

Entanglement in the Majumdar-Ghosh model

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We present an analysis of the entanglement characteristics in the Majumdar-Ghosh (MG) or J_1 - J_2 Heisenberg model. For a system consisting of up to 28 spins, there is a deviation from the scaling behavior of the entanglement entropy characterizing the unfrustrated Heisenberg chain above $J_2 \approx 0.25$. This feature can be used as an indicator of the dimer phase transition occurring in this model. Additionally, we also consider entanglement at the MG point $J_2 = 0.5J_1$.

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I. INTRODUCTION

Entanglement has come to be seen as a prime resource for various quantum-information processing tasks [1]. From another angle, entanglement describes quantum correlations of many-body systems, which on their part are responsible for various interesting physical phenomena, e.g., quantum-phase transitions. In recent years, entanglement has been fruitfully used to give an alternate view on quantum-phase transitions, especially in low-dimensional quantum systems (see Refs. [2,3], and references therein). Frustrated quantum systems have, however, been largely left out of the picture in such discussions so far.

In this paper, we consider the entanglement in a prototypical one-dimensional (1D) frustrated spin system—the Majumdar Ghosh or J_1 - J_2 Heisenberg chain [4]. The spin-1/2 Hamiltonian is described by

$$H = J_1 \sum_{\langle mn \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle nmn \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (1)$$

where the sums run over nearest neighbor (nn) and next-nearest neighbor (nnn) spins, and \mathbf{S}_i are spin-1/2 operators. In what follows, we set $J_1 = 1$ as the energy scale and consider antiferromagnetic $J_2 > 0$ interaction (Fig. 1). The ground-state properties of this system have been studied so far with the use of many methods such as exact diagonalization, DMRG, field-theoretical approach (see Refs. [5,6] for an overview). It is known that the model is critical (i.e., the spin-spin correlation function decays algebraically) and gapless for $J_2 \leq J_2^* \approx 0.2411$ [6,7]. A gap to triplet excitations opens beyond the quantum critical point J_2^* accompanied also by the stabilization of a dimerized phase. Interestingly, for $J_2 = 0.5$ (known as the MG point), the ground-state manifold is exactly known. It is spanned by two degenerate nearest-neighbor dimer states given by

$$|R\rangle = (1,2)(3,4) \dots (N-1,N), \quad |L\rangle = (2,3)(4,5) \dots (N,1), \quad (2)$$

where (i,j) denotes a singlet between spins i and j .

In the following, we will demonstrate that the entanglement, as quantified by the entanglement entropy, exhibits characteristic scaling properties in the critical region. The entanglement entropy, by definition, captures the large-scale entanglement or quantum correlations, in the ground-state of

the system, between two complementary groups of spins on the lattice. We will show that the ground-state entanglement scales not only with respect to the subsystem size n in an infinite system (this possibility was examined carefully in the case of exactly solvable models [2]), but in finite systems for fixed n also with respect to the total size N of the system. The gapped phase is characterized by a deviation from this scaling behavior. This is to be contrasted with the fact that the phase-transition region is not distinguished in the dependence of standard entanglement measures such as entanglement entropy or pairwise concurrence on the control parameter J_2 .

In the second part of this paper, we consider the entanglement at the MG point. This has been considered earlier in Ref. [4], where it was shown that the nearest-neighbor concurrence exhibits a jump at the MG point in finite systems. However, this jump disappears exponentially as the total size of the system increases. We derive a simple formula for the change of concurrence as the parameter J_2 is made to pass through the MG point. Furthermore, we consider a different quantity, the entanglement of a pair of next-nearest-neighbor spins, as a potential indicator of the MG point. This quantity is maximal at the MG point for any size of the system. Furthermore, we analytically show that in the thermodynamic limit this entanglement entropy is invariant in the MG manifold, and thus is a robust maximum. Interestingly as a by-product, in the small size limit, the two translationally invariant (or “quasimomentum”) states turn out to have entanglement entropies that are local minima in this manifold.

