Quantum chaos in spin 1/2 chain

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Abstract

The chaotic behavior in quantum system has a long history for research but is still a controversial topic. Quantum many-body system like spin ½ chain is believed to be a good environment for research for both theoretical and practical significance, and recently the evolving interests on many-body localization in spin chain also made many important progress: by introducing different patterns of defects to spin chain, one can observe different chaotic or nonchaotic phases. Here I employ the powerful pattern generation tool ε-Machine to study quantum chaos in spin ½ chain, and focus on the relationship between measurement information decomposition of different machines and corresponding phases in spin chain. Bound information is found to have potential to link the two parts together.

1 Motivation

The problems of chaos and relaxation have a fundamental importance in the study of many-body classical and quantum systems. The most notable signatures that define the phenomena of chaos in classical mechanics is deterministic randomness and exponential sensitivity to initial conditions, both are related to the concept of unpredictability, caused by the nonlinearity of the system dynamics. However, quantum dynamics are fully described by Schrodinger's Equation, which is linear[1]. And bounded quantum system has discrete energy levels, which prevents the appearance of exponential sensitivity in some ways by breaking the continuity of phase space. In this case, could there still exists chaos in quantum many-body systems? If so, how could we define it? How should we describe it?

Quantum spin chains are prototype quantum many-body systems. They are employed in the description of various complex physical phenomena because of its computational simplicity. By focusing on the time evolution of a Heisenberg spin-1/2 chain and interpreting the results based on the analysis of the eigenvalues, eigenstates, and symmetries of the system, we could study how these properties indicate chaos. Moreover, by introducing different Zeeman splitting on different spin sites[2],[3], we could trigger chaos in the system, and the introduce process could be done by the powerful tool ε-machine. How could different patterns lead to different types of chaotic/nonchaotic systems? How are the properties of machine in terms of information theory affect the resulted quantum system? Could we predict the possible system behavior directly from the machine?

2 Background

2.1 Classic and Quantum Chaos

The unpredictable randomness behavior, known as chaos has been studied since long time ago. Edward Lorenz, a notable researcher in this field describe chaos by the following: "When the present determines the future, but the approximate present does not approximately determine the future." The first part of his description indicates that the dynamics of the system is fully determined, and all the dynamics could be written down in closed form. For a classic chaotic system, whose states could be represented by a point in continuous phase space, if the evolution starts at two slightly different initial conditions, the leading future will be totally different. As the second part of Lorenz's description, without specification of the initial conditions up to arbitrary accuracy, we could not accurately predict the future. This property of classic chaos is known as the exponential sensitivity of initial conditions. One can quantitively describe this behavior by the well-known Lyapunov exponents, which measure the rate of divergence of a bunch of trajectories along several directions in phase space, and hence characterize the sensitivity to initial conditions. Positive and negative Lyapunov exponents correspond to directions of expansions and contractions in phase space respectively. A conservative system has an equal number of positive and negative Lyapunov exponents. If the system is ergodic, then the Lyapunov spectrum does not depend on where the trajectory is started from. The directions in phase space corresponding to conservative quantities (integrals of motion) are associated with zero Lyapunov exponents. A system is technically called chaotic if it has at least one positive Lyapunov exponent.

In classic system, chaotic phenomena require intrinsic nonlinearity inside the dynamics that make the system nonintegrable. Quantum dynamics, on the other hand, are fully described by Schrödinger equation which is fundamentally linear. A bounded quantum system possesses a set of discrete energy levels and hence the evolution is quasi-periodic. The occupancies of those levels are time-invariant and play the role of the integrals of motion in an integrable classical system. In classical chaotic systems, the exponential sensitivity is driven by the continuity of the underlying phase space, which allows to specify the initial conditions up to an arbitrary accuracy. On the other hand, the notion of a point in phase space does not exist in quantum mechanics. Furthermore, the definition of integrability in a quantum system is controversial until today[4]. Therefore, it's difficult to find a widely acknowledged definition of quantum chaos. Instead, for different quantum systems, there are indeed different indicators of quantum chaos, or signatures of quantum chaos. For example, one could also describe the quantum chaos in terms of sensitivity in time-dependent systems. Since the initial conditions of quantum system are vectors in Hilbert space, one could measure the sensitivity to initial conditions by calculate the overlap between two slightly different vectors and the rate of spread of an initial wave packet. Besides, another possible generalization can be given in terms of the stability of the wavefunction of the system under perturbations to the Hamiltonian itself, known as quantum fidelity:

$$\vartheta = < \varphi(t) | \varphi'(t) >$$

In which $\varphi(t)$ evolved by the Hamiltonian H and $\varphi'(t)$ by $H + \delta H$.

