

Level statistics of multispin-coupling models with first- and second-order phase transitions

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We consider self-dual transverse-field Ising spin chains with m -spin interaction, where the phase transition is of second and first order, for $m \leq 3$ and $m > 3$, respectively. We present a statistical analysis of the spectra of the Hamiltonians on relatively large $L \leq 18$ finite lattices. Outside the critical point we found level repulsion close to the Wigner distribution and the same rigidity as for the Gaussian orthogonal ensemble. At the transition point the level statistics in the self-dual sector is shown to be the superposition of two independent Wigner distributions. This is explained by the existence of an extra symmetry, which is connected to level crossing in the thermodynamic limit. Our study has given no evidence for the possible integrability of the models for $m > 2$, even at the transition point. [S1063-651X(98)05907-8]

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I. INTRODUCTION

There are many problems in physics in which multiparticle interactions play an important role. One may mention nuclear forces, solid ^3He [1], adsorbed systems [2], and plasmas [3]. It is known from some exact results [4] that the critical properties of models with many body forces generally depend on the range of interaction. Recently considerable effort has been made to clarify the properties of a simple one-dimensional quantum model described by the Hamiltonian [5,6]

$$\mathcal{H} = -J \sum_l \sigma_l^x \sigma_{l+1}^x \cdots \sigma_{l+m-1}^x - h \sum_l \sigma_l^z \equiv -JH_x - hH_z. \quad (1)$$

Here the σ_l^x, σ_l^z are Pauli matrices at site l and J and h are the exchange coupling and the transverse field, respectively. The classical statistical mechanical equivalent of this model is a two-dimensional square lattice Ising model with mixed m -spin and two-spin interactions [7].

The Hamiltonian Eq. (1) is self-dual [5,6] and the self-dual point is $J=h$ independent of m . According to numerical studies [6–14] there is one phase transition in the system, which takes place at the self-dual point, and the transition changes from second to first order, when $m > m_c = 3$. In the borderline case $m = 3$ the transition is conjectured [7] to belong to the four-state Potts universality class, a conjecture which is supported by an approximate mapping [15] and by numerical studies [10,13,14,16].

Concerning the simple structure of the model, its self-dual symmetry, and the expected relation to Q -state Potts models, one can also pose the question, whether the model is integrable, at least in its self-dual point. To find an answer to this question in this paper we are going to study the statistical properties of the spectrum of the Hamiltonian. As it has been established in a series of papers [17–23] the spectrum of a Hamiltonian (or the transfer matrix for classical statistical

mechanical models) has different statistical properties for integrable and nonintegrable models and one can make a close connection to the theory of the spectral properties of random matrices. In the actual calculation we first make use of all those symmetries of the Hamiltonian which do not depend on the value of the couplings, and for large finite lattices we block diagonalize the eigenvalue matrix of the problem. The statistical analysis of the energy levels is then performed for each block separately. In a nonintegrable model, in which no further internal symmetry is present, the matrix elements of a block matrix are expected to be loosely correlated, so that they can be approximately represented by random entries. Indeed the spectrum of nonintegrable models is found to belong to the class of orthogonal random matrices, to the so-called Gaussian orthogonal ensemble (GOE) and the level spacing distribution is described by the Wigner surmise [24]:

$$P(s) = \frac{\pi}{2} s \exp(-\pi s^2/4). \quad (2)$$

On the other hand, if the Hamiltonian is integrable by the Bethe ansatz there is an infinite number of internal symmetries and consequently the matrix elements of a block matrix are strongly correlated. Loosely speaking integrable Hamiltonians are so peculiar that they are not well described by an ‘‘average Hamiltonian.’’ Then one expects that in this case the eigenvalues themselves behave like independent random numbers, so that the spectrum of integrable models belongs to the ensemble of diagonal random matrices and the level spacing distribution is described by the Poissonian (exponential) distribution: $P(s) = \exp(-s)$. Numerical studies of integrable models [17–23] are indeed in agreement with this assumption.

In this paper we are going to perform the analysis of the level statistics of the multispin-coupling Hamiltonian in Eq. (1). We are going to answer two questions. The first question is whether or not the Hamiltonian is integrable, at least at the transition (self-dual) point. Our second question concerns the

TABLE I. Dimensions of the irreducible representations (i.e., degeneracy) and size of the corresponding block.

