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Quantum chaos: an introduction via chains of spins-1/2

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The purpose of this work is to serve as an introduction to quantum chaos. We avoid the usual path of dealing with ensembles of random matrices and instead consider clean one-dimensional systems of spins-1/2. Quantum systems whose classical counterparts are chaotic have properties that differ from those of quantum systems whose classical counterparts are regular. One of the main signatures of what became known as quantum chaos is a spectrum showing repulsion of the energy levels, as commonly observed in ensembles of random matrices. Here, however, we show how quantum chaos may develop in more realistic systems of spins-1/2, which are devoid of random elements and involve only two-body interactions. Spin-1/2 chains are prototype quantum many-body systems. They are used to study subjects as diverse as quantum computing, quantum phase transition, and quantum transport. Nonetheless, they are simple enough to be accessible to undergraduate students. Our analysis goes beyond the statistics of eigenvalues and exploits also how the structure of the eigenstates may indicate chaos. We make available online all computer codes used to obtain the data for the figures of this work. This should allow students and professors to easily reproduce our results and to further explore new questions.

I. INTRODUCTION

Classical chaos is related to the extreme sensitivity of the dynamics of a system to its initial conditions. In a chaotic classical system, the phase-space trajectories of two particles with very close initial conditions diverge exponentially in time. The rate of this separation is characterized by the so-called Lyapunov exponent [1]. In the quantum world, however, the notion of trajectory loses its meaning. Still, since classical physics is but a limit of quantum physics, it is natural to search for quantum signatures of classical chaos [2, 3].

The energy levels of a quantum system whose classical counterpart is chaotic are highly correlated and they repel each other. This is reflected in various quantities associated with the eigenvalues of the system, such as the distribution of the spacings between neighboring levels, the level number variance, and the spectral rigidity [4]. The energy levels of a quantum system whose classical counterpart is regular (integrable), on the other hand, can cross; they are uncorrelated and randomly distributed. Level repulsion is therefore one of the main features of what became known as quantum chaos. But in addition to the analysis of the eigenvalues, quantum chaos is reflected also in the structure of the eigenstates [5, 6]. Chaotic eigenstates are highly delocalized and their components are random variables.

Already in the 1980s, it was realized that the fluctuation properties of the spectrum of chaotic quantum systems match those of random matrices [7, 8]. Random matrices are matrices filled with random elements whose only constraint is to satisfy some particular symmetries of the system they are trying to model. Starting with Wigner's efforts to understand the statistics of the energy levels of highly excited nuclei [9], random matrix theory [10] was soon employed in the analysis of the spectrum of other quantum many-body systems, such as atoms, molecules, and quantum dots, as well as various other systems, ranging from the quantum Sinai billiard to sequence of prime numbers [4, 7, 8, 11–13].

Real systems, however, are not described by random matrices. Random matrices imply long-range and many-body interactions, whereas real systems have few-body (most commonly only two-body) interactions. Real systems are better described by sparse matrices where only the elements corresponding to two-body interactions are nonzero, as in two-body random ensembles (TBREs) [14, 15]. The elements of TBREs are random variables, which is justified as a way to describe imperfections and noise. However, even though imperfections and noise permeate real systems, they are becoming more and more controllable, which makes pertinent the question of whether systems devoid of randomness may still develop chaos.

In this work, we study clean one-dimensional systems of spins-1/2, where random elements are nonexistent. The systems involve only two-body interactions taking place between nearest-neighbors and in certain cases also between next-nearest-neighbors. Chains of spins-1/2 are accessible systems and may be used to expose students to a multitude of subjects. In addition to the crossover from integrability to chaos, they may be used, for example, to introduce current topics of research such as the metal-insulator transition, quantum phase transition, entanglement, spintronic and methods of quantum control. They have been considered as models for quantum computers, magnetic compounds and have recently been simulated in optical lattices [16].

The paper is organized as follows. Section II provides a detailed description of the Hamiltonian of a spin-1/2 chain. Section III explains how to compute two quantities capable of capturing the crossover from regular to chaotic motion, the level spacing distribution and the number of principal components. Section IV discusses how remaining symmetries of the system may hinder the signatures of chaos even when the system is chaotic. Concluding remarks are given in Sec. V.