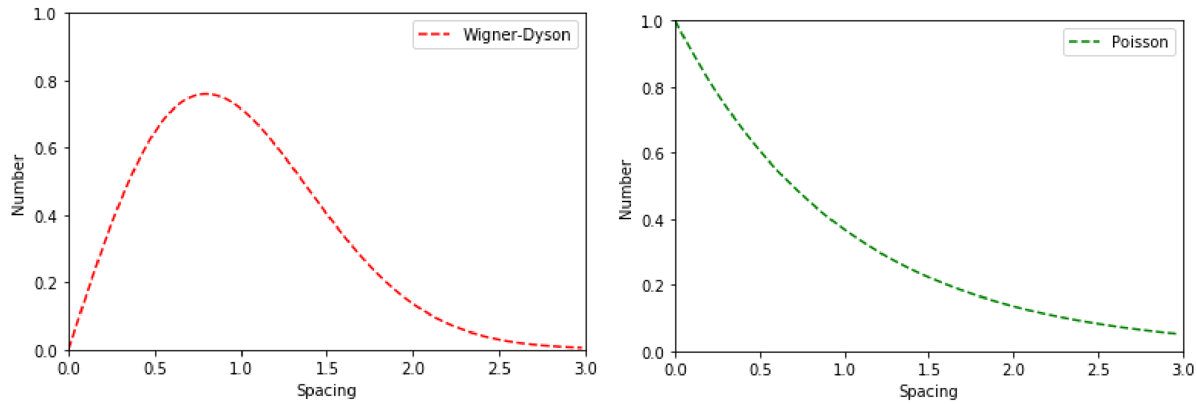

Fig. 1: Wigner-Dyson (left) and Poisson (right) distribution.

Except for that, another good way to describe quantum chaos would rely in the distribution of systems' energy level. The energy levels of chaotic quantum systems and the eigenvalues of random matrices exhibit similar statistical properties, such as level repulsion. The quantity of level spacing $P(s)$, where s is the spacing between two adjacent levels, depends on the universality class to which this system belongs, which, in turn, depends on its underlying symmetries. For example, systems exhibiting time reversal symmetry exhibit the same statistics as the Gaussian Orthogonal Ensemble (GOE) of real symmetric matrices. The spacings of their eigenvalues is characterized by the Wigner-Dyson distribution $P(s) = \frac{\pi s}{2} e^{-\pi s^2/4}$(see Fig.1). Integrable systems, on the other hand, exhibit level clustering. The statistics of their energy level spacings follow a Poisson distribution, $P(s) = e^{-s}$. This property is sometimes used as a definition for quantum integrability, especially in quantum systems lacking a corresponding classical limit.

2.2 Spin ½ Chain

The spin ½ Heisenberg model finds applications in several other contexts. It is a key model in studies of quantum phase transition, superconductivity, localization in disordered systems, as well as the dynamics and thermalization of correlated one-dimensional lattice systems. The interplay of disorder and interactions in quantum systems can lead to several intriguing phenomena, amongst which the so-called many-body localization has attracted a huge interest in recent years[5]. Specially, in the spin ½ chain, the disorder is described by different Zeeman splitting energy at different spin sites. The whole Hamiltonian could be written as below:

$$H = \sum_{i\in[1,L]} S_i \cdot S_{i+1} - h_i S_i^Z$$

where S_i is the spin at site i and h_i is the Zeeman splitting energy.

With the introduce of defects, the spin chain could have two different phases. The chaotic phase will be nonintegrable and have an important behavior: thermalization. Thermalization requires that different parts of the system exchange energy efficiently, such that states with spatially non-uniform energy density can relax to thermal states. Thus, energy transport is necessary and thermalizing systems are expected to be conducting. Often, thermalizing quantum systems are referred to as ergodic, because during their evolution they explore all configurations allowed by the global conservation laws. In contrast to chaotic systems, another many-body localization(MBL) phase has a general mechanism by which quantum systems can avoid thermalization. The localization and the breakdown of ergodicity in MBL systems occur because strong quenched disorder effectively makes energy exchange processes between different degrees of freedom "off-resonant"[6].