$M=3, L=18$																		
Label R	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Dimension	1	1	1	1	2	2	2	2	2	2	2	2	3	3	3	3	6	6
Size	2029	1871	1645	1743	3613	3671	3612	3668	3668	3612	3612	3668	5656	5272	5400	5528	10920	10920

characteristics of the level distribution at a first-order transition point. The paper is organized as follows. The symmetries of the Hamiltonian in Eq. (1), which are essential to perform a block diagonalization, are presented in Sec. II. The statistical analysis of the spectrum of the block-diagonalized Hamiltonian is given in Sec. III, while the results are discussed in the final section.

II. SYMMETRIES OF THE HAMILTONIAN

As described in the Introduction the first step in a statistical analysis of the energy eigenvalues is to block diagonalize the Hamiltonian in Eq. (1) using all those symmetries of the model which do not depend on the actual values of the couplings. Before analyzing these symmetries, let us first notice that if $E(J, h) = \{E_0(J, h), E_1(J, h), \dots, E_{2L-1}(J, h)\}$ denotes the set of energies of the Hamiltonian Eq. (1), one has $E(J, h) = E(\pm J, \pm h)$. This can be seen introducing the operators $O^x = \prod_{i=0}^{L-1} \sigma_i^x$ and $O^z = \prod_{i=0}^{L/m-1} \sigma_{im}^z$ and noting that $H_\alpha O^\beta = \epsilon_{\alpha\beta} O^\beta H_\alpha$, where $\alpha, \beta = x, z$ and $\epsilon_{\alpha, \beta} = 1$ if $\alpha = \beta$ and -1 otherwise. On a finite lattice this symmetry holds for periodic boundary conditions and if the length of the chain is a multiple of m . In what follows we consider this type of lattices and restrict ourselves to the case $h > 0$ and $J > 0$.

The symmetries of the model are of three types: (i) *space-like symmetries*, which describe invariance of the system under geometrical transformations (translation, inversion, etc.); (ii) *gauge symmetries*, which are connected to invariance of the Hamiltonian under internal transformations; and finally (iii) *duality symmetries*, which make a connection between the strong- and weak-coupling regimes of the Hamiltonian.

(i) The *space symmetry* of the model on a finite lattice depends on the boundary condition. In a statistical analysis of the spectrum of finite systems it is desired to use the most symmetric boundary condition to get a block structure, which well represents the statistical behavior of the spectrum in the thermodynamic limit. Therefore, as already mentioned, we apply periodic boundary conditions, which can be formally expressed as $\sigma_{L+i}^x = \sigma_i^x$. The space symmetry group is then the automorphy group of a ring, irrespective of the range of the interaction m . This is the dihedral group generated by the translation T and the reflection R ($T^L = R^2 = \text{identity}$ and $TR = RT^{L-1}$), which both commute with \mathcal{H} .

(ii) The *gauge symmetries* are generalizations of the spin-reversal symmetry for the well known $m=2$ case. Recalling that we take L to be a multiple of m , let us introduce a set of $n = 2^{m-1}$ operators O_k for $k=0, 1, \dots, n-1$:

$$O_k = \prod_{\alpha=0}^{L/m-1} \prod_{i=\alpha m}^{\alpha m+m-1} (\sigma_i^z)^{k_i}, \quad (3)$$

where k_0, k_1, \dots, k_{m-2} are the bits of the binary representation of k , and k_{m-1} is such that

