Lecture Notes

Random matrix theory and eigenstate thermalization

Many-body Quantum Dynamics: Lectures III & IV

October 17 & 19 2023

Contents

1 Selected bibliography

These notes are based on the following references:

- F. H. L. Essler and M. Fagotti, "Quench dynamics and relaxation in isolated integrable quantum spin chains," J. Stat. Mech. **2016**, 064002 (2016)
- L. D'Alessio, Y. Kafri, A. Polkovnikov, and M. Rigol, "From quantum chaos and eigenstate thermalization to statistical mechanics and thermodynamics," Adv. Phys. **65**, 239 (2016)
- S. Pappalardi, Lecture notes on "Introduction to the Eigenstate Thermalization Hypothesis and Beyond"
- For more details on Random Matrix Theory, this book presents an accessible introduction: G. Livan, M. Novaes, and P. Vivo, Introduction to Random Matrices, Springer Briefs in Mathematical Physics, Vol. 26 (2018).

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2 Introduction

In these lectures, we will consider how many-body quantum systems relax to equilibrium, and how the resulting equilibrium properties return the expected behavior from (classical) statistical mechanics.

Classically, our understanding of statistical mechanics starts from the notions of chaos and *ergodicity*. The ergodic hypothesis says that, if we evolve a system in time, it will visit every region in the accessible phase space, and the time spend in any region of the phase space is proportional to the volume of the region. Every microstate in phase space results in a specific value of the observable, but some microstates are much more likely to be visited than others (as quantified through the notion of entropy), and the long-time behaviour of any observable will correspond to the behaviour of these microstates. Such microstates can be found by maximizing the entropy, resulting in a Gibbs ensemble describing the long-time behaviour.

Quantum mechanically, the dynamics of an isolated system follows from the time-dependent Schrödinger equation:

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle \ . \tag{1}$$

For any initial state $|\psi_0\rangle$, this equation can be formally solved as

$$|\psi(t)\rangle = e^{-i\hat{H}t} |\psi_0\rangle = \sum_n e^{-iE_n t} |n\rangle \langle n|\psi_0\rangle \ , \tag{2}$$

where we have set $\hbar = 1$ and introduced an eigenvalue decomposition of the Hamiltonian as

$$\hat{H} |n\rangle = E_n |n\rangle \, . \tag{3}$$

Clearly, all dynamics is encoded in the eigenvalues and eigenstates of the Hamiltonian. There are now two apparent issues.

First, on the practical level, we are interested in the dynamics of *generic* many-body systems – by which we mean that these models cannot be solved analytically and we need to resort to numerical approaches. However, for a system consisting of L spin-1/2 particles, we are faced with the issue that the resulting Hilbert space has a dimension of 2^L. Exact diagonalization of the Hamiltonian matrix rapidly falls out of reach of any computational method for even relatively modest system sizes, and it becomes impossible to exactly obtain the eigenstates.

On a more fundamental level, this dynamics corresponds to a unitary transformation of the initial state with $U(t) = e^{-i\hat{H}t}$. In principle, it is possible to undo this transformation, and the state at $t = 0$ can be exactly recovered from the state at an arbitrary time t by acting with the operator $U^\dagger(t)$. The unitarity clearly precludes any relaxation of the quantum state to equilibrium, since different initial states should give rise to the same equilibrium states. Furthermore, statistical physics tells us that these equilibrium states should not depend on any microscopic properties of the initial states (e.g. the overlaps with eigenstates of a Hamiltonian), but only on the macroscopic properties encoded in the conservation laws (e.g. conservation of energy).

These issues can be resolved simultaneously: quantum mechanical systems relax *locally* rather than *globally*, and for local observables the excited eigenstates of a chaotic Hamiltonian can be treated as the eigenstates of random matrix. This local relaxation implies that, even if the (global) state exhibits nontrivial dynamics, the system can be static if we focus on local observables. Furthermore, eigenstates at a fixed energy behave as thermal states at the same energy, in a way that will be made precise later. As such, rather than making exact statements about specific eigenstates, within chaotic systems it is possible to make exact statements about the statistical properties of many eigenstates. Chaotic Hamiltonians behave like random matrices in many ways, and this emergent randomness gives rise to relaxation to equilibrium and

the emergence of universal behavior at late times. Effectively, the full wave function acts as a thermal bath for any local subsystem.

3 Local thermalization

As mentioned, quantum dynamics corresponds to the unitary transformation of an initial state. However, these states are not physical observables. Consider a physical observable $\hat{O}$, then its dynamics is given by

$$\langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle = \sum_{m,n} c_n^* c_m O_{nm} e^{-i(E_m-E_n)t}\,, \tag{4}$$

with $O_{nm} = \langle n|\,\hat{O}\,|m\rangle$ and $c_n = \langle n|\psi(t=0)\rangle$. We can separate the static part from the dynamic part, writing

$$\langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle = \sum_n |c_n|^2 O_{nn} + \sum_{n,m\neq n} c_n^* c_m O_{nm} e^{i(E_n-E_m)t}, \tag{5}$$

assuming that there are no degeneracies in the spectrum, i.e. $E_n \neq E_m$ if $n \neq m$. At long times, we could expect that oscillations dephase and cancel out, such that

$$\lim_{t\to\infty} \langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle = \sum_n |c_n|^2 O_{nn}. \tag{6}$$

In this way relaxation can be obtained. However, this is still far from thermalization: The final value of the observable depends on the overlap of the initial state with all eigenstates of the Hamiltonian, not just on the energy, and we have also assumed that the oscillations cancel out in some way, which is not a given. For example, if there are a large amount of states for which $E_n - E_m$ is approximately equal, these will not cancel out. So we need some further information about both the eigenstates and the matrix elements of the observable. Additionally, dephasing only can not be responsible for relaxation: the time scale for dephasing is set by the closest energy difference (recall the Heisenberg uncertainty principle for time and energy), which is exponentially small in system size. Still, any steady-state value should correspond to the above result.

Eq. (5) also highlights that relaxation depends on the observable under consideration and can not be generically expected for any Hermitian operator. If we consider e.g. a Hermitian operator of the form $\hat{O} = |p\rangle\langle q| + |q\rangle\langle p|$ and consider its time evolution from a random initial state $|\psi(t=0)\rangle$, we will have

$$\langle\psi(t)|\,\hat{O}\,|\psi(t)\rangle = c_p^* c_q e^{i(E_p-E_q)t} + c.c., \tag{7}$$

which is pure oscillation and hence never reaches a steady-state value. If we wish to see thermalization, we need to restrict ourselves in some way. This is usually done by considering local observables, i.e. if we have a full lattice of L spins, we focus on operators that only act on a local subset of these spins. The projection operators from the above equation are horribly nonlocal, acting on the full system, whereas quantum systems typically relax locally. In this way only 'physical' observables are expected to thermalize.

