$ GOE with $N = 1000$ GOE with $N = 5000$

Figure 4: Empirical cumulative distribution function of eigenvalues (blue) for GOE matrices of increasing size, compared to the theoretical CDF (red) from Wigner's semicircle law.

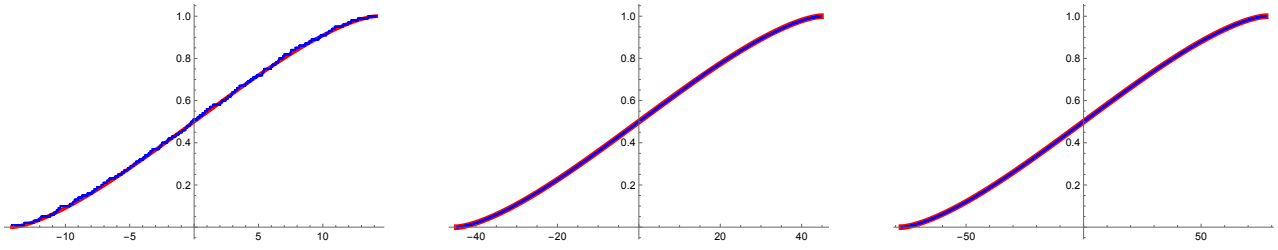
To verify this prediction, we computed the empirical CDFs using again *Mathematica*. For each ensemble (GOE, GUE, and GSE), we generated random matrices of different sizes, extracted their eigenvalues and sorted them to construct the empirical distribution function using (11). The resulting graphs were then compared to the theoretical CDF, $\xi_N(x)$, obtained from the semicircle law, and can be seen in Figures 4, 5 and 6 for the orthogonal, symplectic and unitary ensembles, respectively.

It is interesting to notice how in the graphs corresponding to $N = 100$ one can easily observe the steps in the empirical cumulative distributions of the eigenvalues, which are well approximated by Wigner's semicircle. In the case of $N = 1000, 3000$ and 5000 this approximation is even better, as the empirical cumulative distribution of the eigenvalues resembles a smooth curve which looks almost identical to the one from the semicircle law.



GSE with $N = 100$ GSE with $N = 1000$ GSE with $N = 3000$

Figure 5: Empirical cumulative distribution function of eigenvalues (blue) for GSE matrices of increasing size, compared to the theoretical CDF (red) from Wigner's semicircle law.



GUE with $N = 100$ GUE with $N = 1000$ GUE with $N = 3000$

Figure 6: Empirical cumulative distribution function of eigenvalues (blue) for GUE matrices of increasing size, compared to the theoretical CDF (red) from Wigner's semicircle law.

8.3 Nearest-neighbors spacing distribution

Once we have described the unfolding process, we can analyze and compute the spacing between consecutive levels of the unfolded spectrum. Instead of just computing the difference between consecutive levels, we define the spacing as

$$s_i = (n-1)\frac{\varepsilon_{i+1} - \varepsilon_i}{\varepsilon_n - \varepsilon_1}.$$

This definition of *normalized spacing* satisfies

$$\langle s_i \rangle = \frac{1}{n-1}\sum_{i=1}^{n-1} s_i = 1,$$

i.e., the average of the normalized spacings is 1.

Once we have defined the normalized spacing, we want to find a continuous probability density function, $p(s)$ with $s \in [0, \infty)$ (notice that $s_i > 0$ always), which approximates the distribution of the discrete variable s_i. Moreover, as this discrete variable s_i has mean 1, this continuous density function must satisfy

$$\langle s \rangle = \int_0^\infty s \cdot p(s)\, ds = 1.$$

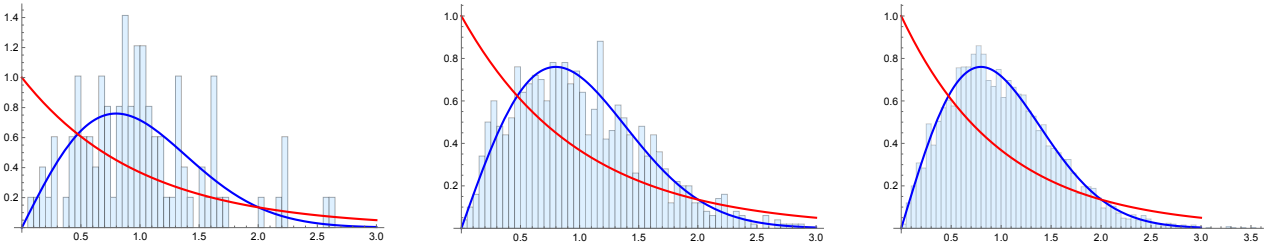
If these energy levels were distributed independently of one another, we could expect that they follow a Poisson distribution $p(s) = ae^{-as}$, where the condition $\langle s \rangle = 1$ implies $a = 1$.