2.3 ε-Machine

A presentation of a given process is any state-based representation that generates the process: it produces all and only the process's word sequences and their probabilities. In the following we consider processes generated by finite hidden Markov models (HMMs). For a given process, while there may be many alternative HMMs, there is a unique, canonical presentation—the process's ε-machine. The recurrent states S of a process's ε-machine are known as the causal states. The causal states are the minimal sufficient statistic of the past for predicting the future. An ε-machine is a type of HMM satisfying three conditions: unifilarity, probabilistically distinct states, and irreducibility. Unifilarity means that from each state there is at most one next state reached on a given symbol. Probabilistically distinct states means that for every pair of states, there is at least one word for which the probabilities of observing word starting from those states differ. Irreducibility implies that the internal Markov chain over the causal states is strongly connected and minimal in the sense that it is not possible to make a smaller unifilar HMM that generates the process.

Therefore, given a pattern of number sequence, the ε-machine generated it could represent its regularity information most efficiently. With our knowledge until now, we know that different patterns of defects in a spin chain could lead to different phases, and the most efficient way to describe and generate patterns is the ε-machines. So could there be any mutual information between ε-machine and resulting chaotic or nonchaotic phases? Or is there any possibility to directly predict the chaos by ε-machine in terms of information theory? That's the main question to explore in this paper(see Fig. 2).

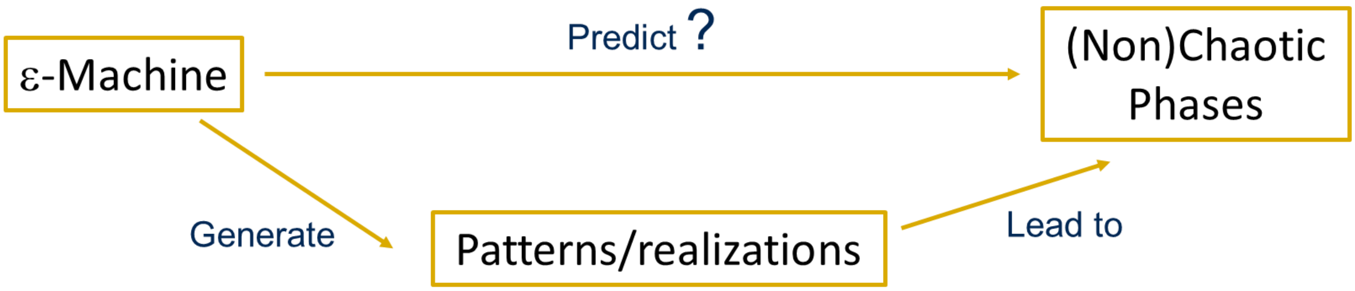

Fig.2: Logic between ε-machine and different phases in spin ½ chain.

3 Methods

All the results and graphs in this work are generated by code in python. For the Hamiltonian of spin ½ chain, Heisenberg interaction model is used (XXX model, J_x=J_y=J_z=1.0), and Nearest-Neighbor Approximation is considered in this work. Besides, open boundary conditions are used for all the calculations (open chain), where the sum goes from site $n = 1$ to site $L - 1$, an excitation on site 1 can move only to site 2 and from site L to $L - 1$.

Considering a spin chain, one could see two extreme cases: all spins up(or down) and half-half. The first one is too trivial for study since its ensemble has only one dimension. In this work, I consider two cases: half-half and one-third spins up(or down, two cases are symmetric). And the system size will be L=15 or 16, which is the biggest number a personal laptop can handle.

Besides, the defect pattern is set to be binary (defect exists or not exists), and defect energy is set to be 0.5 if exists. All patterns are generated by ε-machines. In this work, three kinds of machines are used: Biased Coin(Noisy), Even and Golden Mean. At least five realizations are calculated for each machine, and then average to avoid coincidence. And for each realization, density of states(DOS) is calculated first(see Fig. 3) and then take the energies which have a DOS over 50% of the maximum number to further calculate the level spacing distribution(LSD), since the energies with lower DOS should play less important role and could be source of errors.