$$\sum_{i=0}^{m-1} k_i \quad \text{even}. \quad (4)$$

The spin-reversal symmetry, which holds when m is even, is O_{n-1} corresponding to $k_i = 1$ for all i . It is straightforward to check that the condition Eq. (4) ensures that all the operators O_i commute with $\mathcal{H}(J, h)$. It is also clear that these operators are diagonal, involutive, and form an Abelian group (O_0 is the identity). This implies that all the $2^{m-1} = n$ representations are one dimensional and the corresponding projectors are of the form $P_R = 1/n \sum_{i=0}^{n-1} \epsilon_i^R O_i$ where $\epsilon_i^R = \pm 1$ for all i and R . All these projectors split the Hilbert space in 2^{m-1} invariant subspaces of size 2^{L-m+1} each. For example, for $m=2$ and L even, $P_0 = (1/2)(O_0 + O_1)$ projects onto the subspace with an even number of up spins, while $P_1 = (1/2)(O_0 - O_1)$ projects onto the subspace with an odd number of up spins. The projector $P_0 = 1/n \sum O_i$ projects onto the most symmetric subspace to which the ground state belongs (we refer now to this subspace as the ground-state sector), whereas the other $2^{m-1} - 1$ sectors become degenerate in the thermodynamic limit. Thus, in this limit, the degeneracy of the ground state in the strong-coupling phase $J > h$ is given by 2^{m-1} . This degeneracy for the $m=3$ model is just four, which led Debierre and Turban [7] to conjecture the same universality class for the transition as that for the $Q=4$ -state Potts model.

The combination of the space symmetry and the gauge symmetry is not obvious, since the operators of these two groups do *not* commute in general. The product of these two groups is a semidirect product (not a direct product), since the gauge group is a normal subgroup. As usual the states are labeled by the number of the representation R to which they belong. We have computed the character table of the symmetry group from which the dimensions of the invariant subspaces are deduced and then the block-diagonal Hamiltonian is constructed. The dimensions of the irreducible representations and the size of the corresponding blocks are given in Tables I–III for different values of m , in the range of $0 \leq R < L/2 + 3$ and $0 \leq R < (L-1)/2 + 2$, for L even and odd, respectively. We note that in the ground-state sector, which is labeled by $R=0$ and corresponds to $P_0 = (1/n) \sum O_i$ all the operators of the space and gauge symmetry group commute, so that *in this sector* we have a representation of the dihedral group. In what follows we use the same labeling convention as in [22].

(iii) As mentioned in the Introduction the Hamiltonian in Eq. (1) has the property of *duality symmetry*. To show this and its consequences in finite lattices, first we define, for an infinite lattice, dual Pauli operators τ_i^x, τ_i^z as

TABLE II. Dimensions of the irreducible representations (i.e., degeneracy) and size of the corresponding block.

		$M=4, L=16$															
Label R	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Dimension	1	1	1	1	1	1	1	1	2	2	2	2	2	2	2	2	2
Size	330	265	202	265	288	288	224	224	529	512	544	480	544	480	496	512	526
Label R	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33
Dimension	2	2	2	2	2	2	2	2	2	4	4	4	4	4	4	4	8
Size	512	496	512	496	512	526	512	496	512	1088	960	1024	1024	1024	1024	1024	2048

$$\tau_i^z = \sigma_i^x \sigma_{i+1}^x \cdots \sigma_{i+m-1}^x, \quad (5)$$

$$\sigma_i^z = \tau_i^x \tau_{i+1}^x \cdots \tau_{i+m-1}^x \quad (6)$$

in terms of which the Hamiltonian in Eq. (1) is expressed as

$$\mathcal{H} = -J \sum_i \tau_i^z - h \sum_i \tau_i^x \tau_{i+1}^x \cdots \tau_{i+m-1}^x. \quad (7)$$

Consequently the two sets of energies $E(J, h)$ and $E(h, J)$ are equal:

$$E(J, h) = E(h, J) \quad (8)$$

and the self-dual point $h=J$ corresponds to the transition point of the system, provided there is one single-phase transition in the system. The duality symmetry, as described above, holds in the thermodynamic limit, i.e., when the length of the system $L \rightarrow \infty$. In a *finite system* duality generally relates sectors of the Hamiltonian with different boundary conditions. With periodic boundary conditions one has the symmetries $\sigma_{L+i}^x = \sigma_i^x$ and $\sigma_{L+1}^z = \sigma_i^z$, which in terms of the dual operators in Eq. (5) and Eq. (6) are only satisfied in the ground-state sector of the Hamiltonian. As a result self-duality holds only in the ground-state sector, which is indeed verified numerically. Based on this observation we expect somewhat different statistical properties of the energy levels in the self-dual and non-self-dual sectors.

III. RESULTS OF THE RANDOM MATRIX THEORY

Using the symmetries as described in the preceding section we have performed the block diagonalization of the eigenvalue matrices for large finite lattices, the size of which was a multiple of the length of the interaction m . We went up to $L=18, 16$, and 15 for $m=3, m=4$, and $m=5$, respectively. The size of the blocks, as seen in Tables I–III, is relatively small; especially for larger values of m their size is reduced by gauge symmetry.

