Eigenstate Thermalization Hypothesis in the Vicinity of the Phase Transition of a 2D Transverse Ising Model

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This paper explores the transition from a purely deterministic quantum state to a statistical ensemble state.[1] We provide motivation for the Eigenstate Thermalization Hypthothesis (ETH) from basic principles and by simulating a multiple integrable and non-integrable systems. First, in 1D, we take the integrable transverse Ising model and compute the fluctuation in the diagonal elements of the system. Then, we add a longitudinal field to make the system non-integrable, following the example of [2]. Second, we move into 2D, utilizing the added dimensions of the system to break the integrability of the transverse Ising model. Then using this model and the results from [3], we build a compelling case for including the correlation length in the ETH formalism, providing the beginnings of such a formalism with a simple classical model.

I. INTRODUCTION

Statistical mechanics was developed to reduce the complexity of large many-body systems and extract useful information from them. In particular, we utilize the microcanonical ensemble for a system with a fixed energy and the canonical ensemble for a system at fixed temperature. In both cases, we assume that the system is in statistical equilibrium. If the system in question is classical, like an ideal gas, we assume that it is chaotic, that it accesses its entire available phase space, and ignore the nuances of particle - particle interactions. We only impose conditions such as conservation of energy and momentum. We spent many lectures in 8.333 developing from basic interactions, for a classical system, the Maxwell-Boltzmann distribution, carefully including relevant terms and ignoring higher order terms. Classically, this all makes sense, we have a system which satisfies the Ergodic hypothesis (any micro-state is equi-probable in its phase space over long periods of time), so the system should reach a statistical equilibrium as $T \to \infty$ [1]. However, a quantum system behaves differently. The Schröedinger equation states that a system in an energy eigenstate undergoes deterministic time evolution:

$$|\psi(t)\rangle = e^{\frac{-iHt}{\hbar}} |\psi\rangle |_{t=0} \tag{1}$$

Reconciling deterministic time evolution with the unpredictable time evolution of an ensemble of states is naively easy; just zoom out from particle-particle interactions, but then any system should thermalize (transition from deterministic to ensemble time evolution). However, it can be shown theoretically and experimentally (1-D condensates) that some integrable quantum systems do not thermalize. Therefore, there must be some set of conditions sufficient for thermalization to occur, beyond simply not keeping track of all particle-particle interactions.[2]

II. EIGENSTATE THERMALIZATION HYPOTHESIS

In 1994, Mark Srednicki proposed a mechanism, eigenstate thermalization, to account for the transition over time from a deterministic quantum system to a statistical ensemble.

II.1. Thermal Average

Making the assumption of a large finite system we can decompose any state $|\psi\rangle$ as (assuming, for simplicity, no degenerate states)

$$\begin{aligned} |\psi\rangle &= \sum_\alpha c_\alpha |\alpha\rangle \\ \Rightarrow |\psi(t)\rangle &= \sum_\alpha c_\alpha e^{\frac{-iE_\alpha t}{\hbar}} |\alpha\rangle \end{aligned} \tag{2}$$

Then, the expectation value of any operator $\hat{A}$ (such as magnetization, M)

$$\langle\psi(t)| A |\psi(t)\rangle = \sum_{\alpha,\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha - E_\beta)t}{\hbar}} \langle\beta| A |\alpha\rangle \tag{3}$$

Now, time averaging the system,

$$\begin{aligned} \bar{A} &= \lim_{t\to\infty} \frac{1}{t} \int_0^t \langle\psi(t')| A |\psi(t')\rangle \, dt' \\ \bar{A} &= \lim_{t\to\infty} \frac{1}{t} \int_0^t \sum_{\alpha,\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha - E_\beta)t'}{\hbar}} \langle\beta| A |\alpha\rangle \, dt' \end{aligned} \tag{4}$$

