Disordered phase of a two-dimensional Heisenberg Model with $S = 1$

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We study an anisotropic version of the $J_1 - J_2$ model with $S = 1$. We find a second order transition from a Néel $Q = (\pi, \pi)$ phase to a disordered phase with a spin gap.

I. INTRODUCTION

The Heisenberg model can be mapped to the non-linear sigma model (NL$\sigma$) with an additional term due to Berry phases. In 1D this term has a dramatic effect which was first discovered by Haldane. Integer spin systems have a gap in their excitation spectrum, while half-integer spin systems are gapless but disordered, with an algebraic decay of spin-spin correlations. In the late 1980s it was found that Berry phases do not seem to play a role in 2D for purely Heisenberg Hamiltonians\cite{1,2,3,4}. Hence, all Heisenberg models on the 2D square lattice are on the ordered side of the NL$\sigma$ model. This is in agreement with a theorem by Dyson, Lieb, and Simon (DLS)\cite{5}, extended to 2D systems by Neves and Pereira\cite{6}, which states that for bipartite lattices with $S \geq 1$, the ground state is ordered. Furthermore, Monte Carlo simulations\cite{7} have convincingly shown that the $S = \frac{1}{2}$ model has Néel order.

Affleck extended to 2D systems a 1D theorem due to Lieb, Schulz, and Mattis (LSM)\cite{8} which applies to half-integer spin systems. He argued that since this theorem does not apply to integer spin systems, there could be a difference between the disordered phases of half-integer and integer spin systems in 2D as well. Haldane\cite{9} argued that if by some mechanism it was possible to drive the Heisenberg model into the disordered phase, singular topological contributions known as hedgehogs may be relevant. Read and Sachdev\cite{10} carried out a systematic study of the 2D Heisenberg model in the large-$N$ limit. Their results were in agreement with Affleck and Haldane’s predictions. They predicted that the nature of the disordered phases in 2D is related to the ‘spin’ value. For odd integer ‘spins’, the ground state breaks the symmetry of rotation of the lattice by 180 degrees, for even integer ‘spins’ the ground state does not break any lattice symmetry, and for half-integer ‘spins’, the lattice symmetry is broken by 90 degrees.

The usual criticism against such predictions is that they are obtained in the limit of large spin and they could be invalid for the more relevant cases of small $S$. It is well possible that a different mechanism can emerge for small $S$. The $J_1 - J_2$ model is the most popular model in which a possible disordered phase has been searched. For $S = \frac{1}{2}$, it is generally accepted that for $0.38 < \frac{J_2}{J_1} < 0.6$, this model has a disordered phase. Among the many disordered phases that were proposed\cite{11,12}, the columnar dimer phase which was predicted in Ref.\cite{13} seems to gain broader acceptance lately. But, we have recently argued\cite{14} that this conclusion, which seems to be supported by numerical experiments using exact diagonalization (ED) or series expansions\cite{15}, may be incorrect. Large scale renormalization group studies on an anisotropic version of the $J_1 - J_2$ model show that in the region where the disordered phase is expected, physical quantities of the 2D model are nearly identical to those of an isolated chain. This suggests that there is instead a direct transition at $\frac{J_2}{J_1} = 0.5$ between the Néel $Q = (\pi, \pi)$ and $Q = (\pi, 0)$ phases. At the transition point, the system is disordered with algebraic decay of the correlations along the chains and exponential decay in the other direction. This state is consistent with the LSM theorem.