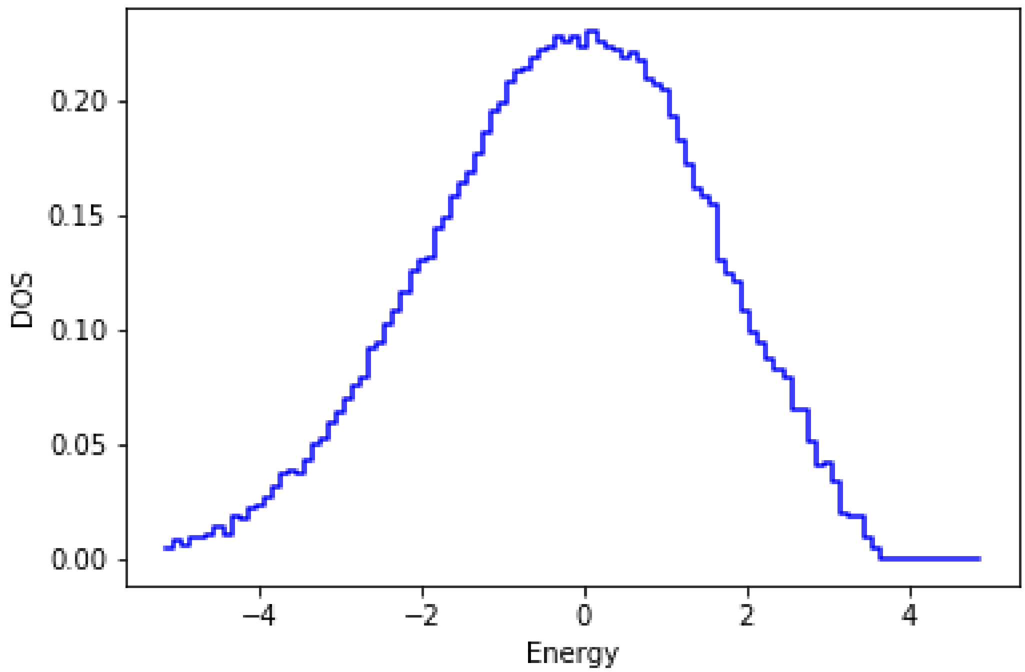

Fig. 3: Example of the DOS of a spin chain (up spin = 7, down spin = 8, defect at 5th site).

4 Results and Discussions

4.1 Simple Realizations

It's important to firstly verify some simple realizations(see Fig. 4) of spin chains, which could provide some reliable references for future work.

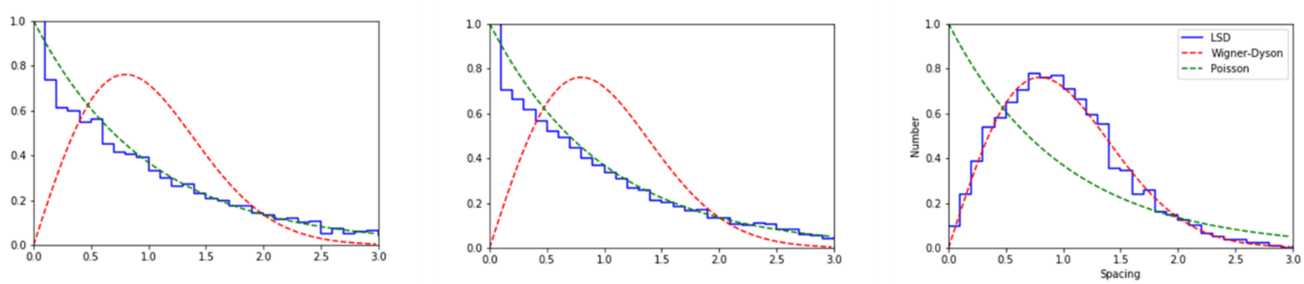

Fig. 4: LSD of some simple realizations(L=16): half-half, no defect, nonchaotic(left); half-half, defect at 1st site, nonchaotic(middle); half-half, defect at middle(8th site), chaotic(right).

First the LSD of a clean chain is calculated, it's not surprising that the distribution follows Poisson distribution and system is not chaotic. Next a defect is added to the first site, since the open boundary condition is used, the excitation on site 1 can move only to site 2. Therefore, the defect effect is localized around the 1st site and could not propagate further to the whole chain, and the system is still nonchaotic. Finally, a single defect is introduced at the very middle site where it could have the most significant influence on the whole chain. And as a result, the LSD becomes Wigner-Dyson distribution and the spin chain becomes chaotic. It's compatible with intuitive thought that unlocalized defect will trigger chaos, other realizations also indicate that single or a few defects introduced except at the first or last site tend to lead to a chaotic system.

4.2 Finite Size Effect

While calculate more realizations, some interesting behaviors are found as below(Fig. 5). The LSD of those system are not obviously nonchaotic or chaotic, instead the distributions are some curve between the two cases.

