

Lecture 11 - Eigenstate thermalization hypothesis cont.

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Ref: L. D'Alessio et al, Advances in Physics, 65, 232 (2016)

Last time we argued that in order for a quantum system to thermalize, it needs to be in a highly-entangled state, such that the reduced density matrix of a small subsystem B is mixed. In this case we can hope that expectation values of observables local to B agree with those of thermal ensembles. If $H = H_A \otimes H_B$, we can think of A as the environment of B. Systems that are thermally coupled to an environment are highly entangled.

So far our arguments have mostly been words and definition, though physically motivated. To make a bit more progress we need to understand when we expect such states and when we expect thermalization. For that we need to venture a bit into quantum chaos and random-matrix theory.

Random-matrix theory

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Take a look at the spectrum of a nuclei and focus on energy levels far above the lowest one. The distribution and spacing of these levels, which are the eigenvalues of the Hamiltonian H_{nuc} describing the nuclei

$$H_{\text{nuc}} |E_i\rangle = E_i |E_i\rangle$$

looks completely random. Solving for the exact levels is complicated and perhaps it is not even useful to know the exact spectrum $\{E_i\}$. Instead, it may suffice to know some statistical properties of the spectrum $\{E_i\}$, such as the mean-level spacing and the level spacing distribution $P(s)$.

This lead Wigner in the 1950's to suggest a statistical theory of energy levels which then evolved into random-matrix theory. Important contributions were also made by Dyson in a series of beautiful J. Math. Phys. papers in 1962.

The essential idea is to replace the complicated matrix H_{nuc} by a random matrix H_{RMT} . With minimal assumptions on the distribution of the levels, we can calculate various things.

Example - 2 levels

We can understand a lot by looking at the example of only two levels. write

$$H = \begin{pmatrix} \epsilon_1 & v/\sqrt{2} \\ v^*/\sqrt{2} & \epsilon_2 \end{pmatrix}$$

The factor of $\sqrt{2}$ is there such that the form of the Hamiltonian is left invariant under a general basis transformation. Assume $\epsilon_1, \epsilon_2, v$ all Gaussian distributed with (assume v real)

$$\langle \epsilon_1 \rangle = \langle \epsilon_2 \rangle = \langle v \rangle = 0$$

$$\langle \epsilon_1^2 \rangle = \langle \epsilon_2^2 \rangle = \langle v^2 \rangle = \sigma$$

H has eigenvalues

$$E_{1,2} = \frac{\epsilon_1 + \epsilon_2}{2} \pm \frac{1}{2} \sqrt{(\epsilon_1 - \epsilon_2)^2 + 2|v|^2}$$

or

$$\bar{E} = \frac{E_1 + E_2}{2} = \frac{\epsilon_1 + \epsilon_2}{2}$$

$$s = E_1 - E_2 = \sqrt{(\epsilon_1 - \epsilon_2)^2 + 2|v|^2}$$

We can now calculate the level spacing distribution

$$P(s) = \langle \delta(s - \sqrt{(\epsilon_1 - \epsilon_2)^2 + 2|v|^2}) \rangle$$

$$= \frac{1}{(2\pi)^{3/2} \sigma^3} \int d\epsilon_1 \int d\epsilon_2 \int dv \delta(s - \sqrt{(\epsilon_1 - \epsilon_2)^2 + 2|v|^2}) \exp\left(-\frac{\epsilon_1^2 + \epsilon_2^2 + |v|^2}{2\sigma^2}\right)$$

This is an gaussian integral that can be performed, see e.g. p. 247 in D'Alessio et al.

with result

$$P(s) = \frac{s}{2\sigma^2} e^{-s^2/4\sigma^2}$$

Note that $\lim_{s \rightarrow 0} P(s) = 0 \Rightarrow$ level repulsion

We assumed V real. Therefore H was real. A real matrix is left invariant (that is, it remains real) under orthogonal transformation

$$OHO^T \sim H$$

with $O O^T = O^T O$. This ensemble of Hamiltonians is therefore called Gaussian orthogonal ensemble (GOE).