In the above figure, suppose we have an operator $\hat{O}_A$ that only acts on the subsystem A. The corresponding operator for the full system can be written as $\hat{O} = \hat{O}_A \otimes \mathbb{1}_B$. We can write the expectation value of this operator as

$$\langle\psi(t)|\hat{O}|\psi(t)\rangle = \mathrm{Tr}\left[\hat{O}\,|\psi(t)\rangle\langle\psi(t)|\right] = \mathrm{Tr}\left[\hat{O}_A \otimes \mathbb{1}_B\,|\psi(t)\rangle\langle\psi(t)|\right] = \mathrm{Tr}_A\left[\hat{O}_A \rho_A\right], \tag{8}$$

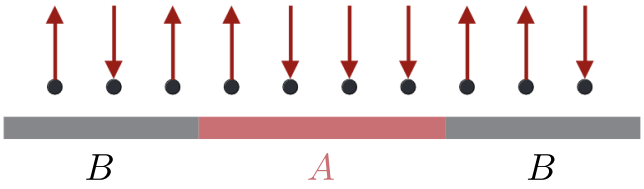

Figure 1: Local relaxation in an isolated many-particle quantum system: we partition the entire system into an arbitrary finite subsystem A and its complement B. We then take the thermodynamic limit while keeping A fixed. Expectation values of all operators that act non-trivially only in A will relax to stationary values at late times.

where we have introduced the *reduced density matrix* ρ_A as

$$\rho_A = \mathrm{Tr}_B \left[|\psi(t)\rangle \langle \psi(t)| \right] . \tag{9}$$

This reduced density matrix fully determines all expectation value of operator that purely act on the local subsystem A. The crucial observation is that ρ_A can be static even if the wave function $|\psi(t)\rangle$ is not.

Local relaxation. A system is said to relax locally if the limit

$$\lim_{t\to\infty} \lim_{L\to\infty} \rho_A(t) \tag{10}$$

exists for any finite subsystem A. Note that the order of limits is important here – these do not commute. For any finite system size L the limit $t \to \infty$ is undefined since there will be recurrences at late times, which is why we first need to take the thermodynamic limit.

Steady-state density matrices. Clearly, if this limit exists for an initial state $|\psi_0\rangle$, it necessarily corresponds to

$$\lim_{t\to\infty} \lim_{L\to\infty} \rho_A(t) = \mathrm{Tr}_B \left[\rho_{\mathrm{DE}} \right] \qquad \text{with} \qquad \rho_{\mathrm{DE}} = \sum_n |\langle n|\psi_0\rangle|^2 |n\rangle \langle n| , \tag{11}$$

which reproduces the time-averaged value of Eq. (5) and where ρ_{DE} is also known as the *diagonal ensemble*. However, this ensemble depends on the overlap of the initial state with all eigenstates of the Hamiltonian, not just on the energy, so we need exponentially many microscopic numbers determining this ensemble.

Thermalization. Crucially, different global operators can give rise to the same reduced density matrices, e.g. different initial states can give rise to the same reduced density matrices (since moving from global to local operators always induces a loss of information). The connection with statistical mechanics is then made by observing that, in general chaotic quantum systems, the steady-state reduced density matrices satisfy

$$\lim_{t\to\infty} \lim_{L\to\infty} \rho_A(t) = \mathrm{Tr}_B \left[\rho_{\mathrm{Gibbs}} \right] \qquad \text{with} \qquad \rho_{\mathrm{Gibbs}} \equiv \frac{e^{-\beta H}}{\mathcal{Z}}, \tag{12}$$

in which the partition function $\mathcal{Z} = \mathrm{Tr}\left[e^{-\beta H}\right] = \sum_n e^{-\beta E_n}$ guarantees the normalization of the reduced density matrices. In other words, the steady-state reduced density matrices and the diagonal ensemble are *locally equivalent* to the thermal Gibbs distribution with a fixed inverse temperature β.

At late times, the expectation value of any local observable $\hat{O}$ should then reproduce the thermal expectation value, i.e.

$$\lim_{t\to\infty} \lim_{L\to\infty} \langle \psi(t)|\hat{O}|\psi(t)\rangle = \mathrm{Tr}\left[\hat{O}\rho_{\mathrm{Gibbs}}\right] = \frac{1}{\mathcal{Z}} \sum_n \langle n|\hat{O}|n\rangle \, e^{-\beta E_n} . \tag{13}$$

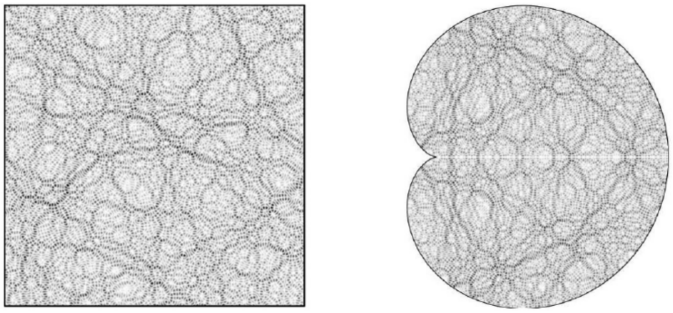

Figure 2: Comparison of the spatial probability density for a highly excited state within a chaotic cardioid billiard (right) and the probability distribution for a random superposition of plane waves (left) at the same energy. From Ref. [1], originally from Ref. [2].

As one particular example, the Hamiltonian is a sum over local observables, so that we can calculate its expectation value from the Gibbs distribution, and we also know that energy should be conserved, $\langle E\rangle = \langle\psi(t)|\hat{H}|\psi(t)\rangle = \langle\psi(0)|\hat{H}|\psi(0)\rangle$. As such, the energy from the Gibbs state should reproduce the initial energy:

$$\mathrm{Tr}\left[\hat{H}\rho_{\mathrm{Gibbs}}\right] = \frac{1}{\mathcal{Z}}\sum_n E_n\, e^{-\beta E_n} = \frac{\sum_n E_n\, e^{-\beta E_n}}{\sum_n e^{-\beta E_n}} = \langle E\rangle\,, \tag{14}$$

which uniquely fixes the inverse temperature β in terms of the energy of the initial state. In this way, we recover the expected result from statistical mechanics.

We emphasize that this equivalence between density matrices only holds locally: the full density matrices are not identical, since they would not reproduce the correct dynamics for e.g. the projectors from Eq. (7). Rather, expectation values of all operators that act non-trivially only in a finite subsystem are identical to the corresponding thermal expectation values. The physical picture underlying thermalization is that the infinitely large complement of our subsystem acts like a heat bath with an effective inverse temperature β. Note also that this inverse temperature need not be positive!

4 Aspects of Random Matrix Theory

In order to obtain a more quantitative understanding of thermalization, it is important to consider the structure of the eigenvalues and eigenstates of generic Hamiltonians and understand in which way we can treat these as random matrices. Here we can start from two numerical observations. A first observation is due to Michael Berry: in Fig. 2 we show the spatial probability density for a single highly excited eigenstate of a single particle in a chaotic cardioid billiard, as compared to a random superposition of plane waves. Locally the two plots are nearly indistinguishable, indicating a high degree of randomness in highly excited eigenstates. A second numerical observation, originally due to Wigner, is that the eigenvalues of highly complicated many-body Hamiltonians exhibit *statistical features* of the eigenvalues of random matrices. Rather than trying to calculate individual eigenvalues, it is possible to make exact statements about the statistical properties of the eigenvalue spectrum. In Fig. 3 we plot the level spacing distribution, i.e. the probability distribution for the distance between subsequent energy levels, $E_{n+1} - E_n$ with $E_{n+1} > E_n$, for the "Nuclear Data Ensemble", which comprises 1726 normalized level spacings for the eigenspectra various heavy nuclei (see Ref. [3] for a

review and references to the original works). This probability distribution can be calculated for an ensemble of random matrices, the so-called Gaussian Orthogonal Ensemble (GOE), and the agreement between the two is remarkable. This distribution is also contrasted with the Poisson distribution that would be obtained if the eigenvalues were statistically independent variables.

