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Integrability of a disordered Heisenberg spin-1/2 chain

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Abstract

We investigate how the transition from integrability to nonintegrability occurs by changing the parameters of the Hamiltonian of a Heisenberg spin-1/2 chain with defects. Randomly distributed defects may lead to quantum chaos. A similar behaviour is obtained in the presence of a single defect out of the edges of the chain, suggesting that randomness is not the cause of chaos in these systems, but the mere presence of a defect.

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1. Introduction

Random matrix theory has long been used to describe the spectra of complex systems, such as nuclei, molecules and mesoscopic solids [1]. Recently it has been used in the study of strongly correlated spin systems [2, 3]. The statistical properties of the quantum energy spectrum are strongly influenced by the underlying classical dynamics. The level spacing distribution of a classical integrable system is Poissonian, $P_{\mathrm{P}}(s) = \exp(-s)$, while the level statistics of a chaotic system is given by the Wigner–Dyson distribution, $P_{\mathrm{WD}}(s) = (\pi s/2)\exp(-\pi s^2/4)$. The Wigner–Dyson distribution is obtained in random matrix theory and it reproduces the level repulsion of chaotic dynamics. These two distributions characterize, respectively, the localized and the metallic phase in the Anderson model of disordered systems. At the critical point between the two phases, an intermediate level spacing statistics occurs [4].

The problem of localization and the statistical properties of the spectra for the case of just one particle has long been understood, but only recently has the problem of many-body systems been addressed [2, 3]. When more than one particle is present in the system, the interaction between them has to be taken into account. The interplay between interaction and disorder is a challenging problem in today's condensed matter physics and it can lead to new and unexpected effects [5].

Here, we consider a one-dimensional Heisenberg spin-1/2 chain with defects and several excitations. A defect corresponds to the site where the energy splitting is different from all the others. It is obtained by applying a different magnetic field in the z direction to the chosen site. A disordered system is characterized by the presence of one or more defects. In the absence of defects this homogeneous system is integrable and is solved with the Bethe ansatz [6]. Its level distribution is therefore Poissonian. As random on-site magnetic fields are turned on and their mean-square amplitude starts increasing, the system undergoes a transition and becomes chaotic. But by further increasing the mean-square amplitude, localization eventually takes place and the distribution becomes Poissonian again. We determine the crossover from integrability to quantum chaos in such a disordered spin chain. In addition, we discuss that the cause for nonintegrability is not the randomness of the system, but the mere presence of defects. If only one defect is placed out of the edges of the chain and if the defect excess energy is of the order of the interaction strength, the system is also chaotic. The same sort of transition integrable–chaotic–integrable is obtained as the defect excess energy increases.

We consider only nearest neighbour interaction. The Hamiltonian describing the system is

$$H = \sum_{n=1}^{L} \left(h_n - \frac{J}{2}\delta_{n,1} - \frac{J}{2}\delta_{n,L} \right) \sigma_n^z + \sum_{n}^{L-1} \frac{J}{4} \vec{\sigma}_n \cdot \vec{\sigma}_{n+1} \tag{1}$$

where $\hbar = 1$ and $\vec{\sigma}$ are Pauli matrices. There are L sites. Each site n is subjected to a magnetic field in the z direction, giving the energy splitting h_n. The chain is ideal whenever all sites have the same energy splitting. A defect corresponds to the site whose energy splitting differs from the others.

For simplicity, we work with an isotropic chain, that is, the coupling constant J for the diagonal Ising interaction $\sigma_n^z \sigma_{n+1}^z$ is equal to the coupling constant for the XY-type interaction $\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y$. This last term is responsible for propagating the excitation through the chain. A single-particle excitation corresponds to a spin pointing up.

In this model, the z component of the total spin $\sum_{n=1}^{L} S_n^z$ is conserved, so states with different number of excitations are not coupled. We therefore look at the level spacing distributions for sectors with the same number of excitations. Since we are interested in determining if the system is integrable or chaotic, we focus on the sector with the largest number of states, that is the sector with $L/2$ excitations. This is the region where chaos should set in first.

