Lecture Notes on Quantum Chaos

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Contents

1 Literature

- [1] Martin C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer, 1990)

  - Classical monography about chaos in physics.
  - Profound physical and mathematical discussion.
  - Sometimes nonstandard notation.

- [2] Fritz Haake, *Quantum Signatures of Chaos* (Springer, 2010)

  - Up-to-date topics, including chaotic dissipative systems and supersymmetric approaches.

- [3] Oriol Bohigas, *Random Matrix Theories and Chaotic Dynamics*, Les Houches LII, ed. M.-J. Gianonni, A. Voros, J. Zinn-Justin, 1989

  - Brief and concise notes on the basics of quantum chaos.

- [4] Madan L. Mehta, *Random Matrices* (Elsevier 2004).

  - Everything you always wanted to know about random matrices (and quantum chaos is from a big part about random matrices).
  - ... and probably even didn't want to know.
  - If you love formulae, you'll be happy reading this book.

- [5] Sandro Wimberger, *Nonlinear Dynamics and Quantum Chaos. An Introduction* (Springer 2023).

  - A modern recent monography.

2 Introduction

2.1 Quantum mechanics is linear

Classical chaos is tightly connected with the nonlinearity of classical equations of motion. On the contrary, quantum mechanics is linear, quantum evolution unitary $\longrightarrow$ no sensitive dependence on "initial conditions", which can be easily proved.

- *Linearity:* Suppose we have a normalized state $|\psi(0)\rangle$ at time $t = 0$ and we add an arbitrary orthogonal perturbation, where ϵ measures the strength of the perturbation,

$$|\psi(0)\rangle \xrightarrow{\text{perturbation}} |\psi(0)\rangle + \epsilon |\psi_\perp(0)\rangle \xrightarrow{\text{normalization}} |\xi(0)\rangle \equiv \sqrt{1 - \epsilon^2} |\psi(0)\rangle + \epsilon |\psi_\perp(0)\rangle, \tag{1}$$

$$\langle\psi(0)|\psi(0)\rangle = \langle\psi_\perp(0)|\psi_\perp(0)\rangle = \langle\xi(0)|\xi(0)\rangle = 1,$$
$$\langle\psi(0)|\psi_\perp(0)\rangle = 0, \tag{2}$$

- *Unitarity:* Time evolution of a ket is (providing the Hamiltonian of the system doesn't depend on time)

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}t} |\psi(0)\rangle \tag{3}$$

and the unitarity guarantees that the orthogonality relations (2) remain valid at any time t:

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi_\perp(t)|\psi_\perp(t)\rangle = \langle\xi(t)|\xi(t)\rangle = 1,$$
$$\langle\psi(t)|\psi_\perp(t)\rangle = 0. \tag{4}$$

A deviation of perturbed and unperturbed vector at time t is hence

$$|\delta(t)\rangle \equiv |\xi(t)\rangle - |\psi(t)\rangle \tag{5}$$

and its norm

$$|\delta(t)| = \sqrt{\langle\delta(t)|\delta(t)\rangle} = \sqrt{\left(\sqrt{1-\epsilon^2}-1\right)^2 \langle\psi(t)|\psi(t)\rangle + \epsilon^2 \langle\psi_\perp(t)|\psi_\perp(t)\rangle} \approx \epsilon\sqrt{1+\frac{\epsilon^2}{4}} \tag{6}$$

doesn't depend on time. Therefore, **a deviation of the state vector doesn't grow in time and can't be used to measure the chaoticity of the state (can't be used to define an analogue of the "Lyapunov exponent").**

2.2   ... So what is chaos in quantum physics?

What can one employ to study and analyze chaos in quantum mechanics? There are two principal approaches how to study quantum chaos:

1. **Semiclassical quantization**

   - Quantize the motion on classical tori via Einstein-Brillouin-Keller quantization or via more advanced techniques (path integral, supersymmetric techniques).

   - Quite a hard theory, but resulting in several highly important theoretical predictions (Gutzwiller formula etc.).

   - Can be used successfully in quantum billiards (systems basically equivalent with classical discrete maps; they are in fact just infinite potential wells with different shapes) and in other simple particular models, but with limited applicability to even slightly more complex quantum systems.

   - Impossible to take use of this method in purely quantum systems like spin systems (Ising model, Heisenberg model, etc.).

   We will touch only a little from this approach.

2. **Spectral correlations**

   - The most fundamental object in quantum mechanics is the energy spectrum.

   - Study of specific statistical properties of quantum levels, especially the correlations between them. It turns out that some simple properties of the spectrum differ significantly if the system is classically chaotic or integrable.

   - The most important mathematical tool here is the **Random matrix theory** [4].

   - Spectral correlations are sometimes even used to define chaos in quantum mechanics. However, the connection between this definition and the ones based on semiclassical approaches is often loose; therefore, Michael Berry proposes to use the term Quantum Chaology instead of Quantum Chaos [6].

   - The mostly cited paper conjecturing a connection between classical chaos and correlations in quantum spectra is the one by Bohigas, Giannoni and Schmit [7].

   This will be the most important part of this introductory course.

3   Integrable systems

3.1   Quantum integrals of motion

In classical physics, integrals of motions $I_j(\boldsymbol{p}, \boldsymbol{q})$ are a set of functions that are conserved throughout the system's time evolution. They are always connected with an additional symmetry of the system. Their Poisson bracket with the Hamiltonian function H is zero, and one usually restricts oneself to the integrals of motion *in involution*, whose mutual Poisson bracket vanishes,

$$\{I_j, H\} = 0, \tag{7a}$$

$$\{I_j, I_k\} = 0. \tag{7b}$$

Suppose we have a quantum system with f degrees of freedom described by a time-independent Hamiltonian $\hat{\mathsf{H}}$. Operators $\hat{\mathsf{I}}_1, \ldots, \hat{\mathsf{I}}_d,\ d \leq f$ that satisfy

$$\left[\hat{\mathsf{I}}_j, \hat{\mathsf{H}}\right] = 0, \tag{8a}$$

$$\left[\hat{\mathsf{I}}_j, \hat{\mathsf{I}}_k\right] = 0, \tag{8b}$$

are the so called *quantum integrals of motion.*[1] Their existence implies that there exists an orthonormal basis $|n_1, \ldots, n_d\rangle$ such that

$$\hat{\mathsf{I}}_j |n_1, \ldots, n_d\rangle = n_j |n_1, \ldots, n_d\rangle, \tag{9}$$

and the Hamiltonian has a block-diagonal structure because

$$\begin{aligned}
0 &= \left\langle n_1, \ldots, n_k, \ldots, n_d \left| \left[\hat{\mathsf{H}}, \hat{\mathsf{I}}_k\right] \right| n_1, \ldots, n'_k, \ldots, n_d \right\rangle \\
&= \left\langle n_1, \ldots, n_k, \ldots, n_d \left| \left(\hat{\mathsf{H}}\hat{\mathsf{I}}_k - \hat{\mathsf{I}}_k\hat{\mathsf{H}}\right) \right| n_1, \ldots, n'_k, \ldots, n_d \right\rangle \\
&= (n_k - n'_k) \left\langle n_1, \ldots, n_k, \ldots, n_d \left| \hat{\mathsf{H}} \right| n_1, \ldots, n'_k, \ldots, n_d \right\rangle,
\end{aligned} \tag{10}$$

hence

$$\left\langle n_1, \ldots, n_d \left| \hat{\mathsf{H}} \right| n'_1, \ldots, n'_d \right\rangle \propto \delta_{n_1 n'_1} \cdots \delta_{n_d n'_d} \tag{11}$$

Eigenstates that correspond to different values of n_k **are not correlated** (the matrix element quantifying the "interaction" between them is identically zero).

3.2   Quantum integrable systems

Again, in analogy with classical physics, when $d = f$ independent quantum integrals of motion exist, the system is called *integrable*. The result of the previous section implies that in such a system, each state can be uniquely labelled with a set of f quantum numbers that are eigenvalues of the f integrals of motion. The typical eigenstates of these operators form a basis for the Hamiltonian, in which the Hamiltonian has a diagonal form. Therefore, **in quantum integrable systems, all the eigenstates are uncorrelated.**

3.3   Einstein-Brillouin-Keller (EBK) quantization

If a classical system is integrable, its Hamiltonian can be expressed in the *action-angle coordinates* $(J_j, \phi_j), j = 1, \ldots, f$ and is independent of the angles ϕ_j, $H = H(\boldsymbol{J})$. This implies that the classical

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[1]A common example of such integrals of motion is the angular momentum and parity, J^π.

motion is confined to f-dimensional tori in the phase space, and the classical dynamics is given by the Hamilton equations of motion

$$\frac{\mathrm{d}J_j}{\mathrm{d}t} = \frac{\partial H}{\partial \phi_j} = 0, \tag{12a}$$

$$\frac{\mathrm{d}\phi_j}{\mathrm{d}t} = \frac{\partial H}{\partial J_j} \equiv \omega_j, \tag{12b}$$

with a simple solution

$$\phi_j(t) = \omega_j t + \phi_j(0), \tag{13a}$$

$$J_j(t) = J_j(0) = \text{const.} \tag{13b}$$

EBK then states that each of the action coordinates can be quantized separately,

$$J_j = \hbar n_j + a_j, \tag{14}$$

where $n_j \in \mathbb{N}$ is a quantum number and a_j a real constant. This result supports the conclusion of the previous section.