We can then integrate the above equation,

$$\begin{aligned} \bar{A} = \lim_{t\to\infty} \Bigg\{ &\sum_\alpha A_{\alpha,\alpha} |c_\alpha|^2 \\ &+ i\hbar \sum_{\alpha\neq\beta} \frac{1}{t} \left(e^{\frac{-i(E_\alpha - E_\beta)t'}{\hbar}} - 1 \right) \frac{A_{\alpha,\beta} c_\alpha c_\beta^*}{E_\alpha - E_\beta} \Bigg\} \end{aligned} \tag{5}$$

$$\bar{A} = \sum_\alpha A_{\alpha,\alpha} |c_\alpha|^2 \tag{6}$$

In step 5 to 6 we have taken the time average of the second term, which is small because of the $1/t$ dependence (we assume the sum over eigenstates is finite, since the system is finite), leaving only the first term which is time independent. Then, imposing the first condition on our system, $A_{\alpha,\alpha} \approx A + \delta A_{\alpha,\alpha}$, with $\delta A_{\alpha,\alpha} \ll A$, for a relevant range of energies,

$$\bar{A} = \sum_{\alpha} A_{\alpha,\alpha}|c_\alpha|^2 \approx A\sum_{\alpha}|c_\alpha|^2 = A \tag{7}$$

Now, take the thermal average in the micro-canonical ensemble:

$$\langle A\rangle_{\mathrm{mc}} = \frac{1}{\Gamma}\sum_{\alpha'}^{\Gamma} A_{\alpha',\alpha'} \approx A\frac{1}{\Gamma}\sum_{\alpha'}^{\Gamma} = A \tag{8}$$

Where $\sum_{\alpha'}$ is the sum over micro-canonical states. Hence, our constraint results in the convenient $\bar{A} = \langle A\rangle_{\mathrm{mc}}$. Therefore, if the components of $\langle\psi|\,A\,|\psi\rangle$ vary in a smooth and controlled manner across different energy eigenstates, our system will thermalize over time such that $\bar{A}$ is the micro-canonical average. However, this constraint does not limit fluctuations about the thermodynamic average; we could have a sinusoidal fluctuation from 0 to $2\bar{A}$ averaging to $\bar{A}$, not consistent with the micro-canonical picture.[1]

II.2. Controlling Fluctuations

If we want fluctuations to be small, we need to look at the temporal variance in $\bar{A}$:

$$\overline{(A(t)-\bar{A})^2} = \lim_{t\to\infty}\frac{1}{t}\int_0^t (\langle A(t)\rangle - \bar{A})^2 \tag{9}$$

We expand the expectation value of A(t):

$$= \lim_{t\to\infty}\frac{1}{t}\int_0^t dt'\left\{\sum_{\alpha,\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta} - \bar{A}\right\}^2$$

$$= \lim_{t\to\infty}\frac{1}{t}\int_0^t dt'\left\{(\sum_{\alpha,\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta})^2 - 2\bar{A}*\sum_{\alpha,\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta} + \bar{A}^2\right\}$$

$$= \lim_{t\to\infty}\frac{1}{t}\int_0^t dt'\left\{(\sum_{\alpha\neq\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta})^2 + 2\bar{A}*\sum_{\alpha\neq\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta} + \bar{A}^2 - 2\bar{A}*\sum_{\alpha\neq\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta} - 2\bar{A}^2 + \bar{A}^2\right\}$$

$$= \lim_{t\to\infty}\frac{1}{t}\int_0^t dt'(\sum_{\alpha\neq\beta} c_\alpha c_\beta^* e^{\frac{-i(E_\alpha-E_\beta)t'}{\hbar}} A_{\alpha,\beta})^2$$

$$= \lim_{t\to\infty}\frac{1}{t}\int_0^t dt'\sum_{\alpha\neq\beta}|c_\alpha|^2|c_\beta|^2|A_{\alpha,\beta}|^2 + 2\sum_{\alpha\neq\beta} c_\alpha c_\beta^* \sum_{\alpha'\neq\beta'} c_{\alpha'} c_{\beta'}^* e^{\frac{-i(E_{\alpha'}+E_\alpha-E_{\beta'}-E_\beta)t'}{\hbar}} A_{\alpha,\beta}A_{\alpha',\beta'}$$

$$\overline{(A(t)-\bar{A})^2} = \sum_{\alpha\neq\beta}|c_\alpha|^2|c_\beta|^2|A_{\alpha,\beta}|^2 \tag{10}$$

Where in the last line, we integrated, cancelling the $\frac{1}{t}$ in the first term, but not in the second. Now looking at the fluctuation regulating terms, we see that these off-diagonal elements of $\langle A\rangle$ must be exponentially small on the scale of the system if our fluctuations are to be small, or else, the sum over all possible energy states can be large. This places yet another constraint for achieving thermalization, $A_{\alpha\neq\beta} \propto e^{-f(L^d)}$, where $F(L^d)$ is an extensive function of the system size, L^d, in d dimensions.[1]

III. CHECKING THERMALIZATION

Our discussion on eigenstate thermalization above constrains the types of systems that can undergo thermalization. In particular, integrable systems are unable to sample a complete phase space and do not thermalize. However, we were unable to reduce the constraints into a set of sufficient conditions, only no-go's. Therefore, checking that a system obeys ETH is not easy because every state in a system that obeys ETH must thermalize. One checks that every state thermalizes by time evolving any given state, a computationally intensive task, and then sampling a sufficient number of random states, adding more complexity.