In a very large system the boundary conditions have no effects, but numerical calculations are limited to a finite number of sites. In a periodic (or closed) chain we found too many degenerate states, so we decided to work with a chain with free boundaries (or open chain). Both systems, closed or open, are known to be integrable in the absence of defects. They are solved with the Bethe ansatz method [6]. An open chain with defects only on the edges is also integrable [7]. Here we choose an open chain with defects of values $-J/2$ on the edges. Such values should diminish border effects.

We work with $L = 12$ sites and 6 excitations, which gives us 924 states. A matrix of such size, 924×924, is sufficient to have good statistics, as illustrated in figure 1. In both plots we have the Poisson distribution (dot-dashed line) and the Wigner–Dyson distribution (long-dashed line). The spacings s correspond to S/M, where M is the mean level spacing and S is the actual spacing. Both histograms are normalized to 1. The histogram at the top of the figure shows that the level spacings of the eigenvalues of a diagonal random matrix of such size are well described by the Poisson distribution. The histogram at the bottom of the figure shows that the level spacings of the eigenvalues of a random matrix of this size agree very well with the Wigner–Dyson distribution. The random elements have a Gaussian distribution.

To find universal statistical properties of a Hamiltonian it is clear that we have to deal with unfolded eigenvalues. Unfolded eigenvalues are renormalized eigenvalues, whose local

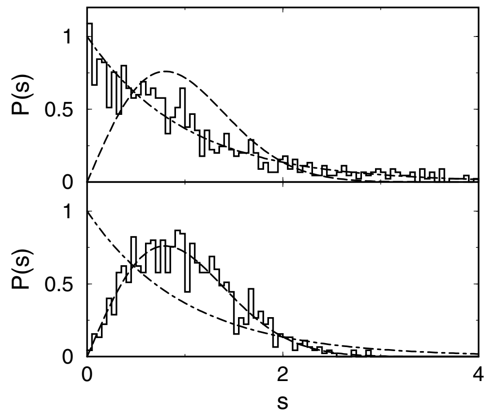

Figure 1. In both graphs, the dot-dashed line gives the Poisson distribution and the long-dashed line corresponds to the Wigner–Dyson distribution. The histogram at the top gives the level spacing distribution for a diagonal random matrix of dimension 924 × 924. The histogram at the bottom gives the level distribution for a random matrix of this size.

density of states is equal to unity everywhere in the spectrum. The exact unfolding procedure consists of finding the system specific mean level density, which is then removed from the data. Sometimes this can be a non-trivial task. An easier and commonly used procedure, which we adopt in this paper, is the following. First, we discard some levels from the edges of the spectrum, where there are large fluctuations. Here, with a spectrum ordered with increasing values of energy, we only consider the energy levels from 13 to 913, and work with 900 level spacings. The spectrum is then divided into 90 pieces of 10 level spacings each and the mean level spacing of each section is computed. The normalized nearest neighbour spacings used to obtain the distributions in figure 1 and in the next figures correspond to energy differences divided by the mean level spacing of their corresponding section.

2. Randomly distributed defects

First we analyse the case of random magnetic fields along the z direction. The energy splitting of each site is given by $h_n = h + d_n$, where d_n are uncorrelated random numbers with a Gaussian distribution: $\langle d_n \rangle = 0$ and $\langle d_n d_m \rangle = d^2 \delta_{n,m}$. When $d = 0$ the system is integrable and a Poisson distribution is obtained, as the histogram at the top of figure 2 shows. As d increases the system undergoes a transition and becomes chaotic; the Wigner–Dyson distribution is obtained, as can be seen from the histogram in the middle of figure 2. However, as we further increase d and it becomes much larger than J, the system becomes localized. As expected, a Poisson distribution reappears (see the bottom of figure 2). Large d/J corresponds to a random diagonal matrix with negligible off-diagonal elements.