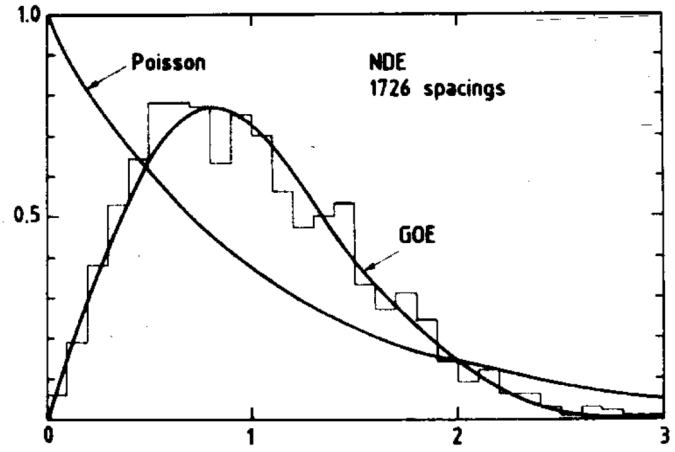

Figure 3: Nearest neighbor spacing distribution for the "Nuclear Data Ensemble" comprising 1726 spacings (histogram) versus $s = S/D$, where D is the mean level spacing and $S_n = E_{n+1} - E_n$ is the actual spacing. Lines represent the GOE and the Poisson distributions. From Ref. [3].

These two pieces of evidence indicate that it is not absurd to treat the (highly structured) Hamiltonians as random matrices. Random matrices have the properties that (a) their eigenvalues obey the so-called *Wigner-Dyson statistics* and (b) their eigenvectors are uncorrelated random unit vectors. We will now briefly review some concepts from random matrix theory (RMT).

Eigenstate properties

If we have eigenstates labelled n, m and expand them in arbitrary basis states labelled i, j (with expansion coefficients $c_n^i, c_m^i, \ldots$), then random matrix theory tells us that the matrix elements are Gaussian random variables satisfying

$$\overline{\left(c_n^i\right)^* \left(c_m^j\right)} = \delta_{ij}\delta_{mn}\frac{1}{\mathcal{D}}, \tag{15}$$

which holds for arbitary basis states, and $\mathcal{D}$ is the dimension of the Hilbert space. Here the overline represent the averaging over different random matrices. Different coefficients of two different states are uncorrelated Gaussian variables, where the variance $|c_i^n|^2$ is independent of both the state and the index. Because of the normalization of the initial state we need that $\sum_{i=1}^{\mathcal{D}} |c_i^n|^2 = 1, \forall n$, which implies the appearance of the factor $1/\mathcal{D}$.

Suppose we have an observable $\hat{O} = \sum_i O_i |i\rangle \langle i|$. The eigenvectors of this operator are a random basis for the eigenstates of the Hamiltonian, so we have

$$\overline{O_{nn}} = \sum_i O_i \overline{\left(c_i^n\right)^* \left(c_i^n\right)} = \frac{1}{\mathcal{D}} \sum_i O_i = \frac{1}{\mathcal{D}} \mathrm{Tr}[\hat{O}] \equiv \overline{O}, \tag{16}$$

$$\overline{O_{mn}} = \sum_i O_i \overline{\left(c_i^m\right)^* \left(c_i^n\right)} = 0, \tag{17}$$

where we have replaced everything with its average value, since we expect fluctuations to be suppressed for large systems. In other words, in the eigenbasis of the Hamiltonian the diagonal matrix elements of an observable are approximately constant, whereas the off-diagonal elements vanish.

Moreover, the fluctuations of the diagonal and off-diagonal matrix elements are suppressed by the size of the Hilbert space. For the diagonal elements

$$\overline{O_{nn}^2} - \left(\overline{O_{nn}}\right)^2 = \sum_{i,j} O_i O_j \overline{\left(c_i^n\right)^* \left(c_i^n\right) \left(c_j^n\right)^* \left(c_j^n\right)} - \sum_{i,j} O_i O_j \overline{\left(c_i^n\right)^* \left(c_i^n\right)} \, \overline{\left(c_j^n\right)^* \left(c_j^n\right)} \tag{18}$$

$$= \sum_i O_i^2 \left(\overline{|c_i^n|^4} - \overline{|c_i^n|^2}^2 \right) = \frac{2}{\mathcal{D}^2} \sum_i O_i^2 \equiv \frac{2}{\mathcal{D}} \overline{O^2} \tag{19}$$

where we have used that these are independent variables for $i \neq j$, and for $i = j$ Gaussian variables satisfy $\overline{|c_i^n|^4} = 3\overline{|c_i^n|^2}^2$ and we have $\overline{|c_i^n|^2} = 1/\mathcal{D}$. Assuming that none of the eigenvalues O_i scales with the size of the Hilbert space, as is the case for physical observables, we see that the fluctuations of the diagonal matrix elements of $\hat{O}$ are inversely proportional to the square root of the size of the Hilbert space.

However, we should be careful with the previous derivation: there exist additional correlations in the overlaps due to the fact that the eigenstates form a complete basis. The effect of these correlations can be seen by choosing $\hat{O} = \mathbb{1}$, for which we would always recover $O_{nn} = 1$ and $O_{mn} = 0$. Crucially, adding any multiple of the identity to the observable should not change the matrix element statistics – whereas it clearly changes $\overline{O^2}$. The issue arises because in the above summations there can be coherent contributions, leading to terms where we can use unitarity. Such coherent contributions are avoided if $\overline{O} = 0$, since then the fact that O_i fluctuates around zero prevents such coherent contributions. These additional correlations can easily be taken into account by redefining $\hat{O} \to \hat{O} - \overline{O}\mathbb{1}$, which does not change the matrix element statistics and corresponds to redefining $\overline{O^2} \to \overline{O^2} - (\overline{O})^2 = \sigma_O^2$ as the variance of the eigenvalues of O. As such, in all results we should read $\overline{O^2}$ as the variance, and the diagonal elements satisfy

$$\overline{O_{nn}^2} - \left(\overline{O_{nn}}\right)^2 = \frac{2}{\mathcal{D}} \sigma_O^2 \,. \tag{20}$$

For off-diagonal elements we similarly find that

$$\overline{O_{mn}^2} - \left(\overline{O_{mn}}\right)^2 = \frac{1}{\mathcal{D}} \sigma_O^2 \,. \tag{21}$$

Combining these expressions we see that, up to leading order in $1/\mathcal{D}$, the matrix elements of any operator in the eigenbasis of the Hamiltonian can be written as

$$O_{mn} = \overline{O}\delta_{mn} + \sqrt{\frac{\sigma_O^2}{\mathcal{D}}} R_{mn}, \tag{22}$$

where R_{mn} is a real variable satisfying $R_{mn} = R_{mn}$ and Gaussian distributed with $\overline{R_{mn}} = 0$ and $\overline{R_{mn}^2} = 1$ if $m \neq n$ and $\overline{R_{nn}^2} = 2$ otherwise. It is straightforward to check that this ansatz reproduces the calculated mean and variance of the matrix elements.

Crucially, this ansatz also results in thermalization! Plugging this ansatz into the diagonal ensemble, we immediately get

$$\lim_{t\to\infty} \langle \psi(t) | \hat{O} | \psi(t) \rangle = \sum_n |c_n|^2 O_{nn} = \sum_n |c_n|^2 \overline{O} = \overline{O} \,. \tag{23}$$

For any initial state, random matrix theory predicts that the steady-state value is given by $\overline{O}$, which is also the Gibbs expectation value at infinite temperature ($\beta = 0$) since $\overline{O} = \mathrm{Tr}[\hat{O}]/\mathcal{D}$. Furthermore, from Eq. (18) it follows that the long-time fluctuations around this steady-state value are suppressed by a factor $1/\mathcal{D}$.

