Entanglement in the Majumdar-Ghosh model

Ravindra W. Chhajlany, Piotr Tomczak, Antoni Wójcik, and Johannes Richter

1 Physics Department, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland
2 Institut für Theoretische Physik, Universität Magdeburg, P.O. Box 4120, D-39016 Magdeburg, Germany
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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 behaviour of the entanglement entropy characterizing the unfrustrated Heisenberg chain as soon as $J_2 > 0.25$. This feature can be used as an indicator of the dimer phase transition that occurs at $J_2 = J_2^* \approx 0.2411 J_1$. Additionally, we also consider entanglement at the MG point $J_2 = 0.5 J_1$.

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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 [2, 3] and references therein). Frustrated quantum systems, have however been largely left out of the picture in such discussions so far.

In this Article, we consider the entanglement in a prototypical 1-D frustrated spin system – the Majumdar Ghosh or $J_1$-$J_2$ Heisenberg chain [4]. The spin-1/2 Hamiltonian is described by

$$ H = J_1 \sum_{\langle n.n. \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle n.n.n. \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, $$

where the sums run over nearest neighbour (n.n.) and next nearest neighbour (n.n.n.) 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. The ground state properties of this system have been studied so far with the use of many methods like exact diagonalization, DMRG, field theoretical approach (see [4] and [5] for an overview). It is known that the model is critical (i.e., the spin-spin correlation function decays algebraically) and gapless for $J_2 \leq J_2^* \approx 0.2411$ [4, 5, 6]. 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 neighbour dimer states given by

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

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. 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 case of models which can be solved exactly [2]), but in finite systems for fixed $n$ also with respect to the total size $N$ of the system. In the gapped phase, a clear deviation from this scaling emerges which can be used to identify the critical point of this system. This is to be contrasted with the fact that the entanglement measured by standard measures such as entanglement entropy or pair-wise concurrence do not detect the critical point of this model, on their own.

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 neighbour 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 neighbour 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 byproduct, in the small size limit, the two translationally invariant (or 'quasi-momentum') 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 conveniently measured by the entanglement entropy. The entanglement entropy is defined as the von Neumann entropy of the chosen subsystem, i.e. if the (reduced) density matrix of the subsystem is $\rho_n$ and $\lambda_j$ 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 entanglement entropy of a block of contiguous spins has been shown to scale differently with the block size $n$, in critical and non-critical 1D systems [2]. In the thermodynamic limit (total system size $N \to \infty$), the entanglement entropy of a non-critical system tends...
to saturate, while it displays universal scaling behaviour for critical systems \[9\]:

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

(4)

where \(c\) is a universal scaling constant and \(c_0\) is model dependent. These two constants take the values 1 and \(\pi\) for the isotropic Heisenberg antiferromagnetic chain. The extension of Eq. (4) to finite critical systems was given in \[10\]:

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

(5)

For small values of \(n/N\), this equation becomes

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

(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.

A. Case 1: Fixed \(N = 28\)

First, let us focus on the scaling of the entanglement entropy w.r.t. 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) or (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. \(n\).

In order to quantitatively characterize the deviation of the entanglement from the scaling relation (5) at finite frustrating \(J_2 > 0\), the value of \(\chi^2\) defined in the standard way, i.e., as a square root of the sum of squares of residuals, is calculated and plotted in Fig. 3. This quantity 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 for \(J_2 \gtrsim J_2^* \approx 0.2411\). The flat minimum for \(J_2 \approx 0.10\) is a result of the competition between a finite size correction and the correction resulting from the presence of interaction \(J_2\).

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
Entanglement entropy $S(n,28)$

For larger subsystem sizes the finite size correction dominates.

control parameter $J_2$, as in certain other models. Indeed, as shown by Osterloh et al., the phase transitions in XY spin-$1/2$ models can be identified explicitly by the dependence of the entanglement between two nearest neighbour 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 [12, 13, 14]).

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 Section III). We have checked that entanglement entropies of variously chosen subsystems, such as block entanglement of consecutive spins, or blocks of next nearest neighbour 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 behaviour [18].

The finite size problem can be circumvented by the usual finite-size scaling techniques. Consider e.g. the entanglement entropy of two nearest neighbour 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 behaviour in Eq. (6). The scaling of blocks of 4, 6 spins are also presented in Fig. [19].

Let us focus on the dependence of the scaling of $n = 2$ entanglement entropy on the control
FIG. 3: The least-square deviation $\sqrt{\chi^2}$ of the calculated values of the entanglement form the line described by Eq. 5 (dashed line in Fig. 2) in dependence on the frustration $J_2$. The system contains 28 spins and $\chi^2$ was calculated for $n \leq 6$. Note that $\sqrt{\chi^2}$ starts to increase as beyond the quantum critical point $J_2^* \approx 0.2411$.

parameter $J_2$. The correction to the $N^{-2}$ scaling can again be characterized by the value of $\chi^2$, describing the difference between the calculated entropies for $J_2 > 0$ and the straight line for $J_2 = 0$, see Fig. 3. Significantly, there is a clear deviation from critical scaling for $J_2 > J_2^*$. The phase transition may thus be detected and 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 point, the general question posed in this section remains open for future discussion.