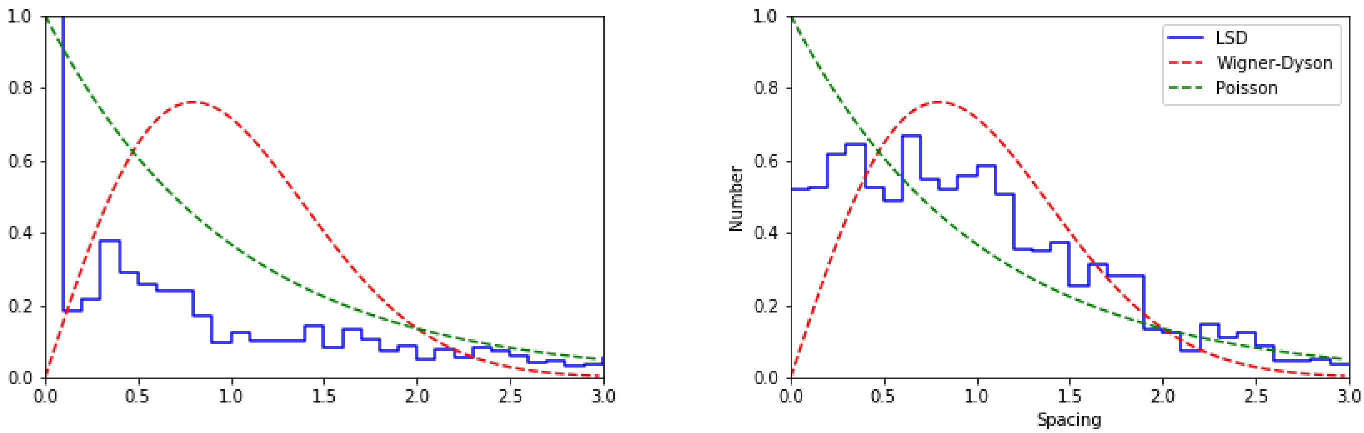

Fig. 5: Examples of finite size results

The effect could be explained by the finite size of the spin systems. In the finite size system, the phase transition happens gradually instead of abruptly, and thus there will be some intermediate states which do not belongs to either phase. And these realizations typically have some short-range symmetries which will disappear if the system size is infinite, but they still could provide some information for us. Here I introduce a deviation of the distribution from Poisson distribution, which sums up the distance from Poisson distribution of every bin at the middle. A bigger deviation indicates more chaotic system.

4.3 Biased Coin(Noisy) Machine

First Biased Coin(Noisy) process is considered(Fig. 6). Biased Coin Machine is one of the most commonly used machines for many situations. Basically it will generate a sequence of random independent variables 0 or 1, and the probability of generating 0 or 1 at each digit is the same. Here I used symbol 1 to indicate defect exists at corresponding site.

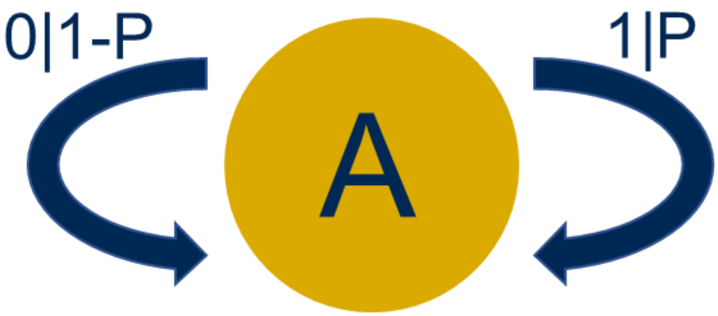

Fig. 6: Scheme of Biased Coin Machine(P: probability of defect at each site)

As one can easily see, if P is close to 0, the generated sequence will be basically a sequence of 0s, and the corresponding spin chain will be clean. Therefore the deviation will decrease with P near P = 0. And similarly, if P is close to 1, there is highly probably that every site is defect and the chain could be another kind of "clean". The deviation should decrease with P increase near P = 1. As a result, the most chaotic case should happen near P = 0.5, and the calculation results could verify the assumption(Fig. 7).