A more convenient way of analysing the evolution of the level spacing distributions with respect to the ratio d/J is by using the parameter $\eta = \int_0^{s_0} [P(s) - P_{\mathrm{WD}}(s)]\, \mathrm{d}s \big/ \int_0^{s_0} [P_{\mathrm{P}}(s) - P_{\mathrm{WD}}(s)]\, \mathrm{d}s$, where $s_0 = 0.4729\ldots$ is the intersection point of $P_{\mathrm{P}}(s)$ and P_{WD} [3, 8]. A regular system has $\eta = 1$ and a chaotic system has $\eta = 0$. The stars in figure 3 show the dependence of η on d/J. There we compute the average of η, $\langle \eta \rangle$, for each value of d/J for 20 different sequences of 12 Gaussian random numbers. The transition integrable–chaotic–integrable is clear. The system is initially integrable, becomes very chaotic in the interval $0.1J < d < 0.5J$ and then reaches integrability again as d becomes much larger than J. At this last step, the

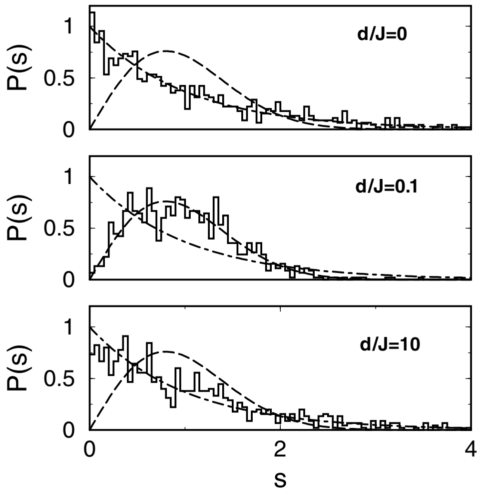

Figure 2. The histograms correspond to the actual level distribution for random on-site magnetic fields. We choose $J = 1$. The dot-dashed line gives the Poisson distribution and the long-dashed line corresponds to the Wigner–Dyson distribution.

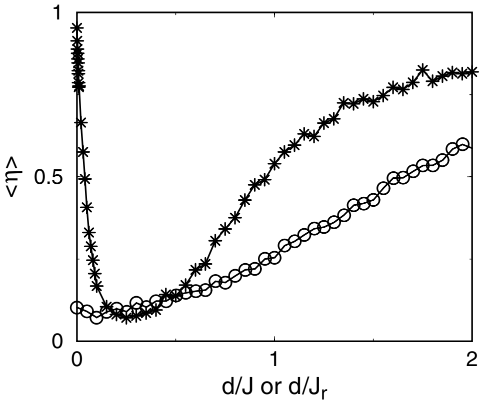

Figure 3. Stars give the dependence of $\langle\eta\rangle$ on the ratio d/J when the on-site magnetic fields are random. Circles give the dependence of $\langle\eta\rangle$ on the ratio d/J_r when both diagonal and non-diagonal elements are random.

energy splitting of each site becomes very different from all the others and the excitations become localized.

Besides considering the site energies as random numbers, another way of introducing disorder is by taking the non-diagonal matrix elements at random. This is shown with circles in figure 3. These are obtained in the following way. The off-diagonal elements, which characterize the hopping of excitations, also have a Gaussian distribution and the mean square is given by J_r. We use a sequence of 2772 random numbers for them. Again 20 different sequences of 12 Gaussian random numbers are used for the diagonal elements, which characterize the energy splittings. The parameter η is averaged over the 20 sequences. The circles in figure 3 give therefore the dependence of $\langle\eta\rangle$ on d/J_r. In contrast to the case discussed before, random coupling leads to chaos even when the energy splittings of all sites

