Plaquette ground state of the Shastry-Sutherland model: Density-matrix renormalization-group calculations

S. Moukouri*

Department of Physics and Michigan Center for Theoretical Physics, University of Michigan, 2477 Randall Laboratory, Ann Arbor, Michigan 48109, USA

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I use the two-step density-matrix renormalization-group (DMRG) method based on two-leg ladder expansion to show numerical evidence of a plaquette ground state for $J_2=1.3J_1$ in the Shastry-Sutherland model. I argue that the DMRG method is very efficient in the strong frustration regime of two-dimensional spin models where a spin-Peierls ground state is expected to occur. It is thus complementary to quantum Monte Carlo algorithms, which are known to work well in the small frustration regime but which are plagued by the sign problem in the strong frustration regime.

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A number of studies have been devoted to the Shastry-Sutherland model (SSM).[1–12] This interest is motivated by the relevance of the SSM to the physics of the two-dimensional (2D) spin gap system $SrCu_2(BO_3)_2$.[13] The SSM is a frustrated antiferromagnetic model on a square lattice whose Hamiltonian is written as

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{[i,j]} \mathbf{S}_i \mathbf{S}_j, \tag{1}$$

where $\langle i,j \rangle$ represents nearest-neighbor sites and $[i,j]$ stands for the next-nearest neighbors on every other plaquette in the pattern shown in Fig. 1. There is a general agreement that in the weak frustration regime $J_1 \gg J_2$, the SSM is Néel ordered while in the strong frustration regime $J_1 \ll J_2$, the model is a valence bond solid. In fact, Shastry and Sutherland showed that for $J_2 > 2J_1$ the wave function made of the product of local orthogonal dimers is an exact ground state. Numerical simulations based on series expansions and exact diagonalization have pushed the dimer phase boundary down to $J_2 \approx 1.5J_1$. The estimated boundary of the Néel phase is $J_2 \approx 1.2J_1$.

However, the nature of the ground state for $1.2J_1 \lesssim J_2 \lesssim 1.5J_1$ so far has remained controversial. A mean-field Schwinger boson approach found that the intermediate phase is helical.[2] Perturbation theory[3] and series expansion[4] studies predicted a direct first-order transition between the Néel and the dimer phases. A large N study[7] also predicted a helical phase. In addition it suggested that a broader phase diagram contains a plaquette phase which might occur if fluctuations were included. A subsequent series-expansion analysis[6] predicted a plaquette phase with a spin gap. This conclusion was criticized in another series-expansion study which suggested a possible gapless phase whose nature was unclear.[8] The existence of the intermediate phase was also suggested in a renormalization-group analysis.[9] An exact diagonalization study on a $N=32$ site system has concluded to a plaquette phase. The Monte Carlo method, which is very effective for spin systems in absence of frustration,[14] is plagued by the sign problem in this regime of strong frustration. Knowledge of the exact ground-state phases is essential; this could serve as a starting point in variational investigations of the nature of superconductivity that might arise upon doping.[12]

In this Brief Report I present numerical evidence of the plaquette phase at $J_2=1.3J_1$. For this purpose, I will use the two-step density-matrix renormalization-group (DMRG) method.[15,16] The DMRG (Ref. 17) has provided a breakthrough in the study of quantum Hamiltonians in one dimension. Extensions of the DMRG to two-dimensional Hamiltonians have been less effective. Liang and Pang[18] found that as the linear dimensions of the system grow, the number of the reduced density-matrix states needed to maintain accuracy grows exponentially. This problem is particularly severe for quantum antiferromagnets in their ordered phase. The spontaneous symmetry breaking which takes place in the thermodynamic limit is due to the collapse of an infinite number of excited states onto the ground state. The implication for finite systems, in the parameter regime where long-range order occurs, is a near degeneracy of a large number of low-lying states with the ground state. Each state within this large set would carry the same weight in the reduced density

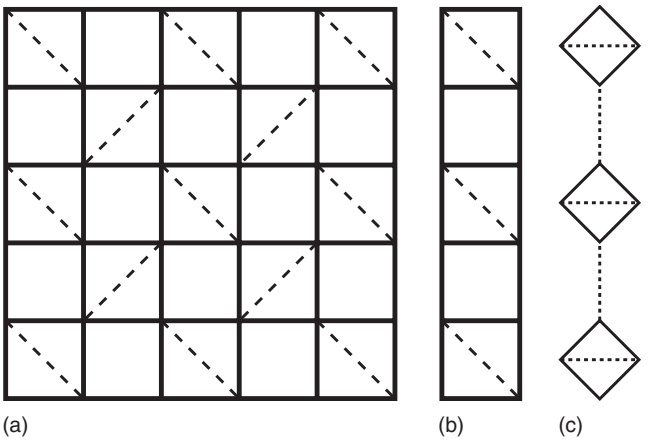

FIG. 1. (a) Bond patterns in the Shastry-Sutherland lattice. The J_1 bonds are between the nearest neighbors. The J_2 bonds are along every other diagonal. (b) The two-leg ladder: starting point of the two-step DMRG approach to the two-dimensional lattice. (c) Orthogonal dimers: starting point more adapted to the dimerized phase. It is obtained by covering the two-dimensional lattice along the diagonals.

matrix. For this reason, standard DMRG simulations of spin Hamiltonians are limited to systems of about ten sites wide.