In order to have a real Hamiltonian requires the presence of time reversal

$$THT^{-1} = H$$

with $T^2 = +1$. For example one can take $T = K$ with K complex conjugation. Then

$$H^* = H.$$

If there is no time-reversal symmetry, then H is in general complex. V is complex, and we can treat $\text{Im } V$ and $\text{Re } V$ as independent variables. We now get, with an analogous calculation

$$P(s) = \frac{s^2}{2\pi\sigma^3} \cdot e^{-s^2/4\sigma^2}$$

As before $P(s) \rightarrow 0$ as $s \rightarrow 0$, but now faster.

That is, there is even more level repulsion. The reason is that there are now more parameters to vary to make $E_1 = E_2$, so the probability is smaller.

Now, a general complex matrix is left invariant under unitary transformations

$$U H U^\dagger \sim H$$

with $U U^\dagger = U^\dagger U = 1$, U is a unitary matrix.

This is the Gaussian unitary ensemble (GUE)

Finally, if $T^2 = -1$ and $THT^{-1} = H$, which happens when you have half-integral spin, then the elements of H are quaternions and it is left invariant under

symplectic transformations: S symplectic if $S^T \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
 \Rightarrow Gaussian symplectic ensemble (GSE). with $11 N \times N$ unit matrix
and S $2N \times 2N$.

Traditionally these ensembles are denoted by an index

β	ens	β
GOE		1
GUE		2
GSE		4

β counts the number of real parameters needed to specify each element.

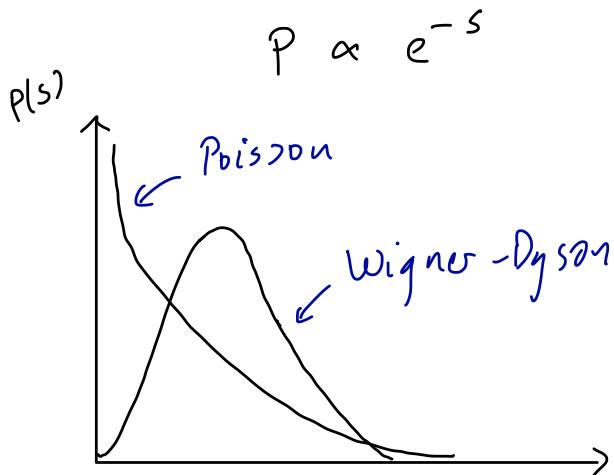
For larger matrices the level spacing distribution is more complicated, but surprisingly well approximated by the so-called Wigner-Dyson distribution:

$$P(s) = A_\beta s^\beta e^{-B_\beta s^2}$$

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A_β and B_β are coefficients found by normalizing $P(s)$ and fixing the mean level spacing.

This should be compared with completely independent levels that have a level spacing distribution that is Poissonian



When do we expect to get each distribution.

Quantum chaos:

$$\begin{array}{ccc} \text{Classical dynamics} & & \text{Quantum level spacing} \\ \text{chaotic} & \rightarrow & \text{Wigner-Dyson} \\ \text{integrable} & \rightarrow & \text{Poisson} \end{array}$$

See: A.O. Stone, "Einstein's unknown insight and the problem of quantizing chaos", Physics Today 58 37, (2005)

More generally, we have a relation

$$\begin{array}{ccc} \text{ergodic} & \rightarrow & \text{Wigner-Dyson} \\ \text{integrable} & \rightarrow & \text{Poisson (or something else)} \end{array}$$

(This may not always be true but is a good first guess)

Wave functions in random matrix theory

The wave functions in RMT are completely random. In a generic basis $\{|i\rangle\}$ we write

$$|\Psi\rangle = \sum_i \psi_i |i\rangle$$

The joint probability distribution of the components ψ_i can be written

$$P_{GOE}(\psi_1, \psi_2, \dots, \psi_N) \propto \delta\left(\sum_i \psi_i^2 - 1\right)$$

$$P_{GUE}(\psi_1, \psi_2, \dots, \psi_N) \propto \delta\left(\sum_i |\psi_i|^2 - 1\right)$$

Matrix elements

Suppose now we have an operator

$$\hat{O} = \sum_i O_i |i\rangle \langle i| \quad \text{with} \quad \hat{O} |i\rangle = O_i |i\rangle$$

For a given Hamiltonian with eigenstates $|m\rangle$ and $|n\rangle$

$$O_{mn} = \langle m | \hat{O} | n \rangle = \sum_i O_i \langle m | i \rangle \langle i | n \rangle = \sum_i O_i \overline{\psi_{m,i}^* \psi_{n,i}}$$