II. SPIN-1/2 CHAIN

We study a one-dimensional spin-1/2 system (spin-1/2 chain) described by the Hamiltonian

$$H = H_z + H_{\rm NN}, \tag{1}$$

where

$$H_z = \sum_{n=1}^{L} \omega_n S_n^z = \left(\sum_{n=1}^{L} \omega S_n^z \right) + \epsilon_d S_d^z,$$

$$H_{\rm NN} = \sum_{n=1}^{L-1} \left[J_{xy} \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y \right) + J_z S_n^z S_{n+1}^z \right] .$$

Above, $\hbar$ is set equal to 1, L is the number of sites, and $S_n^{x,y,z} = \sigma_n^{x,y,z}/2$ are the spin operators at site n, $\sigma_n^{x,y,z}$ being the Pauli matrices. The term H_z gives the Zeeman splitting of each spin n, as determined by a static magnetic field in the z direction. A spin up in the z direction is indicated as $|\uparrow\rangle$ or with the vector $\binom{1}{0}$ and a spin down $|\downarrow\rangle$ with $\binom{0}{1}$. An up-spin on site n has energy $+\omega_n/2$, while a down-spin has energy $-\omega_n/2$. A spin up corresponds then to an excitation. All sites are assumed to have the same energy splitting ω, except a single site d, whose energy splitting $\omega + \epsilon_d$ is caused by a magnetic field slightly larger than the others. This site is referred to as defect.

The second term, $H_{\rm NN}$, is known as the XXZ Hamiltonian. It describes the couplings between nearest-neighbor (NN) spins; J_{xy} is the strength of the flip-flop term $S_n^x S_{n+1}^x + S_n^y S_{n+1}^y$ and J_z the strength of the Ising interaction $S_n^z S_{n+1}^z$.

The flip-flop term exchanges the position of neighboring up and down spins according to

$$J_{xy}(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y)|\uparrow_n\downarrow_{n+1}\rangle = (J_{xy}/2)|\downarrow_n\uparrow_{n+1}\rangle$$

or, equivalently, it moves the excitations through the chain. Notice that we have assumed open boundary conditions, as indicated by the sum in $H_{\rm NN}$ which goes from $n = 1$ to site $L - 1$. This means that an excitation in site 1 (or L) can only move to site 2 (or to site $L - 1$). The scenario of a ring where an excitation on site L can also move to site 1 corresponds to closed boundary conditions and is mentioned briefly in Sec. V.

The Ising interaction implies that pairs of parallel spins have higher energy than pairs of anti-parallel spins, that is

$$J_z S_n^z S_{n+1}^z|\uparrow_n\uparrow_{n+1}\rangle = +(J_z/4)|\uparrow_n\uparrow_{n+1}\rangle, \qquad (2)$$

whereas

$$J_z S_n^z S_{n+1}^z|\uparrow_n\downarrow_{n+1}\rangle = -(J_z/4)|\uparrow_n\downarrow_{n+1}\rangle. \qquad (3)$$

For the chain described by H (1), the total spin in the z direction, $S^z = \sum_{n=1}^{L} S_n^z$, is conserved, *i.e.* $[H, S^z] = 0$. This is a symmetry of the system. It means that the total number of excitations is fixed; the Hamiltonian cannot create or annihilate excitations, it can only move them through the chain.

In order to write the Hamiltonian in the matrix form and then diagonalize it to find its eigenvalues and eigenstates, we need first to choose a basis. The most natural choice is the one we have used so far to describe the terms of H, that is arrays of up and down spins in the z-direction. We refer to it as the site-basis. In this basis, H_z and the Ising interaction contribute to the diagonal elements of the matrix, whereas the flip-flop term leads to the off-diagonal elements.

In the absence of disorder, the system is said to be clean. A clean spin-1/2 chain with NN exchange only (the XXZ model) is integrable and can be solved with the Bethe Ansatz method [17]. The addition of disorder [18], even if just one defect in the middle of the chain [19], as considered here, may lead to the onset of quantum chaos. The source of chaos is the interplay between the Ising interaction and the defect.