3.4 Nearest neighbour spacing distribution

This is one of the most used spectral statistics. It measures the probability of finding two neighbouring levels at a distance s from each other.

Let us now derive the Nearest Neighbour Spacing Distribution (NNSD) of a generic quantum integrable system. Suppose there is a quantum level at $E = E_0$, and $p(s)$ is the probability density that we find the next level at a distance s from E_0. Without the loss of generality, we can set $E_0 = 0$. Now we can schematically write

$$p(s)\mathrm{d}s = \underbrace{\text{Probability}\left(\frac{\text{a level in }\mathrm{d}I}{\text{no level in }I}\right)}_{\mu(s)\mathrm{d}s} \underbrace{\text{Probability (no level in }I)}_{1 - \int_0^s p(s')\mathrm{d}s' = \int_s^\infty p(s')\mathrm{d}s'}, \tag{15}$$

where $I = (0, s)$ is an interval spanning from $E = E_0 = 0$ to $E = E_0 + s$ and $\mathrm{d}I = (s, s + \mathrm{d}s)$. Number $p(s)\mathrm{d}s$ is the probability that we find a level neighbouring to E_0 at interval $\mathrm{d}s$. We come to an integral equation[2] for $p(s)$,

$$p(s) = \mu(s) \int_s^\infty p(s')\mathrm{d}s'. \tag{16}$$

Solution: Let us define

$$P(s) \equiv \int_s^\infty p(s')\mathrm{d}s'. \tag{17}$$

Then

$$\frac{\mathrm{d}P}{\mathrm{d}s} = -p(s) = -\mu(s)P(s), \tag{18}$$

which is a differential equation for $P(s)$, whose solution is

$$P(s) = P_0\, \mathrm{e}^{-\int_0^s \mu(s')\mathrm{d}s'}. \tag{19}$$

Substituting back into (18) leads to

$$p(s) = P_0 \mu(s)\, \mathrm{e}^{-\int_0^s \mu(s')\mathrm{d}s'}, \tag{20}$$

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[2] A separable Volterra integral equation of the 2nd kind.

where P_0 is fixed by the normalisation of probability. On top of that, the mean spacing is normalised to one. It leads to the following two conditions:

$$\int_0^\infty p(s)\mathrm{d}s = 1,$$
$$\int_0^\infty sp(s)\mathrm{d}s = 1. \tag{21}$$

If the levels E are completely uncorrelated, then $\mu(s) = \text{const}$ and (20)–(21) gives the **Poisson distribution**[3]

$$\boxed{p_{\text{int}}(s) = \mathrm{e}^{-s}} \tag{23}$$

(the subscript "int" indicates this is the NNSD for integrable systems).

The simplest quantum integrable systems that you have encountered (isotropic harmonic oscillator, hydrogen atom) are, in fact, exceptions from the generic situation, with NNSD different from the one just derived. Why? The reason is that these systems are what is sometimes called *superintegrable*: Their symmetry is higher than necessary, and they have more integrals of motion than $f = 3$ (for the hydrogen atom, it is the Runge-Lenz vector; isotropic harmonic oscillator has an additional analogous integral of motion). In other words, they are invariant with respect to a higher symmetry group than necessary: For an isotropic system, it is sufficient to be invariant with respect to SO(3), while the isotropic harmonic oscillator is invariant with respect to U(3) group, and the hydrogen atom to SO(4).

Task 3.1: *One of the generic systems with an almost Poissonian spectrum that can be calculated easily is the 2D incommensurate rectangular infinite potential well.[4] It is an integrable system because it is fully separable. It means that it can be solved in each dimension separately. The appropriate Hilbert space for the entire system can be written as a product of the Hilbert spaces of the subsystems. The Hamiltonian of each subsystem is an integral of motion on its own. Its spectrum is given by the formula*

$$E_{n_1,n_2} = \frac{\pi^2\hbar^2}{2M}\left[\left(\frac{n_1}{a}\right)^2 + \left(\frac{n_2}{b}\right)^2\right], \tag{24}$$

where $n_1, n_2 \in \mathbb{N}$ are two independent quantum numbers and a, b are the dimensions of the box. Incommensurate means that their ratio $\alpha = a/b$ is not a rational number. The best choice of α is something close to 1.

Calculate a whole part of the spectrum of this system with a sufficient number of eigenenergies (at least 1000 lowest-lying states, but it is easy and fast to reach up to 10^6 states) and plot a histogram of the nearest neighbour spacing distribution. Compare this histogram with the theoretical prediction (23). You can choose

$$\alpha = \sqrt{\frac{\pi}{3}} \qquad or \qquad \alpha = \sqrt{\frac{\mathrm{e}^3}{21}} \tag{25}$$

or any random number close to 1.

Play a little with this simple model; you can, for example, use a rational number for α and test how sensitive the NNSD is to "resonances" in the spectrum caused by the commensurate box dimensions.

A detailed discussion of this system (concluding that the levels in the infinite well are, in fact, correlated) is given in Ref. [8].

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[3]It is in fact the well-known Poisson distribution

$$P(k; s) = \frac{s^k}{k!}\,\mathrm{e}^{-s}, \tag{22}$$

which gives the probability that an event occurs k times on an interval s, but here restricted to $k = 0$ (we ask for no level at interval s). In the quantum chaos theory, it is (23) what is usually called Poisson distribution.

[4]It is also an example of a billiard system.

Solution 3.1: *A Python code with the solution is in the public GitHub repository of this project. It consists of these files:*

- `box2D.py`*: A file with the model specification. It contains functions to calculate the energy spectrum and the smooth part of the level density.*

- `statistics.py`*: Functions to unfold the spectrum (more about the unfolding in Section 6.2) and obtain unit average level density; functions to calculate the nearest neighbour spacing distribution of the unfolded spectrum and the Poisson and Wigner distribution functions.*

- `plots.py`*: Functions that plot histograms and compare numerically obtained distributions with exact ones.*

The results (level density and nearest neighbour spacing distribution) are displayed in Figure 1. There are three configurations:

1. *The incommensurate ratio of a, b, $\alpha = \sqrt{\pi/3}$ (first line of the Figure) with almost perfectly Poissonian NNSD. A slight deviation from formula (23) is observed at the smallest spacings. The level density is almost uniform, with a small lack of states at the lowest energies. The NNSD will be improved if the lowest part of the spectrum is disregarded.*

2. *2D box with a strong resonance, $\alpha = 3/2$ (second line of the Figure). No irregularity is observed in the level dynamics, but the NNSD is not Poissonian. The resonance introduces correlations among the levels, which disturb the Poisson distribution.*

3. *2D box with a weak resonance, $\alpha = 11/10$ (third line of the Figure). There is still a deviation in the NNSD from the Poissonian distribution. However, the figure is much more improved compared with the strongly resonant case.*

4   Chaotic systems

Here only a very brief overview of the history of quantum chaos is sketched. For more details, I strongly recommend reading the first chapter of Mehta's monography [4].

4.1   Wigner surmise

The field of quantum chaos started developing with the work of Eugene Wigner in the 1950s. At that time, a lack of close states was observed in high-lying slow nuclear resonances. At first, it was being explained by imperfect measuring techniques, but then Wigner [9, 10, 11] proposed and succeeded in using the Random Matrix Theory (RMT) to describe this suspicious behaviour of the resonances, and he formulated the so-called

Theorem 4.1: (Wigner surmise) *Suppose we have a complicated and complex system with an (often high) unknown number of degrees of freedom (such as a highly excited atomic nucleus[5]) and we do not know anything about the interaction among the constituents. The only thing we know about the Hamiltonian is the symmetry it satisfies (rotational invariance, time-reversal invariance etc.). Then a sequence of consecutive energy levels with the same spin and parity will have the same statistical properties as the spectrum of a random matrix whose elements are independent numbers taken from the Gaussian normal distribution. Levels of different spin and parity are not correlated.[6]*

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[5]A plethora of models successfully explains low-lying nuclear excitations, *e.g.* nuclear collective models, shell model, etc., with only a relatively small number of degrees of freedom. These models become more and more inaccurate as the excitation energy increases, making the approximation of the complicated nucleon interactions impossible.