Now use

$$\overline{\psi_{m,i}^* \psi_{n,j}} = \frac{1}{D} \delta_{mn} \delta_{ij}$$

where the overbar means an average over the distribution of ψ_m and ψ_n . D is the dimension of H . Using this

$$\bar{O}_{mn} = \frac{1}{D} \sum_i O_i \equiv \bar{O}$$

and

$$\bar{O}_{mn} = 0 \quad \text{if } m \neq n$$

Fluctuations of matrix elements about their mean are also suppressed

$$\begin{aligned}\overline{\delta O_{mm}^2} &= \overline{O_{mm}^2} - \overline{O_{mm}}^2 \\ &= \sum_{ij} O_i O_j \overline{\Psi_{m,i}^* \Psi_{m,i} \Psi_{m,j}^* \Psi_{m,j}} - \sum_{ij} O_i O_j \overline{\Psi_{m,i}^* \Psi_{m,i}} \overline{\Psi_{m,j}^* \Psi_{m,j}}\end{aligned}$$

To calculate the expectation value of 4 wave functions $\overline{\Psi_i^* \Psi_j^* \Psi_k^* \Psi_l}$, we use Wick's theorem that states that such expectation values are given by all possible pairings of wave functions into products of expectation values of the pairs: (This is true for Gaussian probability distributions)

Complex case:

$$\overline{\Psi_{i_1}^* \Psi_{i_2}^* \dots \Psi_{i_N}^* \Psi_{j_1} \Psi_{j_2} \dots \Psi_{j_N}} = \sum_p \overline{\Psi_{i_{p_1}}^* \Psi_{j_1}} \overline{\Psi_{i_{p_2}}^* \Psi_{j_2}} \dots \overline{\Psi_{i_{p_N}}^* \Psi_{j_N}}$$

Real case:

$$\overline{\Psi_{i_1} \Psi_{i_2} \dots \Psi_{i_{2N}}} = \sum_{\substack{\text{pairings} \\ \{i_1, \dots, i_{2N}\}}} \overline{\Psi_{i_{k_1}} \Psi_{i_{k_2}}} \overline{\Psi_{i_{k_3}} \Psi_{i_{k_4}}} \dots \overline{\Psi_{i_{k_{2N-1}}} \Psi_{i_{k_{2N}}}}$$

Sketch of a proof:

Let's do the real case. For a general gaussian probability distribution of N variables $\vec{\Psi} = (\Psi_1, \dots, \Psi_N)$ we have

$$P(\vec{\Psi}) = \frac{\sqrt{\det A}}{(2\pi)^{N/2}} e^{-\frac{1}{2} \vec{\Psi}^T A \vec{\Psi}}$$

with A a real positive-definite symmetric $N \times N$ matrix. We then have

$$\int d\vec{\Psi} P(\vec{\Psi}) = 1.$$

You can show this by diagonalizing A and change variables to this diagonal basis. The N -dimensional integral is then a product of N gaussian integrals

$$\int_{-\infty}^{\infty} dx_i e^{-\frac{a_i}{2} x_i^2} = \sqrt{\frac{2\pi}{a_i}}$$

with a_i eigenvalues of A . Remember also that $\det A = \prod a_i$.

We can further show that

$$\int d\bar{\psi} P(\bar{\psi}) e^{\bar{j}^T \cdot \bar{\psi}} = e^{\frac{1}{2} \bar{j}^T \cdot \bar{A}^{-1} \bar{j}} \quad (*)$$

where \bar{j} is an arbitrary N -component vector. This is obtained by a shift in the integration variables $\bar{\psi} \rightarrow \bar{\psi} + \bar{A}^{-1} \bar{j}$. This integral serves as a generator of correlation functions. For example, acting on the right hand side with

$$\begin{aligned} \frac{\partial^2}{\partial j_m \partial j_n} \int d\bar{\psi} P(\bar{\psi}) e^{\bar{j}^T \cdot \bar{\psi}} \Big|_{\bar{j}=0} &= \int d\bar{\psi} P(\bar{\psi}) \psi_m \psi_n e^{\bar{j}^T \cdot \bar{\psi}} \Big|_{\bar{j}=0} \\ &= \int d\bar{\psi} P(\bar{\psi}) \psi_m \psi_n = \overline{\psi_m \psi_n} \end{aligned}$$