Alternatively, we could only test every "eigenstate" for thermalization; ideally, without time evolving each one. Fortunately, we can say something special about the energy eigenstates. We know from equation (7) above that the variations in the expectation value of an operator across different eigenstates must be small. In fact, for $\sum_\alpha A_{\alpha,\alpha}|c_\alpha|^2 \approx A\sum_\alpha|c_\alpha|^2$ to hold, $\delta A_{\alpha,\alpha} = A - \delta A_{\alpha,\alpha}$ must exponentially small in the system size.

The above constraint implies that

$$\langle n+1|\,\hat{A}\,|n+1\rangle - \langle n|\,\hat{A}\,|n\rangle \equiv r_n \approx \mathcal{O}(e^{-L^d}) \tag{11}$$

We can now apply this constraint and greatly simplify the hunt for thermalizable systems. In particular, if we can show that $|r_n| \to 0$ for all n as $L\to\infty$, then it follows that the eigenstates which evolve deterministically in time exhibit a time-averaged expectation value equal to their thermal expectation value.

Phrased more clearly, we need only compute r_n to strongly suggest that a system is undergoing eigenstate thermalization. While diagonalizing a matrix is not computationally easy, it is easier than tracking time evolution.[2]

III.1. 1D Transverse Field Ising Model

It is well known that the simple 1D transverse field Ising model is integrable, however a transverse Ising model with longitudinal and transverse fields is not. These provide an ideal test case; if the constraint above is satisfied for the simple Ising model, then it is not a constraint on thermalization, but if it is failed by the simple transverse Ising model and passed by the complicated Ising model, then (while not a proof) this provides compelling evidence for the occurrence of eigenstate thermalization.

Utilizing the Hamiltonian and numbers provided by [2], we created the following model:

$$H = \sum_i (J\sigma_{z,i}\sigma_{z,i+1} + g\sigma_{x,i} + h\sigma_{z,i}) \qquad (12)$$

By tuning h, we are able to add and remove the longitudinal field. Then, by diagonalizing the matrix H and computing the local operator expectation value $\langle n|\,\sigma_{x,1}\,|n\rangle$, we can obtain $|r_n|$ for many eigenvalue pairs.

In figure 1, we compute $|r_n|$ for both models and plot the distribution of $|r_n|$'s. As expected, the more complicated transverse Ising model (non-integrable Ising model) demonstrates the behavior described above; $\delta A_{\alpha,\alpha}$ was exponentially small in the system size. In the integrable transverse model case, this was not true and thermalization does not occur.