[6]Spin and parity are conserved quantities (integrals of motion), and following the conclusions of Section 3 they must be uncorrelated.
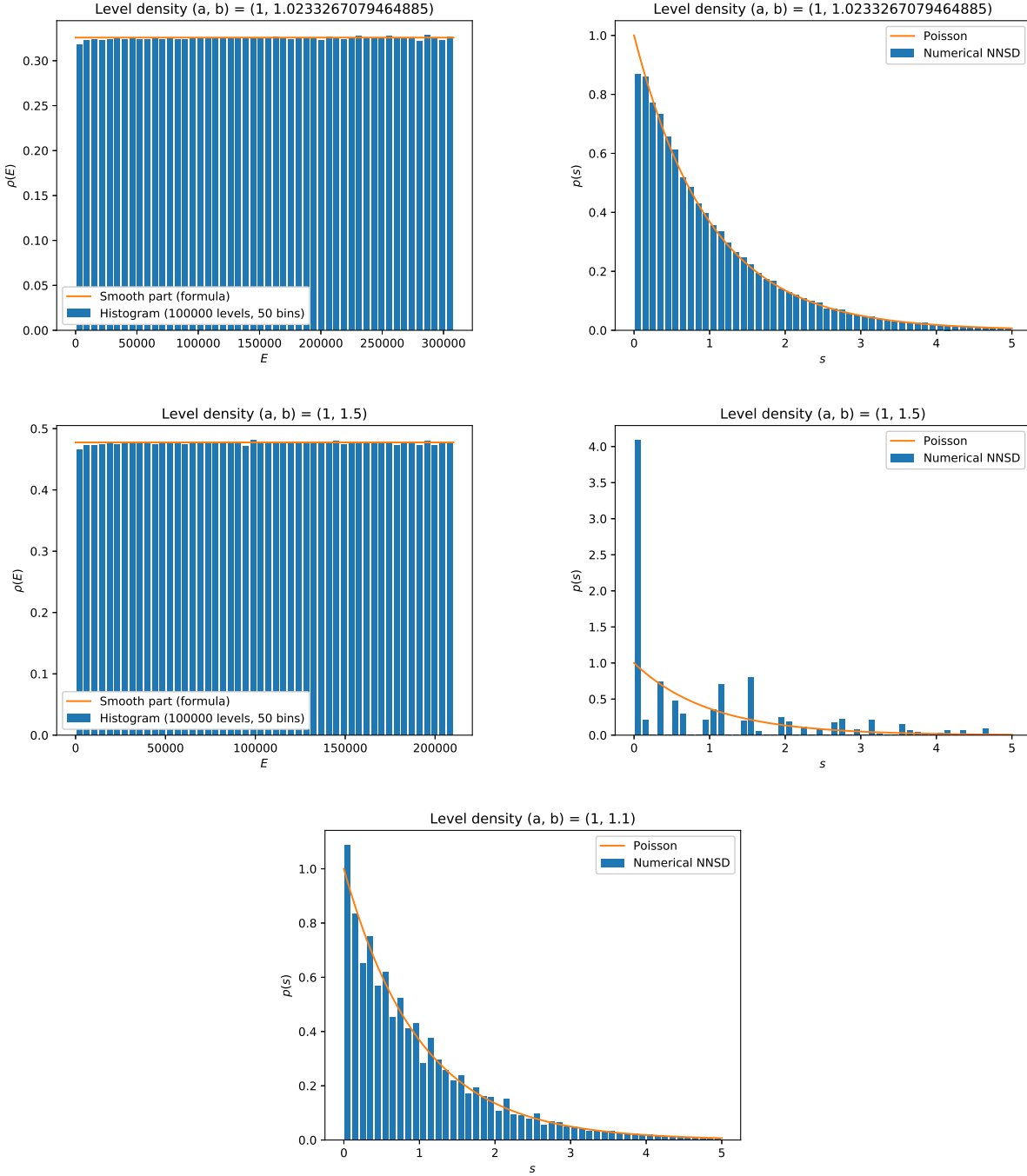
Figure 1: Level density and nearest neighbour spacing distribution for the 2D rectangular infinite-well potential with $\hbar = M = 1$ and (a) incommensurate lengths of the edges, (b) lengths in a strong resonance, and (c) lengths in a weak resonance. The resonance introduces correlations among the levels.

Soon after, Wigner derived the formula for the Nearest Neighbour Spacing Distribution of 2×2 random matrices invariant under rotations:

$$p_w(s) = \frac{\pi}{2} s \, e^{-\frac{\pi}{4} s^2}, \tag{26}$$

which is often called **Wigner(-Dyson) distribution**[7] (the derivation will be presented later in Sec. 5.2). Compared with the Poisson distribution for an integrable system (23), which has a maximum at $s = 0$, *i.e.* the eigenlevels tend to bunch together, the spectrum satisfying the Wigner distribution exhibits clear **level repulsion** (the probability of coinciding levels is $p_w(0) = 0$[8]).

4.2 Bohigas conjecture

In the beginning, the theory of quantum matrices was just a tool to study the statistical spectral properties of many-body systems under unknown interactions. In contrast, quantum counterparts of classically chaotic systems were studied by semiclassical methods in systems with only a few degrees of freedom. But then, in 1984, Bohigas, Giannoni and Schmit published a ground-breaking paper [7] stating:

Theorem 4.2: (Bohigas (-Giannoni-Schmit) conjecture) **All quantum systems whose classical analogues are chaotic exhibit the same spectral fluctuation properties as predicted by the theory of random matrices.** *On the contrary, quantum systems with stable classical analogues (not necessarily integrable) have uncorrelated energy levels.*

This paper established the field that is since then called quantum chaos.
Now some remarks:

1. Until now, the conjecture has not been proved in its generality.[9] However, there is a vast list of numerical studies based on a wide variety of systems that support its validity (but there are also several counter-examples of systems that are classically regular but have random-matrix-like quantum spectrum,[10] and vice versa).

5 Gaussian random matrix ensembles

The main question now is the following: What are some significant properties of an ensemble of matrices whose elements are random variables with a specific probability law? What can we say about correlations among the eigenlevels and eigenvectors?

As with many theories, their pioneers are often forgotten and scarcely mentioned. The development of the random matrix theory began in the 1920s [13] but did not draw much attention then. The theory became more popular when Wigner formulated his surmise, see Section 4.1, but mathematically rigorous foundations of the so-called Random Matrix Theory (RMT) were established in a series of beautiful papers by Dyson [14][11] (the distribution (26) is sometimes called the *Wigner-Dyson distribution*). He introduced the classification of the Gaussian random matrix ensembles

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[7]Beware, there is another quantity in quantum mechanics called Wigner distribution (also called Wigner quasiprobability distribution or Wigner function).

[8]This phenomenon is tightly related with the quantum *no-crossing theorem.*

[9]There are several different classes of classically chaotic systems:

| Ergodic | $\supset$ | Weakly Mixing (WM) | $\supset$ | Strongly Mixing (SM) | $\supset$ | Kolmogorov (K-) | $\supset$ | Bernoulli (B-) |

The complete discussion of this classification is beyond the scope of this lecture (and it belongs to the area of classical chaos theory); you can find it in [12]. It has been proved, though, that mixing at the classical level is sufficient to generate random matrix statistics.

[10]For example the Šeba's billiard: a circular billiard with a δ-function sitting in the middle.

[11]Freeman John Dyson, who passed away in 2020, was an author or co-author of many seminal ideas and theorems in mathematics and physics. However, only a few are named after him, probably due to his modesty (the most famous is the Dyson series, leading to Feynman-Dyson diagrams). As a curiosity, he became a professor without having finished his PhD studies. He is a laureate of the Templeton Prize.

according to their invariance properties under time reversal. He proved that there are only three classes of them (universality classes), and he aptly stated: "What is here required is a new kind of statistical mechanics, in which we renounce exact knowledge not of the state of the system but of the system itself. We picture a complex nucleus as a 'black box' in which a large number of particles interact according to unknown laws. The problem then is to define in a mathematically precise way an ensemble of systems in which all possible laws of interaction are equally possible."

So what is the Gaussian random matrix, and what are the available ensembles?