Taking the same derivative on the right hand side, we get

$$\begin{aligned} \frac{\partial^2}{\partial j_m \partial j_n} e^{\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j}} \Big|_{\bar{j}=0} &= \frac{\partial}{\partial j_m} \left(\frac{\partial}{\partial j_n} \left(\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j} \right) e^{\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j}} \right) \Big|_{\bar{j}=0} \\ &= \left[\frac{\partial^2}{\partial j_m \partial j_n} \left(\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j} \right) e^{\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j}} + \frac{\partial}{\partial j_n} \left(\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j} \right) \frac{\partial}{\partial j_m} \left(\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j} \right) e^{\frac{1}{2} \bar{j}^T \bar{A}^{-1} \bar{j}} \right] \Big|_{\bar{j}=0} \end{aligned}$$

Only the first term is nonzero at $\bar{j}=0$ and we get

$$= \frac{1}{2} (\bar{A}_{mn}^{-1} + \bar{A}_{nm}^{-1}) = \bar{A}_{mn}^{-1}$$

Since A is symmetric. We have obtained:

$$\overline{\psi_m \psi_n} = \bar{A}_{mn}^{-1}$$

This can now be iterated. For example

$$\overline{\psi_m \psi_n \psi_q \psi_p} = \bar{A}_{mn}^{-1} \bar{A}_{qp}^{-1} + \bar{A}_{mq}^{-1} \bar{A}_{np}^{-1} + \bar{A}_{mp}^{-1} \bar{A}_{nq}^{-1}$$

Convince yourself that this is true by explicit derivation on both sides of (*). By then replacing \bar{A}_{mn}^{-1} by $\overline{\psi_m \psi_n}$ we get the result we wrote before. The complex case works similarly, with the integral

$$\frac{\det A}{\pi^n} \int d\bar{\psi}^+ d\bar{\psi}^- e^{-\bar{\psi}^+ A \bar{\psi}^- + \bar{\omega}^+ \cdot \bar{\psi}^- + \bar{\psi}^+ \cdot \bar{\omega}^-} = e^{\bar{\omega}^+ A^- \bar{\psi}^-}$$

assuming A hermitian.

Now, let's us this to calculate the expectation values we need:

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ψ real:

$$\overline{\psi_i \psi_i \psi_j \psi_j} = \overline{\psi_i^2} \overline{\psi_j^2} + 2\delta_{ij} \overline{\psi_i^2}$$

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$$so \quad \overline{\delta O_{mm}^2} = 2 \sum_i O_i^2 \overline{\Psi_i^2} = \frac{2}{D^2} \sum_i O_i^2 \equiv \frac{2}{D} \overline{O^2}$$

ψ complex

$$\underbrace{\psi_i^* \psi_i \psi_j^* \psi_j}_{\text{Pex}} = |\overline{\psi_i}|^2 |\overline{\psi_j}|^2 + \delta_{ij} \overline{|\psi_i|^2}$$

$$\text{so } \overline{\delta O_{mm}^2} = \frac{1}{D} \overline{O^2} \quad \text{or} \quad \overline{\delta O_{mm}^2} = \frac{3\beta}{D} \overline{O^2} \quad \text{for } \beta=1, 2.$$

$$\text{Similarly : } \overline{|O_{mn}|^2} - \overline{|O_{mn}|}^2 = \frac{1}{D} \overline{O^2}$$

$$\begin{aligned}
 & \frac{\psi_{m_1}^n \psi_{m_2}^n \psi_{p_1}^{n_1} \psi_{p_2}^{n_2}}{\psi_{a_1} \psi_{a_2} \psi_{p_1} \psi_{p_2}} \\
 &= \frac{1}{\beta^2 - 1} (\delta_{m_1 n_1} \delta_{a_1 p_1} \delta_{m_2 n_2} \delta_{a_2 p_2} + \delta_{m_1 n_2} \delta_{a_1 p_2} \delta_{m_2 n_1} \delta_{a_2 p_1}) \\
 & - \frac{1}{(\beta \alpha^2 - 1)} (\delta_{m_1 n_1} \delta_{a_1 p_2} \delta_{m_2 n_2} \delta_{a_2 p_1} + \delta_{m_1 n_2} \delta_{a_1 p_1} \delta_{m_2 n_1} \delta_{a_2 p_2})
 \end{aligned}$$