However, we are not there yet. Because of the randomness, the final value of the observable has become completely independent of the initial state, and does not depend on the initial energy! So, apparently eigenstates of physical Hamiltonians have some more structure than a random matrix. This structure is the subject of the Eigenstate Thermalisation Hypothesis (ETH), as proposed by Mark Srednicki in Ref. [4].

The Wigner surmise

Before moving on to ETH, we will first derive an important result on the eigenvalue spacing statistics of random matrices. The Gaussian Orthogonal Ensemble (GOE) is a model for random symmetric matrices (i.e. matrices M satisfying $M^T = M$) whose entries are independent (up to the symmetricity constraint) normal random variables. These matrices are randomly distributed, and the probability of obtaining a given matrix is invariant under orthogonal transformations, i.e. $P(O^T M O) = P(M)$ for $OO^T = \mathbb{1}$. For the GOE the probability density of a matrix M is given by

$$P(M) = \frac{1}{\mathcal{Z}_{\mathrm{GOE}}} \exp\left[-\frac{\mathcal{D}}{4}\mathrm{Tr}(M^2)\right], \tag{24}$$

with normalization obtained as

$$\mathcal{Z}_{\mathrm{GOE}} = \int\!\!\int \prod_{m\leq n} dM_{mn} \exp\left[-\frac{\mathcal{D}}{4}\mathrm{Tr}(M^2)\right]. \tag{25}$$

Note that other ensembles exist, the Gaussian Unitary Ensemble and the Gaussian Symplectic Ensemble, defined for complex matrices and quaternionic ensembles respectively, but here we focus on the GOE. The GOE models real Hamiltonians with time-reversal symmetry, whereas the GUE is appropriate when time-reversal symmetry is broken.

Remarkably, the results from Fig. 3 can be derived already from a simple random matrix with $\mathcal{D} = 2$. Suppose we have a 2×2 random matrix

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{pmatrix}, \tag{26}$$

where the matrix elements are random variables with Gaussian distribution

$$P(M) \propto \exp\left[-\frac{1}{2}\left(M_{11}^2 + M_{22}^2 + 2M_{12}^2\right)\right]. \tag{27}$$

In other words, the diagonal elements are random variables from a Gaussian distribution $\mathcal{N}(\mu, \sigma^2)$ with mean $\mu = 0$ and variance $\sigma^2 = 1$, whereas the off-diagonal element is a random variable from a Gaussian distribution $\mathcal{N}(\mu = 0, \sigma^2 = 1/2)$.

This matrix has two eigenvalues $E_\pm$, which can be directly obtained from the characteristic equation

$$\begin{vmatrix} M_{11} - E & M_{12} \\ M_{12} & M_{22} - E \end{vmatrix} = 0 \qquad \Rightarrow \qquad E^2 - (M_{11} + M_{22})E + (M_{11}M_{22} - M_{12}^2) = 0, \tag{28}$$

leading to

$$E_\pm = \frac{M_{11} + M_{22}}{2} \pm \frac{1}{2}\sqrt{(M_{11} - M_{22})^2 + 4M_{12}^2}, \tag{29}$$

from which we can now calculate the probability density $P(s) = P(E_+ - E_- = s)$ for the level spacing s. We see that $M_{11} + M_{22} = \mathrm{Tr}[M]$ only results in a constant shift for both eigenvalues, since we can subtract $\mathrm{Tr}[M]\mathbb{1}$ from the initial matrix without changing the eigenvalue spacing, and the diagonal elements only appear through $(M_{11} - M_{22})$. The difference of two Gaussian variables with variance $\sigma^2 = 1$ is a Gaussian variable with variance $\sigma^2 = 2$. Writing $\lambda = M_{11} - M_{22}$ and $v = M_{12}$, we have

$$P(s) = \frac{1}{2\pi} \int d\lambda \int dv\, e^{-v^2 - \lambda^2/4} \delta\left(s - \sqrt{\lambda^2 + 4v^2}\right). \tag{30}$$

This integral can be evaluated by introducing polar coordinates $v = r\cos(\theta)/2$ and $\lambda = r\sin(\theta)$, resulting in a Jacobian $dvd\lambda = rdrd\theta/2$ and returning

$$P(s) = \frac{1}{4\pi} \int_0^{2\pi} d\theta \int_0^{\infty} dr\, re^{-r^2/4}\, \delta(s - r) = \frac{s}{2} e^{-s^2/4}. \tag{31}$$

It is often convenient to rescale s in terms of the average level spacing ratio $\int_0^\infty dss P(s)$. Redefining $P(s)$ for this normalized level spacing ratio, we find that

$$P(s) = \frac{\pi s}{2} \exp(-\pi s^2/4). \tag{32}$$

This result is also known as the *Wigner surmise* and is illustrated in Fig. 4. While this expression is not exact for $\mathcal{D} > 2$, it is clearly a very good approximation to the general GOE level spacing statistics also observed in Fig. 3. This statistical behavior is also known as Wigner-Dyson level statistics, and the emergence of Wigner-Dyson statistics for level spacings is often considered as a defining property of quantum chaotic systems.

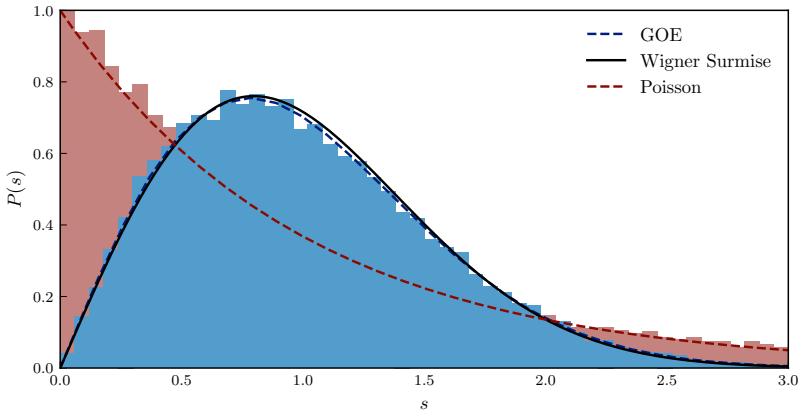

Figure 4: Comparison of the Wigner surmise with the numerically obtained level spacing distribution for a GOE of random matrices and a Poissonian distribution. The histogram represents the spacing for the eigenvalues of a chaotic Hamiltonian (GOE) and for purely random variables (Poisson). In both cases the distributions have been normalized to return an average value of unity.

Level repulsion. One important result from Eq. (32) is that the probability of observing a level spacing s vanishes as $s \to 0$. Effectively, chaotic models exhibit level repulsion. This can be made apparent by showing the eigenstate spectrum of a chaotic Hamiltonian as a variable in this Hamiltonian is smoothly changed, as illustrated in Fig. 8 below. Clearly, the eigenvalues 'repel' each other and exhibit *avoided crossings*. Physically, this highlights the difficulty of preparing systems in excited eigenstates of chaotic systems, since each avoided crossing will

result in Landau-Zener dynamics (see later) and excited states can not be smoothly connected to eigenstates in a simple, e.g. noninteracting, limit.