Theorem 5.1: *The Gaussian random matrix* H *is a matrix from an ensemble of matrices with probability distribution* $P(\mathsf{H})$, *satisfying*

1. *The probability distribution is invariant under a given transformation* W,

$$P(\mathsf{H}) = P(\mathsf{H}'), \quad where \ \mathsf{H}' = \mathsf{W}^{-1}\mathsf{H}\mathsf{W} \tag{27}$$

(necessary if we want matrix H *to correspond with the Hamiltonian of a physical system).*

2. *Matrix elements of* H *are statistically independent.*

From these two requirements, it follows that the distribution of matrix elements is Gaussian (this statement will be proved in Section 5.2).

The three available ensembles are[12]:

1. **Gaussian Orthogonal Ensemble (GOE),** $\beta = 1$: Time-reversal invariant systems with $\hat{\mathsf{T}}^2 = 1$. This ensemble is invariant under orthogonal transformation,

$$P(\mathsf{H}) = P\left(\mathsf{O}^\mathsf{T}\mathsf{H}\mathsf{O}\right), \quad \mathsf{O}^\mathsf{T}\mathsf{O} = 1. \tag{28}$$

The matrix H modelling the Hamiltonian of our system is real symmetric and has $N(N+1)/2$ independent real components. The majority of quantum systems belong to the GOE.

2. **Gaussian Unitary Ensemble (GUE),** $\beta = 2$: Systems not invariant under time reversal. This ensemble is invariant under unitary transformation,

$$P(\mathsf{H}) = P\left(\mathsf{U}^{-1}\mathsf{H}\mathsf{U}\right), \quad \mathsf{U}^{-1}\mathsf{U} = 1. \tag{29}$$

The matrix H is complex Hermitian and has N^2 independent real components. GUE is suitable, *e.g.*, for systems in external magnetic field.

3. **Gaussian Symplectic Ensemble (GSE),** $\beta = 4$: Time-reversal invariant systems with $\hat{\mathsf{T}}^2 = -1$. This ensemble is invariant under symplectic transformation,

$$P(\mathsf{H}) = P\left(\mathsf{S}^{-1}\mathsf{H}\mathsf{S}\right), \quad \mathsf{S}^{-1}\mathsf{S} = 1. \tag{30}$$

The matrix H is quaternionic Hermitian and has $N(2N-1)$ independent components.[13] This is the least common case to encounter. Systems in this class have half-integer spins and exhibit Kramers's degeneracy. Note that the first experiment to obtain the GSE-like spectrum was performed quite recently [15] using specially designed quantum graphs.

Index β is called the **Dyson number**. Examples of spectra of matrices belonging to these three ensembles are given in Figure 2(a).

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[12]From a mathematical point of view, these three classes exhaust the distinct real associative normed division algebras (in effect, number systems). That is why there are just these three ensembles.

[13]Quaternionic $N \times N$ matrix can be modelled by $2N \times 2N$ complex matrices.

5.1   Other ensembles

If we weaken any of the conditions of Theorem 5.1, we may extend the number of universality classes and introduce new ensembles:

- Altland-Zirnbauer universality classes [16] (7 additional classes by relaxing Equation (28), taking into account particle-hole symmetry or chiral symmetry).

- Random unitary matrices (Gaussian Circular Ensembles) for modelling the scattering S-matrix instead of the Hamiltonian matrix.

- Random band matrices.

- Ginibre ensembles [17] (condition (28) completely disregarded).

In these notes, we shall restrict ourselves on the Gaussian ensembles only.

5.2 2×2 GOE matrices

Many properties of random matrix ensembles can be demonstrated on the smallest nontrivial matrices possible (and some of the properties can be explicitly derived only for these matrices).

5.2.1   Probability distribution

In this section, we will derive the properties of a 2×2 random matrix from the Gaussian Orthogonal Ensemble (usually abbreviated as GOE random matrix). We will follow the requirements given in Theorem 5.1.

The matrix $\mathsf{H} \in \mathsf{GOE}(2)$ is real and symmetric, so it has only three independent elements H_{11}, H_{22}, H_{12}. The probability is normalized,

$$\int \mathrm{d}H_{11}\mathrm{d}H_{12}\mathrm{d}H_{22}P(\mathsf{H}) = 1 \tag{31}$$

1. The probability distribution has to be invariant under orthogonal transformation,

$$P(\mathsf{H}) = P(\mathsf{H}'), \qquad \text{where} \quad \mathsf{H}' = \mathsf{O}^{\mathsf{T}}\mathsf{H}\mathsf{O}, \tag{32}$$

where a general 2×2 orthogonal matrix can be written as

$$\mathsf{O}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \approx \begin{pmatrix} 1 & \theta \\ -\theta & 1 \end{pmatrix}, \tag{33}$$

$$\mathsf{O}^{\mathsf{T}}(\theta) = \mathsf{O}^{-1}(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \approx \begin{pmatrix} 1 & -\theta \\ \theta & 1 \end{pmatrix}, \tag{34}$$

and depends on just one parameter (angle) θ. Without the loss of generality, we can consider infinitesimal rotations $\theta \approx 0$ only. Then it follows from (32) that

$$\begin{aligned} \begin{pmatrix} H_{11}' & H_{12}' \\ H_{21}' & H_{22}' \end{pmatrix} &= \begin{pmatrix} 1 & -\theta \\ \theta & 1 \end{pmatrix} \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} 1 & \theta \\ -\theta & 1 \end{pmatrix} \\ &= \begin{pmatrix} H_{11} - 2\theta H_{12} + \theta^2 H_{22} & \theta H_{11} + H_{12} - \theta^2 H_{12} - \theta H_{22} \\ \theta H_{11} - \theta^2 H_{12} + H_{12} - \theta H_{22} & \theta^2 H_{11} + 2\theta H_{12} + H_{22} \end{pmatrix} \\ &\approx \begin{pmatrix} H_{11} - 2\theta H_{12} & H_{12} + \theta\,(H_{11} - H_{22}) \\ H_{12} + \theta\,(H_{11} - H_{22}) & H_{22} + 2\theta H_{12} \end{pmatrix} \end{aligned} \tag{35}$$

(up to the 1st order in θ).

2. The matrix elements are statistically independent, which means that the probability $P(\mathsf{H})$ is given by the product of probabilities of individual elements,

$$P(\mathsf{H}) = P_{11}(H_{11})P_{12}(H_{12})P_{22}(H_{22}). \tag{36}$$

Substituting from (32) and (35) we get

$$
\begin{aligned}
P(\mathsf{H}) &= P_{11}(H'_{11})P_{12}(H'_{12})P_{22}(H'_{22}) \\
&= P_{11}\left(H_{11} - 2\theta H_{12}\right)P_{12}\left(H_{12} + \theta(H_{11} - H_{22})\right)P_{22}\left(H_{22} + 2\theta H_{12}\right) \\
&\quad \left|1^{\text{st}} \text{ order Taylor expansion}\right| \\
&\approx \left[P_{11}(H_{11}) - 2\theta H_{12}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}}\right]\left[P_{12}(H_{12}) + \theta(H_{11} - H_{22})\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}}\right]\left[P_{22}(H_{22}) + 2\theta H_{12}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}}\right] \\
&= P(\mathsf{H})\left\{\left[1 - 2\theta\frac{H_{12}}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}}\right]\left[1 + \theta\frac{H_{11} - H_{22}}{P_{12}}\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}}\right]\left[1 + 2\theta\frac{H_{12}}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}}\right]\right\} \\
&\quad \left|1^{\text{st}} \text{ order terms in } \theta\right| \\
&\approx P(\mathsf{H})\left\{1 - \theta\left[2\frac{H_{12}}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}} - 2\frac{H_{12}}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}} - \frac{H_{11} - H_{22}}{P_{12}}\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}}\right]\right\}.
\end{aligned} \tag{37}
$$

The last expression has to be invariant with respect to θ, so the bracket must vanish:

$$2\frac{H_{12}}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}} - 2\frac{H_{12}}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}} - \frac{H_{11} - H_{22}}{P_{12}}\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}} = 0 \tag{38}$$

$$\frac{1}{P_{12}H_{12}}\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}} - \frac{2}{H_{11} - H_{22}}\left(\frac{1}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}} - \frac{1}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}}\right) = 0 \tag{39}$$

We obtain an equation for the distributions P_{11}, P_{12}, P_{22}, which can be separated into two independent equations,

$$
\begin{aligned}
\frac{1}{P_{12}H_{12}}\frac{\mathrm{d}P_{12}}{\mathrm{d}H_{12}} &= -4A \\
\left(\frac{1}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}} - \frac{1}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}}\right) &= -2A\left(H_{11} - H_{22}\right)
\end{aligned} \tag{40}
$$

(we called the arbitrary separation constant $-4A$). The second equation can be further separated into

$$
\begin{aligned}
\frac{1}{P_{11}}\frac{\mathrm{d}P_{11}}{\mathrm{d}H_{11}} + 2AH_{11} &= -B \\
\frac{1}{P_{22}}\frac{\mathrm{d}P_{22}}{\mathrm{d}H_{22}} + 2AH_{22} &= -B.
\end{aligned} \tag{41}
$$

The solutions of the separated 1st differential equations are

$$
\begin{aligned}
P_{12} &= C_{12}\,\mathrm{e}^{-2AH_{12}^2}, \\
P_{11} &= C_{11}\,\mathrm{e}^{-AH_{11}^2 - BH_{11}}, \tag{42} \\
P_{22} &= C_{22}\,\mathrm{e}^{-AH_{22}^2 - BH_{22}}, \tag{43}
\end{aligned}
$$

where C_{11}, C_{12}, and C_{22} are integration constant.