Having the block-diagonalized Hamiltonian we solved

their spectrum by standard numerical methods, which are contained in the LAPACK library. The next step, before performing the analysis, is to unfold the spectrum, i.e., to subtract the average tendency and to keep only the fluctuations, which are normalized in the same manner at each part of the spectrum. Technical details relating to unfolding the spectrum are given in Refs. [22,23].

The unfolded spectrum is then analyzed and several spectral quantities are determined and compared with the predictions of random matrix theory. First, we consider the level spacing distribution $P(s)$, which is expected to be of the Wigner form in Eq. (2) for nonintegrable models, whereas it is generally of the Poissonian form for integrable models. To analyze realistic spectra it is often useful to consider Brody's interpolation formula:

$$P_\beta(s) = c(1 + \beta)s^\beta \exp(-cs^{\beta+1}), \quad (9)$$

with $c = [\Gamma((\beta+2)/(\beta+1))]^{1+\beta}$, which corresponds to the Wigner and the Poisson form for $\beta=1$ and $\beta=0$, respectively. The interpolation parameter β , which is determined by an optimization fit, proved itself to be a useful indicator for the localization of integrable varieties [22,23].

Another quantity characterizing the independence of the eigenvalues is the spectral rigidity in an interval of length l :

$$\Delta_3(l) = \left\langle \frac{1}{l} \min_{a,b} \int_{\alpha-l/2}^{\alpha+l/2} [N_u(\epsilon) - a\epsilon - b]^2 d\epsilon \right\rangle_\alpha, \quad (10)$$

where $N_u(\epsilon) \equiv \sum_i \Theta(\epsilon - \epsilon_i)$ is the integrated density of unfolded eigenvalues and $\langle \rangle_\alpha$ denotes an average over α . Finally, we shall also consider the number variance $\Sigma^2(l)$ defined as the variance of the number of unfolded eigenvalues in an interval of length l :

$$\Sigma^2(l) = \langle [N_u(\epsilon+l/2) - N_u(\epsilon-l/2) - l]^2 \rangle_\epsilon, \quad (11)$$

where the angle brackets denote an averaging over ϵ .

First we present the results of the statistical analysis of the spectra *outside the transition point*. As seen in Figs. 1 and 2

TABLE III. Dimensions of the irreducible representations (i.e., degeneracy) and size of the corresponding block.

		$M=5, L=15$																
Label R	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
Dimension	1	1	2	2	2	2	2	2	2	5	5	5	5	5	5	10	10	10
Size		102	38	138	136	136	136	136	136	374	310	374	310	374	310	682	682	682

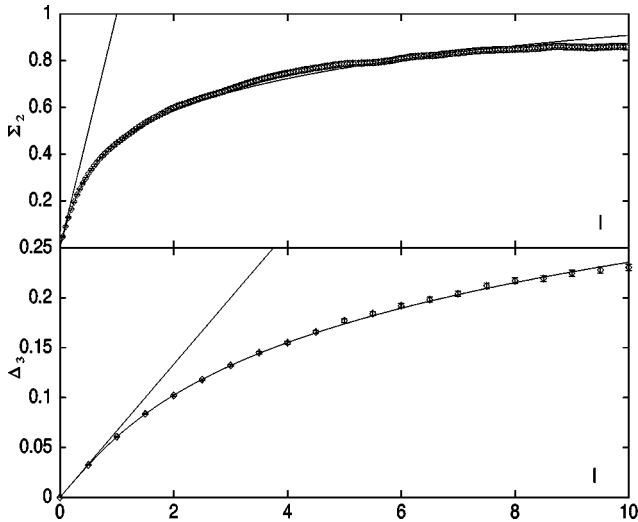


FIG. 1. Level spacing distribution for $L=15$, $M=3$, $h/J=1.36$, and *all* the representations. The exponential (E) and the Wigner (W) distributions are shown (full line), together with the Brody distribution (broken line) for the fitted best value of the parameter $\beta=1.01$ (see text).