Taken together, to leading order in $\frac{t}{D}$

$$O_{mn} = \bar{O} \delta_{mn} + \sqrt{\frac{O^2}{D}} R_{mn}$$

$$O_{mn} = \bar{O} \delta_{mn} + \sqrt{\frac{1}{D} (\bar{O}^2 - \bar{o}^2)} R_{mi}$$

See details in the note for exercise class 5

where R_{nn} is a random variable with zero mean and unit variance (2 for diagonal part of GOE)

Entanglement entropy

Page ('93) calculated the entanglement entropy of a random state and showed it follows a volume law — see problem set 3.

Quantum quench

Prepare system in pure state $|\psi_0\rangle = \sum_m c_m |m\rangle$ with $|m\rangle$ the eigenvectors of Hamiltonian $H|m\rangle = E_m |m\rangle$. Time evolve with

$$H: \quad |\psi(t)\rangle = \sum_m c_m e^{-iE_m t} |m\rangle$$

Time evolution of observable \hat{O} :

$$\begin{aligned} O(t) &= \langle \psi(t) | \hat{O} | \psi(t) \rangle = \sum_{m,n} c_m^* c_n e^{i(E_m - E_n)t} O_{mn} \\ &= \sum_m |c_m|^2 O_{mm} + \sum_{m \neq n} c_m^* c_n e^{i(E_m - E_n)t} O_{mn} \end{aligned}$$

At long times second term dephases to zero

$$O(+ \rightarrow \sum_m |c_m|^2 O_{mm}$$

If O thermalizes, this should agree with the microcanonical expectation value. How can it? Seems to depend on details of initial state. But if H a random matrix, then $O_{mm} \approx \bar{O}$ and

$$\sum_m |c_m|^2 O_{mm} \approx \bar{O} \sum_m |c_m|^2 = \bar{O}$$

in agreement with microcanonical ensemble at $\beta=0$, i.e., infinite temperature.

Then $S_{th} = \frac{1}{2} e^{-\beta \hat{H}} \rightarrow \frac{1}{D} \mathbb{1}$ with D the Hilbert space dimension, and $\langle \hat{O} \rangle_{th} = \text{tr}(\hat{\rho} \hat{O}) = \frac{1}{D} \text{tr}(\hat{O}) = \bar{O}$.

The eigenstate thermalization hypothesis

Random matrix theory can not generally describe observables in experiments since these do depend on temperature. The eigenstate thermalization hypothesis is a generalization which takes the form of an ansatz for matrix elements:

$$O_{mn} = O(\bar{E}) \delta_{mn} + e^{-S(\bar{E})/2} f_o(\bar{E}, \omega) R_{mn}$$

Here $\bar{E} = \frac{E_n + E_m}{2}$ and $\omega = E_n - E_m$

$S(\bar{E})$ thermodynamic entropy at \bar{E}

f_0 and O smooth functions of their arguments

Why $e^{-S/2}$? Compare with RMT where random term $\sim \frac{1}{D^{1/2}}$. Here fluctuations of all states Ω consistent with the microcanonical ensemble: $\frac{1}{D^{1/2}} \rightarrow \frac{1}{\Omega^{1/2}}$

but $S = \ln \Omega$ or $\Omega = e^S$

If we look at a very small energy window such that in that window $O(\bar{E}) = \bar{O}$ and $f_0(\bar{E}, \omega)$ are constants the ETH \rightarrow RMT.

Relevant energy scale: Thouless energy $E_T = \frac{\hbar D}{L^2}$

with D the diffusion constant $E_T \sim \frac{1}{\tau_T}$ when τ_T the time it takes to diffuse to the size of the system

$$L^2 \sim D \tau_T$$

ETH and thermalization

$\bar{O}(\bar{E})$ agrees with statistical mechanics ensembles provided

$$\langle E \rangle = \langle \psi_0 | H | \psi_0 \rangle = \text{tr} (\hat{S}_{\text{th}} H)$$

That is: the temperature is determined by the energy density in the initial state.