The probability distribution is, therefore,

$$P(\mathsf{H}) = C\,\mathrm{e}^{-A\left(H_{11}^2 + H_{22}^2 + 2H_{12}^2\right) - B(H_{11} + H_{22})}, \tag{44}$$

where $C = C_{11}C_{12}C_{22}$ is a normalisation constant constrained by condition (31), A fixes the unit of energy, and B gives the shift of energy (can be made 0 by an appropriate choice of zero energy), so the distribution can finally be written in the form

$$\boxed{P(\mathsf{H}) = C\,\mathrm{e}^{-A\operatorname{Tr}\mathsf{H}^2}}. \tag{45}$$

A couple of observations and comments:

1. From the distribution (44), it follows that the nondiagonal elements have half the dispersion that the diagonal elements. This is important for the numerical generation of GOE random matrices.

2. The expression (45) is valid for other Gaussian matrix ensembles (GUE and GSE) and an arbitrary matrix dimension N.

5.2.2   Eigenvalues distribution

Here we want to move from the matrix element probability distribution (45) to the probability distribution of finding a particular pair of eigenvalues (for a $N = 2$ matrix). The eigenvalues of the 2×2 matrix are

$$E_\pm = \frac{1}{2}\left(H_{11} + H_{22}\right) \pm \frac{1}{2}\sqrt{\left(H_{11} - H_{22}\right)^2 + 4H_{12}^2}. \tag{46}$$

The original matrix is then

$$\mathsf{H} = \mathsf{O}^{\mathsf{T}} \operatorname{diag}\left(E_+, E_-\right)\mathsf{O}, \tag{47}$$

where the eigenvectors matrix O is the orthogonal transformation matrix (33). Substitution gives

$$\begin{aligned}
H_{11} &= E_+ \cos^2\theta + E_- \sin^2\theta \\
H_{22} &= E_+ \sin^2\theta + E_- \cos^2\theta \\
H_{12} &= \left(E_+ - E_-\right)\sin\theta\cos\theta.
\end{aligned} \tag{48}$$

This specifies the transformation $(E_+, E_-, \theta) \leftrightarrow (H_{11}, H_{22}, H_{12})$ whose Jacobian is

$$\begin{aligned}
J &= \det \frac{\partial(H_{11}, H_{22}, H_{12})}{\partial(E_+, E_-, \theta)} \\
&= \det \begin{pmatrix}
\cos^2\theta & \sin^2\theta & -2(E_+ - E_-)\sin\theta\cos\theta \\
\sin^2\theta & \cos^2\theta & 2(E_+ - E_-)\sin\theta\cos\theta \\
\sin\theta\cos\theta & -\sin\theta\cos\theta & (E_+ - E_-)\left(\cos^2\theta - \sin^2\theta\right)
\end{pmatrix} \\
&= (E_+ - E_-)\left[cos^4\theta\left(\cos^2\theta - \sin^2\theta\right) + 2\sin^4\theta\cos^2\theta + 2\sin^4\theta\cos^2\theta \right. \\
&\qquad \left. + 2\sin^2\theta\cos^4\theta + 2\sin^2\theta\cos^4\theta - \sin^4\theta\left(\cos^2\theta - \sin^2\theta\right)\right] \\
&= (E_+ - E_-)\left[cos^4\theta\cos 2\theta + \sin^2 2\theta - \sin^4\theta\cos 2\theta\right] \\
&= (E_+ - E_-)\left[\left(cos^2\theta + \sin^2\theta\right)\left(cos^2\theta - \sin^2\theta\right)\cos 2\theta + \sin^2 2\theta\right] \\
&= (E_+ - E_-)\left[\cos^2 2\theta + \sin^2 2\theta\right] \\
&= E_+ - E_-,
\end{aligned} \tag{49}$$

so the desired (joint) probability density is

$$\begin{aligned}
P\left(E_+, E_-\right) &= \left.P(H_{11}, H_{22}, H_{12})\right|_{(H_{11}, H_{22}, H_{12}) \mapsto (E_+, E_-, \theta)} \\
&= C\left|J\right|\mathrm{e}^{-A\operatorname{Tr}\mathsf{H}^2} \\
&= C\left|E_+ - E_-\right|\mathrm{e}^{-A\left(E_+^2 + E_-^2\right)}.
\end{aligned} \tag{50}$$

Some comments:

1. The eigenvalue distribution is independent of the angle θ.

2. For a general N-dimensinal matrix from a Gaussian ensemble with Dyson index β, the joint probability distribution for eigenvalues is

$$P(E_1, \ldots, P_N) = C \prod_{j<k}^{1\cdots N} \left|E_j - E_k\right|^\beta \, \mathrm{e}^{-A\sum_{j=1}^N E_j^2}. \tag{51}$$

5.2.3   Nearest neighbour spacing distribution

NNSD is obtained from (50) via

$$
\begin{aligned}
p(s) &= \int_{-\infty}^{\infty} \mathrm{d}E_+ \int_{-\infty}^{\infty} \mathrm{d}E_- \, \delta\left(s - |E_+ - E_-|\right) P(E_+, E_-) \\
&= C \int_{-\infty}^{\infty} \mathrm{d}E_+ \int_{-\infty}^{\infty} \mathrm{d}E_- \, \delta\left(s - |E_+ - E_-|\right) |E_+ - E_-| \, \mathrm{e}^{-A\left(E_+^2 + E_-^2\right)} \\
&\quad \left|
\begin{array}{c}
\text{We suppose that } E_+ > E_- \text{ and substitute } E_+ \to \sigma: \\
\sigma = E_+ - E_-, \\
\mathrm{d}\sigma = \mathrm{d}E_+
\end{array}
\right| \\
&= C \int_{0}^{\infty} \mathrm{d}\sigma \int_{-\infty}^{\infty} \mathrm{d}E_- \delta(s - \sigma)\sigma \, \mathrm{e}^{-A\left[(\sigma + E_-)^2 + E_-^2\right]} \\
&= C \int_{-\infty}^{\infty} \mathrm{d}E_- \, s \, \mathrm{e}^{-A\left(s^2 + 2sE_- + 2E_-^2\right)} \\
&= C \int_{-\infty}^{\infty} \mathrm{d}E_- \, s \, \mathrm{e}^{-A\left[\frac{s^2}{2} + \left(\sqrt{2}E_- + \frac{s}{\sqrt{2}}\right)^2\right]} \\
&= C \int_{-\infty}^{\infty} \frac{\mathrm{d}e}{\sqrt{2}} s \, \mathrm{e}^{-A\frac{s^2}{2}} \, \mathrm{e}^{-Ae^2} \\
&= D s \, \mathrm{e}^{-\frac{A}{2}s^2} .
\end{aligned}
\tag{52}
$$

After normalizing and rescaling to have a unit mean level spacing (21), we land to the already discussed Wigner distribution (26),

$$
p_w(s) = \frac{\pi}{2} \, s \, \mathrm{e}^{-\frac{\pi}{4}s^2} .
\tag{53}
$$

Comments:

1. Distribution (53) is valid for matrices 2×2 only. For higher-dimensional matrices, it is impossible to get a closed formula for the spacing density; it can be found only numerically. However, the deviation from p_w is at most in the order of a few per cent, even when $N \to \infty$, see Figure 2(c). For practical purposes, the distribution (53) is good enough. Hence, it is widely used for matrices of an arbitrary dimension.

