Quantum chaos in spin chains with a tunable impurity

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Abstract: We analyze the spectral properties of one-dimensional spin chains, that can be described with a simplification of the Heisenberg model, the XXZ model, in order to study the transition from a regular to a chaotic behaviour. The spectrum of the system is obtained by direct diagonalization of the Hamiltonian matrix. We describe the onset of quantum chaos, in terms of the spectral properties, for a XXZ chain when only one of the spins is subjected to the influence of an external magnetic field of variable intensity.

I. INTRODUCTION

Classical chaos is referred to the non-deterministic evolution of a dynamical system. Systems whose time evolution is very sensitive to its initial conditions, in which smooth variations on these can induce exponential divergences on the trajectories in the phase space, are classically called chaotic systems [1]. However, it is well known that the concept of trajectories is not applicable to quantum systems. Thus, to introduce the concept of chaos in quantum systems, one needs to find an alternative approach.
Quantum chaos studies the properties of the spectrum that appear when the classical analogous of the system would be in a chaotic regime. Following the work of Bohigas-Giannoni-Schmit (BGS) [2], a way to characterize the chaoticity of a quantum system relies on studying the statistical properties of the many-body spectrum [3]. In this work we discuss the appearance of quantum chaos in spin chains analyzing the spectra of the many-body system. First of all, in Sec II, we discuss some spectral properties of a quantum system and how they are related to chaos. Then, in Sec III, we introduce one-dimensional spin chains. Finally in Sec IV, we study the transition from a regular domain to a chaotic regime of a chain with 15 spins by introducing an impurity of variable intensity but fixed in the 7th site.

II. DESCRIPTION OF THE SPECTRUM

A. Unfolding the spectrum

In order to compare different systems of many sizes we need to unfold their spectra. As explained in Ref. [3], locally rescaling the energies we make the local density of the renormalized states be 1, and we can compare the level repulsion of spectra that initially could have different densities. A way to proceed is sorting the eigenvalues in increasing values of energy and then separate them into several sets, computing the mean level spacing of each set and finally dividing each eigenvalue by this averaged value. Additionally, we can also discard a certain amount eigenvalues at the edges of the spectrum.

B. Level spacing distribution

The most common way to study the chaoticity of a quantum system is by the distribution of consecutive energy gaps. An energy gap is the difference between two consecutive eigenvalues of the Hamiltonian, $s_i = E_{i+1} - E_i$. One can build a probability distribution for these energy gaps, $P(s)$.
A system is said to be integrable when the eigenvalues of its Hamiltonian are uncorrelated. In these cases the expected level spacing distribution is a Poissonian [4],

$$P_{\mathrm{P}}(s) = e^{-s}. \tag{1}$$

On the other hand, when a system is chaotic we must appeal to the BGS conjecture. The distribution of level spacings of a chaotic system is known to be a Wigner-Dyson one, just like for the Gaussian orthogonal ensemble [2]. The level repulsion is manifested in the distribution of spacings by having $P(s) \sim s^{\beta}$ for $s \to 0$ [4], with $\beta = 1$ in the Wigner-Dyson case. The distribution function can be written as

$$P_{\mathrm{WD}}(s) = \frac{\pi}{2} s e^{-\frac{\pi}{4}s^2}. \tag{2}$$

This distribution has a maximum at $s_{\max} = \sqrt{2/\pi}$, while in the integrable regime it always decays. The level repulsion is manifested by not having two identical consecutive energies, i.e., $P(s=0) = 0$. In chaotic systems there are no energy degenerations. We must remember that the spectrum is ordered in increasing values of energy.

C. Ratios of consecutive level spacings

There are other ways to determine in which regime a system is found. A quantity that can be defined in order to capture the level repulsion is the following average ratios of level spacings $\langle r \rangle$; where the ratios r_i are defined as,

$$r_i = \min\left\{ \frac{E_{i+1} - E_i}{E_i - E_{i-1}}, \frac{E_i - E_{i-1}}{E_{i+1} - E_i} \right\}, \tag{3}$$

and E_i is the ith eigenvalue of the system [5]. This quantity is able to summarize spectral properties such as the level spacing distribution. We can see in Ref. [5] that the Poisson distribution translates to the ensemble average $\langle r\rangle \approx 0.38629$, while the Wigner-Dyson distribution translates to $\langle r\rangle \approx 0.53070$. Computing this value for a given spectrum, we can see how close it is to a Poisson or a Wigner-Dyson distribution. One must be careful because obtaining those numbers does not necessarily implies having a Poisson or a Wigner-Dyson, respectively, so we must always check that the average ratio obtained fits with the corresponding distribution. This magnitude allows us to avoid unfolding the spectrum, and summarizes its distribution with a single quantity.