While the case $S = \frac{1}{2}$ has generated numerous studies\cite{16,17,18,19}, other values of $S$ have not been studied to the author’s knowledge. Thus, the role of topological effects in the $J_1 - J_2$ model for small $S$ remains unknown. In this letter, we propose to study the case $S = 1$. We will apply the two-step density-matrix renormalization group\cite{20,21} (TSDMRG) to study the spatially anisotropic Heisenberg Hamiltonian in 2D,

$$H = J_\parallel \sum_{i,l} S_{i,l}S_{i+1,l} + J_\perp \sum_{i,l} S_{i,l}S_{i,l+1} + J_d \sum_{i,l} (S_{i,l}S_{i+1,l+1} + S_{i+1,l}S_{i,l+1})$$

where $J_\parallel$ is the in-chain exchange parameter and is set to 1; $J_\perp$ and $J_d$ are respectively the transverse and diagonal interchain exchanges. Although the Hamiltonian\cite{22} is anisotropic, it retains the basic physics of $J_1 - J_2$ model. In the absence of $J_d$, the ground state is a Néel ordered state with $Q = (\pi, \pi)$. When $J_d \gg J_\perp$, another Néel state with $Q = (\pi, 0)$ becomes the ground state.

A disordered ground state is expected in the vicinity of $J_d = \frac{J_\perp}{2}$. In this study, we will only be concerned with the transition from $Q = (\pi, \pi)$ Néel phase to the disordered phase. The lattice size is fixed to $32 \times 33$; the transverse coupling is set to $J_\perp = 0.2$ and $J_d$ is varied from $J_d = 0$ up to the maximally frustrated point $J_d = 0.102$, i.e., the point where the ground state energy is maximal (see Ref.\cite{23}). We use periodic boundary conditions (PBC) in the direction of the chains and open boundary conditions (OBC) in the transverse direction. This short paper will be followed by a more extensive work\cite{14}, where a finite size analysis is performed.
II. METHOD

We used the TSDMRG\textsuperscript{15,16} to study the Hamiltonian (1). The TSDMRG is an extension two 2D anisotropic lattices of the DMRG method of White\textsuperscript{18}. In the first step of the method, ED or the usual DMRG method are applied to generate a low energy Hamiltonian of an isolated chain of length $L$ keeping $m_1$ states. Thus the superblock size is $9 \times m_1^2$ for an $S = 1$ system. Then $m_2$ low-lying states of these superblock states, the corresponding energies, and all the local spin operators are kept. These describe the renormalized low energy Hamiltonian of a single chain. They form the starting point of the second step in which $J_\perp$ and $J_d$ are switched on. The coupled chains are studied again by the DMRG method. Like the original DMRG method, the TSDMRG is variational. Its convergence depends on $m_1$ and $m_2$, the error is given by $\max(\rho_1, \rho_2)$, where $\rho_1$ and $\rho_2$ are the truncation errors in the first and second steps respectively.

Since the TSDMRG starts with an isolated chain, a possible criticism of the method is that it could not effectively couple the chains. This means that it would eventually miss an ordered magnetic phase. The source of this criticism is the observation that the DMRG was introduced to cure the incorrect treatment of the interblock coupling in the old RG. But this criticism misses the fact that, in the old RG treatment, dividing the lattice into blocks and treating the interblock as a perturbation was doomed to failure because both the intra and inter-block couplings are equal. In the coupled chain problem, however, when the interchain coupling is small, it is imperative as Wilson\textsuperscript{19} put it long ago to separate the different energy scales.

III. RESULTS

The low energy Hamiltonian for an isolated chain is relatively easy to obtain, we keep $m_1 = 162$ states and $L = 32$. For this size the finite size gap is $\Delta = 0.4117$ which is very close to its value in the thermodynamic limit $\Delta_H = 0.4105$. This is because we used PBC and the correlation length is about six lattice spacings. The truncation error during this first step was $\rho_1 = 5 \times 10^{-5}$. We then kept $m_2 = 64$ lowest states of the chain to start the second step. During the second step, the ground state with one of the first excited triplet states with $S_z = 1$ were targeted. The truncation error during this second step varies from $\rho_2 = 1. \times 10^{-3}$ in the magnetic phase to $\rho_2 = 1. \times 10^{-7}$ in the disordered phase. This behavior of $\rho_2$ is consistent with previous tests in $S = 1$ systems in Ref.\textsuperscript{20} where we find that the accuracy of the TSDMRG increases in the highly frustrated regime.