Recent developments by the author[15,16,19] have shown that the DMRG could be very useful for 2D models in the region of the parameter space where this technical difficulty is less severe or even absent. This occurs, for instance, for spatially anisotropic antiferromagnets or in the highly frustrated regime of isotropic magnets. In this latter case, general arguments from the large N approach[20] suggest that the ground state is a collection of weakly coupled dimers or plaquettes. Presumably deep in the disordered phase because of the presence of a spin gap, the ground state would be dominant in the reduced density matrix. This is more favorable to a DMRG simulation. It is usually in this regime that the sign problem is most severe in quantum Monte Carlo (QMC) simulations. Hence the DMRG would be complementary to QMC for frustrated models with disordered phases with broken translational symmetry. The excited states would become more and more important as the coupling is moved toward the boundary with the magnetically ordered phase. An approach based on these ideas recently has been applied to find the ground-state phase diagram of the checkerboard model.[19] The same approach is applied here to the SSM.

I start with a single two-leg ladder with L rungs as shown in Fig. 1. By doing so, I implicitly assume that the interladder interactions are small. Strictly, this is true only in the magnetically disordered phase and will be justified *a posteriori*. However, such a starting point could also be justified qualitatively even for the magnetically ordered phase where interladder interactions are not small. In the valence bond representation of quantum antifferomagnets, the wave function is written as

$$\Psi = \sum_{\alpha} c_{\alpha} \prod_{(ij)\in\{\alpha\}} |(\mathbf{ij})\rangle, \tag{2}$$

where $|(\mathbf{ij})\rangle = (|\uparrow\downarrow\rangle_{ij} - |\downarrow\uparrow\rangle_{ij})/\sqrt{2}$ is a dimer wave function between the sites i and j and $\{\alpha\}$ is a configuration of dimers. Such valence bond representations are qualitatively good for both the disordered and ordered phases.[21] In the present approach, two-leg ladders are the building blocks. The wave function is written as

$$\tilde{\Psi} = \sum_{\text{ladders}} \tilde{c}_{\text{ladders}} \prod_{\text{ladders}} \Phi_{\text{ladder}}, \tag{3}$$

where Φ_{ladder} is an eigenfunction of a single ladder Hamiltonian. Given that the lowest Φ_{ladder} is dominated by a product of dimers, $\tilde{\Psi}$ bears some similarity with Ψ. However, the set of Φ_{ladder}'s includes excited states on the ladder; the structure of $\tilde{\Psi}$ is thus much more complex than a simple short-range dimer expansion. When the ground state is made of weakly coupled plaquettes or dimers, it would be expected that this representation would yield quantitatively good results as well. But the essential point is that this approximation does not necessarily assume that the ground state is disordered. It will be shown below that a magnetically ordered state can be reached as well, though with less accuracy than in the disordered phase.

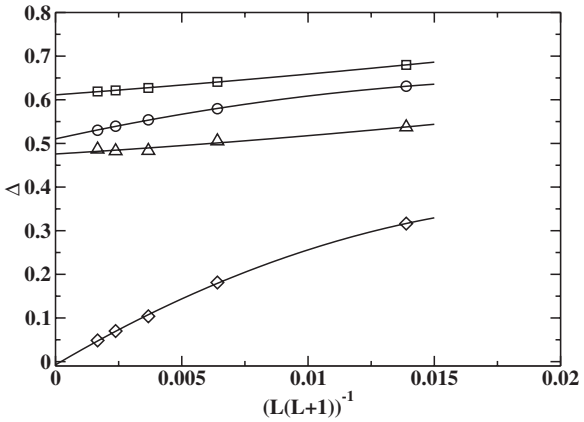

FIG. 2. Gaps as a function of L for a single ladder for $J_2=0$ (circles) and $J_2=1.3J_1$ (squares) and for two-dimensional systems for $J_2=0$ (diamonds) and $J_2=1.3J_1$ (triangles).