III. ONE-DIMENSIONAL SPIN-1/2 CHAINS

A. States of the system

A single spin-1/2 can be represented by the spin operators $\hat{S}^i = \frac{1}{2}\hat{\sigma}^i$ $(i = x, y, z)$, where $\hat{\sigma}^i$ are the Pauli matrices. A quantum state of an spin can be represented through spinors, that usually are written in terms of the basis vectors, which are eigenvectors of the $\hat{\sigma}^z$ operator. Now let us take a chain of L spins. Each spin can be found in both up and down states. As we have 2 possible configurations for each spin, the total number of combinations that our system can have is 2^L, which fixes the dimension of the Hilbert space.
We can also divide the system in subspaces setting restrictions of a certain number of up-spins (N_{up}). The dimension of each subspace can be calculated by the combinatorial number $\binom{N}{N_{up}}$ [3], which tells us in how many ways we can achieve a configuration with a fixed number of spins pointing up. By using the binomial theorem, we recover the total dimension as,

$$2^L = \sum_{N_{up}=0}^{L} \binom{L}{N_{up}}. \tag{4}$$

B. The XXZ Hamiltonian

1. The Heisenberg model

When the spins are located on a chain, the states of each one can be affected by the presence of other spins. We consider the following XXZ Hamiltonian [3],

$$\hat{H}_{\mathrm{XXZ}} \equiv J\sum_n (\hat{S}^x_n\hat{S}^x_{n+1} + \hat{S}^y_n\hat{S}^y_{n+1} + \Delta\hat{S}^z_n\hat{S}^z_{n+1}), \tag{5}$$

where n labels the site of the chain. The sum over n is extended from 1 to $L-1$ when open boundary conditions are imposed, and from 1 to L when we have periodic boundary conditions and the first spin can interact with the last one. J is the strength of the interaction between neighbouring spins and Δ is a symmetry breaking parameter. We are working with a simplification of the Heisenberg model.
This Hamiltonian can be decomposed in two terms. On one hand we have the Ising interaction,

$$\hat{H}_{\mathrm{ZZ}} \equiv J\sum_n \hat{S}^z_n\hat{S}^z_{n+1}. \tag{6}$$

We are considering interactions only between first neighbours and neglecting the magnetic field contribution. The Ising interaction is diagonal, so it is not properly a quantum model since the eigenstates of this Hamiltonian are uncorrelated:

$$\hat{S}^z_n\hat{S}^z_{n+1}\left|\uparrow_n\uparrow_{n+1}\right\rangle = \frac{1}{4}\left|\uparrow_n\uparrow_{n+1}\right\rangle \tag{7}$$

and

$$\hat{S}^z_n\hat{S}^z_{n+1}\left|\uparrow_n\downarrow_{n+1}\right\rangle = -\frac{1}{4}\left|\uparrow_n\downarrow_{n+1}\right\rangle. \tag{8}$$

On the other hand, we have the flip-flop term,

$$\hat{H}_{\mathrm{flip-flop}} = J\sum_n \hat{S}^x_n\hat{S}^x_{n+1} + \hat{S}^y_n\hat{S}^y_{n+1}, \tag{9}$$

which introduces the truly quantum effects on the system. It can be seen that it interchanges the spins of two anti-parallel adjacent spins, thus mixing the basis:

$$(\hat{S}^x_n\hat{S}^x_{n+1} + \hat{S}^y_n\hat{S}^y_{n+1})\left|\uparrow_n\downarrow_{n+1}\right\rangle = \frac{1}{2}\left|\downarrow_n\uparrow_{n+1}\right\rangle, \tag{10}$$

$$(\hat{S}^x_n\hat{S}^x_{n+1} + \hat{S}^y_n\hat{S}^y_{n+1})\left|\downarrow_n\uparrow_{n+1}\right\rangle = \frac{1}{2}\left|\uparrow_n\downarrow_{n+1}\right\rangle. \tag{11}$$

While the Ising term does not couple any state, the nearest-neighbour flip-flop contribution correlates states that are similar except for both orientations in a pair of consecutive antiparallel spins, as seen in Eqs. (10) and (11). This is translated in a tridiagonal structure for the Hamiltonian matrix.