II. ENTANGLEMENT ENTROPY SCALING

Given a pure state of a quantum many-body system, the entanglement of a given subsystem with its complement is uniquely measured by the entanglement entropy. The entanglement entropy is defined as the von Neumann entropy

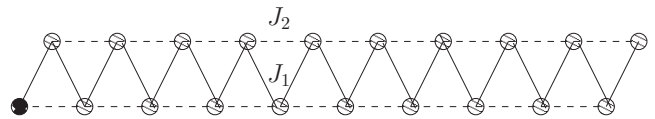


FIG. 1. Model system with nearest J_1 and next-nearest-neighbor interaction J_2 .

of the chosen subsystem, i.e., if the (reduced) density matrix of the subsystem is ρ_n and λ_j are its eigenvalues, then the entanglement entropy is defined as

$$S(\rho_n) \equiv - \sum_j \lambda_j \log_2 \lambda_j. \quad (3)$$

The physical properties of quantum many-body systems are influenced by the spatial extent of correlations present. This is usually described by the correlation length of two-particle correlators. A quantum-phase transition is induced by diverging correlation length. Physically, the entanglement entropy of a group of n spins depends on the properties of all relevant correlators of $2, 3, \dots, n$ spins and also single spin averages and thus contains much more information about the nature of correlations in the system (e.g., for the ground state of the Hamiltonian (1), the entanglement between two spins and the rest of the lattice depends only on the correlation between the two spins (see Sec. III) while the entanglement entropy of any three spins depends only on all three pair correlators and the helicity of the considered spins). It is thus expected that the entanglement entropy should be a potential indicator of quantum-phase transitions.

Indeed, the entanglement entropy of a block of contiguous spins has been shown to scale differently with the block size n , in critical and noncritical 1D systems [2]. In the thermodynamic limit (total system size $N \rightarrow \infty$), the entanglement entropy of a noncritical system tends to saturate, giving rise to a length scale that can be associated with an “entanglement length” [8]. On the other hand, for critical systems, the entanglement entropy diverges logarithmically and importantly displays universal scaling behavior [9],

$$S(n) = \frac{c_0}{3} + \frac{c}{3} \log_2 n, \quad (4)$$

where c is a universal scaling constant that is the central charge of the corresponding conformal field theory and c_0 is model dependent. At criticality, the entanglement length thus effectively becomes infinite. The two constants take the values 1 and π , respectively, for the isotropic Heisenberg antiferromagnetic chain. The extension of Eq. (4) to finite critical systems was given in Ref. [10],

$$S(n, N) = \frac{c_0}{3} + \frac{c}{3} \log_2 \left[\frac{N}{\pi} \sin \left(\frac{\pi n}{N} \right) \right]. \quad (5)$$

For small values of n/N , this equation becomes

$$S(n, N) = \frac{c_0}{3} + \frac{c}{3} \log_2 n - \frac{c}{18 \ln 2} \pi^2 \left(\frac{n}{N} \right)^2 - \frac{c}{540 \ln 2} \pi^4 \left(\frac{n}{N} \right)^4 + \mathcal{O} \left(\frac{n}{N} \right)^6. \quad (6)$$

In the rest of this section, we consider the scaling of the block entanglement entropy in the ground state of the MG model. The ground state is calculated via exact diagonalization (Lanczos method) of systems of up to 28 spins on imposing periodic boundary conditions. This model has recently been considered by Laflorencie *et al.* [11] using

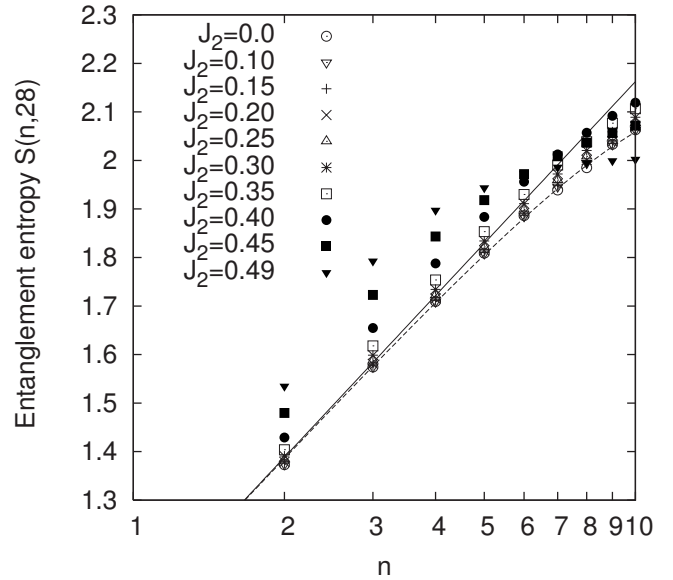


FIG. 2. Scaling of the entanglement entropy of the MG model. The system contains 28 spins and the length of the subsystem changes from $n=2$ to $n=10$. The full line represents the logarithmic scaling of an infinite system—Eq. (4). The dashed line shows the finite-size correction given by Eq. (5). Note that the correction resulting due to $J_2 > 0$ is most pronounced for small n . For larger subsystem sizes the finite size correction dominates.

