

PHY511: Eigenstate Thermalization Hypothesis

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Abstract

In this paper, we motivate and provide an overview of the Eigenstate Thermalization Hypothesis and its relation to ergodicity in quantum mechanics. This formalism is applied to the anisotropic $S = 1/2$ Heisenberg spin chain, and we compare properties of expectation values as well as thermalization of observables in both integrable and non-integrable regimes.

1 Classical Statistical Physics

We would like to compute the time-average of a classical observable O , but calculating the momentum over a large range of time is generally challenging. We consider extra assumptions to make this problem less challenging. Consider the path of a particle in phase space. In general, the model may have symmetries which confines the surface Σ on which the particle is constrained. If this particle's path is dense in the surface Σ , or in other words the path gets arbitrarily close to every point contained in Σ , then the system is called ergodic. On the other hand, if the system is integrable, or has a sufficient number of constants of motion so that there is an analytic solution to the equations of motion, then the system is not ergodic. From Louisville's Theorem, we know that a state spends an equal amount of time in equal volumes of phase space. Combining ergodicity and Louisville's theorem, we can express the time-average of a classical observable in terms of its spatial average [2]

$$\overline{O} = \frac{1}{A(\Sigma)} \int_{\Sigma} d\sigma \cdot O(\sigma) \quad (1)$$

where $A(\Sigma)$ is the area of the surface Σ . It is apparent that this is precisely the result of the microcanonical ensemble, which we will now review. We consider a system with fixed number of particles N , volume V , and energy E , referred to as the microcanonical ensemble. The microcanonical ensemble assumes a uniform probability distribution over the domain $I_{\Delta} = [\varepsilon - \Delta, \varepsilon)$, and then takes the limit $\Delta \rightarrow 0$ to obtain I_0 . The probability distribution is simply $P = 1/W$ where W is the number of microstates with energy E , and fixed number of particles and volume. We can compute expectation values of observables in the microcanonical ensemble as simply the average over the allowed states [1]

$$\langle O \rangle_{mc} \equiv \sum_{m \in I_0} P(m) \cdot O_{mm} = \frac{1}{W} \sum_{m \in I_0} O_{mm} \quad (2)$$

where we use the standard matrix element notation $O_{mm} \equiv \langle m | O | m \rangle$. In assigning an equal probability to all states within the energy shell, we discard all information about the initial state.

Chaos is characterized by a system's extreme sensitivity to initial conditions. Ergodic and chaotic systems are closely related, but the latter is stronger than the former. We are well-justified in applying the microcanonical ensemble, and statistical mechanics in general (since the other

ensembles are equivalent), given that we can prove that our system is chaotic, or more generally ergodic.

2 Eigenstate Thermalization Hypothesis

Thermalization in quantum mechanics is a natural question that arises when we look at macroscopic phenomena from the lens of quantum mechanics. As motivation, consider a brick which consists of roughly an Avogadro's number of particles and initial conditions. Modelling this system exactly, and keeping track of the dynamics and all of these initial conditions is computationally infeasible. Nonetheless, these plentiful interactions lead to a single macroscopic state, a brick. If one were to more-or-less change the initial conditions of the atoms comprising the brick, you would still have a brick with the same thermodynamics. It is not clear why you can roughly ignore the initial conditions.

2.1 Quantum Statistical Physics

We provide a brief overview of quantum mechanics to emphasize that the theory is typically strongly dependent on the initial conditions. Given a wavefunction $|\psi(t)\rangle = \sum_m c_m e^{-i\varepsilon_m t} |m\rangle$ ($\hbar = 1$) with initial conditions $c_m = \langle\psi(0)|m\rangle$ and eigenstates $|m\rangle$, we compute the expectation value of a (quantum) observable

$$\langle O \rangle_{\psi(t)} \equiv \langle \psi | O | \psi \rangle = \sum_{m,n} c_n^* c_m O_{nm} e^{i(\varepsilon_n - \varepsilon_m)t}. \quad (3)$$

We then average over time and let $T \rightarrow \infty$ to obtain [1, 3]

$$\begin{aligned} O_\infty &\equiv \lim_{T \rightarrow \infty} \overline{\langle O \rangle_{\psi(t)}} \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \cdot \langle O \rangle_{\psi(t)} \\ &= \sum_m |c_m|^2 O_{mm} + i \lim_{T \rightarrow \infty} \left[\sum_{n \neq m} \frac{c_n^* c_m O_{nm}}{\varepsilon_m - \varepsilon_n} \left(\frac{e^{-i(\varepsilon_m - \varepsilon_n)T} - 1}{T} \right) \right]. \end{aligned} \quad (4)$$

If we assume that the phase factors in the second term are sufficiently small, so that it does not rival the $1/T$ decay [3], then the second term then vanishes in the limit and we obtain

$$O_\infty = \sum_m |c_m|^2 O_{mm}. \quad (5)$$

This value of the observable in the infinite-time limit is called the diagonal ensemble. It is clear from the above expression that the observable depends strongly on the initial conditions c_m , unlike in the microcanonical ensemble. Comparing the two approaches, the microcanonical ensemble depends solely on the total energy, while the quantum approach depends on the initial conditions. Therefore, thermalization cannot generally manifest in quantum systems.