2. Symmetries of the Hamiltonian

The Hamiltonian of the system commutes with $\hat{S}^z$, where $\hat{S}^z = \sum_n \hat{S}^z_n$ is the third component of the total angular momentum. Each eigenstate of the XXZ Hamiltonian can be constructed with a linear combination of states with a fixed number of up-spins [3], since each one has to be also an eigenstate of $\hat{S}^z$. Thus, the matrix can be organized in boxes, which only the diagonal ones are different from zero. For this, the subspaces with different N_{up} can be treated independently. The whole system is the union of all these subspaces, as expressed in Eq. (4). Realizing that the configuration of lowest energy corresponds to a configuration with all the spins pointing

down, we could understand an up-spin as an excitation, but as a consequence of the total spin number conservation, we can not create nor annihilate these excitations. In this model they only can be moved on the chain [1]. Then, we talk about excited states for those whose configurations let the system be in a larger energy without changing N_{up}.
If we make a reflection transformation, then the Hamiltonian remains invariant [3]. The parity ($\hat{\Pi}$) is a conserved quantity, where

$$\hat{\Pi} = \begin{cases} \hat{\mathcal{P}}_{1,L}\hat{\mathcal{P}}_{2,L-1}\cdots\hat{\mathcal{P}}_{\frac{L}{2},\frac{L}{2}+1} \text{ if } L{=}\text{even} \\ \hat{\mathcal{P}}_{1,L}\hat{\mathcal{P}}_{2,L-1}\cdots\hat{\mathcal{P}}_{\frac{L-1}{2},\frac{L+3}{2}} \text{ if } L{=}\text{odd} \end{cases}, \tag{12}$$

and

$$\hat{\mathcal{P}}_{n,m} = \hat{S}^x_n\hat{S}^x_m + \hat{S}^y_n\hat{S}^y_m + \hat{S}^z_n\hat{S}^z_m + \frac{1}{2}\mathbb{1}. \tag{13}$$

IV. CHAOTICITY IN 1D SPIN-1/2 SYSTEMS

From now on, we are going to consider a chain of $L = 15$ spins governed by the XXZ model, Eq. (5). The number of up-spins is set to $N_{up} = 5$, so the dimension of this subspace is $\binom{15}{5} = 3003$, which allows to obtain enough statistics of the consecutive gaps. In this case, the system is known to be integrable and the level spacing distribution should follow a Poissonian one [3]. We take the anisotropy parameter as $\Delta = 0.5$. Large values of this parameter make the flip-flop term negligible and we may lose quantum effects; correlations between states may disappear.

A. Achieving the chaotic regime

If we want to lead the system into chaos we must add some perturbation on the system that can make such an important change on the spectrum that the level spacing distribution becomes a Wigner-Dyson one. An easy way to achieve that would be by allowing the spins to have interactions with 2nd neighbours [1]. But, the one we are studying in this article is just adding a single impurity (or defect) on a site of the chain. This impurity can turn an integrable system into a chaotic one if it is added in the proper site of the chain and it has a reasonable intensity. The Hamiltonian of a system with a single impurity located at site "α" ($1 < \alpha < L$) is

$$\hat{H}_{\text{impurity}} = \hat{H}_{XXZ} + \varepsilon J\hat{S}^z_\alpha. \tag{14}$$

We have added a magnetic field, of magnitude εJ, that only interacts with that spin α. We call ε the strength, or intensity, of the impurity.
We can see in Fig. 1 that there is a correspondence between the difference average ratio of level spacings computed with respect to the theoretical ones and how similar is each distribution to the respective ones. In Fig. 1