DMRG techniques in the context of open boundary conditions.

A. Case 1: Fixed N

First, let us focus on the scaling of the entanglement entropy with respect to the block size n of consecutive spins for a system with a fixed number N of spins. This case, for $N \leq 20$ and $J_2=0$, has been analyzed previously [2]. Our results for $N=28$ are shown in Fig. 2. As expected the numerical data for $J_2=0$ (open circles) are well described by Eqs. (5) and (6) describing the saturation of von Neumann entropy for finite N . But there is also good agreement of the calculated entanglement for finite J_2 up to $J_2 \approx 0.25$ with the line given by Eq. (5). Fitting the values of $S(n, 28)$ to Eq. (5) yields $c_0=3.131$ and $c=1.017$. For comparison, the logarithmic divergence of the entanglement in the thermodynamic limit is also drawn.

The correction to this scaling due to the frustrating J_2 in the finite system of 28 spins can be most clearly seen for small n . For larger n the finite-size correction [see Eq. (6)] and the frustration effect show opposite tendencies and cancel each other partially. However, for strong frustration near the Majumdar-Gosh point, i.e., for $J_2=0.49$, the frustration effect is clearly visible for all n considered. It is thus reasonable to argue that the presence of $J_2 \neq 0$ will produce a saturation of the entanglement vs n .

As mentioned in the Introduction, the considered model has an extended critical region from $J_2=0$ to $J_2=J_2^* \approx 0.2411$ [6,7]. In the weak frustration limit $J_2 < J_2^*$, this model belongs to the universality class of the isotropic Heisenberg model. Due to this, the change in the scaling of

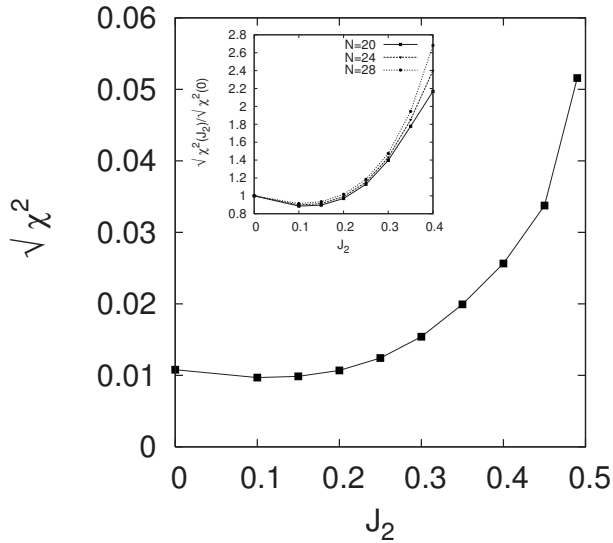


FIG. 3. Least-square deviation $\sqrt{\chi^2}$ of the calculated values of the entanglement from the line described by Eq. (5) (dashed line in Fig. 2) in dependence on the frustration J_2 . The system contains 28 spins and $\sqrt{\chi^2}$ was calculated for $n \leq 6$. Note that $\sqrt{\chi^2}$ starts to increase in the gapped phase where the scaling relations Eqs. (5) and (6) do not hold. Inset: A comparison of normalized least-square deviations for systems containing 20, 24, 28 spins.

the entanglement in this region is expected to be governed by the model-dependent c_0 term. Physically, the weak frustration is not expected to drastically influence the entanglement (or other physical properties) as compared to the isotropic case. In particular, the dependence of c_0 on J_2 in this regime is also expected to be weak, in the thermodynamic limit.