To bring the system to chaotic regime, we set $J_{xy} = 1$ (arbitrary unit), choose $J_z = \epsilon = 0.5$ (arbitrary unit), and place the defect on site $d = \lfloor L/2 \rfloor$. This choice is based on the following factors. (i) The strength of the Ising interaction cannot be much larger than J_{xy}, because this would localize the excitations by limiting the number of effectively coupled states. For instance, basis vectors with several pairs of parallel spins would have energy much higher than states with few pairs of parallel spins [cf. Eqs.(2), (3)] and J_{xy} would not be able to effectively couple them. Chaos cannot occur in a localized system. (ii) The defect cannot be placed on the edges of the chain, because in this case the system is still integrable [20]. (iii) The defect should not be too large, because it would simply break the chain in two, that is an excitation on the left of the defect would not have enough energy to overcome it and then reach the right side of the chain, and vice versa.

III. QUANTUM CHAOS

Different quantities exist to identify the crossover from the regular to the chaotic regime in quantum systems. We consider the level spacing distribution, which is associated with the eigenvalues, and the number of principal components, which measures the complexity of the eigenstates.

A. Level spacing distribution

The distribution of spacings s of neighboring energy levels [4, 10–12] is the most frequently used quantity to study short-range fluctuations in the spectrum. Quantum levels of regular systems are not prohibited from crossing and the distribution is Poissonian,

$$P_P(s) = \exp(-s). \qquad (4)$$

In chaotic systems, crossings are avoided; there is level repulsion and the level spacing distribution is given by the Wigner-Dyson distribution, as predicted by random matrix theory. The form of the Wigner-Dyson distribution depends on the symmetry properties of the Hamiltonian. Systems with time reversal invariance are described by Gaussian orthogonal ensembles (GOEs). A GOE corresponds to an ensemble of real symmetric matrices, whose elements H_{ij} are independent random numbers from a Gaussian distribution. The average of the elements and the variance satisfy $\langle H_{ij}\rangle = 0$ and $\langle H_{ij}^2\rangle = 1+\delta_{ij}$. The level spacing distribution of a GOE is given by

$$P_{WD}(s) = (\pi s/2)\exp(-\pi s^2/4). \qquad (5)$$

The same distribution is achieved for model (1) in the chaotic limit. However, our system differs from GOEs in two ways, it

has only two-body interactions and does not contain random elements.

In order to obtain the level spacing distribution, we need first to separate the eigenvalues according to their symmetry sectors. If we mix eigenvalues from different symmetry sectors, we may not achieve a Wigner-Dyson distribution even if the system is chaotic. This is because eigenvalues from different subspaces are independent and therefore have no reason to repel each other. The conservation of S^z in H (1) implies that the Hamiltonian is separated into uncoupled blocks, each corresponding to a subspace with a particular number of spins pointing up. In the studies below, we focus on the subspace that has $L/3$ up-spins and dimension $dim = L!/[(L/3)!(L-L/3)!]$.

The second essential step before computing the histogram of neighboring level spacings is to unfold the spectrum. The procedure consists of locally rescaling the energies, so that the local density of states of the renormalized eigenvalues is 1. There are different methods to achieving this. Here we describe a pedagogical one.

First, we make sure that our spectrum $\{E_1, E_2, \ldots, E_{dim}\}$ is ordered in increasing values of energy. We then discard some levels from the edges of the spectrum, where the fluctuations are large. Let us remove at least 10% of the eigenvalues, approximately half of them from very low energies and half from very high energies. The lowest energy that we will consider is $E_l = E_{\lfloor dim/20 \rfloor}$. Next, we divide the eigenvalues in groups of 11, the last eigenvalue of one group always reappearing as first element of the next group. We then have $q = \lfloor 90\% \times dim/10 \rfloor$ sets of energy levels corresponding to

$$\begin{aligned}
&\text{Set } 1 : \{E_l, E_{l+1} \ldots E_{l+10}\} \\
&\text{Set } 2 : \{E_{l+10}, E_{l+11} \ldots E_{l+20}\} \\
&\ldots \\
&\text{Set } q : \{E_{l+10(q-1)}, E_{l+10(q-1)+1} \ldots E_{l+10q}\}
\end{aligned}$$

For each set i, with $i = 1, 2, \ldots, q$, we compute the mean level spacing D_i according to

$$D_i = [E_{l+10i} - E_{l+10(i-1)}]/10.$$

Each eigenvalue $E_{l+10(i-1)+j}$, with $j = 0, 1, \ldots 10$, is renormalized as $e_{l+10(i-1)+j} = E_{l+10(i-1)+j}/D_i$. The mean level spacing of each new set of energies e's is therefore 1. Since the density of states is the number of states in an interval of energy, that is the reciprocal of the mean level spacing, the renormalized energies ensures also that the local density of states is unity.