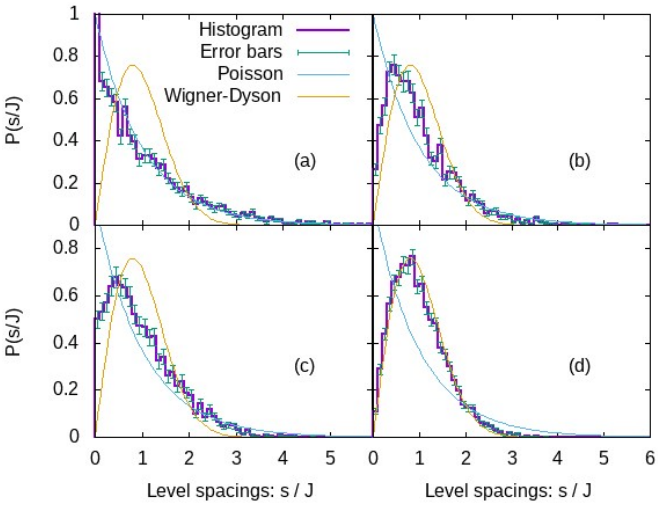

FIG. 1: Four examples of the level spacing distributions. (a) $\langle r\rangle = 0.36987$, no impurity (integrable domain); (b) $\langle r\rangle = 0.47914$, impurity at 7 with $\varepsilon = 0.05$; (c) $\langle r\rangle = 0.42485$, impurity at 8 with $\varepsilon = 0.5$; (d) $\langle r\rangle = 0.50745$, impurity at 7 with $\varepsilon = 0.1$ (chaotic domain).

panels (b) and (c) we can see that the distributions are something in between a chaotic and a non-chaotic regime, what tells us that the transition is implemented in a progressive way.
As we discuss below, the presence of this local magnetic field has large consequences for the whole system. Additionally, we can notice that if we apply the same magnetic field on every site of the chain we will not see any effect, since it only would produce a displacement on the diagonal elements of the matrix. Note that the original Heisenberg model includes a magnetic field term that we neglected, in which the impurity would increase the Zeeman splitting on the site where it is located [6].

B. Dependence on the position of the impurity

Unlike in a closed chain, in an open one the position where we locate the impurity is very important because, as we can see below, depending on its position, the chaoticity of the system changes. For example, if we have an impurity at an edge of the chain it is difficult for the one on the opposite edge to see any influence. In fact, if we locate it at an edge of the chain there is an analytical proof of the integrability of the system [1]. We should expect to find the system nearer to chaos as the more centered the impurity is located. Although the magnetic field only affects to a single spin, the polarization of that spin inevitably influences on its neighbours, since they are correlated.
In Fig. 2 we see that there is a symmetric behaviour due to the parity conservation and there is what seems an anomaly on the central spin (8th site) that we can also see in Fig. 1 panel (b). The most chaotic situation, for

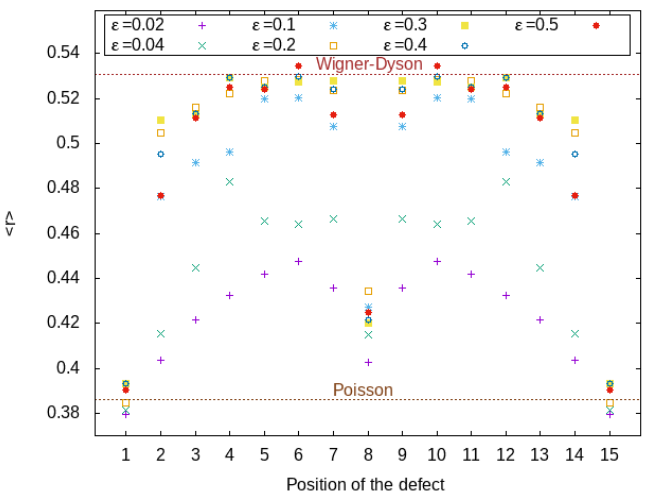

FIG. 2: Representation of the average ratio $\langle r \rangle$ for the different locations of the impurities in the chain. The different symbols correspond to different values of the impurity strength, ε, see Eq. (14). The corresponding values for the Poisson and Wigner Dyson distributions are marked with dotted lines.