The deviation of the entanglement from the scaling relations is a natural indicator of quantum-phase transitions. We define this deviation of entanglement from the scaling relation (5) at finite frustrating $J_2 > 0$, in the standard way, as a square root of the sum of squares of residuals $\sqrt{\chi^2}$. This quantity is calculated and plotted in Fig. 3. It measures the differences between the calculated entropies for $J_2 > 0$ and the line given by Eq. (5). Notably, one can observe a significant deviation from the critical scaling above the interval $J_2 \in \{0.2, 0.3\}$, containing the dimer transition point. The behavior in the entire critical region is expected to be flat with a sharp deviation above the critical point J_2^* , in the thermodynamic limit. Indeed, for finite systems the deviation from scaling becomes more pronounced above $J_2 \geq 0.25$ with an increase of the system size, as seen in the inset of Fig. 3. The dependence on J_2 , in particular, the flat minimum for $J_2 \approx 0.10$ is a finite-size effect which, by the argument given in the preceding paragraph, should disappear for larger systems [12].

B. Case 2: Fixed n

The question arises as to whether the quantum-phase transition in the MG model can be identified directly from the dependence of “sufficiently local” entanglement measures on the control parameter J_2 , as in certain other models. Indeed, as shown by Osterloh *et al.* [13], the phase transitions in XY

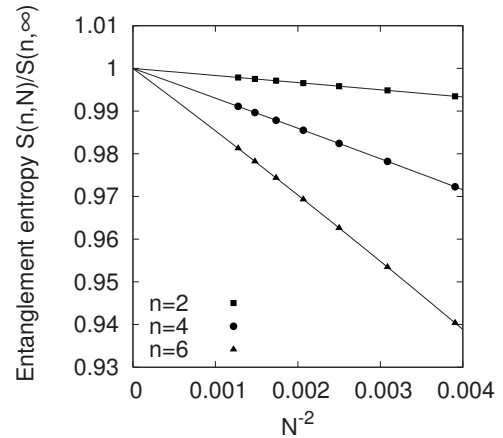


FIG. 4. Finite-size scaling of the von Neumann entropy $S(n, N)$ of the unfrustrated Heisenberg chain, i.e., for $J_2=0$, for fixed subsystem size n . The system size N changes from 16 to 28 spins.

spin-1/2 models can be identified explicitly by the dependence of the entanglement between two nearest-neighbor spins, as measured by the concurrence, on the control parameter. On the other hand, single and two-spin entanglement entropy of XY models have been shown to detect quantum-phase transitions (see Refs. [14–16]).

The concurrence does not visually detect the dimer phase transition of the MG model, as seen in Ref. [4]. The single spin entropy is always equal to 1, since the ground state remains rotationally invariant (see Sec. III). We have checked that entanglement entropies of variously chosen subsystems, such as block entanglement of consecutive spins, or blocks of next-nearest-neighbor spins also do not identify the phase transition in this model. The reason for this may be that: either local entanglement measures do not detect this phase transition or the small system sizes considered do not capture this behavior [17].

The finite-size problem can be circumvented by the usual finite-size scaling techniques. Consider, e.g., the entanglement entropy of two nearest-neighbor spins ($n=2$) for different total system sizes N . For the isotropic Heisenberg antiferromagnet ($J_2=0$) this quantity scales as N^{-2} as shown in Fig. 4 (the scaling is given by a perfect line with correlation better than 0.9999 for N ranging from 16 to 28). This fully agrees with the dominating behavior in Eq. (6). The scaling of blocks of 4,6 spins are also presented in Fig. 4 [18].

Let us focus on the dependence of the scaling of $n=2$ entanglement entropy on the control parameter J_2 . The correction to the N^{-2} scaling can again be characterized by the value of $\sqrt{\chi^2}$, describing the difference between the calculated entropies for $J_2 > 0$ and the straight line for $J_2=0$ (see Fig. 5). Significantly, there is a clear deviation from critical scaling for $J_2 \geq 0.25$, which is remarkably close to the critical point J_2^* considering the examined system sizes. Furthermore, finite-size effects are much less apparent in this case of scaling as compared with the results of the previous section. The phase transition may thus be located by the dependence of $\sqrt{\chi^2}$ on the control parameter.