2. Similar formulae can be derived for other ensembles. Normalised NNSD for all three ensembles of Gaussian matrices are

$$
\begin{aligned}
\text{GOE}: &\qquad p_w^{(\beta=1)}(s) = \frac{\pi}{2} \, s \, \mathrm{e}^{-\frac{\pi}{4}s^2} \\
\text{GUE}: &\qquad p_w^{(\beta=2)}(s) = \frac{32}{\pi^2} \, s^2 \, \mathrm{e}^{-\frac{4}{\pi}s^2} \\
\text{GSE}: &\qquad p_w^{(\beta=4)}(s) = \left(\frac{64}{9\pi}\right)^3 s^4 \, \mathrm{e}^{-\frac{64}{9\pi}s^2}
\end{aligned}
\tag{54}
$$

and they are displayed in Figure 2(b). An important observation is that the strength of the repulsion depends on the Dyson number,

$$
p_w^{(\beta)} \approx s^\beta \quad \text{for } s \ll 1.
\tag{55}
$$

5.3   Wigner semicircle law

A final remark related to the spectra of random matrices is the average level density. It is given by integral

$$
\overline{\rho}(E) = \int \mathrm{d}E_2 \cdots \mathrm{d}E_N P(E, E_2, \ldots, E_N),
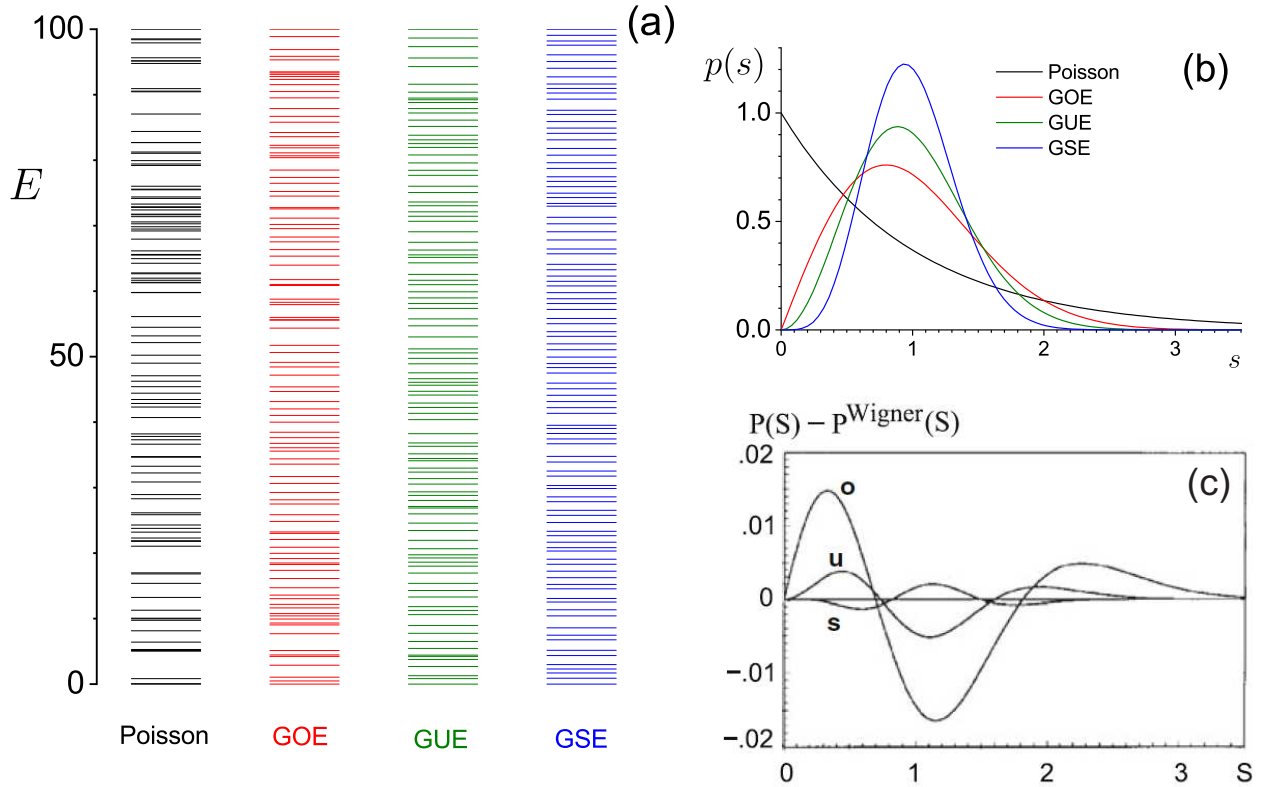\tag{56}
$$

Figure 2: (a) Example of spectra with different NNSD. The spectra are normalised to $\langle s \rangle = 1$. The stronger the level repulsion given by the Dyson number, the more uniform the spectrum looks. For levels with Poisson distribution, there are both bunches of levels and wide gaps. (b) Probability distributions (54) corresponding to chaotic systems compared with the Poisson distribution (23) corresponding to an integrable system. (c) Absolute deviation of $p_w(s)$ for 2×2 matrices from the NNSD for infinite-size matrices. The most significant deviation is observed for GOE at $s \approx 0.4$. However, the deviation does not exceed 4%. This panel is taken from [2].

where P is the joint probability density (51).

When matrix dimension N is high, $N \to \infty$, the integral[14] converges to the **Wigner semicircle law** [11]

$$\overline{\rho}(E) = \begin{cases} \frac{1}{2\pi}\sqrt{1-E^2} & |E| \leq 1, \\ 0 & |E| > 1, \end{cases} \tag{57}$$

where, to secure convergence of the integral, we impose the following condition,

$$\overline{H_{jk}H_{kj}} = \overline{H_{jj}^2} = \frac{1}{4N}. \tag{58}$$

If we go back to (45), we see that the variance σ^2 of matrix elements is related with A via

$$A = \frac{1}{2\sigma^2}. \tag{59}$$

Hence condition (58) is satisfied if

$$\sigma = \frac{1}{2\sqrt{N}}. \tag{60}$$

Comments:

- The semicircle law (57) is only valid in the limit $N \to \infty$. For smaller matrix sizes, the behaviour of the level distribution at $E = \pm 1$ is not abrupt (*i.e.*, changing from $\overline{\rho} = 0$ to $\overline{\rho} > 0$ with an infinite jump in the derivative $\overline{\rho}'$), but smooth. Even though for large matrices, these finite-size effects are rather tiny, they must be taken into account in the unfolding process discussed in Section 6.2.

- The semicircle law is valid also for GUE and GSE.

- For practical numerical purposes, the level density $\overline{\rho}(E)$ is approximated by a histogram. In a physical system given by one particular Hamiltonian, we have just one spectrum; therefore, it is necessary to have the highest number of converging levels possible to get a reasonably precise approximation of $\overline{\rho}(E)$. On the other hand, random matrices are taken from the ensemble, so one can calculate an ensemble average of all the matrix properties, including the level density $\overline{\rho}(E)$.

- While the fluctuation properties, such as the NNSD, have universal validity, the semicircle law of level density is a specific property of the Gaussian matrix ensembles. More about it in the following section.

5.4   Generating a GOE matrix

A matrix from the Gaussian matrix ensembles can be generated numerically by using the distribution (45). Namely, a GOE matrix is a symmetric matrix whose elements are normally distributed values with variance σ^2 of the non-diagonal items and $2\sigma^2$ for the diagonal items:

$$H_{jk} = H_{kj} = N\left(0, (1 + \delta_{jk})\sigma^2\right), \tag{61}$$

where δ_{kj} is the Kronecker delta. The same matrix is achieved when one takes a matrix A with elements

$$A_{jk} \in N(0, 2\sigma^2) \tag{62}$$

and symmetrise it,

$$\mathsf{H} \equiv \frac{\mathsf{A} + \mathsf{A}^\dagger}{2}. \tag{63}$$

---

[14]This integral requires relatively advanced mathematical tools. The most straightforward way to perform it is via Grassmann integration.

Task 5.1: *Make a routine to generate a* GOE *matrix and calculate its eigenvalues. Show that for sufficiently large matrices,* $N \gtrsim 1000$,[15] *the level density is very well approximated by the Wigner semicircle law. In order to get a more precise estimate of the level density, calculate an average over a sample of several random matrices.*

6   Statistical analysis of a quantum spectrum

In this section, it will be assumed that we have a spectrum of a general quantum system, and our goal is to prepare the spectrum so that we can use spectral statistics to distinguish whether the levels are correlated or not.