In hand of the unfolded spacings of neighboring levels, the histogram can now be computed. Notice that to compare it with the theoretical curves, the distribution needs to be normalized, so that its total area is equal to 1.

Figure 1 shows the level spacing distribution for the cases where the defect is placed on site 1 (left panel) and on site $\lfloor L/2 \rfloor$ (right panel). The first corresponds to an integrable model and the distribution is Poissonian, while the second is a chaotic system, so the distribution is Wigner-Dyson.

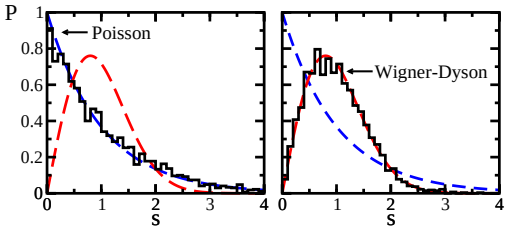

FIG. 1: (Color online.) Level spacing distribution for H (1) with $L = 15$, 5 spins up, $\omega = 0$, $\epsilon = 0.5$, $J_{xy} = 1$, and $J_z = 0.5$ (arbitrary unit); bin size = 0.1. Left panel: defect on site $d = 1$; right panel: defect on site $d = 7$. Dashed lines: theoretical curves.

B. Number of principal components

Delocalization measures [5, 6], such as the number of principal components (NPC), determine how much spread the eigenstates are in a particular basis. For an eigenstate $|\psi_i\rangle$ written in the basis vectors $|\xi_k\rangle$ as $|\psi_i\rangle = \sum_{k=1}^{dim} c_{ik}|\xi_k\rangle$, NPC is defined as

$$\text{NPC}_i \equiv \frac{1}{\sum_{k=1}^{dim} |c_{ik}|^4}. \tag{6}$$

This quantity gives the number of basis vectors that contribute to each eigenstate. It is small when the state is localized and large when the state is delocalized.

For GOEs, the eigenstates are simply random vectors, *i.e.* the amplitudes c_{ik} are independent random variables. These states are completely delocalized. Complete delocalization does not mean, however, that NPC=dim. Because the weights $|c_{ik}|^2$ fluctuate, the average over the ensemble gives NPC $\sim dim/3$ [5, 6].

In our case, since model (1) has only two-body interactions, NPC does not reach $dim/3$. Moreover, the largest values appear only in the middle of the spectrum of the system in the chaotic regime. This is because the level density of systems with two-body interactions has a Gaussian shape. This indicates that the highest concentration of states appears in the middle of the spectrum. It is there that strong mixing of states can happen leading to widely spread eigenstates.

The values of NPC are also intimately related to the basis used. The basis considered depends on the question one is after. In studies of spatial localization, for example, the site-basis is an appropriate one. In order to separate regular from chaotic behavior, on the other hand, a more appropriate basis corresponds to the eigenstates of the integrable limit of the model. This basis is referred to as the mean-field basis [6]. In our model, there are different integrable limits. We chose to consider the case where $\epsilon_d \neq 0$ and $J_z = 0$, because the presence of the defect ensures the breaking of possible remaining symmetries (see Sec. IV). The crossover to chaos is then caused by the addition of Ising interaction.