While the above results show that there is a change in scaling of local entanglement entropy around the critical

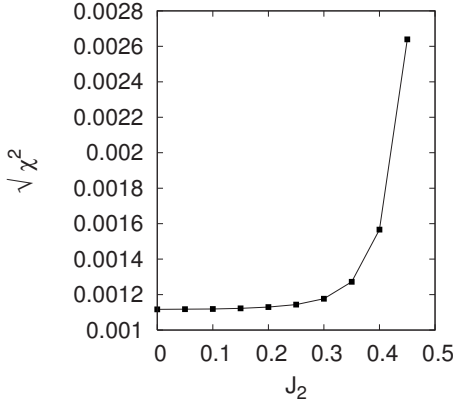


FIG. 5. The deviation (measured by $\sqrt{\chi^2}$) from the straight line scaling for $J_2=0$ and $n=2$ (the upper line in Fig. 4) for larger values J_2 .

point, the general question posed in this section remains open for future discussion.

III. MAJUMDAR-GHOSH POINT

We now turn to the entanglement at the MG point $J_2=1/2$. In particular, we are going to consider two measures of entanglement, viz., the concurrence of two spins (which was recently analyzed in Ref. [19]) and the entanglement entropy of two spins.

To fix notions, recall that the model Hamiltonian [Eq. (1)] possesses rotational [SU(2)] symmetry. It is widely believed that the ground state $|g\rangle$ of 1D Heisenberg antiferromagnets also exhibits this symmetry, i.e., is a total singlet $S=0$ state. This implies that any subset of spins chosen from the whole system is also rotationally invariant. This follows from the following simple identity for the reduced state of n arbitrary spins:

$$\begin{aligned} \rho_n &= \text{Tr}' \rho_g = \text{Tr}' U^{\otimes N} \rho_g (U^\dagger)^{\otimes N} \\ &= U^{\otimes n} (\text{Tr}' U^{\otimes N-n} \rho_g (U^\dagger)^{\otimes N-n}) (U^\dagger)^{\otimes n} \\ &= U^{\otimes n} \rho_n (U^\dagger)^{\otimes n}, \end{aligned} \quad (7)$$

which holds provided $\rho_g = |g\rangle\langle g|$ is rotationally invariant, i.e., $\rho_g = U^{\otimes N} \rho_g (U^\dagger)^{\otimes N}$ for an arbitrary single-spin unitary operator U (the symbol Tr' denotes the partial trace over the unwanted spins). In particular, the reduced state of each individual spin in the ground state of the MG model is maximally mixed $\rho_1 = \mathbb{1}/2$ implying that a single spin is maximally entangled with either all or some of the remaining spins in the lattice. Similarly, any state of two spins belongs to the one parameter family of so-called Werner states [20], that can be represented as

$$\rho_2 = p |\Psi^-\rangle\langle\Psi^-| + \frac{1-p}{4} \mathbb{1}, \quad (8)$$

where $|\Psi^-\rangle$ denotes a singlet and $p = -(4/3)\langle S_i \cdot S_j \rangle$ is just the (rescaled) isotropic correlation function of the involved spins.

The entanglement between two spins, characterized by the concurrence [21] $C(\rho_2)$, can be checked to be given by a simple formula for Werner states

$$C(\rho_2) = \max\left(0, \frac{3}{2}p - \frac{1}{2}\right). \quad (9)$$

Thus, two spins are entangled with each other as long as the correlations between them are sufficiently antiferromagnetic, $\langle S_i \cdot S_j \rangle < -1/4$ [22]. The entanglement entropy [see Eq. (3)] of two spins in a Werner state, on the other hand, is given by the relation

$$S(\rho_2) = 2 - \frac{1+3p}{4} \log(1+3p) - 3 \frac{1-p}{4} \log(1-p). \quad (10)$$