2.2 Diagonal Elements

We now motivate criteria for which thermalization will manifest in quantum systems. Note the structure of the diagonal and microcanonical ensembles appear similar if we assume that the diagonal elements O_{mm} are sufficiently smooth in energy, or $O_{mm} \approx O$ for some O [1]. From this we obtain the simplification of the diagonal ensemble expectation value

$$O_\infty = \sum_m |c_m|^2 O_{mm} \approx O \sum_m |c_m|^2 = O. \quad (6)$$

On the other hand, note that the microcanonical ensemble considers energy levels sufficiently close to the energy of the system, and therefore, the diagonal elements should also approximate $O_{mm} \approx O$, to obtain

$$\langle O \rangle_{mc} = \frac{1}{W} \sum_{m \in I_0} O_{mm} \approx \frac{O}{W} \sum_{m \in I_0} 1 = O, \quad (7)$$

and hence we have $\langle O \rangle_{mc} \approx O_\infty$, as intended. We can summarize the assumption on the observable by requiring the diagonal case of [1]

$$O_{mn} \approx \bar{O}(m) \cdot \delta_{mn} + \sqrt{\frac{\bar{O^2}(m, n)}{D}} \cdot R_{mn}$$

(8)

where $D = \exp(sV)$ is the Hilbert space dimension and V is the volume of the system. In the second term, R_{mn} is a random variable that satisfies $\overline{R_{mn}} = 0$ and $\sigma_R^{mn} = 1$. The second term represents a perturbation (violation) to the smoothness of O_{mn} , exponentially suppressed by the volume of the system. The two functions of the observable, $\bar{O}(m)$ and $\bar{O^2}(m, n)$ are smooth functions of the energy.

2.3 Off-Diagonal Elements

We will see that it is important to suppress the off-diagonal terms when considering temporal fluctuations in the observable. We define the variance in temporal fluctuations from the steady state [1]

$$\begin{aligned} \sigma_\infty^2 &\equiv \lim_{T \rightarrow \infty} \overline{(\langle O \rangle_{\psi(t)} - O_\infty)^2} \equiv \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^\infty dt \cdot (\langle O \rangle_{\psi(t)} - O_\infty)^2 \\ &= \sum_{m \neq n} |c_m|^2 |c_n|^2 |O_{mn}|^2. \end{aligned} \quad (9)$$

Applying the assumed form of the off-diagonal elements, we have [1]

$$\sigma_\infty^2 = \frac{1}{D} \sum_{m \neq n} |c_m|^2 |c_n|^2 \cdot \overline{O^2(m, n)} \cdot R_{mn}^2 \approx \frac{1}{D}, \quad (10)$$

and we see that temporal fluctuations are suppressed given the off-diagonal case of Eqn. (8) . To recap, diagonal elements are responsible for ensuring the convergence of O_∞ and its agreement with the microcanonical ensemble, while the off-diagonal elements are responsible for ensuring sufficiently small temporal fluctuations in the observable with respect to O_∞ .

3 Anisotropic $S = 1/2$ Heisenberg Spin Chain

We introduce the anisotropic $S = 1/2$ Heisenberg spin chain as a model to study the implications of the Eigenvalue Thermalization Hypothesis, and its dependence on integrability.

3.1 Model

The model consists of a spin-chain of length L (in the \hat{z} direction), with the Hamiltonian [4]

$$H = J \sum_{i=1}^L (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + \Delta_2 S_i^z S_{i+2}^z) \quad (11)$$

where Δ represents the anisotropy in the interaction, and $\Delta_2 \neq 0$ breaks integrability. In other words, if $\Delta_2 = 0$ then we have a macroscopic number of conserved quantities $\{Q_n\}_{n=1}^L$ so that $[H, Q_n] = 0$. For general Δ_2 , we can map the model to a system of interacting spinless fermions with hopping, nearest and next-nearest ($\approx \Delta_2$) neighbor interactions.