III. THE 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 [4]) 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 1-dimensional 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.
Entanglement entropy $S(n,N) / S(n,\infty)$

**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.

This follows from the following simple identity for the reduced state of $n$ arbitrary spins:

$$\rho_n = \text{Tr}' \rho_g = \text{Tr}' U^\otimes N \rho_g (U^\dagger)^\otimes N = U^\otimes n (\text{Tr}' U^\otimes N - n \rho_g (U^\dagger)^\otimes N - n) (U^\dagger)^\otimes n = U^\otimes n \rho_n (U^\dagger)^\otimes n,$$

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 $\text{Tr}'$ 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 $\rho_1 = 1/2$ 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 $\rho_2$, that can be represented as

$$\rho_2 = p|\Psi^-\rangle \langle \Psi^-| + \frac{1-p}{4} 1,$$

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 $C(\rho_2)$, can be checked to be given by a simple formula for Werner states

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

Thus, two spins are entangled with each other as long as the correlations between them are sufficiently antiferromagnetic, $\langle S_i \cdot S_j \rangle < -1/4$. The entanglement entropy (see Eq.
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 bigger values $J_2$.

The deviation ($\chi^2$) of two spins in a Werner state, on the other hand, is given by the relation

\[ S(\rho_2) = 2 - \frac{1+3p}{4} \log(1+3p) - \frac{1-p}{4} \log(1-p). \]  

(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 neighbour concurrence is either 0 or 1 depending on whether the considered pair resides on the same or different singlets. The average nearest neighbour 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

\[ |\pm\rangle = \frac{1}{\sqrt{\Omega_{\pm}}}(|R\rangle \pm |L\rangle), \]

(11)

where the normalizing factors are

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

(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 [17]). It is thus interesting to characterize the entanglement in the momentum basis $|\pm\rangle$. 

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First, consider the entanglement of two nearest neighbour spins, say 1 and 2 (the same end result holds for all nearest neighbour 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

$$\rho_{(1,2)}^{(\pm)} = \text{Tr}^r|\pm\rangle\langle \pm| = \frac{1}{\Omega_{\pm}}\text{Tr}^r(|R\rangle\langle R| \pm |R\rangle\langle L| \pm |L\rangle\langle R| + |L\rangle\langle L|) =$$

$$= \frac{1}{\Omega_{\pm}}((1 \pm 2x)|\Psi^-\rangle\langle \Psi^-| + \mathbb{I}/4). \quad (13)$$

The entanglement between two neighbouring spins in the 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. (13)

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

The absolute value of this expression gives the “jump” in the nearest neighbour 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. 4. However, for large $N$, $\Delta C$ approaches zero exponentially. Additionally, two spins that are not nearest neighbours are not entangled with each other, since the correlation function drops rapidly with distance. Thus a more general measure considered in Ref. 4, viz. the total concurrence being the sum of concurrences of all pairs contains only one non-zero contribution coming from nearest neighbours 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

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

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 supplemented 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 $J_2 \approx 0.5781$ [6]. 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 neighbour 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 n.n.n 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 $\theta$ flattens out to the maximal possible value exponentially fast, since $x \to 0$ (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 n.n.n. entanglement entropy for 16 spins) as the sole maximum in the diagram.

**IV. CONCLUDING REMARKS**

We have focussed on the entanglement properties in the Majumdar-Ghosh model. Based on data from numerical calculations of finite chains (up to 28 spins), we have discussed the
scaling of the entanglement entropy of blocks of consecutive spins and shown 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 behaviour 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 non-critical gapped phase appears in the characteristic change in scaling of the local entanglement measures w.r.t. 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 neighbour pair entanglement 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 Article, 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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[1] M.A. Nielsen and I.L. Chuang, *Quantum Computation Quantum Information*, Cambridge University Press, Cambridge, 2000.
[2] G. Vidal, J.I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[3] T. Roscilde, P. Verrucchi, A. Fubini, S. Haas, and V. Tognetti Phys. Rev. Lett. 94, 147208 (2005).
[4] X-F Qian, T. Shi, Y. Li, Z. Song and C-P. Sun, Phys. Rev. A 72, 012333 (2005).
[5] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. 10, 1388 (1969); C. K. Majumdar and D. K. Ghosh, J. Math. Phys. 10, 1399 (1969).
[6] S. R. White and I. Affleck, Phys. Rev. B 54, 9862 (1996).
[7] H.-J. Mikeska, A.K. Kolezhuk, in *Quantum Magnetism*, Lecture Notes in Physics 645, U. Schollwöck, J. Richter, D.J.J. Farnell, R.F. Bishop, Eds. (Springer-Verlag, Berlin, 2004), p. 1 - 83.
[8] K. Okamoto, and K. Nomura, Phys. Lett. A 169, 433 (1992).
[9] C. Holzhey, F. Larsen, and F. Wilczek, Nucl. Phys. B424, 443 (1994).
[10] P. Calabrese and J. Cardy, J. Stat. Mech., P06002 (2004).
[11] A. Osterloh, L. Amico, G. Falci and R. Fazio, Nature 416, 608 (2002).
[12] L. Campos Venuti, C. Degli Esposti Boschi, M. Roncaglia and A. Scaramucci, Phys. Rev. A 73, 010303(R) (2006).
[13] T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 032110 (2002).
[14] S-Q Su, J-L Song, S-J Gu and H-Q Lin, Los Alamos archive preprint quant-ph/0606133 (2006).
[15] R. F. Werner, Phys. Rev. A 40, 4277 (1989).
[16] W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
[17] W. Marshall, Proc. Roy. Soc. A 232, 48 (1955).
[18] The systems sizes studied in Ref. 4 range from $N = 6$ to 12, while we have densely checked for up to $N = 18$.
[19] For these and larger blocks, effects of terms of the order $O(n/N)^4$ become important.
[20] Interestingly, $\langle S_i \cdot S_j \rangle = -1/4$ is the classically optimal antiferromagnetic correlation corresponding to the Néel state. So, enhanced antiferromagnetic correlations are a manifestation of quantum entanglement.