Returning now to the MG point, one of the states $|R\rangle$ or $|L\rangle$ is realized as the ground state, with broken translation symmetry, in the thermodynamic limit. In these states, the nearest-neighbor concurrence is either 0 or 1 depending on whether the considered pair resides on the same or different singlets. The average nearest-neighbor concurrence in both these states is $C(|R(L)\rangle)_{av} = 1/2$. For finite chains, however, in the absence of an additional symmetry-breaking field, it is more natural to revert to an orthogonal ‘‘qubit’’ basis of the ground-state manifold, which can be chosen to be the eigenstates of the momentum operator

$$|\pm\rangle = \frac{1}{\sqrt{\Omega_\pm}} (|R\rangle \pm |L\rangle), \quad (11)$$

where the normalizing factors are

$$\Omega_\pm = 2(1 \pm x), \quad x \equiv \langle R|L\rangle = (-1)^{N/2} 2^{1-N/2}, \quad (12)$$

and x is the overlap of the two dimer states. On traversing the MG point from left to right, the ground state changes from $|+\rangle$ ($|-\rangle$) to $|-\rangle$ ($|+\rangle$) for a translationally invariant system with even (odd) $N/2$ (this is related to Marshall’s sign law [23]). It is thus interesting to characterize the entanglement in the momentum basis $|\pm\rangle$.

First, consider the entanglement of two nearest-neighbor spins, say 1 and 2 (the same end result holds for all nearest-neighbor spins in these states, due to translational invariance). The parameter p could be determined by calculating the corresponding correlation functions. Equivalently, we calculate the form of the state $\rho_{(1,2)}$ of these two spins explicitly. Notice that the two spins are bound into a singlet in the state $|R\rangle$, while they belong to different singlets in the state $|L\rangle$, thus yielding a maximally mixed reduced state. Hence,

$$\begin{aligned} \rho_{(1,2)}^{(\pm)} &= \text{Tr}' |\pm\rangle\langle\pm| \\ &= \frac{1}{\Omega_\pm} \text{Tr}' (|R\rangle\langle R| \pm |R\rangle\langle L| \pm |L\rangle\langle R| + |L\rangle\langle L|) \\ &= \frac{1}{\Omega_\pm} [(1 \pm 2x) |\Psi^-\rangle\langle\Psi^-| + \mathbb{1}/4]. \end{aligned} \quad (13)$$

The entanglement between two neighboring spins in the

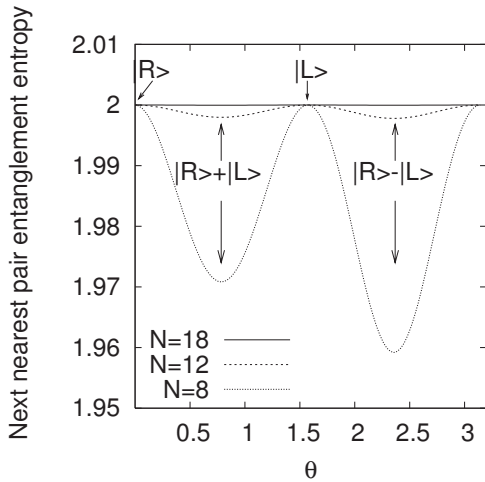


FIG. 6. Entropy of a pair of nnn spins in the ground-state manifold at the MG point.

symmetric and antisymmetric states is determined by the parameters

$$p_{\pm} = \frac{1 \pm 2x}{2(1 \pm x)}. \quad (14)$$

For $N > 6$, both states are entangled ($p_{\pm} > 1/3$), and so the difference in the concurrence between them can be calculated from Eq. (9),

$$\Delta C = C(\rho_{12}^{(+)}) - C(\rho_{12}^{(-)}) = \frac{3}{2}(p_{+} - p_{-}) = \frac{3x}{2(1-x^2)}. \quad (15)$$

The absolute value of this expression gives the “jump” in the nearest-neighbor concurrence on traversing the MG point from left to right (the sign of this difference depends on N , which is consistent with the ground states in the vicinity of the MG point). This quantity has been proposed to be an indicator of the MG point in the concurrence diagram in Ref. [19]. However, for large N , ΔC approaches zero exponentially. Additionally, two spins that are not nearest neighbors are not entangled with each other, since the correlation function drops rapidly with distance. Thus a more general measure considered in Ref. [19], viz., the total concurrence being the sum of concurrences of all pairs contains only one non-zero contribution coming from nearest neighbors and hence cannot detect the MG point.