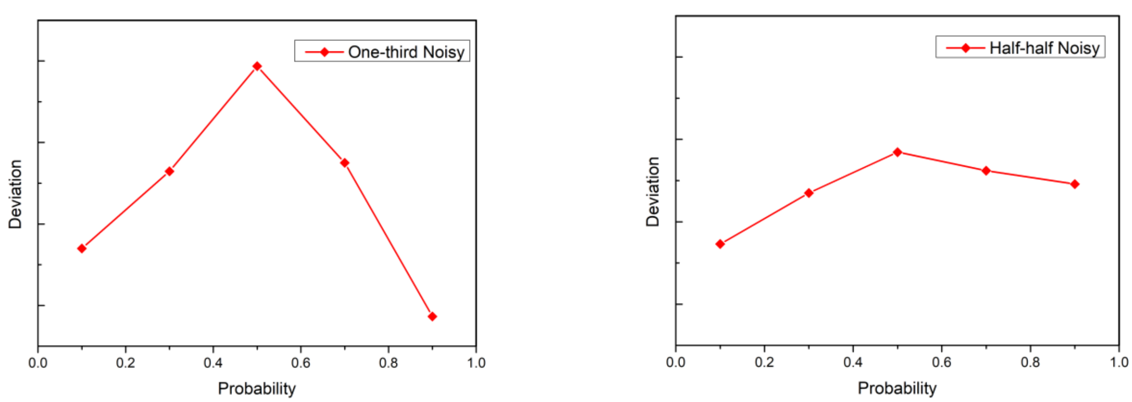

Fig. 7: Deviation of Noisy chain versus probability

4.4 Golden Mean Machine

Golden Mean Process is another common process worth studied(Fig. 8). Biased Coin Machine is one of the most commonly used machines for many situations. The rule for Golden Mean Process is that generated sequence will have no consecutive 1s: if the current symbol is 1, the next symbol will be 0 with 100% probability. When applied this rule to the spin chain, the chain will have no consecutive site of defects.

Fig. 8: Scheme of Golden Mean Machine.

As the P becomes larger, the generated sequence will have more occurrence of 10 pairs. The 10 pairs could be regarded as a bigger single site with mean field approximation, and the system will become more clean and symmetric with more occurrence of 10 pairs. Actually a chain of recurrence 01 pairs is nonchaotic based on the calculation results. The deviation will monotonically decrease with P increases, which is verified by calculation(Fig. 9). The slightly bigger case at P = 0.3 in one-third case could be explained by the limited number of realizations.

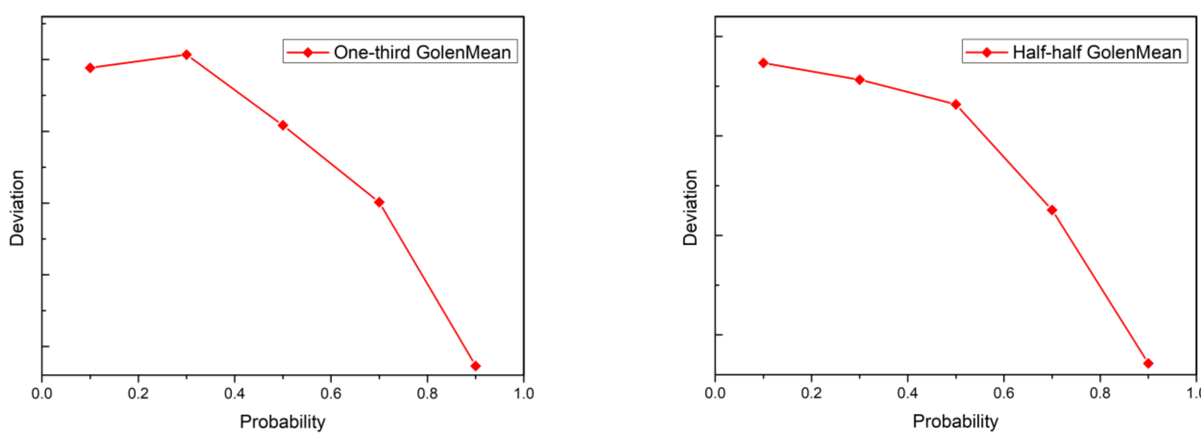

Fig. 9: Calculation results of Golden Mean chain

4.5 Even Machine

Even Process(Fig. 10) is like a counterpart of Golden Mean: the rule for Even Process is that all sequence of 1s will have even number. If the current symbol is 1 and previous symbol is 0, the next symbol must be a 1. The property could be seen as consecutive 11 pairs, and the corresponding spin chain will have only consecutive defects.

Fig. 10: Scheme of Even Machine

If P is close to 0, the chain will be basically clean and nonchaotic. And if P is close to 1, there will be more occurrence of 11 pairs, making the whole chain consists of mostly 1s. Therefore the deviation should decrease with P when P is close to 1. The two cases are verified by calculation results(Fig. 11).