on the example of the $m=3$ model at a coupling $J/h=1.36$ for a 15-site chain, all the three characteristic quantities of the spectrum are very well described by the Wigner distribution [24]. Figure 2 presents the rigidity and the number variance for the same parameters. The expected behavior for independent random energies and for the eigenvalues of the GOE is also shown. The GOE behavior is observed up to quite large values of L , indicating that GOE matrices provide a good description of the Hamiltonian. The data shown are obtained averaging over all the representations. However, very similar results are obtained averaging only over the self-dual sector. The characteristic parameters of the spectrum do not depend on whether the sector under consideration is self-dual or non-self-dual. We also note that very similar behavior is found for other ranges of the interaction $m>3$ or for other values of $J/h>1$. Consequently, there is no evidence for the integrability of the model with $m>2$ away from the critical point.

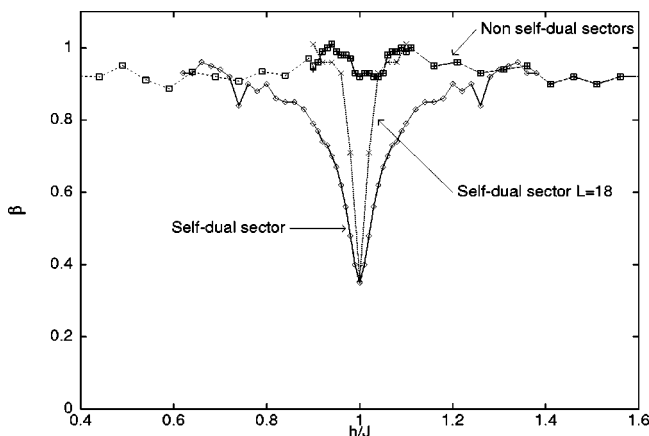


FIG. 2. Rigidity (a) and variance (b) for $L=15$, $M=3$, $h/J=1.36$, and *all* the representations. The corresponding quantities for the GOE matrices and for random diagonal matrices are also shown in full lines.

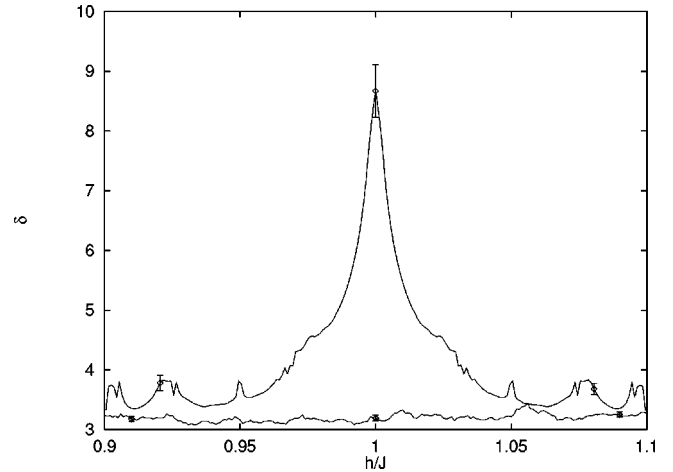


FIG. 3. Parameter β as a function of h/J for $m=3$. For $L=15$ the data are averaged separately over all self-dual sectors or over all non-self-dual sectors. For $L=18$ only the representation R_0 to which the ground state belongs is taken into account.

In the following we investigate the level statistics of the model as a function of the ratio h/J and calculate the interpolation parameter β in Eq. (9) as a best fit over the self-dual and non-self-dual sectors. The results are shown in Fig. 3 for $L=15$ and $m=3$, whereas data for the largest system size are only included in the self-dual sector. We note that the corresponding data for $m=4$, $m=5$, and a less extensive calculation for $m=6$, lead us to very similar conclusions. One can see in Fig. 3 that Brody's parameter β has different behavior in the self-dual and in the non-self-dual sectors. While in the non-self-dual sectors β is approximately constant and its value $\beta\approx 1$ corresponds to the GOE result, in the self-dual sector there is a change in the value of β around the self-dual point. Actually its value drops from $\beta=1$ to about $\beta\approx 0.45$ at the transition point. The region where the change in β takes place seems to shrink only to the self-dual point in the thermodynamic limit, as can be seen in Fig. 3 by comparing the results with $L=15$ and $L=18$.