The question thus arises concerning other indicators of this special point. For the infinite system, a simple candidate could be the dimer order parameter given by the difference

$$d = \frac{1}{N} \left| \left(\sum_i \langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle - \langle \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2} \rangle \right) \right|. \quad (16)$$

At the MG point, d takes the value $3/8$. Considering the notion of dimerization, one could naively assume that this is the largest possible value as it corresponds to exact dimers. However, the states $|R\rangle$, $|L\rangle$ are not eigenstates of the dimer operator and as such d cannot take on extremal values for these states. Physically, one could expect that high but not perfect antiferromagnetic correlations on one bond supple-

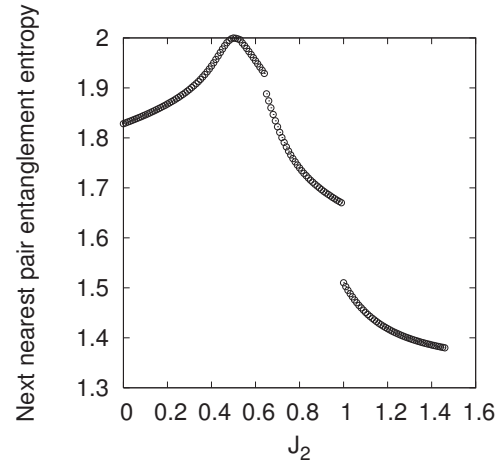


FIG. 7. The nnn pair entanglement entropy for $N=16$ spins. The two jumps, which are finite-size effects, connected to energy-level crossings for this system. These discontinuities vanish as the system size grows.

mented by slightly ferromagnetic correlations on the other could create a larger value of the dimerization. Using DMRG techniques, it has been shown that indeed the maximum dimerization does not occur at the MG point but at $J_2 \approx 0.5781$ [5]. Additionally, this quantity depends largely on the working basis: for translationally invariant states like $|\pm\rangle$, the value of this parameter is always zero. Thus, the dimer order parameter also does not distinguish the MG point satisfactorily.

The entanglement entropy of a pair of next-nearest-neighbor spins is a much more appropriate quantity that distinguishes the MG point. Due to degeneracy at the MG point, the general form of the ground state is

$$|\Psi_g\rangle = \frac{1}{\sqrt{1+x \sin \theta}} \left(\cos \frac{\theta}{2} |R\rangle + \sin \frac{\theta}{2} |L\rangle \right). \quad (17)$$

The parameter $p_{i,i+2}$ for a pair of nnn spins in the above state is given by

$$p_{i,i+2} = - \frac{x \sin \theta}{1 + x \sin \theta}. \quad (18)$$

For finite systems, the dimer states $|R\rangle$, $|L\rangle$ obviously maximize the entropy of entanglement, which is equal to 2. Moreover, as the size of the system increases, the dependence of the entropy on θ flattens out to the maximal possible value exponentially fast, since $x \rightarrow 0$ (see Fig. 6). This further justifies the choice of this quantity as a universal indicator of the MG point. Interestingly, the momentum states $|\pm\rangle$ are distinguished as local minima in the ground-state entanglement diagram. In the wider range of values of J_2 , the pair entropy of the MG point is indeed uniquely distinguished (see Fig. 7, for the nnn entanglement entropy for 16 spins) as the sole maximum in the diagram.

IV. CONCLUDING REMARKS

We have focused on the entanglement properties in the Majumdar-Ghosh model. Based on data from numerical cal-

culations of finite chains (up to 28 spins), we have discussed the scaling of the entanglement entropy of blocks of consecutive spins and argued that it can be used as a tool to identify the quantum critical point of this model. In contrast with other numerically studied models, the critical behavior of the system does not manifest itself directly in the dependence of “local” entanglement on the control parameter, for the considered system sizes. However, the transition from the critical gapless phase to the noncritical gapped phase appears clearly in the characteristic change in scaling of the local entanglement measures with respect to total system sizes. Furthermore, we have shown that the Majumdar-Ghosh point of this model can be identified as a maximum in the dependence of next-nearest neighbor pair entanglement entropy on the control parameter.

In the end, we would like to add that one can heuristically consider the entanglement entropy of the lower rail of spins with the upper rail of the considered system (Fig. 1) as a

natural candidate for distinguishing the phases of this model. Indeed, the dimer phase is expected to be characterized by enhanced correlations between the lower and upper rails of spins. Once again however, for the system sizes considered there is no “characteristic change” in the dependence of this quantity on the control parameter. The results have not been provided in this paper, since they resemble the results presented in Fig. 7. At the MG point, again the “momentum” eigenstates reside in local minima, as in Fig. 6.

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