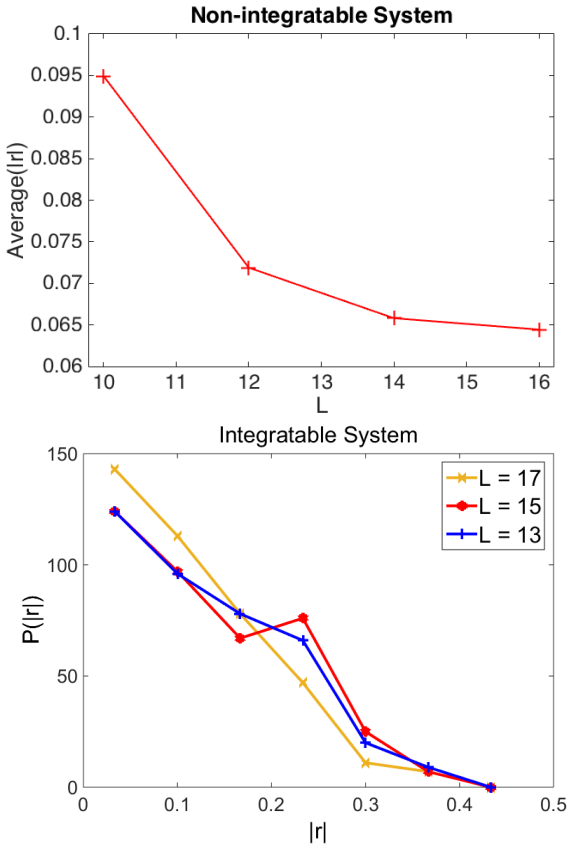

FIG. 1. In Figures 1 (a) above, we see a direct comparison of the average r_n value for a transverse Ising model with a longitudinal field. r_n was computed with the 400 lowest eigenstates in both figures. Notice the exponential decay of $\bar{r}$ in the system size, L (number of spins). In Figure 1 (b) we plot the distribution of $|r_n|$ for a transverse Ising models without a longitudinal field contribution, notice it's independence of the system size. Both systems obey the Hamiltonian in 12 with periodic boundary conditions and L spins, but with the following constants: in Figure 1 (a), J = 1, g = .9045, h = .809; in Figure 1 (b), J = 1, g = .9045, h = 0.

III.2. 2D Transverse Ising Model

Extending the above Hamiltonian to a 2D square lattice system, we were once again able to demonstrate clear thermalization relative to Ising model shown in Figure 1 (b). Looking at Figure 2, we see a a clear dependence on system size (N = 9 → N = 16). Furthermore, in the 2D case, the longitudinal field is no longer necessary (see Figure 2) to ensure thermalization. So, we were able to construct a simpler thermalizable transverse Ising model with a perturbative transverse field $h\sigma_{z,i}$ (see Figure 2).

The simple transverse Ising model presents a clear advantage over the previous 1D case. In particular we know the critical temperature of the XZ model, $h/J \approx 3$ [3, 5]. Therefore, we should be able to approach a phase transition by fixing J and varying h. Looking at Figure 3, as we approach the phase transition $|r_n|$ grows dramatically and is no longer exponentially small in the system size. This is indicative of and ETH violation. However, a system far from the critical point does thermalize. We are able to conclude that the 2D XZ model does not thermalize at its phase transition.

III.2.1. Phase Transitions in 2D Transverse Ising Model

The 2D Transverse Ising Model is a well studied system.[3] It has the Hamiltonian, with σ are the Pauli matrices

$$H = \sum_{i,j} (-J\sigma_{x,i,j}(\sigma_{x,i+1,j} + \sigma_{x,i,j+1}) + h\sigma_{z,i,j}) \qquad (13)$$

The ground state in the limit of small h is that of a 2D Ising model with all spins up or down. However for larger h, all spins point down. This implies that the first available excitation involves a spin flip, breaking $\mathbb{Z}_2$ symmetry and creating a gapped excitation. The transverse 2D Ising model can be mapped to an anisotropic 3D Ising model to solve for the critical ratio $h/J \approx 3$ and exponent for $\xi \propto (T - T_c)^{-.66}$. [3] This provides a good check for our ETH results.

However, it is difficult to extract more information from $|r_n|$ in this case, beyond the initial conclusions. $|r_n|$ only predicts large fluctuations across the expectation value of an operator in different energy eigenstates. However, as mentioned in section II.2, we can further

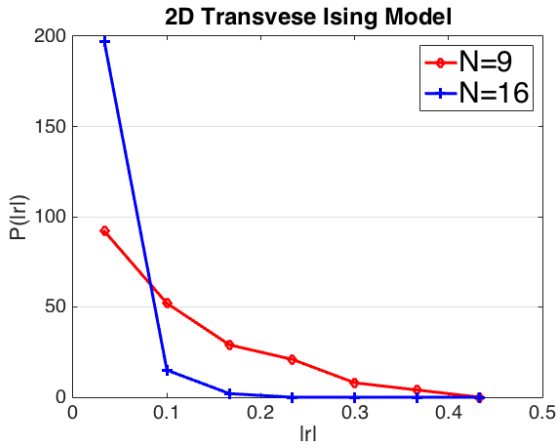

FIG. 2. In the figure above, we take the 2D version of the transverse Ising model, removing the longitudinal term previously required to prevent integrability. Here we use the smallest 200 eigenvalues and move from a system size of 9 spins to 16 spins, again periodic boundary conditions. Unfortunately, larger systems require too much computational power.