6.1   Level density

The level density can always be written as a sum of two parts: the smooth part $\overline{\rho}(E)$ and the oscillatory part $\tilde{\rho}(E)$,

$$\rho(E) \equiv \overline{\rho}(E) + \tilde{\rho}(E). \tag{64}$$

The smooth part gives an average number of levels in an interval dE. It is system dependent, expressed by the semiclassical **Weyl fomula**[16]

$$\overline{\rho}(E) = \frac{1}{(2\pi\hbar)^f} \int d^f\boldsymbol{p}d^f\boldsymbol{q}\, \delta\left(E - H(\boldsymbol{p}, \boldsymbol{q})\right), \tag{65}$$

where f is the number of degrees of freedom and $H(\boldsymbol{p}, \boldsymbol{q})$ the classical Hamiltonian. This formula consists of a ratio of the volume of the energy "hypersurface" in the classical phase space,[17] and the volume of a quantum elementary "cell" $(2\pi\hbar)^f$. Since the smooth part does not depend on the dynamics, it cannot give any account of the system's chaoticity.

The oscillatory part carries information about the spectral correlations. It is given by the *Gutzwiller trace formula* [1]

$$\tilde{\rho}(E) = \sum_p \sum_{r=1}^{\infty} \frac{rT_p}{\sqrt{\|\det\left(1 - \mathsf{M}_p\right)\|}} \cos\left[\frac{1}{\hbar}rS_p(E) - \frac{\pi}{2}r\nu_p\right] \tag{66}$$

where p indexes all the simple periodic orbits of the system, r specifies the number of repetitions, T_p is the period of the orbit, M_p is the stability (monodromy) matrix, $S_p(E)$ is the action of the orbit, and ν_p is a phase connected with the orbit (the *Maslov index*).

6.1.1   Smooth level density of a potential well

The potential well is an important example of a simple integrable system. Suppose we have a particle moving in an infinite cuboid-like f dimensional potential well (billiard)

$$H = \begin{cases} \frac{1}{2M}\boldsymbol{p}^2 & \boldsymbol{q} \in \mathcal{C}, \\ \infty & \text{elsewhere,} \end{cases} \tag{67}$$

---

[15]Standard routines based on LAPACK library can diagonalise matrices up to $N \approx 20000$ in a PC with 16 GB RAM. However, since the computational complexity of the diagonalisation algorithm is $\mathcal{O}(N^3)$, it takes enormous time to diagonalise such large matrices (usually several hours), while matrices of $N \approx 1000$ are usually calculated within seconds.

[16]It is worth mentioning a related work by Mark Kac, discussing general properties of a vibrational spectrum of a "drum": a membrane of an arbitrary shape with a fixed boundary [18].

[17]Liouville measure of the phase space.

where $\mathcal{C}$ is a cuboid of side lengths $a, b, c, \ldots$ and M a mass of the particle. Following (65), the smooth part of the level density is

$$
\begin{aligned}
\overline{\rho}(E) &= \frac{1}{(2\pi\hbar)^f} \frac{\partial}{\partial E} \int_{E \geq H(\boldsymbol{P},\boldsymbol{q})} \mathrm{d}^f \boldsymbol{p} \, \mathrm{d}^f \boldsymbol{q} \\
&= \frac{1}{(2\pi\hbar)^f} \frac{\partial}{\partial E} \underbrace{\int_{\mathcal{C}} \mathrm{d}^f \boldsymbol{q}}_{V \equiv \text{vol } \mathcal{C} = abc \cdots} \underbrace{\int_{E \geq \frac{p^2}{2M}} \mathrm{d}^f \boldsymbol{p}}_{\text{volume of a } f\text{-dimensional ball}} \\
&= \frac{V}{(2\pi\hbar)^f} \frac{\partial}{\partial E} \left. \frac{\pi^{\frac{f}{2}}}{\Gamma\left(\frac{f}{2}+1\right)} p^f \right|_{p=\sqrt{2ME}} \\
&= \frac{V}{(2\pi\hbar)^f} \frac{f}{2} \frac{(2\pi M)^{\frac{f}{2}}}{\Gamma\left(\frac{f}{2}+1\right)} E^{\frac{f}{2}-1},
\end{aligned}
\tag{68}
$$

where Γ is the Gamma function. Specifically,

$$
\overline{\rho}^{(f=1)}(E) = a\sqrt{\frac{M}{2}} \frac{1}{\pi\hbar} \frac{1}{\sqrt{E}},
\tag{69}
$$

$$
\overline{\rho}^{(f=2)}(E) = ab\frac{M}{2\pi\hbar^2},
\tag{70}
$$

$$
\overline{\rho}^{(f=3)}(E) = abc\frac{M}{\pi^2\hbar^3}\sqrt{\frac{M}{2}}\sqrt{E}.
\tag{71}
$$

An important observation is that **the smooth level density of the 2D potential well is constant, independent of energy**. We silently made use of this vital property in Task 3.1.

6.2   Unfolding

The information about the spectral correlations is encoded in the oscillating level density only. We must find a procedure for rescaling the spectrum to eliminate the smooth part and stay with the oscillatory part. This procedure is called unfolding, and it consists of a transformation

$$
E_j \longrightarrow e_j = f(E_i),
\tag{72}
$$

where $\overline{\rho}(e) \equiv 1$. What is the appropriate form of the function f? It is required that

$$
\begin{aligned}
1 = \frac{1}{\overline{\rho}(e)} &= \frac{\Delta e}{\Delta N} \\
&= \frac{1}{\Delta N}\left[f\left(E + \frac{\Delta E}{2}\right) - f\left(E - \frac{\Delta E}{2}\right) \right] \\
&= \frac{\Delta E}{\Delta N} f'(E) = \frac{f'(E)}{\overline{\rho}(E)},
\end{aligned}
\tag{73}
$$

so that

$$
f(E) \equiv \overline{N}(E) = \int_{-\infty}^{E} \overline{\rho}(E')\mathrm{d}E',
\tag{74}
$$

where $\overline{N}(E)$ is the cumulative level density.

Let us distinguish now two situations:

1. The smooth level density is known and, most preferably, given by an analytic formula. We can integrate it using (74) and employ the resulting cumulative level density to perform the unfolding. Examples of such systems are:

- The infinite cuboid-like potential well (68)

$$\overline{N}(E) = \frac{V}{(2\pi\hbar)^f} \frac{(2\pi M)^{\frac{f}{2}}}{\Gamma\left(\frac{f}{2}+1\right)} E^{\frac{f}{2}}. \tag{75}$$

- The large GOE matrix (57)

$$\overline{N}(E) = \frac{1}{8\pi}\left[2E\sqrt{1-E^2} + 2\arcsin E + \pi\right]. \tag{76}$$

2. If we are not able to calculate the phase space integral (65), because we either do not know the semiclassical Hamiltonian, or the integration is too laborious, we have to find an approximation of the smooth level density. The accumulated level density calculated from the spectrum is

$$N(E) = \sum_j \Theta\left(E - E_j\right), \tag{77}$$

where θ is the Heaviside step function. Its smooth part is obtained by a least-square fit of an appropriate function, usually by a polynomial of a rather small degree (usually between 3 and 7).

One must be extra cautious here: by taking a function that does not fit well to $N(E)$, a part of the smooth level density will remain in the unfolded spectrum and distort the correlation statistics. On the other hand, if we "overfit" the accumulated level density, we eliminate the interesting oscillatory part of the spectrum, and we may even end up with an equidistant "picket-fence" spectrum. Extra care must also be taken at the outer limits of the fitted spectrum, where any approximating function usually has the highest deviation (it is also a common practice to disregard a small part of the lowest and highest energy levels after unfolding). The approximate unfolding is thus a very delicate procedure, requiring some experience and feeling to get it right.

Note that there are ways to bypass the unfolding procedure by either studying statistics unaffected by the smooth part of the level density. There are also simple unfolding procedures on the market, suitable only for a subset of correlation statistics (for example, simple unfolding via moving average breaks the long-range correlations).

Task 6.1: *Repeat the calculations of Task 3.1, but for a 3D box with incommensurate edge lengths. Plot the level density and the accumulated level density, carry out the unfolding, and show the NNSD for the unfolded levels. Try to do the unfolding both by means of the exact formula (75) and by a polynomial fit.*

Task 6.2: *Use the routine of Task 6.2 and calculate the spectrum of a random matrix. Unfold it via the exact formula (76) and via a polynomial approximation. Calculate and compare the NNSD with the expected Wigner distribution (53). Play with the degree of the unfolding polynomial. Try to cut the "head" and "tail" of the unfolded spectrum and observe changes (improvements) in the resulting NNSD.*

6.3 Brody distribution

Physical systems, especially those with low number of degrees of freedom, usually exhibit mixed-type of dynamics. In the classical physics it means that at given energy E there are islands in the phase space with regular dynamics (zero Lyapunov exponent) surrounded by chaotic sea (positive Lyapunov exponent). Hence we cannot expect purely Poissonian or Gaussian-Ensemble-like level statistics in the quantum mechanics, but some kind of mixture of both.