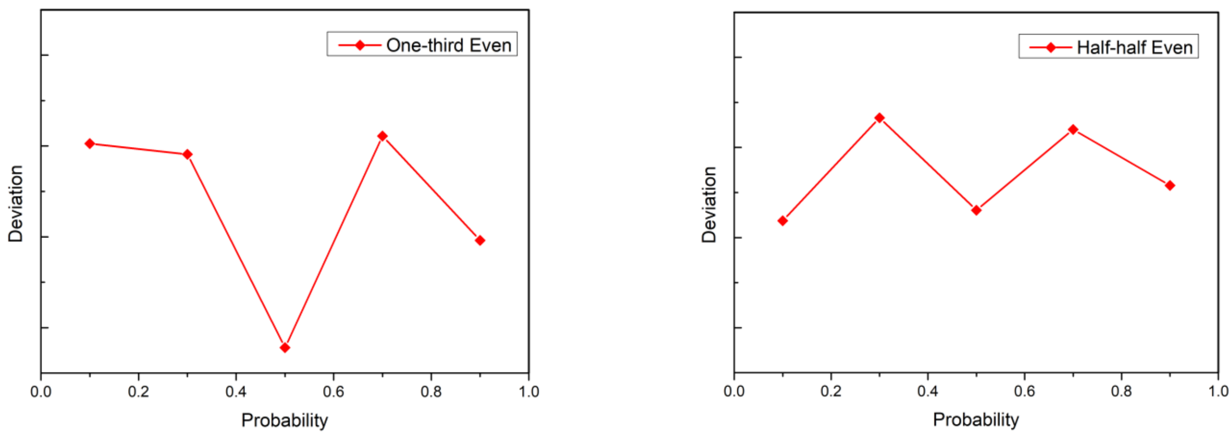

Fig. 11: Calculation results of Even chain

Another interesting part is that the deviation will have a drop at the middle in both cases. After observing the specific realizations, one can find that at P = 0.5, it is highly probable that the chain will have a few 11 pairs separated by 0s. This kind of realizations might have some symmetry due to the finite size of chains, which suppresses the chaotic behaviors. On the other hand, separated 11 pairs could act as localization centers, which gives rise to nonchaotic many-body localization phases.

5 Conclusion and Prospective

Although there is currently not an agreement on the definition of chaos in quantum world, quantum chaos indeed has different important signatures in different systems. For many-body system like spin chain, the statistical properties of energy level such as level spacing distribution have quiet significance for describing quantum chaos. By direct calculation of Hamiltonians for different spin chains, one can prove that the introduce of defect could lead to phase transition between MBL phase and ergodic phase in this system, and different patterns of defects can lead to different phases.

By utilizing the powerful tool ε-Machines, one can see that different machines will give rise to different phases. Even the topological structures of machines are the same, like Golden Mean and Even machines, the resulting chaotic behaviors are totally different, which requires us to explore deeper by views of information behind the topological structure and relate the properties of machine to the resulting different phases. The information decomposition of a process[7](Fig. 12) proposed by Crutchfield could provide meaningful methods for this research.