We have shown in Ref.\textsuperscript{20} for $S = 1$ that: (i) the TSDMRG shows a good agreement with QMC for lattices of up to $32 \times 33$, even if a modest number of states are kept; (ii) spin-spin correlations extrapolate to a finite value in the thermodynamic limit. However, because of the strong quantum fluctuations present for $S = 1$, the extrapolated quantities were small and thus could be doubted. Furthermore, our prediction of a gapless disordered state between the two magnetic phases has been regarded with a certain skepticism\textsuperscript{21,22,23} because it would be expected that such a state would be unstable against some relevant perturbation at low energies not reached in our simulation. This is not the case for $S = 1$, where quantum fluctuations are weaker. We thus expect larger extrapolated values $C_{x=\infty}$ and $C_{y=\infty}$. The results in Fig.\textsuperscript{11} for the correlation function along the chains,

$$C_x = \frac{1}{3} \langle S_{L/2,L/2+1} S_{L/2+x,L/2+1} \rangle,$$

FIG. 1: Longitudinal spin-spin correlations (full line) and their extrapolation (dotted line) for $J_d = 0$ (top), 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.075, 0.08, 0.085, 0.09, 0.101 (bottom) as function of distance.

FIG. 2: Transverse spin-spin correlations (full line) and their extrapolation (dotted line) for $J_d = 0$ (top), 0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.075, 0.08, 0.085, 0.09, 0.101 (bottom) as function of distance.
and in Fig. (2) for the correlation function in the transverse direction,

\[ C_y = \frac{1}{3} \langle S_{L/2,L/2+1} S_{L/2,L/2+y} \rangle, \quad (3) \]

unambiguously show that in the weakly frustrated regime, the system is ordered. Despite the strong anisotropy, \( C_{x=\infty} \) and \( C_{y=\infty} \) are not very different. The anisotropy is larger for small \( x \) and \( y \). But, due to the difference in the boundary conditions, \( C_x \) seems to reach a plateau while \( C_y \) bends downward. This behavior of \( C_y \) is indeed related to the fact that the spins at the edge do not feel the bulk mean-field created by other chains.

As \( J_d \) increases, \( C_{x=\infty} \) and \( C_{y=\infty} \) decreases and vanish at \( J_d \approx 0.085 \) and \( J_d \approx 0.075 \) respectively. The difference in the value of \( J_d \) in the two directions is probably due to the difference in the boundary conditions.

In Fig. (3) and Fig. (4) we plot the corresponding order parameters \( m_x = \sqrt{C_{x=\infty}} \) and \( m_y = \sqrt{C_{y=\infty}} \). The two curves display the typical form of a second order phase transition. However, we have not extracted any exponent because even though we believe our results will remain true in the thermodynamic limit, finite size effects may nevertheless be important close to the transition. A systematic analysis of this region is left for a future study.

The phase transition is also seen in the spin gap shown in Fig. (5). In the ordered state, the system is gapless. The finite size spin gap is nearly independent of \( J_d \) and is in the order of the truncation error \( \rho_2 \). At the transition which occurs at \( J_d \approx 0.075 \), \( \Delta \) sharply increases and becomes close to the Haldane gap at the maximally frustrated point where we find \( \Delta = 0.3854 \) for \( J_d = 0.102 \).

Néel ordered phase is destroyed and the system enters into a disordered phase with a spin gap. The value of the gap at the maximally frustrated point is close to that of the Haldane gap of an isolated chain. This disordered phase is consistent with the large \( N \) prediction of Ref. (11). This study shows the striking difference between integer and half-integer spin systems. For \( S = \frac{1}{2} \), the TSDMRG predicted a direct transition between the two Néel phases with a disordered gapless state at the critical point. Thus, as we have recently found (17), despite the fact that the mechanism of the destruction of the Néel phase is independent of the value of the spins, at the transition point, topological effects become important leading to the distinction between integer and half-integer spins.

IV. CONCLUSION

In this letter, we have studied an anisotropic version of the \( J_1 - J_2 \) model with \( S = 1 \) using the TSDMRG. We find that for a critical value of the frustration, the

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