To study thermalization in this model, we define local operators, composed of products of two and three spin operators. The so-called spin-current operator is defined as

$$J^s = J \sum_{i=1}^L (S_i^y S_{i+1}^y - S_i^y S_{i+1}^y) \quad (12)$$

which is not a conserved quantity for the integrable case. We also consider the kinetic part of the Hamiltonian, corresponding to the first two terms

$$H^{\text{kin}} = J \sum_{i=1}^L (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) \quad (13)$$

As a representative of products of three operators, we consider the energy-current operator

$$J^\varepsilon = J^2 \sum_{i=1}^L ((S_i^x S_{i+2}^y - S_i^y S_{i+2}^x) S_{i+1}^z - \Delta (S_i^x S_{i+1}^y - S_i^y S_{i+1}^x) (S_{i-1}^z + S_{i+2}^z)) \quad (14)$$

which is a conserved quantity in the integrable case [4]. These operators represent operators of a variety of properties. We will not motivate their particular expressions for sake of brevity.

3.2 Exact-Diagonalization Study

We numerically compute the diagonal matrix elements O_{mm} of these three operators using exact diagonalization to test the validity of the diagonal case of Eqn. (8). In our computations, we set $S_{\text{tot}}^z = -1$ to break particle-hole symmetry, and define two spin chains with lengths $L \in \{12, 15\}$ and parameters $J = 1$, $D = 0.5$, $D_2 \in \{0, 0.5\}$ where $D_2 = 0(0.5)$ corresponds to the integrable (non-integrable) case. Recall that the Eigenstate Thermalization Hypothesis (ETH) relies on thermodynamic system size, and thus if our model satisfies the assumptions, we should see the sensitivity to initial conditions diminish with length L , which is precisely the observation, see Figure (1).

We also study temporal fluctuations, with initial state $|\psi_0\rangle = |100\dots\rangle$ and lengths $L \in \{12, 14, 16, 18\}$. Note that this initial state is not an eigenstate of the Hamiltonian(s). The initial state is time-evolved from $t_0 = 0$ to $t_1 = 400$ by exponentiating the Hamiltonian. We see that with increasing length, the temporal fluctuations of $\langle H^{\text{kin}} \rangle_\psi$ diminishes as expected and convergence is more pronounced.

4 Conclusion

In this paper, we provided a theoretical overview of the Eigenstate Thermalization Hypothesis (ETH) and motivated its understanding with respect to classical statistical mechanics and ergodicity. This framework was then applied to the anisotropic $S = 1/2$ Heisenberg spin chain to understand the impact of non-integrability on thermalization of expectation values. Through exact-diagonalization calculations, it is suggested that this model satisfies the assumptions of the ETH, and we see that the temporal fluctuation in expectation value of a particular operator, H^{kin} representing the kinetic energy of the spin chain, diminishes with chain length and convergence is more pronounced.