Suppose that $|\xi\rangle$ represents the mean-field basis and $|\phi\rangle$ the site-basis. If we obtain the eigenstates $|\psi\rangle$ in the site-basis, $|\psi_i\rangle = \sum_{j=1}^{dim} a_{ij}|\phi_j\rangle$, and we know the relation between the two bases, $|\xi_k\rangle = \sum_{j=1}^{dim} b_{kj}|\phi_j\rangle$, we may rewrite the eigen-

states in the mean-field basis as

$$|\psi_i\rangle = \sum_{k=1}^{dim} \left(\sum_{j=1}^{dim} a_{ij} b^*_{kj} \right) |\xi_k\rangle = \sum_{k=1}^{dim} c_{ik} |\xi_k\rangle. \qquad (7)$$

Figure 2 depicts NPC of the eigenstates in both the site-basis (top panels) and the mean-field basis (bottom panels) for the cases where the defect is placed on site 1 (left panels) and on site $\lfloor L/2 \rfloor$ (right panels). For the regular system (left panels), NPC shows large fluctuations, whereas in the chaotic regime (right panels), NPC becomes a smooth function of energy. The onset of chaos leads to the uniformization of the eigenstates; in the middle of the spectrum they approach random vectors. Thus, chaotic eigenstates close in energy have similar structures and consequently similar values of NPC.

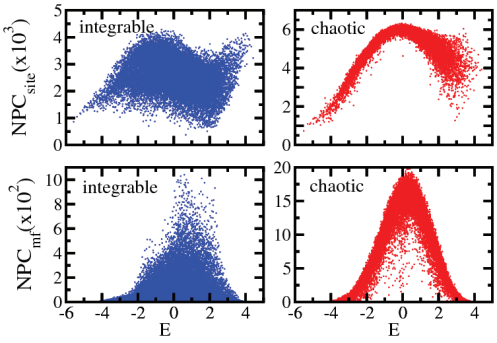

FIG. 2: (Color online.) Number of principal components for the eigenstates of H (1) vs energy; $L = 18$, 6 spins up, $\omega = 0$, $\epsilon = 0.5$, $J_{xy} = 1$, and $J_z = 0.5$ (arbitrary unit). Top panels: site-basis; bottom panels: mean-field basis. Left panels: defect on site $d = 1$; right panels: defect on site $d = 9$.

These results have important consequences for the problem of thermalization in isolated quantum systems, a subject that has received much attention recently, especially due the possibility of testing the theory with experiments in optical lattices [21]. Basically, thermalization in the sense of agreement with the predictions from statistical mechanics is expected to happen only when eigenstates close in energy show the same level of complexity, that is when they become chaotic [22].

IV. SYMMETRIES

The onset of chaos may happen also in a clean spin-1/2 chain if we add further couplings, for example between next-nearest-neighbors (NNNs) [22–24]. The Hamiltonian now becomes

$$H = H_{\rm NN} + \alpha H_{\rm NNN}, \qquad (8)$$

where

$$H_{\rm NNN} = \sum_{n=1}^{L-2} \left[J'_{xy} \left(S^x_n S^x_{n+2} + S^y_n S^y_{n+2} \right) + J'_z S^z_n S^z_{n+2} \right] .$$

For α sufficiently large ($\alpha \gtrsim 0.2$ when $L = 15$), there are various scenarios where chaos may develop: (i) in the absence of Ising interactions, $Jz = Jz' = 0$; (ii) in the absence of flip-flop term between NNNs, $J'_{xy} = 0$; (iii) in the absence of Ising interaction between NNNs, $J'_z = 0$, and (iv) in the presence of all four terms.

Depending on the parameters of H (8), however, we may not obtain a Wigner-Dyson distribution even if the system is chaotic. This happens if not all symmetries of the system are taken into account [24, 25]. We have already mentioned conservation of total spin in the z direction. In the absence of defect, other symmetries of H (8) include [26]:

• *Parity*. Parity may be understood by imagining a mirror in one edge of the chain. For the eigenstates written in the site-basis, the probability of each basis vector is equal to that of its reflection. For example, suppose we have $L = 4$ and one excitation. The eigenstates are given by $|\psi_i\rangle = a_{i1}|\uparrow\downarrow\downarrow\downarrow\rangle + a_{i2}|\downarrow\uparrow\downarrow\downarrow\rangle + a_{i3}|\downarrow\downarrow\uparrow\downarrow\rangle + a_{i4}|\downarrow\downarrow\downarrow\uparrow\rangle$. The amplitudes will either be $a_{i1} = a_{i4}$ and $a_{i2} = a_{i3}$ in the case of even parity, or $a_{i1} = -a_{i4}$ and $a_{i2} = -a_{i3}$ in the case of odd parity. The level spacing distribution needs to be independently obtained for each parity sector.