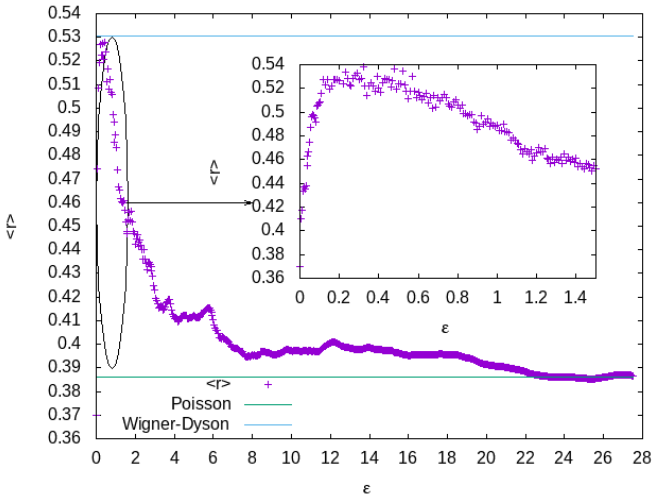

FIG. 3: Representations of the evolution of the average ratios of level spacings with the strength of an impurity located at the site 7 of a chain of 15 spins. The inset shows a zoom on the lower ε region.

every intensity, occurs when the impurity is located in sites 7 and 9, in a chain of 15 spins. Previously we had commented that the chaotic behaviour should be more prominent the more centered the defect is located. This hypothesis is surprisingly broken when the impurity is found on the 8th site. It happens because when the impurity is located just in the center, the system is able to be split in two parts that can be statistically studied separately, thus breaking the chaoticity. When the impurity fixes the polarization of the spin, forbidding this one to flip, then the spins on the right side of the one with the defect become uncorrelated with the ones on the left side. The strength necessary to let it happen is much smaller if the location of this impurity is exactly in the center. Later we will see that it can also happen for other positions depending on the intensity of the applied magnetic field.

C. Evolution of the system depending on the impurity strength

Starting with a non-chaotic chain of 15 spins where there would not be any impurity, i.e. $\varepsilon = 0$, we can study the evolution as the intensity of an impurity located at the 7th site of the chain (or by the parity symmetry it is equivalent to locate it at the 9th site) is increased. In Fig. 3 we can see how a system evolves with ε, and we can observe that the chaotic domain is present for a finite range of the strengths of the impurity. At first, the transition from a regular to chaotic behaviour is very fast. Further increasing ε, the system returns to the non-chaotic domain, but the transition is much softer than the first one.

For the case of $\varepsilon = 0$, we obtain an exponential decay of the level spacing distribution, see Fig. 1 panel (a). As we increase the value of ε, we expect to reach a chaotic regime. Representing an histogram of the level spacings we can see that, for small values of ε, the distribution starts diverging from a Poissonian and the distribution progressively changes until reaching a Wigner-Dyson distribution, see Fig. 1 panel (d). Between both regimes we see that there is a range of strengths of the impurity that leads the system into a kind of intermediate state, as the ones seen in Fig. 1 panel (b). The average of the ratios of level spacings gets values in between the expected ones for a Poisson and a Wigner-Dyson.

Once the chaotic regime is achieved, the system does not remain there forever. If we continue increasing ε, the system returns to the non-chaotic behaviour. The external magnetic field tries to align the spin where it is located. When that external interaction is large enough to make the interaction between the spin where it is applied and its neighbours negligible, we can consider that that spin has no other choice but to be parallel to the external field and the system loses the chaoticity. When the strength of the impurity becomes much bigger than the interaction between neighbours, then the chain is broken in two [1]. We can see in Fig. 4 (a) the evolution of the average magnetization, for a given intensity of the defect, of the 7th spin in the ground state, and notice that this magnitude converges to $\langle \hat{S}_z \rangle = \hbar/2$. If we set the restriction that the 7th spin must always point up, then for all the values of the strength we do obtain $\langle r \rangle = 0.37940$, what lets us verify the last discussion. If the 7th spin is always polarized in the same direction, then the strength does not affect the system. Since the 6th and 8th spins no longer influence the 7th one, and they can not interact between them, then we can consider the system is formed