It has been conjectured [19] (*Percival conjecture*) that the parts of the quantum spectrum that correspond to the remnants of classical tori (regions with classical stable dynamics) are statistically independent of the parts related with the chaotic classical regions, so that the energy level sequence is a mixture of levels with Wigner and with Poissonian statistics. Mathematically it is described by the *Berry-Robnik distribution* [20]. However, in practice, it is much more common to use the *Brody distribution* [21], which is, in fact, an artificial distribution obtained by assuming level repulsion

$$\mu(s) = s^\omega \tag{78}$$

in formula (20). It leads to the nearest neighbour level distribution in the form

$$P_{\text{Brody}}(s; \omega) = N_\omega(\omega + 1)s^\omega \, \mathrm{e}^{-N_\omega s^{\omega+1}} \tag{79}$$

$$N_\omega = \left[\Gamma\left(\frac{\omega + 2}{\omega + 1} \right) \right]^{\omega+1},$$

where Γ is the Euler Gamma function and $\omega \in [0, 1]$ is a parameter that measures the chaoticity of the system: When $\omega = 0$, Brody distribution coincides with Poissonian distribution, whereas for $\omega = 1$ it gives Wigner GOE distribution. This parameter is usually fitted from the unfolded NNSD by means of the least-square fit. Brody distribution for various values of parameter ω is depicted in Figure 3.
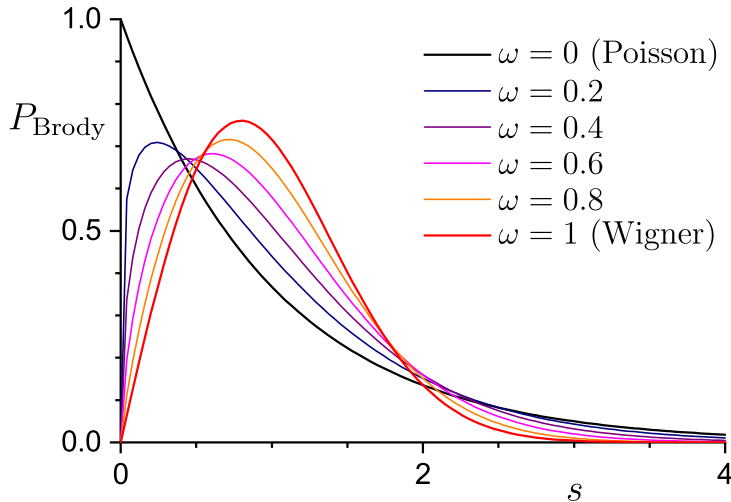

Figure 3: Brody distribution (79) for various values of parameter ω.

Despite having known conflicts with theoretical predictions for the NNSD behaviour, Brody distribution is highly successful and often gives better estimate of the degree of system's chaoticity than other more firmly founded theoretical distributions.[18]

6.4   Long-range correlations

Short-range correlations, such as NNSD, are usually the first choice to study the chaotic properties of a system. They are easy to work with and quite resistant to unsuitably performed unfolding procedures. However, we may need a more sensitive indicator of deviation from the Random Matrix Theory in the spectral statistic, and that is when the long-range correlations come in handy.

---

[18]Apart from the Berry-Robnik distribution, there is also Izrailev distribution [22], Caurier-Grammaticos-Ramani distribution and Lenz-Haake distribution on the market. The last two have been constructed for 2×2 matrices only. The main difference between various distributions is in the form of chaotic perturbation they assume.

6.4.1 Δ_3 statistics

This is one of the most commonly used long-range statistics. It consists of approximating the unfolded cumulative level density $\overline{N}(e)$ with line segments of length L and taking the average square deviation,

$$\Delta_3(E_0; L) = \frac{1}{L} \left\langle \min_{a,b} \int_{e_0 - \frac{L}{2}}^{E_0 + \frac{L}{2}} \left[\overline{N}(e) - ae - b \right]^2 \mathrm{d}e \right\rangle, \tag{80}$$

where $\langle \bullet \rangle$ denotes averaging over the ensemble (it is also possible to average over E_0 if the dynamics depends weakly on the energy). For discrete set of unfolded levels e_j there exists a practical formula to calculate Δ_3 [23],

$$\Delta_3(L) = \frac{n^2}{16} - \frac{1}{L^2} \left[\sum_{j=1}^{n} \tilde{e}_j \right]^2 + \frac{3n}{2L^2} \sum_{j=1}^{n} \tilde{e}_j^2 - \frac{3}{L^4} \left[\sum_{j=1}^{n} \tilde{e}_j^2 \right]^2 + \frac{1}{L} \left[\sum_{j=1}^{n} (n - 2j + 1) \tilde{e}_j \right], \tag{81}$$

$$\tilde{e}_j = e_j - E_0,$$

where $n \approx L$ is the number of levels within the interval $[E_0 - L/2, E_0 + L/2]$. For L large, this statistic behaves like

$$\Delta_3(L) = \begin{cases} \frac{1}{12} & \text{for equidistant spectrum,} \\ \frac{L}{15} & \text{for integrable (Poissonian) spectrum,} \\ \frac{1}{\pi^2 \beta} \ln L + c_\beta + \mathcal{O}(L^{-1}) & \text{for spectrum of Gaussian random matrices,} \end{cases} \tag{82}$$

where β is the Dyson index and

$$c_1 = \ln 2\pi + \gamma - \frac{\pi^2}{8} - \frac{5}{4}, \tag{83}$$

γ being the Euler-Mascheroni constant.[19]

6.4.2 Σ^2 statistics

This statistic is also often called *number variance*, and it is the variance of the number of levels on intervals of length L,

$$\sigma^2(E_0; L) = \left\langle [\#(E_0; L) - L]^2 \right\rangle = \left\langle \left[\overline{N}\left(E_0 + \frac{L}{2} \right) - \overline{N}\left(E_0 - \frac{L}{2} \right) - L \right]^2 \right\rangle, \tag{85}$$

where $\#(E_0; L)$ is the number of levels on interval $[E_0 - L/2, E_0 + L/2]$. This statistics is easier to calculate, but it fluctuates more than the statistics Δ_3. Therefore, it is more suitable if we have a large set of levels or if we can perform the averaging $\langle \bullet \rangle$ over many realisations.

For large L, this statistic behaves like

$$\Sigma^2(L) = \begin{cases} 0 & \text{for equidistant spectrum,} \\ L & \text{for integrable (Poissonian) spectrum,} \\ \frac{2}{\pi^2 \beta} \ln L + d_\beta + \mathcal{O}(L^{-1}) & \text{for spectrum of Gaussian random matrices,} \end{cases} \tag{86}$$

where

$$d_1 = \ln 2\pi + \gamma - \frac{\pi^2}{8} + 1. \tag{87}$$

Task 6.3: *Calculate the Δ_3 and Σ^2 statistics for the integrable 2D box with spectrum (24) and for the unfolded* GOE *spectra obtained in Task 6.2 and compare numerical results with theretical asymptotic formulae (82) and (85). Show that a wrong unfolding leads to high deviations in the long-range correlations.*

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[19]

$$\gamma = \lim_{n \to \infty} \left(-\ln n + \sum_{j=1}^{n} \frac{1}{k} \right) = -\int_0^\infty \mathrm{e}^{-x} \ln x \, \mathrm{d}x \approx 0.577216 \tag{84}$$

7 Quantum standard map

Quantum standard map models, for example, atoms and molecules under short pulses of a laser beam. Hamiltonian of the standard map

$$H = \frac{p^2}{2} + V(q) \sum_{n=-\infty}^{\infty} \delta(t - n), \tag{88}$$

where (p, q) are canonically conjugate momentum and coordinate. The potential is periodic in q,

$$V(q + k) = V(q), \quad k \in \mathbb{Z}. \tag{89}$$

and for the standard map, it reads as

$$V(q) = \frac{K}{(2\pi)^2} \cos 2\pi q. \tag{90}$$

The coordinate at n-th kick, and the momentum just before and just after the n-th kick, are

$$p_{n+1} = p_n - \frac{\mathrm{d}V}{\mathrm{d}q}(q_n) = p_n + \frac{K}{2\pi} \sin 2\pi q, \tag{91a}$$

$$q_{n+1} = (q_n + p_{n+1}) \mod 1 \tag{91b}$$

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