• *Spin reversal*. If the chain has an even number of sites and $L/2$ up-spins, then $S^z = 0$. Here, pairs of equivalent basis vectors correspond to those which become equal if we rotate all the spins from one vector by 180^o. For example, state $|\uparrow\downarrow\downarrow\uparrow\rangle$ pairs with state $|\downarrow\uparrow\uparrow\downarrow\rangle$.

• *Total spin*. If the system is isotropic, *i.e.* $J_{xy} = J_z$ and $J'_{xy} = J'_z$, total spin, $S^2 = (\sum_{n=1}^{L} \vec{S}_n)^2$, is conserved.

Notice that in the case of closed boundary conditions, there is also momentum conservation. The more symmetries the system has, the smaller the subspaces, which is not good for statistics. This explains why in panels (b), (c), (d), and (e) of Fig. 3 we deal with open boundary conditions, avoid the $S^z = 0$ subspace, and choose $J_z \neq J_{xy}$. In doing so, the only symmetries we need to take into account when studying the clean systems are S^z and parity.

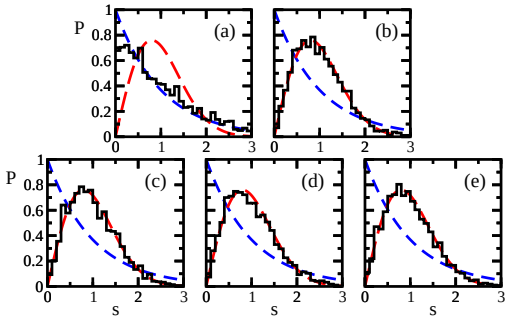

FIG. 3: (Color online.) Level spacing distribution for H (8) with $\alpha = 0.5$. Panel (a): $L = 14$, 7 spins up, $J_{xy} = J'_{xy} = J_z = J'_z = 1$; all eigenvalues of the subspace $S^z = 0$ are considered. Panels (b), (c), (d) and (e): $L = 15$, 5 spins up, $J_{xy} = 1$. The eigenvalues are separated according to the parity of the corresponding eigenstates; $P(s)$ is the average of the distributions of the two parity sectors. Panel (b): $J'_{xy} = 1$, $J_z = J'_z = 0.5$. Panel (c): $J'_{xy} = 1$, $J_z = J'_z = 0$. Panel (d): $J'_{xy} = 0$, $J_z = J'_z = 0.5$. Panel (e): $J'_{xy} = 1$, $J_z = 0.5$, $J'_z = 0$. Arbitrary unit and bin size = 0.1.

The top panels of Fig. 3 compare the level spacing distribution of two chaotic spin-1/2 chains from category (iv). The one on the left panel contains the three symmetries itemized above which are not taken into account, so $P(s)$ becomes a misleading Poisson distribution. The one on the right panel has only parity and this symmetry is taken into account, so $P(s)$ becomes a clear Wigner-Dyson.

The bottom panels show the level spacing distribution for chaotic spin-1/2 chains from the categories (i), (ii), and (iii) above. Parity is properly taken into account, leading to the expected Wigner-Dyson distributions.

V. CONCLUSION

We provided a detailed procedure to verify whether a one-dimensional system of spins-1/2 is in the chaotic regime. Two quantities were considered: the level spacing distribution, obtained with the eigenvalues, and the number of principal components of the eigenstates. A simple recipe to unfold the spectrum and the importance of taking into account the symmetries of the system before making the histogram were discussed. The number of principal components were computed in two different bases and an expression to change the basis in which the eigenstates are written was given.

Spin-1/2 chains are excellent models to introduce undergraduate students to basic concepts of linear algebra and quantum mechanics, from matrix diagonalization to the time evolution of the wave functions. They serve also as a starting point to explore various topics of current research in physical, biological and computer science. To motivate further studies and to facilitate the understanding of the present paper, the computer programs used to obtain the data for Figs. 1, 2, and 3 are available online in [27]. There, the reader will also find suggestions for exercises.

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