Non-chaotic models. As one comment, we note that integrable (i.e. non-chaotic) systems do not exhibit Wigner-Dyson statistics. This is the subject of the *Berry-Tabor conjecture*: Berry and Tabor postulated that the energy spectra in "generic" integrable systems satisfies Poisson statistics with $P(s) = e^{-s}$ [5]. The qualitative argument underlying the conjecture is very intuitive and can be illustrated using the simple example of N harmonic oscillators with incommensurate frequencies. The incommensurability here is precisely the condition defining that this system is "generic" integrable, and we can consider a Hamiltonian

$$\hat{H} = \sum_{k=1}^{N} \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k \,. \tag{33}$$

The frequencies ω_k can e.g. represent the normal modes of a harmonic chain. The energy spectrum of this model immediately follows as the sum of the energies of different modes:

$$E_{n_1,\ldots n_N} = \sum_k \hbar\omega_k n_k, \tag{34}$$

where n_k are arbitrary integers. Unless the frequencies ω_k are commensurate with each other, the high-energy states are completely uncorrelated because states with a similar energy can arise from very different combinations of the occupation numbers n_k. Such a lack of correlations between nearby levels is characteristic of a Poisson process, where energy levels are randomly chosen.

Poissonian statistics would also be observed in models with additional symmetries, even if Wigner-Dyson statistics appears within individual symmetry sectors, as evidenced by the possibility of level crossings between states corresponding to different symmetry sectors.

5 Eigenstate Thermalization Hypothesis

If the Hamiltonian were completely random, any observable expressed in the eigenstate basis of the Hamiltonian would become completely diagonal, with all diagonal elements equal to the average value of the operator. ETH proposes a different structure for observables in the eigenstate basis of a Hamiltonian, given by

$$O_{mn} = \overline{O}(E)\delta_{mn} + e^{-S(\overline{E})/2} f_O(E,\omega) R_{mn}, \tag{35}$$

with $\overline{O}(E)$ the microcanonical expectation value and $f_O(E,\omega)$ smooth functions of the average energy $E = (E_m + E_n)/2$ and the energy difference $\omega = E_m - E_n$, and R_{mn} a random variable with zero mean, unit variance, and satisfying $R_{mn} = R_{nm}$. The thermodynamic entropy $S(E)$ is defined as the logarithm of the (coarse-grained) density of states, i.e. the number of eigenstates with energy E is given by $e^{S(E)}$. The function $f_O(E,\omega)$ is also known as the *spectral function* and satisfies $f_O(E,-\omega) = f_O(E,\omega)$ for real Hamiltonians.

What does this say? The matrix elements of an observable, expressed in the eigenbasis of a Hamiltonian, have a specific structure. **(1)** The diagonal elements vary smoothly with the energy of the states. **(2)** The off-diagonal elements are much smaller than the diagonal elements, and fluctuate with a structure determined by a smooth envelope function $f_O(E,\omega)$. Furthermore, off-diagonal elements vanish exponentially for large entropy. So if many states have a similar energy, their off-diagonal elements will be exponentially suppressed.

Quantum mechanically, ergodicity and thermalization is essentially translated into properties of eigenstates. This reproduces the RMT result if we focus on a region for fixed E where

$f_O(E,\omega)$ is constant. So RMT predicts the correct substructure of observables in narrow energy windows, but the energy variations are only captured by the ETH. The energy scale at which ETH simplifies to RMT is known as the *Thouless energy*.

5.1 Thermalization

The diagonal elements encode the connection with the Gibbs ensemble. Consider thermal expectation values of the form

$$\langle \hat{O} \rangle_\beta \equiv \mathrm{Tr}\left[\hat{O} e^{-\beta \hat{H}}\right]/\mathcal{Z}. \tag{36}$$

Introducing an eigenvalue decomposition of the Hamiltonian, we find that

$$\langle \hat{O} \rangle_\beta = \frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} O_{nn} = \frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} \overline{O}(E_n), \tag{37}$$

where in the last equality we plugged in the ETH ansatz. The discrete sum can be replaced by an integral, taking into account the density of states, $\sum_n \to \int dE_n e^{S(E_n)}$, leading to

$$\langle \hat{O} \rangle_\beta = \frac{1}{\mathcal{Z}} \int dE\, \overline{O}(E)\, e^{S(E)-\beta E}. \tag{38}$$

Both terms in the exponential are extensive, i.e. scale with system size, such that for large system sizes we can evaluate this integral to extremely good approximation using a saddle point approximation. This fixes the energy and the entropy according to the standard thermodynamic prescription as $S'(E) = \beta$ at the thermodynamic energy $E = E_\beta$. Here we also recognize the *thermodynamic free energy* $F = E - \beta^{-1} S$.

Taking into account the proper normalization, we find that

$$\langle \hat{O} \rangle_\beta \approx \overline{O}(E_\beta). \tag{39}$$

In other words, the smooth function necessarily corresponds to the thermal expectation value of the operator at the corresponding thermal energy. In this way the diagonal elements lead to the thermal distribution.

We can now show that the ETH reproduces the expected thermalization. For the steady-state value we find that

$$\lim_{t\to\infty} \langle \psi(t)|\, \hat{O}\, |\psi(t)\rangle = \sum_n |c_n|^2 \overline{O}(E_n). \tag{40}$$

Suppose that energy fluctuations in the initial state are small, e.g. the initial state has an extensive energy and sub-extensive energy fluctuations $\delta E^2 = \langle \psi_0|\hat{H}^2|\psi_0\rangle - \langle \psi_0|\hat{H}|\psi_0\rangle^2$. Within ETH we can do a Taylor expansion around the average energy of the initial state $\langle E\rangle$ and say

$$O(E_n) \approx \overline{O}(\langle E\rangle) + (E_n - \langle E\rangle)\overline{O}'(\langle E\rangle) + \frac{1}{2}(E_n - \langle E\rangle)^2 \overline{O}''(\langle E\rangle), \tag{41}$$

such that

$$\lim_{t\to\infty} \langle \psi(t)|\, \hat{O}\, |\psi(t)\rangle \tag{42}$$

$$= \sum_n |c_n|^2 \overline{O}(\langle E\rangle) + \sum_n |c_n|^2 (E_n - \langle E\rangle)\overline{O}'(\langle E\rangle) + \frac{1}{2}\sum_n |c_n|^2 (E_n - \langle E\rangle)^2\, \overline{O}''(\langle E\rangle) \tag{43}$$

$$= \overline{O}(\langle E\rangle) + \frac{\delta E^2}{2}\overline{O}''(\langle E\rangle), \tag{44}$$

In the first equality we have introduced the Taylor expansion, and in the second equality the definition of the average and energy variance. since we have assumed that the energy variance of the initial state is sufficiently small, we find that the steady-state value reproduces the microcanonical expectation value $\overline{O}(\langle E\rangle)$ at the average energy.

Observables satisfying the ETH thermalize to a limiting value only determined by the average energy of the initial state, as is known classically! Since everything only depends on the average energy, the Gibbs ensemble will correctly reproduce the values of the observables, since this state is fully determined by the average energy. Furthermore, while ETH reduces the microcanonical expectation values, in the presence of 'equivalence of ensembles' as established for e.g. spin chains with short-range interactions, the microcanonical expectation values reproduce the expectation values from the Gibbs ensemble. In this way, the Gibbs state can be seen as some kind of 'representative state' for all states with a given energy. From the ETH ansatz, higher-order fluctuations can also be calculated, showing that fluctuations vanish as $e^{-S(\langle E\rangle)}$.