This observation leads us to study carefully the spectral properties of the models *at the transition point*, the results of which are shown in Fig. 4(a). As seen in the figure the level spacing distribution could not be well fitted by the interpolation formula in Eq. (9), at least with the symmetries we have taken into account. However, it is given approximately by the arithmetic average of the Wigner and Poisson distributions, which is also shown in the figure. We argue that the measured spectral quantities in the self-dual sector can be interpreted as if the spectrum is composed of two independent Wigner distributions. To check our assumption we have taken two non-self-dual blocks of roughly the same size each of which has Wigner characteristics and merged the levels of the two blocks. Then we analyzed the level statistics of the combined blocks and the obtained results in Fig. 4(b) look very similar to those we found for the self-dual sector and presented in Fig. 4(a).

Thus at this point we conclude that the spectrum of the self-dual sector at the self-dual point is seemingly composed of two independent parts, each having Wigner-type characteristics. This type of behavior is the result of an extra symmetry, the *self-duality*, which is just seen in the self-dual

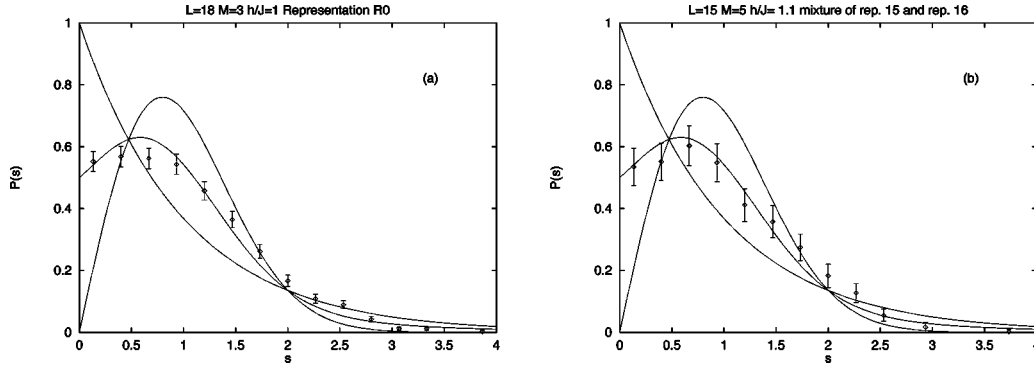


FIG. 4. (a) Level spacing distribution for $L=18$, $M=3$ and for the representation to which the ground state belongs. (b) Combination of the spectrum of two different representations R_{15} and R_{16} of the $m=5$ model for $L=15$.

sector. Furthermore, we argue that this extra symmetry is manifested by the crossing of energy levels at the self-dual point in the thermodynamic limit $L \rightarrow \infty$. To see this we have calculated the quantity

$$\delta = \left\langle \frac{\max(s_i, s_{i-1})}{\min(s_i, s_{i-1})} \right\rangle_i, \quad (12)$$

which measures the asymmetry in the level spacing distribution. For *independent* random variables chosen according to a Wigner distribution one has $P(\delta) = 4\delta/(1+\delta^2)^2$ yielding a mean value $\langle \delta \rangle = 1 + \pi/2 \approx 2.5708$. For matrices from the GOE, the correlation between spacings s_i modifies this value. We have numerically found that this value does not vary considerably with the size of the matrix, and is very close to

$$\langle \delta \rangle_{\text{GOE}} \approx 3. \quad (13)$$

(Diagonalizing 1000 GOE random matrices of size ranging from 3 up to 2000.) As seen in Fig. 5 for non-self-dual sectors δ is indeed close to the GOE result in Eq. (13). Similarly, $\delta \approx 3$ is found in the self-dual sector far from the self-dual point, however, there is a sharp increase in δ in the neighborhood of $h/J=1$ [25]. Since the value of δ at the self-dual point is monotonically increasing with the size of the system (see Table IV), one expects that in the thermody-