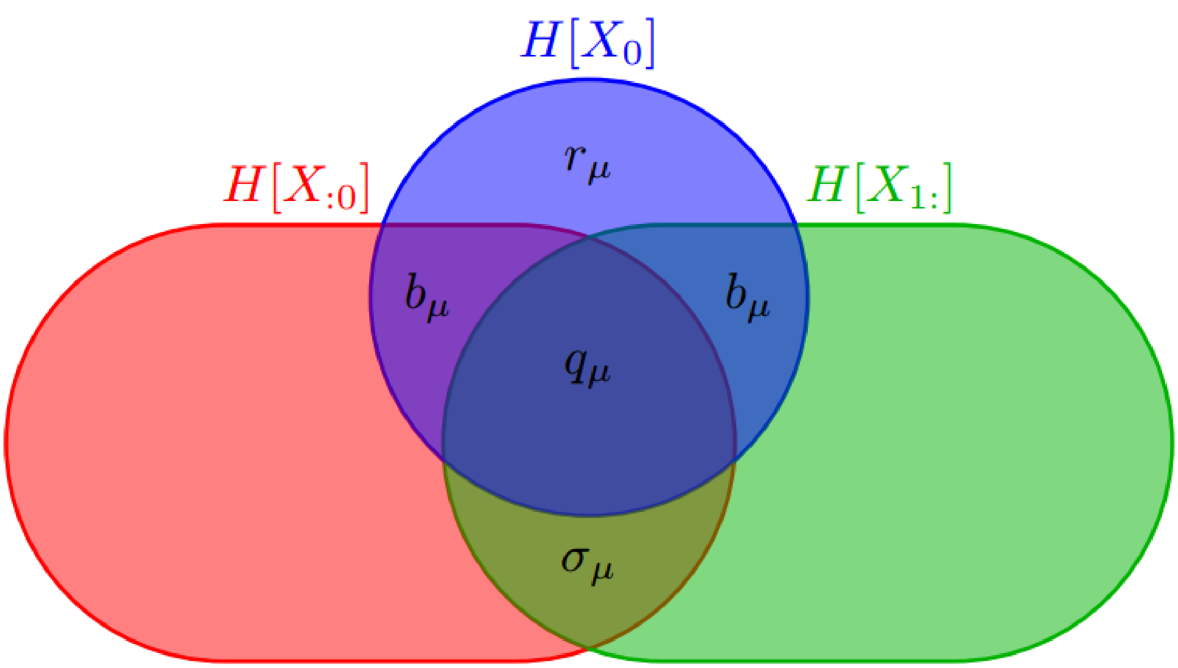

Fig. 12: Measurement decomposition diagram of a process

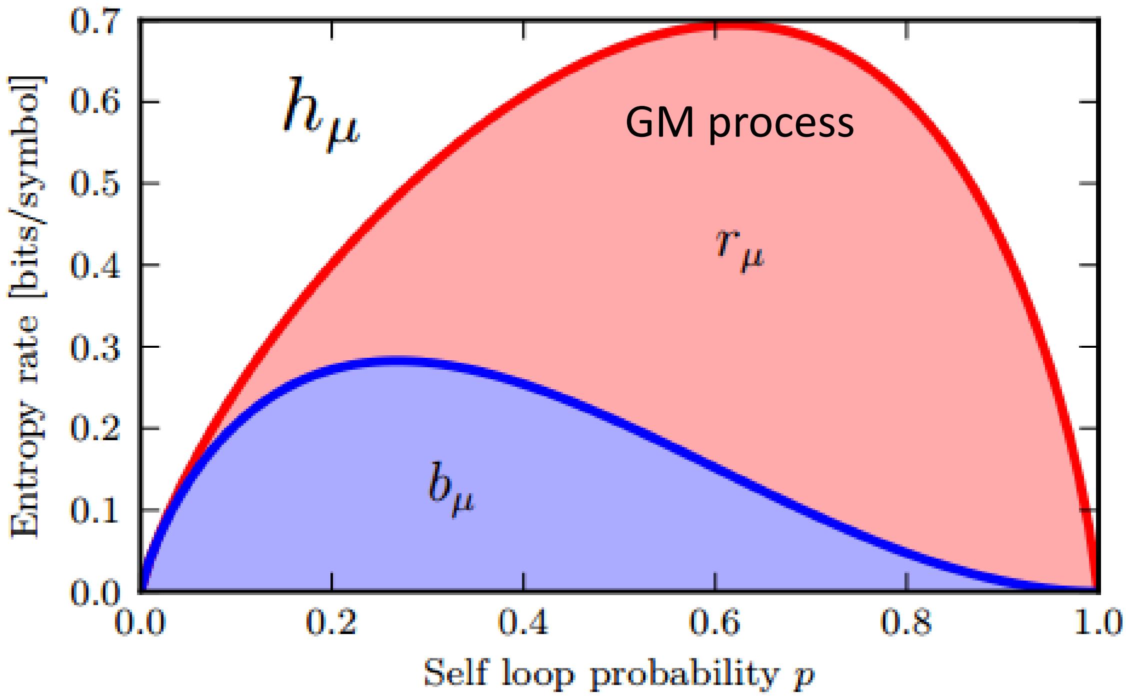

Fig. 13: Measurement decomposition of h_μ of Golden Mean Process as edge probability p changes

In terms of information theory, the Golden Mean and Even process have same entropy rate h_μ but different decompositions bound information b_μ and residual information r_μ, which leads to difference on the way of information sharing between current and future. And furthermore, decompositions b_μ and r_μ won't be a constant for a process when the edge probability changes(Fig. 13). For the Golden Mean process, one could see that as P increases, r_μ also increases, which means the ephemeral information existing only for the present would occupy a bigger part of entropy rate and the information relevant to predict the future decreases. Therefore, the unknown part, or randomness of the process decreases as P increases, and less randomness means less chaotic, which is consistent with the calculated results.

However, to strictly prove the relationship between bound information and chaos, there are more concrete work need to do. This work only shows the potential relation in an intuitive way and provide more possibilities for this research field.

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