However, as we have discussed earlier, this is not the case for Gaussian matrices, where adjacent levels tend to avoid each other. In these cases, the spacing distribution is given by

$$\rho(s) = \begin{cases} \frac{\pi}{2} s \exp\left(-\frac{\pi}{4}s^2\right) & \text{(GOE)}, \\ \frac{32}{\pi^2} s^2 \exp\left(-\frac{4}{\pi}s^2\right) & \text{(GUE)}, \\ \frac{2^{18}}{3^6\pi^3} s^4 \exp\left(-\frac{64}{9\pi}s^2\right) & \text{(GSE)}, \end{cases}$$

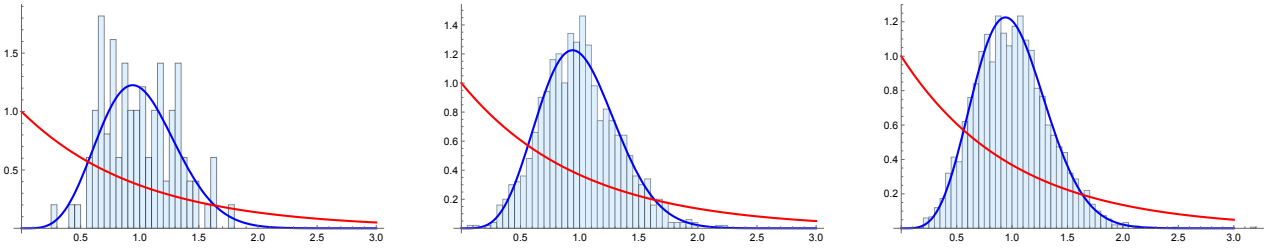
which is known as *Wigner's surmise*.

We can check these distributions using our *Mathematica* notebook again. In this case, after computing the sorted spectrum of our random matrix, we unfolded it using Wigner's semicircle law as described in the previous section, and then computed the normalized spacings between consecutive unfolded eigenvalues. The results we obtained were plotted together with their predicted distributions and the results are displayed in Figures 7, 8 and 9 for the orthogonal, symplectic and unitary ensembles, respectively.



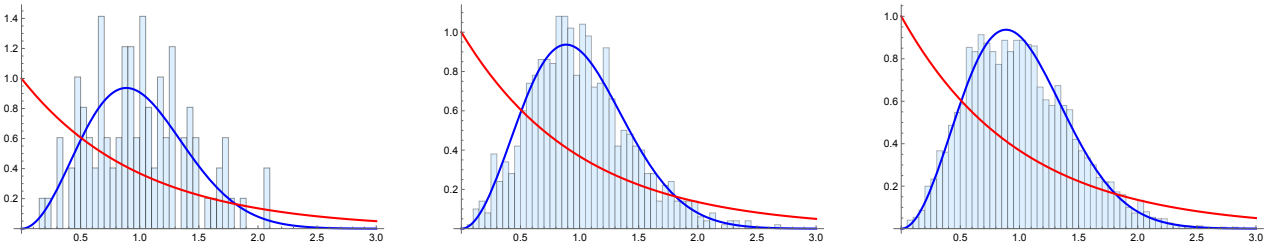
GOE with $N = 100$ GOE with $N = 1000$ GOE with $N = 5000$

Figure 7: Empirical spacings of the unfolded spectrum of GOE matrices of increasing size, compared to Poisson distribution (in red) and Wigner's surmise (in blue).



GSE with $N = 100$ GSE with $N = 1000$ GSE with $N = 3000$

Figure 8: Empirical spacings of the unfolded spectrum of GSE matrices of increasing size, compared to Poisson distribution (in red) and Wigner's surmise (in blue).