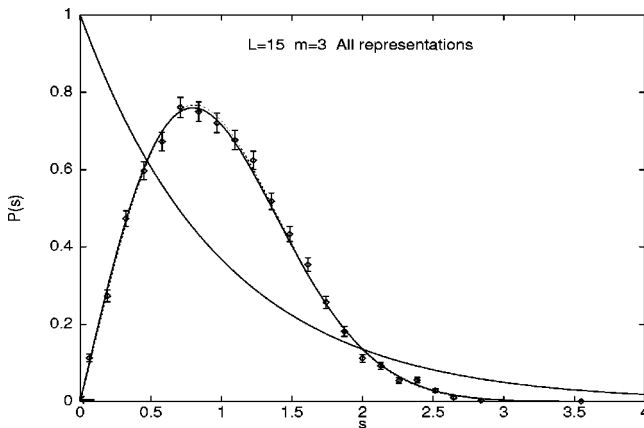


FIG. 5. The asymmetry parameter δ in Eq. (12) as a function of h/J for $L=16$ and $m=4$. The upper curve corresponds to the self-dual sector and the lower curve to non-self-dual sectors. The error bars are calculated as the variance divided by the square root of the number of spacing ratios.

amic limit $\delta \rightarrow \infty$. Thus there is an exact degeneracy in the self-dual sector at the transition point, which should be connected with the presence of an extra symmetry. The possible origin of this extra symmetry is discussed in the final section.

IV. LEVEL STATISTICS AT A FIRST-ORDER TRANSITION POINT

In this paper we have studied the statistical properties of the spectrum of a transverse-field Ising spin chain with m -spin interactions and compared to the predictions of random matrix theory. Away from the transition point, which is known exactly from duality symmetry, the spectrum is shown to be a Gaussian orthogonal ensemble and its properties are well described by the Wigner distribution. On the other hand, at the transition point the spectral properties of the self-dual and non-self-dual sectors are different. While the spectra of non-self-dual sectors are close to the Wigner distribution the same for the self-dual sector can be described as the composition of two independent Wigner distributions. Furthermore, we have shown that this special behavior at the transition point is the result of level crossing in the thermodynamic limit.

This observation can be compared with the known exact [26] and numerical [27] results on the two-dimensional $Q > 4$ Potts model. As known exactly [28], this model is also self-dual and there is a first-order transition in the system. As an analogous quantity to the Hamiltonian in Eq. (1) we consider the \mathcal{T} transfer matrix of the Potts model, which in the Hamiltonian limit [29,30] is given by $\mathcal{T} = \exp(-\tau H_P)$, where τ denotes the lattice spacing and H_P is the Hamiltonian of the one-dimensional quantum Potts model. According to exact results [26] in the thermodynamic limit the ground state of H_P at the transition point is $(Q+1)$ -fold degenerate. At

TABLE IV. The asymmetry parameter δ in Eq. (12) as a function of L for $m=3, 4$, and 5 in the ground-state sector. When present the number in parentheses refers to the asymmetry calculated for the *entire* self-dual sector.

	$L=10$	$L=12$	$L=15$	$L=16$	$L=18$
$m=3$		4.79	6.54 (9.63)		11.31
$m=4$		4.58		5.09 (8.67)	
$m=5$	1.76		4.33		

this point the first two levels of the self-dual sector, as well as the first levels of the $Q-1$ other, non-self-dual sectors are degenerate. Thus the first order nature of the transition is manifested by a level crossing in the self-dual sector. (For finite rings one observes a hybridization gap in the self-dual sector, which vanishes exponentially with the size of the system [27].) As shown by numerical calculations [27] the same type of level crossing phenomena takes place for the higher lying levels, too. Thus, for finite systems, the spectrum at the transition point is expected to decompose into two parts, which are going to be degenerate in the thermodynamic limit.

Our numerical results on the multispin-coupling model are in agreement with the above picture, thus we expect a similar scenario. The self-dual symmetry at the transition point, which is connected to a level crossing in the self-dual sector in the thermodynamic limit, is responsible for the unusual spectral properties of the multispin-coupling models for $m > 3$. The $m = 3$ model, in which the transition is expected to be second order, is assumed to represent the border limit of continuous models. Thus one expects that the above

scenario, which stays valid as $m \rightarrow 3^+$, could hold also for $m = 3$, perhaps with another type of functional form for the size dependence of the hybridization gap. Indeed, this type of behavior has been found by our numerical studies.

Finally, we discuss possible integrability of the multispin-coupling model in Eq. (1). As a result of our numerical studies of spectral properties of the model we conclude that there is no evidence in favor of integrability of the Hamiltonian in Eq. (1) for $m > 2$, even at the transition point.

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