constrain these fluctuations. We know that in the case of a thermalizable system, the off diagonal matrix elements must be exponentially small in the system size so

$$v(N) = \frac{\sum_{i\neq j}^{N} |\langle i|A|j\rangle|^2}{N^2 - N} \propto e^{-F(L^d)} \tag{14}$$

Where $F(L^d)$ is some function of the system size. However, we can plot v as we approach the phase transition. Statistical mechanics predicts that fluctuations will grow as the system approaches criticality which implies that at the critical point $v \approx \mathcal{O}(1)$, where $\mathcal{O}(1)$ implies no exponential suppression. Looking at Figure 4, we see the same phase transition outlined by the $\mathcal{O}(1)$ v's as in Figure 3. This implies that at the critical point, the system will not thermalize for two different reasons. First, the variations in the expectation values of the system's eigenstates in an arbitrarily small energy window are too large, preventing the temporal expectation value for an operator A from matching its thermal expectation value, ($\bar{A} \neq \langle A\rangle_{\text{mc}}$). And second, the variations in $\langle A(t)\rangle$ also becomes very large. So, even if $\bar{A} \approx \langle A\rangle_{\text{mc}}$, an initial state $|\psi\rangle$ can vary arbitrarily far from the thermal average, never thermalizing. Furthermore, this divergence is not sharp; fluctuations, both r and v, grow relatively smoothly as the system approaches a phase transition. Therefore, there must be some mechanic within the ETH constraints to allow for this. In particular, $v \propto e^{-F(L^d)/x^l}$, where x^l is some variable related to the scale of fluctuations. Luckily, we also know that ξ diverges near the critical point and gives the relevant scale for fluctuations. This is very suggestive, we could imagine a dependence $v \propto e^{-F(L^d)/\xi^l}$, such that as $\xi \to \infty$, $v \to 1$. If our model were more accurate (more spins and a larger N in $v(N)$), we could attempt to vary $T - T_c$ ($\approx 1/J$) while taking $h \to 0$ and plot v vs. ξ and find l.

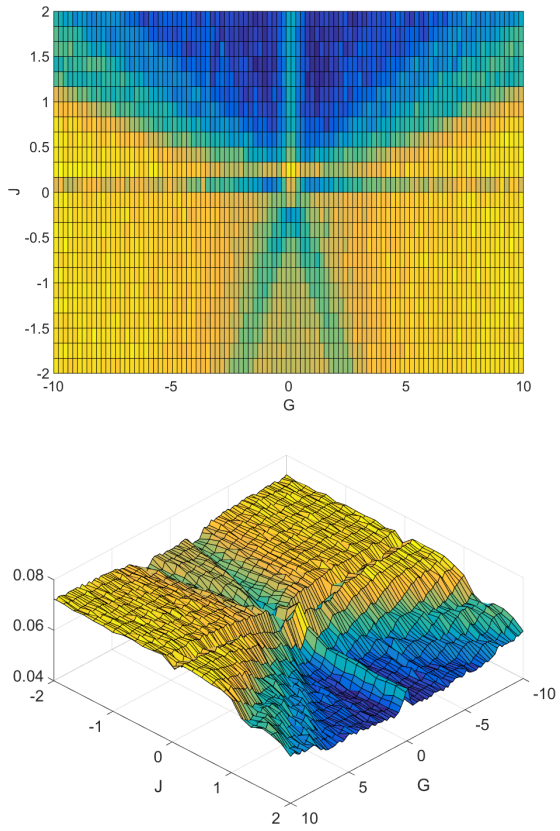

FIG. 3. The above figure shows a 3D plot of the $|\bar{r}|$ while varying the magnetic field strength in the z direction with G (transverse field) corresponding to the h used above; the brighter color corresponds to a larger $|\bar{r}|$. Notice the ridge along the line $G \approx 3J$; it corresponds to the Ferromagnetic to Paramagnetic phase transition. Furthermore, the paramagnetic phase has large fluctuations in $|\bar{r}|$ since its diagonal elements vary greatly from spin to spin, influencing $|\bar{r}|$ beyond the phase transition.