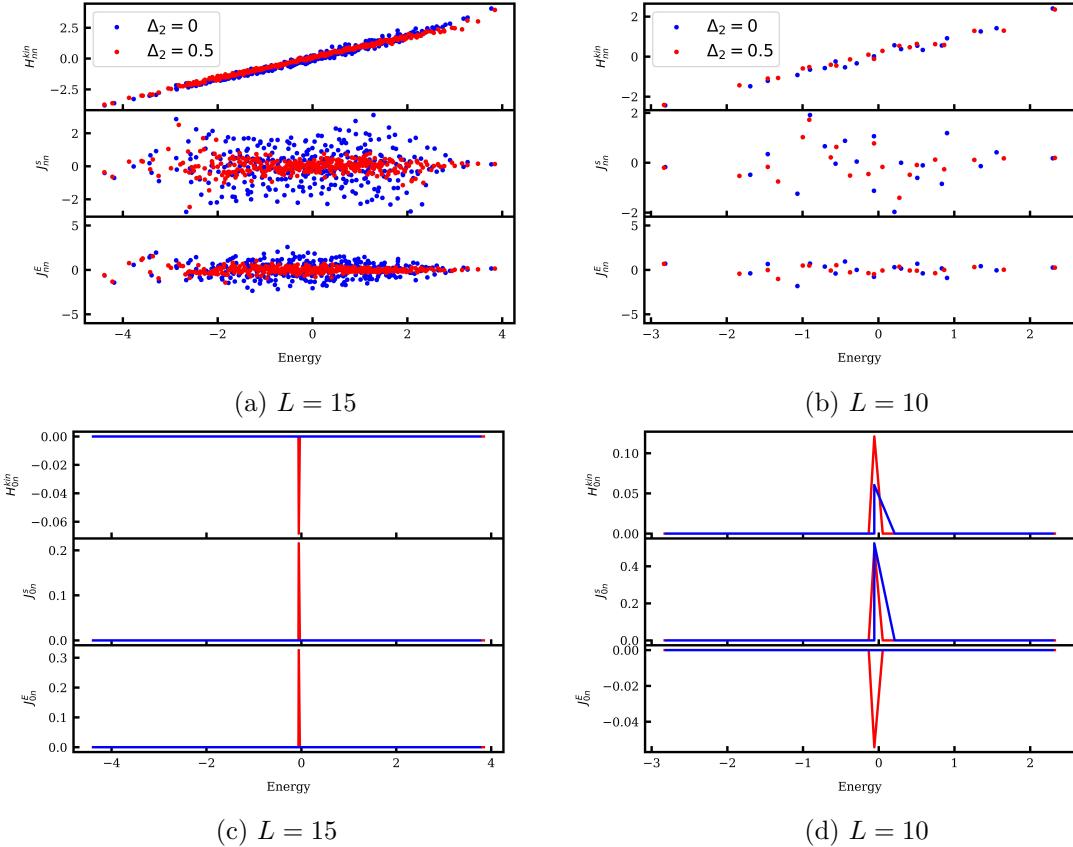


Figure 1: Exact-diagonalization simulation of the expectation values of the three operators defined above. The integrable(non-integrable) case corresponds to blue(red) for all plots. (a,b) The diagonal case is studied and we compute the diagonal matrix elements O_{mm} for all values of energy, or m . In sub-figure (a(b)) we have $L = 15(10)$. It is qualitatively clear that for $L = 15$ in the non-integrable case, the diagonal matrix elements are less sensitive to energy compared to the integrable case; this statement is much less strong in the case of $L = 10$ where the sensitivities are comparable. (c,d) The off-diagonal case is studied and we compute the off-diagonal matrix elements O_{0m} . In both the $L = 10$ and $L = 15$ non-integrable cases, the ETH assumption holds well as we expect the off-diagonal matrix elements to be proportional to a delta-function centered at $m = 0$.

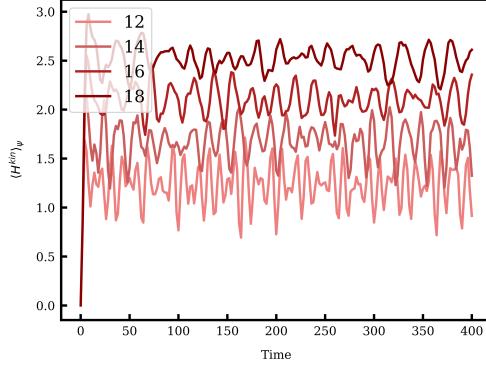


Figure 2: The initial state $|\psi\rangle$ is time-evolved in the non-integrable case, $\Delta_2 = 0.5$. We see that with larger length L (see legend), the fluctuations of the expectation value $\langle H^{\text{kin}} \rangle_\psi$ diminish and convergence is more pronounced.

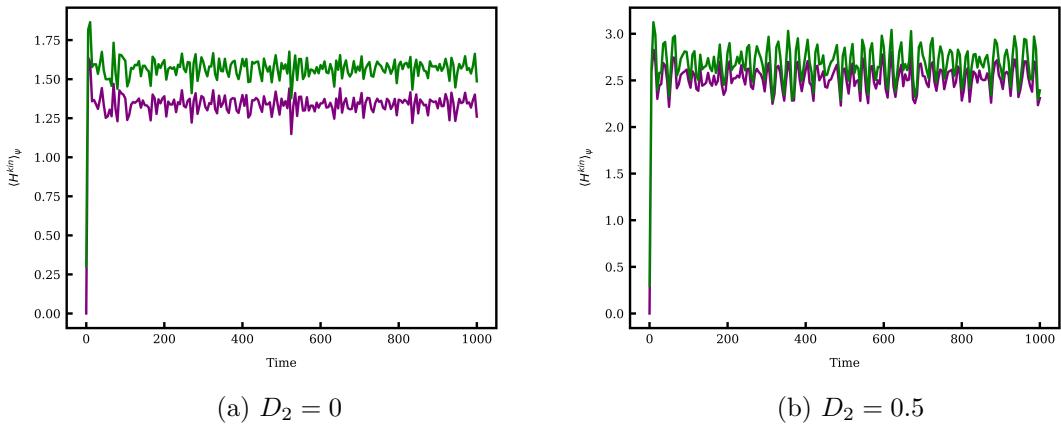


Figure 3: Purple represents the time evolution of the initial state $|100\dots\rangle$, and green represents that of $\sqrt{0.9}|100\dots\rangle + \sqrt{0.1}|010\dots\rangle$. We simulate with length $L = 18$. (a) In the integrable case, we see large deviation in the thermalized expectation value H_∞^{kin} with respect to initial state. (b) In the non-integrable case, we see much less deviation.

References

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This paper represents my own work in accordance with University regulations.

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