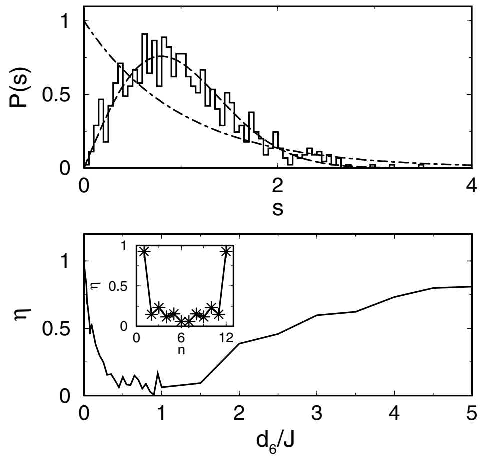

Figure 4. Top panel: the histogram corresponds to the level distribution of the Heisenberg spin-1/2 chain with a defect in the middle of the chain, on site 6. The defect excess energy is equal to the interaction strength J. Dot-dashed and long-dashed lines give the Poisson and the Wigner–Dyson distributions, respectively. Bottom panel: dependence of the parameter η on the ratio d_6/J. The defect is placed on site 6. The inset gives the dependence of η on the position of the defect; the defect excess energy is J.

are the same ($d = 0$). Large chaoticity is kept up to $d \sim 0.5J_r$ and there is now only one transition, from chaoticity to integrability. Such transition takes a little longer to happen than in the previous case, though localization is also attained once the ratio d/J_r becomes large.

3. One single defect

In the system treated here, chaos can be associated with randomness only when the coupling is random. In the case of a constant interaction strength, what is really responsible for the nonintegrability of the system is not the randomness of the energy splittings, but the mere existence of a defect, as we now discuss in this section. Let us consider again a constant coupling. The top of figure 4 shows that a Wigner–Dyson distribution can also be obtained when there is only one defect in the middle of the chain and the defect excess energy is of the order of the interaction strength. For this histogram all sites have the same energy splitting $h_n = h$, except site 6, which has $h_6 = h + J$.

Here too we use the parameter η to study the evolution of the level spacing distribution with respect to the ratio d_6/J. The bottom of figure 4 indicates a transitional behaviour very similar to the case of constant coupling and random diagonal elements. The one-defect system is initially regular, but by increasing d_6 it becomes chaotic. The highest degree of chaoticity happens when $d_6 \sim J$. The level repulsion now settles in more slowly than in the previous situation of random magnetic fields. As d_6 is further increased, an excitation on site 6 will become site-localized. This means that when the ratio d_6/J becomes very large there are two kinds of states in the system: states with a localized excitation on site 6 and states with no excitation on the defect. These two types of states are not coupled. This system becomes equivalent to two smaller and uncoupled ideal chains, and integrability is therefore recovered.

In the inset at the bottom of figure 4, we again consider one single defect, whose excess energy is equal to J. It shows how the parameter η depends on the position of the defect and confirms that the Heisenberg spin-$1/2$ system is integrable when it has defects placed on its edges.

Similar results are obtained for a chain with 14 sites and one defect on site 7, but as an illustration the smaller system with 12 sites is enough.

4. Conclusion

We have shown that in a Heisenberg spin-$1/2$ chain, randomly distributed defects lead to the transition integrable–chaotic–integrable, according to the ratio d/J. When random off-diagonal elements are also considered, there is only one transition from nonintegrability to integrability. The transition integrable–chaotic–integrable is also observed when the coupling is constant and there is only one defect out of the edges of the chain. The level spacing distribution obtained in this case depends on how large the defect excess energy is in relation to the interaction strength.

Obtaining analytical solutions for disordered spin chains is not an easy task and in many cases is simply impossible. The algebraic version of the Bethe ansatz is often used to *construct* integrable Hamiltonians [9]. The analysis of level spacing distributions should therefore be useful to identify which real or constructed Hamiltonians are indeed integrable.

Understanding under what conditions disordered spin systems become integrable is not just relevant for condensed matter physics, but also for quantum computation, since these systems are commonly used to model different proposals of quantum computers (see [5] and references therein). Chaos is a source of serious concern in quantum computation, for it can completely destroy the operability of a quantum computer [10, 11].

Also in the context of entanglement there is great interest in disordered spin systems [12]. Using them to study how the entanglement between qubits may be affected by chaos and localization would be very important for quantum information. This is what we intend to do next.

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