III.2.2. ξ and ETH

While we weren't able to compute l numerically, it maybe possible to make an educated guess. Consider a classical system of spins in 1D. Intuitively for the system to thermalize, the initial state must lose coherence. While the system is initially uncorrelated, as the spins interact they become entangled with each other, however, the correlation between two spins, i, j, cannot occur faster than the speed of sound in the system. Therefore the time it takes for the system to decohere or self-correlate is on the order of the correlation length divided by the speed of sound, or

$$\mathcal{O}(\Delta t) = \frac{\xi}{v_s} \tag{15}$$

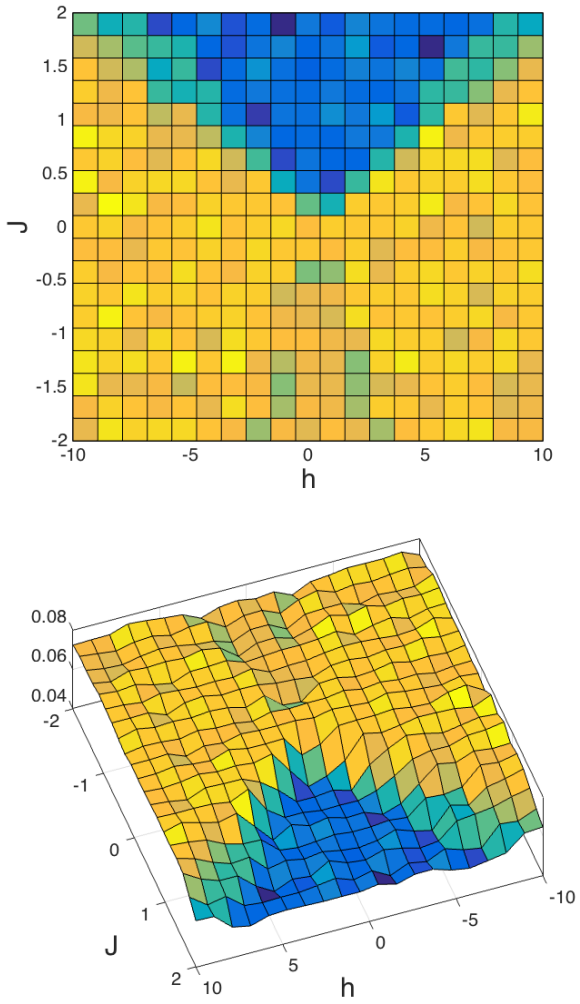

FIG. 4. The above figure shows a 3D plot of the v for N = 200, while varying the magnetic field strength in the z direction with G corresponding to the h used above; the brighter color corresponds to a larger v. Again, notice the ridge along the line $G \approx 3J$.

Naively, one would expect $l \propto d$, but in this picture the 2D case is no different. The maximum correlation distance becomes $\xi\sqrt{2}$ if there are diagonal interactions, or 2ξ if each spin can only interact with its nearest neighbor. By induction, it is clear that in this classical picture $l = 1$ and is independent of dimension, d.

Beyond an intuitive argument for $l = 1$, the classical picture also provides a clear reasoning behind the lack of thermalization in critical systems. As it approaches the critical point, any initial state $|\psi\rangle$ will take $\mathcal{O}(\xi/v_s)$ time to thermalize, but as mentioned above, ξ diverges as one approaches a critical point.

IV. CONCLUSION

While far from a proof, the above simulations make a compelling argument for the existence of eigenstate thermalization in those non-integrable systems. By utilizing both an integrable and non-integrable 1D transverse Ising model, we add some numerical validity to the $|r_n|$ approach described above.[2] Then, by transitioning into a 2D square lattice transverse Ising model, we utilized a well described system to explore eigenstate thermalization near phase transitions. While unable to implement time evolution in our system due to computational limitations, we developed another metric by which a system's ETH constraints could be evaluated. Combined with the r_n approach, the $v(N)$ indicator demonstrated the existence of large fluctuations in both the diagonal and off diagonal elements of $A_{\alpha,\beta}$ for any operator $\hat{A}$ near the critical point of a system.

The increasing off diagonal elements of $A_{\alpha,\beta}$ upon approaching a critical point were suggestive of a dependence on the correlation length of the system. In particular, that the off diagonal elements

$$A_{\alpha\neq\beta} \propto e^{\frac{-F(L^d)}{\xi^l}} \tag{16}$$

Moreover, using only simple classical reasoning, we make the educated guess that $l = 1$ by considering the time required for our system to thermalize. The suggested dependence on the correlation length of the system would create yet another constraint a system must satisfy to undergo eigenstate thermalization.