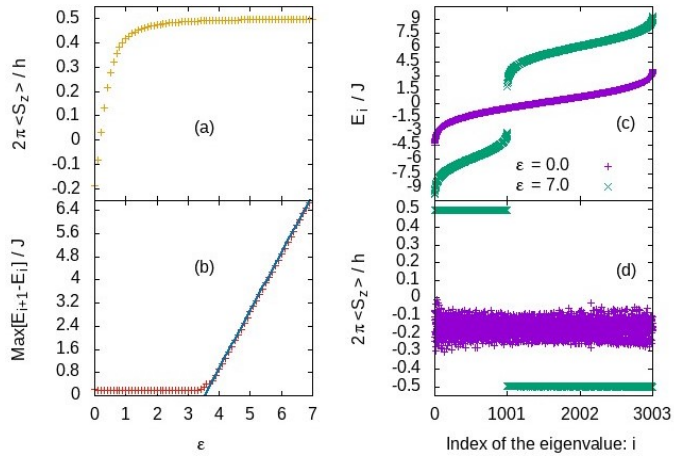

FIG. 4: (a) Dependence on the strength of the impurity, ε, located at the 7th site of the chain of the magnetization of that spin (for the ground state). (b) Dependence on ε of the maximum gap (energy difference between eigenstates) of each spectrum. (c) Representation of the eigenvalues, for 2 different strengths of the impurity, in terms of its index (they are ordered in increasing values). (d) Magnetization of the 7th spin for all the excited states of the system.

by 2 chains, one of 6 spins, and another of 7 spins.
For different intensities we can represent the spectrum just by plotting all the eigenvalues as a function of the spectral index, see Fig. 4 panels (c) and (d). Then we can notice that, for $\varepsilon \simeq 3.3$, a considerable large gap appears just in a third of the spectrum. When it happens we can see that the spectrum is divided in two sets of eigenvalues that have similar shapes. We can study the evolution of the maximum gap in the spectrum as a function of the impurity strength, see Fig. 4(b). Below strengths of $\varepsilon \simeq 3.3$, the maximum gap is smaller than the order of J. Above that value, the maximum gap of all the spectrum increases linearly with ε as $f(\varepsilon) = (1.99476 \pm 0.00017)\varepsilon - (7.0787 \pm 0.0012)$ (with a correlation coefficient of $R^2 = 0.9999996$) . By plotting the magnetization for each eigenstate, for a given strength, we can notice that this term corresponds to the amount of energy required in order to flip the spin from up to down, see Fig. 4 panel (d), $2\varepsilon J$.
The ground state for a chain with a large ε has the 7th spin pointing up. All the configurations that have this spin pointing down, for these strengths, are excited states. We can notice that the first set of eigenstates, see figure 4 (d), contains every state that have the 7th spin pointing up, while the second set has that spin pointing down. We have 2/3 of combinations with the spins pointing down and a third pointing up, as seen in Fig. 4 (d). The index where the gap appears is the fraction of eigenstates that have the spins pointing up,

$$i_{gap} = \frac{N_{up}}{L}\binom{L}{N_{up}} = \frac{(L-1)!}{(N_{up}-1)!(L-N_{up})!}. \qquad (15)$$

V. SUMMARY & CONCLUSIONS

We have studied some notions about quantum chaos on a chain of spins induced by the presence of an impurity that only affects on one site of the chain. A regular chain can suffer a transition to chaos if we set the strength of the impurity properly.
We have considered a well known spin model, the XXZ model. By introducing a perturbation, i.e. an impurity, on one of the spins we have been able to characterize the transition from an integrable regime to a chaotic one. Interestingly, as the strength of the magnetic field associated to the impurity is increased further, the system turns integrable again. This has been explained by noting, in that case, that the perturbed spin gets pinned and the system divides in two similar to the original XXZ chain. When the intensity of the impurity is large enough to fix an spin, it can not be considered only as a perturbation. Thus, we conclude that an appropriate range for the strength of the impurity, in order to study the chaoticity of spin chains, is $|\varepsilon| \lesssim 1$. For the same reason we must avoid locating the impurity at the edges and the center of the chain.

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