Quantum quenches. One specific setup in which the above argument to hold is in quantum quenches. In a so-called quantum quench the system is prepared in the ground state $|\psi_0\rangle$ of an initial (local) Hamiltonian $\hat{H}_0$, and at $t=0$ the Hamiltonian is abruptly changed ('quenched') to a Hamiltonian $\hat{H}_0+\hat{H}_1$ and the system is left to evolve under this new Hamiltonian. In such a quench setting we find that the energy fluctuations in the original state in the eigenbasis of the new Hamiltonian are given by

$$\begin{aligned}\delta E^2 &= \langle\psi_0|(\hat{H}_0+\hat{H}_1)^2|\psi_0\rangle - \langle\psi_0|(\hat{H}_0+\hat{H}_1)|\psi_0\rangle^2 \\ &= \langle\psi_0|(\hat{H}_1)^2|\psi_0\rangle - \langle\psi_0|\hat{H}_1|\psi_0\rangle^2,\end{aligned} \tag{45}$$

using that $|\psi_0\rangle$ is an eigenstate of $\hat{H}_0$. For a local Hamiltonian we can write $\hat{H}_1=\sum_j \hat{h}_j$, where $\hat{h}_j$ are local operators indexed by lattice sites j, to obtain

$$\delta E^2 = \sum_{j_1,j_2}\left[\langle\psi_0|\hat{h}_{j_1}\hat{h}_{j_2}|\psi_0\rangle - \langle\psi_0|\hat{h}_{j_1}|\psi_0\rangle\,\langle\psi_0|\hat{h}_{j_2}|\psi_0\rangle\right]. \tag{46}$$

In the absence of long-range connected correlations in the ground state (which is typically the case for ground states of gapped systems), the contributions to these summations decay exponentially as $|j_1-j_2|$ increases, such that the number of terms that contribute to this summation will scale as L (with L the number of lattice sites). We find that $\Delta E \propto L^{1/2}$ and since $E\propto L$ the relative energy fluctuations vanish as $\delta E/E \propto L^{-1/2}$.

5.2 Fluctuations

The spectral function $f_O(E,\omega)$ appearing in the off-diagonal matrix elements encodes all fluctuations of the operator, both static and dynamic.

Let us first consider the dynamic fluctuations. While our previous discussion showed that the diagonal ensemble is equivalent to the Gibbs ensemble, the diagonal ensemble in principle only follows as the long-time average of the observable. It could be possible that the system does not equilibrate but rather keeps exhibiting large fluctuations around the time-average thermal value. However, ETH additionally predicts that this is not the case and we can think of the thermal value as the constant equilibrium value. Consider the long-time average of the fluctuations, i.e. we quantify how much the expectation value of $\hat{O}(t)$ deviates from the thermal prediction at each time and average this quantity:

$$\delta O_t^2 = \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\left[\langle\hat{O}(t)\rangle - \langle\hat{O}\rangle_\beta\right]^2 = \lim_{T\to\infty}\frac{1}{T}\int_0^T dt\left|\sum_{n,m\neq n} c_n^* c_m O_{nm} e^{i(E_n-E_m)t}\right|^2. \tag{47}$$

Assuming that $E_m - E_n = E_{m'} - E_{n'}$ only if $m = m'$ and $n = n'$ (recall that we made a similar assumption, $E_m = E_n$ only if $m = n$, in deriving the diagonal ensemble), we find that

$$\delta O_t^2 = \sum_{n,m\neq n} |c_n|^2 |c_m|^2 |O_{nm}|^2 \leq \max |O_{nm}|^2 \propto e^{-S(E)} . \tag{48}$$

Fluctuations around the thermal value are hence exponentially suppressed!

Let us next consider the static fluctuations. Suppose we are able to prepare the system in an eigenstate $|n\rangle$ of the Hamiltonian. If we measure the observable, we will obtain different measurement outcomes and the expectation value of the operator corresponds to the average value of the measurement outcomes. The fluctuations on these measurement outcomes follow as

$$\delta O_n^2 = \langle n|\hat{O}^2|n\rangle - \langle n|\hat{O}|n\rangle^2 = \sum_{m\neq n} |O_{mn}|^2 . \tag{49}$$

It is natural that the off-diagonal elements appear here, since if the observable was diagonal in the eigenbasis of the Hamiltonian all eigenstates would have a fixed value of the observable and we would observe no fluctuations. Plugging in the ETH ansatz, we find that

$$\delta O_n^2 = \sum_{m\neq n} e^{-S(E_n+\omega/2)} |f_O(E_n + \omega/2, \omega)|^2 R_{mn}^2 . \tag{50}$$

Here we introduced $\omega = (E_m - E_n)/2$ such that $E = (E_m + E_n)/2 = E_n + \omega/2$. For a sufficiently large density of states we can replace R_{mn}^2 with its average value. Replacing the summation with an integral and introducing the corresponding density of states, we have that

$$\delta O_n^2 = \int d\omega\, e^{S(E_n+\omega)-S(E_n+\omega/2)} |f_O(E_n + \omega/2, \omega)|^2 . \tag{51}$$

This expression can be simplified by introducing a Taylor expansion, writing

$$S(E_n + \omega) - S(E_n + \omega/2) \approx S'(E_n)\frac{\omega}{2} = \frac{\beta\omega}{2}, \tag{52}$$

where we have again defined $\beta = S'(E_n)$, and similar for the spectral function, to obtain

$$\delta O_n^2 = \int d\omega\, e^{\beta\omega/2} \left(|f_O(E_n, \omega)|^2 + \frac{\omega}{2}\frac{\partial}{\partial E} |f_O(E_n, \omega)|^2 \right) . \tag{53}$$

This Taylor expansion can be motivated from the fact that the spectral function decays exponentially for large ω. Crucially, we observe that the fluctuations of the observable are a smooth function of their energy, and can be written as an appropriately weighted integrable over all possible fluctuation frequencies. As such, if we have small energy fluctuations, we can approximate the fluctuations in the steady state by the fluctuations of an eigenstate with the same energy as the initial state. This is an example of the equivalence of ensembles: thermal fluctuations (canonical ensemble) correspond to single-eigenstate fluctuations (microcanonical ensemble).

Comments. ETH is only expected to be valid from states in the bulk of the spectrum, so away from the edges, precluding the ground state and the low-lying excited states. ETH is said to be satisfied in a strong (weak) sense if all (almost all) eigenstates obey Eq. (35). Similarly, ETH is only expected to hold for physical observables, which is here guaranteed by the restriction to local operators. ETH also makes clear that exponentially long times may not be needed for relaxation. By destroying phase coherence between a finite fraction of the eigenstates, we can average over the random variables appearing in the off-diagonal matrix elements within ETH, such it is possible to approach the infinite-time prediction with high accuracy in a time much shorter than the inverse (many-body) level spacing – which is required to destroy coherence between all eigenstates.

6 Numerical verification

Using QuSpin, it is now straightforward to verify ETH. We consider a representative chaotic Hamiltonian as given by the mixed-field Ising model

$$\hat{H} = J\sum_{j=1}^{L}\sigma_j^z\sigma_{j+1}^z + h_x\sum_{j=1}^{L}\sigma_j^x + h_z\sum_{j=1}^{L}\sigma_j^z\,, \tag{54}$$

where we impose periodic boundary conditions $\sigma_{L+1}^z \equiv \sigma_1^z$ and fix the parameters $(J, h_x, h_z) = (1.0, 0.9045, 0.8090)$. These parameters are generic but often appear in numerical studies of this model as a testbed of quantum chaos. In order to avoid the effect of unwanted symmetries, we restrict ourself to the symmetry subsector with even parity and zero momentum. Within this symmetry sector, the eigenspectrum exhibits Wigner-Dyson statistics.