GUE with $N = 100$ GUE with $N = 1000$ GUE with $N = 3000$

Figure 9: Empirical spacings of the unfolded spectrum of GUE matrices of increasing size, compared to Poisson distribution (in red) and Wigner's surmise (in blue).

Analyzing these graphs we can clearly see the repulsion behavior and how the distribution of the spacings is very well approximated by the Wigner's surmise of the corresponding distribution (especially for bigger N).

8.4 Quantum chaos. Berry-Tabor and Bohigas-Giannoni-Schmit conjectures

The fact that the energy levels of Gaussian matrices repel each other is no coincidence. This is because these models represent quantum systems whose classical analogues are *chaotic*. On the other hand, random matrices which represent systems that are classically integrable do not present this behavior. Their eigenvalues are independently distributed, and hence the spacings follow a Poisson distribution.

In order to understand the reasons behind this, we need to recall that for integrable classical systems we can find some invariant tori (corresponding to the level sets of the integrals of motion), which are invariant under the Hamiltonian flow, i.e., trajectories with different values of the integral of motions live in different tori. The quantum analogue of this is a Hamiltonian which can be diagonalized by eigenstates labelled as $|\mathbf{k}\rangle$, where $\mathbf{k} = (k_1, \dots, k_n)$ is an eigenstate of each of the integrals of motion I_j with eigenvalue k_j. Therefore, if we introduce a random perturbation H_{rand} that respects the integrals of motion, we get

$$\langle \mathbf{k}|H_{\text{rand}}|\mathbf{k}'\rangle = 0, \text{ for } \mathbf{k} \neq \mathbf{k}'.$$

This means that the randomized Hamiltonian is block-diagonal, and eigenstates from different levels do not interact with each other due to this randomness. In other words, the distribution of their energies levels are not affected by each other, they feel no repulsion, and hence the spacing between consecutive levels follows a Poisson distribution.

On the other hand, if we are dealing with a chaotic classical system, we know that the trajectories will be dense in the energy shell, being arbitrarily close to any other trajectory with the same energy.

This behavior is the complete opposite to the one present in integrable systems. When transitioning to the quantum context, this means that if we introduce a randomized Hamiltonian, eigenstates will interact with each other through this perturbation, which will in general create some repulsion between the new energy levels. That is why quantum systems whose classical analogues are chaotic, such as those represented by the Gaussian ensembles, present some repulsion between their energy levels, leading to spacing distributions different from Poisson distribution.

These ideas and intuitions led Berry and Tabor formulate in [1] the following conjecture

Conjecture (Berry and Tabor)**.** *If a quantum system has a classically integrable Hamiltonian, then its quantum energy levels (after unfolding) are independently distributed. In particular, the level spacings follow a Poisson distribution.*

The chaotic analogue of this conjecture was formulated by Bohigas, Giannoni and Schmit in [2]:

Conjecture (Bohigas-Giannoni-Schmit)**.** *For a quantum Hamiltonian whose classical counterpart is fully chaotic, the fluctuations of its unfolded energy spectrum coincide with those of a Gaussian ensemble chosen according to the system's discrete symmetries (GOE, GUE, or GSE). In particular, the level spacings follow Wigner's surmise.*

These conjectures are widely believed to be true and they have been verified in many solvable and chaotic models. However, they have not been fully proved yet and it is expected that they will be difficult to rigorously prove due to the subtle semiclassical connections between classical integrability and chaos, and their quantum analogues.

References

[1] M. V. Berry and M. Tabor. Level clustering in the regular spectrum. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, 356(1686):375–394, 1977.

[2] O. Bohigas, M. J. Giannoni, and C. Schmit. Characterization of chaotic quantum spectra and universality of level fluctuation laws. *Phys. Rev. Lett.*, 52:1–4, Jan 1984.

[3] P.J. Forrester. *Log-Gases and Random Matrices (LMS-34)*. Princeton University Press, 2010.

[4] M. L. Mehta, editor. *Random Matrices*. Academic Press, San Diego, revised and enlarged second edition edition, 1991.

[5] J. J. Sakurai and Jim Napolitano. *Modern Quantum Mechanics*. Cambridge University Press, 3 edition, 2020.

[6] H.J. Stöckmann. *Quantum Chaos: An Introduction*. Cambridge University Press, 1999.

Mathematica notebook and appendix

The *Mathematica* notebook used for this project, as well as the appendix with the proof of Proposition 4, can be found in this repository.