Therefore, we propose the study of time evolution in some of these non-integrable systems with the goal of further expanding the ETH formalism in the vicinity of phase transitions.

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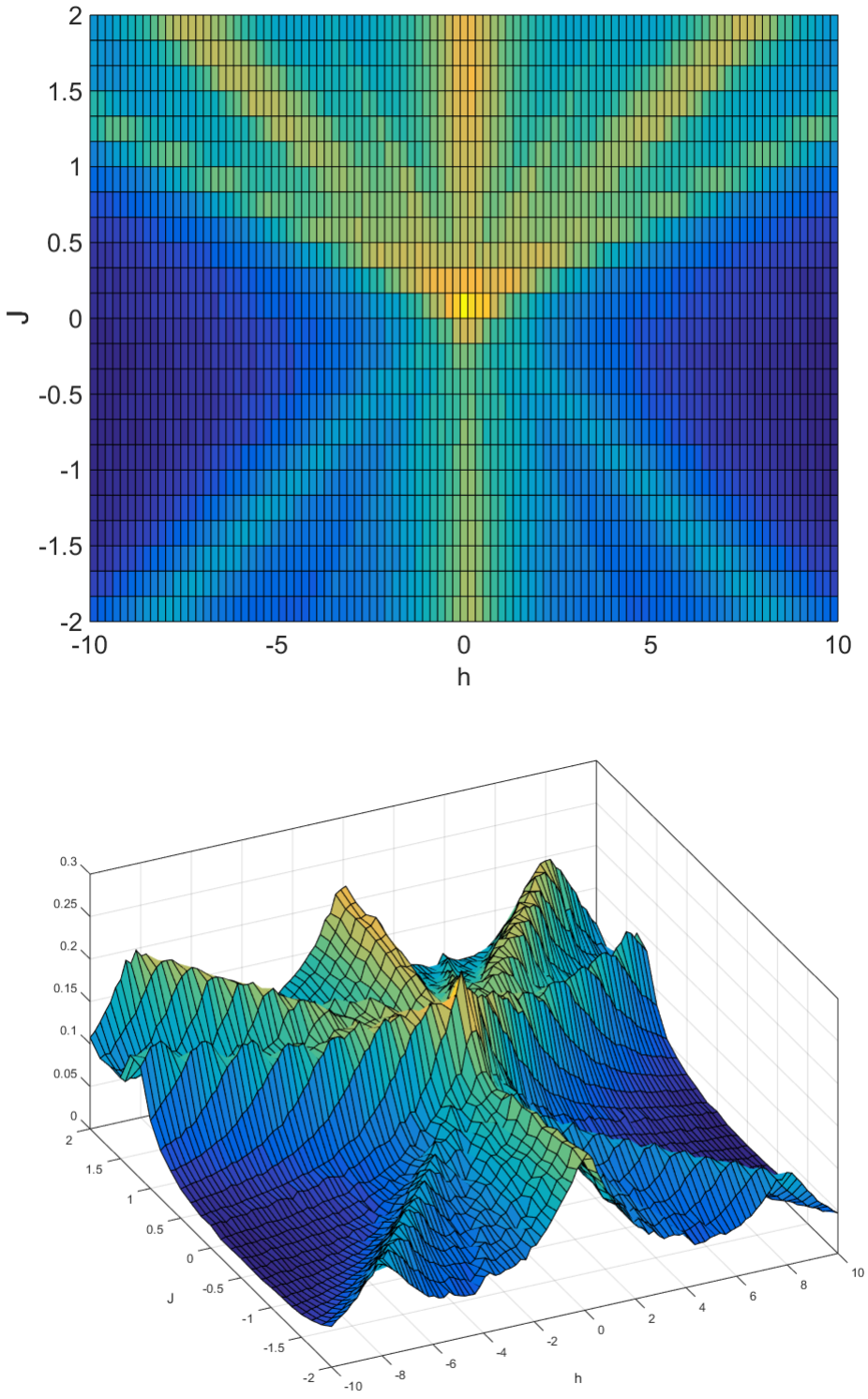

FIG. 5. In this figure we fix G = 0, and allow h to vary in the 2D version of the the following Hamiltonian $H = \sum_i \left(J\sigma_{z,i}\sigma_{z,i+1} + g\sigma_{x,i} + h\sigma_{z,i}\right)$