As a representative observable, we consider a local hopping term along the x direction,

$$\hat{O} = \frac{1}{L}\sum_{j=1}^{L}\sigma_j^x\sigma_{j+1}^x\,. \tag{55}$$

The diagonal matrix elements are illustrated in Fig. 5, and we can clearly observe that these behave as a smooth function of the energy, becoming increasingly narrow as the system size L is increased. The off-diagonal matrix elements are illustrated in Fig. 6 for $E = 0$. These matrix elements clearly exhibit large fluctuations, with a smooth enveloping function.

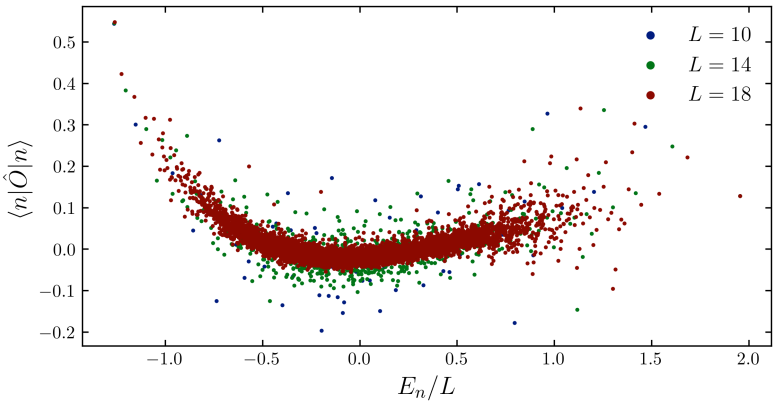

Figure 5: Expectation values of $\hat{O} = \sum_{j=1}^{L}\sigma_j^z$ in the eigenstates of the mixed-field Ising Hamiltonian (54) as a function of the energy of the corresponding eigenstate.

It is also possible to verify whether the off-diagonal matrix elements satisfy a Gaussian distributoin. For Gaussian variables R_{mn} with zero mean, it is a straightforward calculation to show that

$$\Gamma \equiv \overline{|R_{mn}|^2}/\overline{|R_{mn}|}^2 = \frac{\pi}{2}. \tag{56}$$

We can perform a similar averaging for O_{mn} at fixed average energy E and for different frequencies ω, and as illustrated in Fig. 7 we observe a value close to the expected value of $\pi/2$ at all frequencies.

To conclude, we can also illustrate the presence of level repulsion and avoided crossings in chaotic many-body systems. In Fig. 8 we show the eigenspectrum of the mixed-field Ising model for a longitudinal field λh_z where we change λ from 0 to 1. It should be apparent

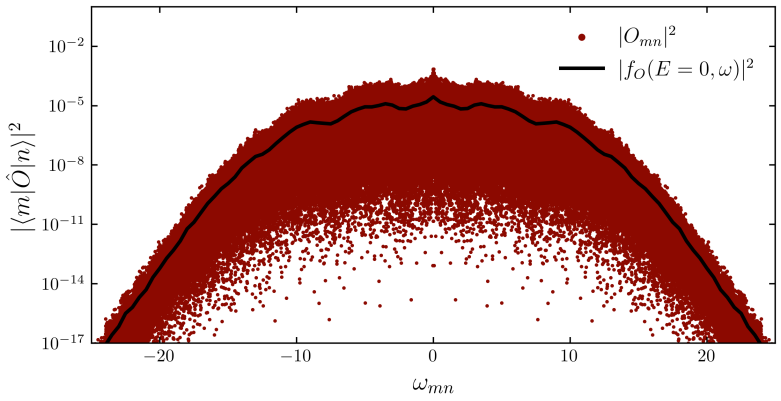

Figure 6: Off-diagonal matrix elements of $\hat{O} = \sum_{j=1}^{L} \sigma_j^z$ in the eigenstates of the mixed-field Ising Hamiltonian (54) as a function of the energy difference ω for average energy $E \in [-0.1, 0.1]$ and system size $L = 18$.

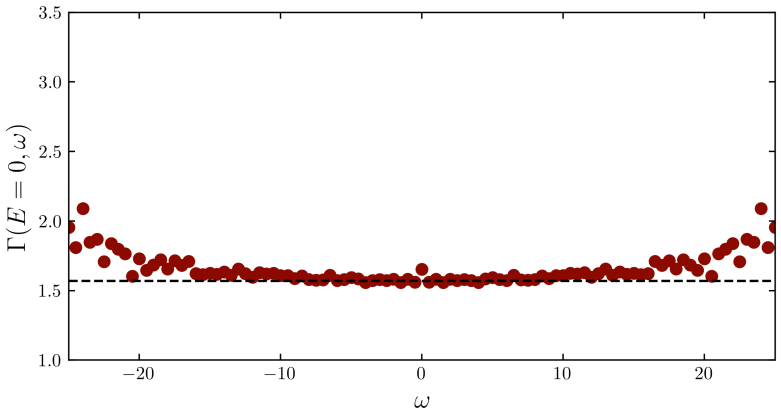

Figure 7: Value of Γ [Eq. (56)] in the off-diagonal eigenstates of the mixed-field Ising Hamiltonian (54) as a function of the energy difference ω for average energy $E \in [-0.1, 0.1]$ and system size $L = 18$. At all frequencies the calculated value is close to $\pi/2$ (dashed black line), consistent with a Gaussian distribution.

that the energy levels exhibit an abundance of avoided crossings as the longitudinal field is changed, and no exact level crossings are present (even if some levels can get arbitrarily close together). Note that ETH also implies that excited eigenstates at the same energy cannot be physically distinguished using local measurements.

7 Fluctuation-dissipation relations.

Let us illustrate how ETH can be used to recover standard results from statistical mechanics. These calculations help to illustrate how the spectral function does not just fully determine the equilibrium fluctuations but also the dynamical fluctuations. Specifically, the spectral function naturally appears in linear response, underlying the important fluctuation-dissipation relation, and determines the nontrivial operator dynamics. Consider two-point autocorrelation func-

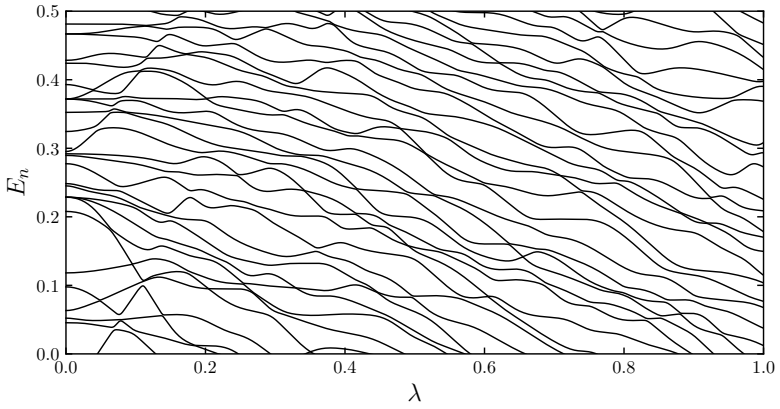

Figure 8: Part of the energy spectrum of the mixed-field Ising Hamiltonian (54) as h_z is varied from 0 to 1 for $L = 14$. As the Hamiltonian is changed the energy levels undergo avoided crossings and exhibit level repulsion.

tions at an inverse temperature β of the form

$$\kappa_2(t) = \langle \hat{O}(t)\hat{O} \rangle_\beta - \langle \hat{O} \rangle_\beta^2 \,. \tag{57}$$

These naturally appear in the anticommutator

$$F(t) = \frac{1}{2} \langle \{ \hat{O}(t), \hat{O} \} \rangle_\beta - \langle \hat{O} \rangle_\beta^2 \,, \tag{58}$$

which quantifies the *fluctuations* of the system in thermal equilibrium, and the commutator

$$\rho(t) = \langle \left[\hat{O}(t), \hat{O} \right] \rangle_\beta \,, \tag{59}$$

which appears in Kubo linear response theory and fully determines the *dissipation* in the system. Their Fourier transforms $\tilde{F}(\omega)$ and $\tilde{\rho}(\omega)$ fully determine the thermal fluctuations at a given frequency and the system's response to an external perturbation at a given frequency respectively. The former corresponds to the quantum equivalent of the power spectrum. Here we define the Fourier transform as $\tilde{F}(\omega) = \frac{1}{2\pi} \int d\omega \, e^{i\omega t} F(t)$.

One cornerstone of statistical mechanics is the *fluctuation-dissipation relation*, relating these two quantities as

$$\tilde{F}(\omega) = \left[\frac{1}{e^{\beta\omega} - 1} + \frac{1}{2} \right] \tilde{\rho}(\omega) \,. \tag{60}$$

On the right we have $\tilde{\rho}(\omega)$, setting the dissipative response to an external perturbation at a fixed frequency ω, and on the left we find the thermal fluctuations $\tilde{F}(\omega)$ at the same frequency ω, where the two are related through a Bose-Einstein distribution (which also appears the classical fluctuation-dissipation relation) as well as a constant $1/2$ that can be thought of as quantum fluctuations. Intuitively, for every process that dissipates energy, turning it into heat (e.g., friction), there is a reverse process related to thermal fluctuations. This holds quantum mechanically as well as classically, e.g. Brownian motion and drag, or thermal noise in a resistor and resistance.

The fluctuation-dissipation equation can also be rewritten in a slightly more compact form as

$$\tilde{F}(\omega) = \frac{1}{2} \coth\left(\frac{\beta\omega}{2} \right) \tilde{\rho}(\omega) \,. \tag{61}$$

Both quantities can be related to the Fourier transform of the autocorrelation function as

$$\tilde{F}(\omega) = \frac{\tilde{\kappa}_2(\omega) + \tilde{\kappa}_2(-\omega)}{2}, \qquad \tilde{\rho}(\omega) = \tilde{\kappa}_2(\omega) - \tilde{\kappa}_2(-\omega)\,. \tag{62}$$

Let us now make these relations explicit within the context ETH and show how the spectral function naturally appears.

Introducing the eigenvalue decomposition of the Hamiltonian, the autocorrelation reads

$$\kappa_2(t) = \frac{1}{\mathcal{Z}} \sum_{m,n} e^{-\beta E_n} e^{i(E_n - E_m)t} |O_{mn}|^2 - \left(\frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} \langle n|\hat{O}|n\rangle \right)^2 . \tag{63}$$

The diagonal contribution in the first term can again be evaluated as

$$\frac{1}{\mathcal{Z}} \sum_n e^{-\beta E_n} |O_{nn}|^2 \approx \frac{1}{\mathcal{Z}} \int dE\, e^{S(E) - \beta E}\, \overline{O}(E)^2 \approx \overline{O}(E_\beta)^2 \approx \langle \hat{O} \rangle_\beta^2 \,, \tag{64}$$

and hence cancels with the contribution $\langle \hat{O} \rangle_\beta^2$.

For the remaining off-diagonal contribution, we find that

$$\kappa_2(t) = \frac{1}{\mathcal{Z}} \sum_{m,n \neq m} e^{-\beta E_n} e^{i(E_n - E_m)t} |O_{mn}|^2 \,. \tag{65}$$

Plugging in the ETH ansatz, we can write

$$\kappa_2(t) = \frac{1}{\mathcal{Z}} \sum_{m,n \neq m} e^{-\beta E_n - S(E_{mn})}\, e^{-i\omega_{mn} t}\, |f_O(E_{mn}, \omega_{mn})|^2 |R_{mn}|^2, \tag{66}$$

with $E_{mn} = (E_m + E_n)/2$ and $\omega_{mn} = E_m - E_n$. If the spectrum is sufficiently dense we can replace $|R_{mn}|^2$ by its average value of 1 and replace the summations by integrals, taking into account the density of states, to obtain

$$\frac{1}{\mathcal{Z}} \int dE_m \int dE_n\, e^{-\beta E_n + S(E_m) + S(E_n) - S(E_{mn})}\, |f_O(E_{mn}, \omega_{mn})|^2\, e^{-i\omega_{mn} t} \tag{67}$$

This integration can be simplified by switching to so-called *Wigner variables* $E \equiv E_{mn}$ and $\omega \equiv \omega_{mn}$, such that $E_{m,n} = E \pm \omega/2$, to return

$$\frac{1}{\mathcal{Z}} \int dE \int d\omega\, e^{-\beta(E - \omega/2)} e^{S(E + \omega/2) + S(E - \omega/2) - S(E)}\, |f_O(E, \omega)|^2\, e^{-i\omega t}, \tag{68}$$

where we can Taylor expand the thermodynamics entropies to return

$$S(E + \omega/2) + S(E - \omega/2) = 2S(E) + S''(E)\frac{\omega^2}{4} + \mathcal{O}(\omega^4)\,. \tag{69}$$

The integral then returns

$$\frac{1}{\mathcal{Z}} \int dE e^{S(E) - \beta E} \int d\omega\, e^{\beta\omega/2} e^{S''(E)\omega^2/4}\, |f_O(E, \omega)|^2\, e^{-i\omega t}. \tag{70}$$

The inverse of the second derivative scales extensively (since both S and E are extensive), such that the term $e^{S''(E)\omega^2/4}$ is only significantly different from 1 for very large frequencies (proportional to system size), where however the spectral function vanishes exponentially. As such,

we can put this term equal to one. The integral over E can again be evaluated using a saddle-point approximation, which again fixes the energy and corresponding inverse temperature to satisfy $\beta = S'(E_\beta)$, and we end up at the final result that

$$\kappa_2(t) = \int d\omega\, e^{\beta\omega/2} |f_O(E_\beta, \omega)|^2\, e^{-i\omega t}. \tag{71}$$

The Fourier transform can be read off as

$$\tilde{\kappa}_2(\omega) = e^{\beta\omega/2} |f_O(E_\beta, \omega)|^2, \tag{72}$$

and we find that

$$\tilde{F}(\omega) = \cosh\left(\frac{\beta\omega}{2}\right) |f_O(E_\beta, \omega)|^2, \qquad \tilde{\rho}(\omega) = 2\sinh\left(\frac{\beta\omega}{2}\right) |f_O(E_\beta, \omega)|^2. \tag{73}$$

The fluctuation-dissipation is clearly satisfied since

$$\tilde{F}(\omega) = \frac{1}{2}\coth\left(\frac{\beta\omega}{2}\right)\tilde{\rho}(\omega). \tag{74}$$

While it it not surprising that the fluctuation-dissipation is satisfied, since this should hold more generally, the remarkable result is that the spectral function naturally appears in these quantities, such that it can also be experimentally determined.

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