The results for an isolated two-leg ladder were obtained for $J_2=0$ and for $J_2=1.3J_1$. The conventional DMRG is known to yield highly accurate results for the ground state and the low-lying states.[22] A set of the low-lying Φ_{ladder} is obtained by targeting the spin sectors from $S=0$ to $S=\pm 4$ and by keeping up to $m=144$ states. This is enough to maintain the truncation error below 10^{-6} in all cases. There is a spin gap in the thermodynamic limit as in two cases seen in Fig. 2. The center-to-end correlation functions $C_L = \langle \mathbf{S}_{L/2+1,r} \mathbf{S}_{L,r} \rangle$, where $r=1,2$ is the leg index, shown in Fig. 3 decay exponentially in both cases. But the short-range correlations in Fig. 4 reveal that $J_2=0$ and $J_2=1.3J_1$ belong to two different phases of the ladder. When $J_2=0$, the dominant short-range correlations are the rung dimers $C_r(i) = \langle \mathbf{S}_{i,1} \mathbf{S}_{i,2} \rangle$. C_r is stronger than the correlations along a leg $C_{l_{n,d}}(i) = \langle \mathbf{S}_{i,r} \mathbf{S}_{i+1,r} \rangle_{n,d}$ for plaquettes with no diagonal bond (n) or with a diagonal bond (d); when $J_2=0$, $C_{l_n} = C_{l_d}$. Both $C_r(i)$ and $C_{l_{n,d}}(i)$ are independent of i, except for small variations at the boundary. For $J_2=1.3J_1$, $|C_{l_n}| > |C_{l_d}|$ and the bond pattern shows strong alternations as a function of i as seen in Fig. 4. At the same time, $C_r \approx C_{l_n}$ indicating that the system is now in the plaquette phase. The plaquette-plaquette inter-

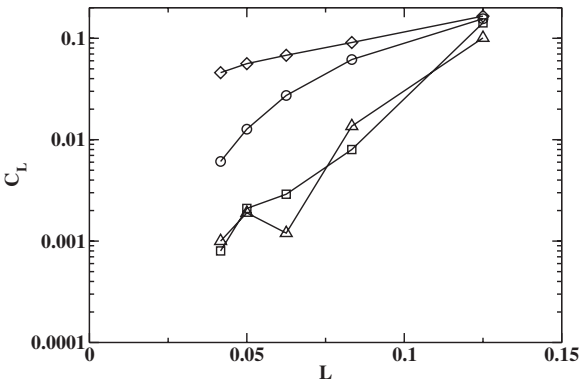

FIG. 3. Edge-to-center correlation as a function of L_y for a single ladder for $J_2=0$ (circles) and $J_2=1.3J_1$ (squares) and for two-dimensional systems for $J_2=0$ (diamonds) and $J_2=1.3J_1$ (triangles).

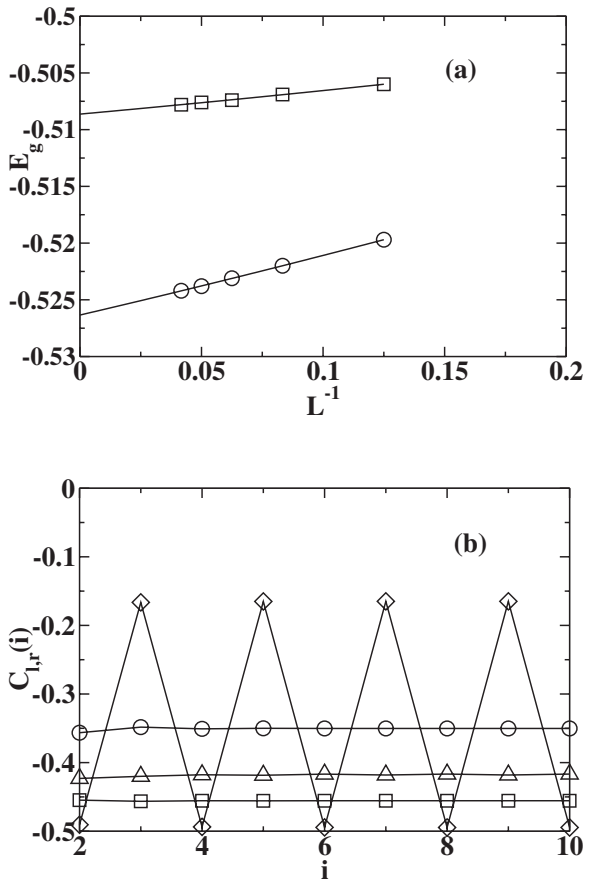

FIG. 4. (a) Ground state energy of two-leg ladders for the Shastry-Sutherland model at $J_2=1.3J_1$ (circles) and for the checkerboard model at $J_2=J_1$ (squares). (b) Short-range correlations for the Shastry-Sutherland two-leg ladder with $L_x=24$ for $J_2=0$, $C_{l_{n,d}}$ (circles), C_r (squares) and for $J_2=1.3J_1$, $C_{l_{n,d}}$ (diamonds), C_r (triangles).

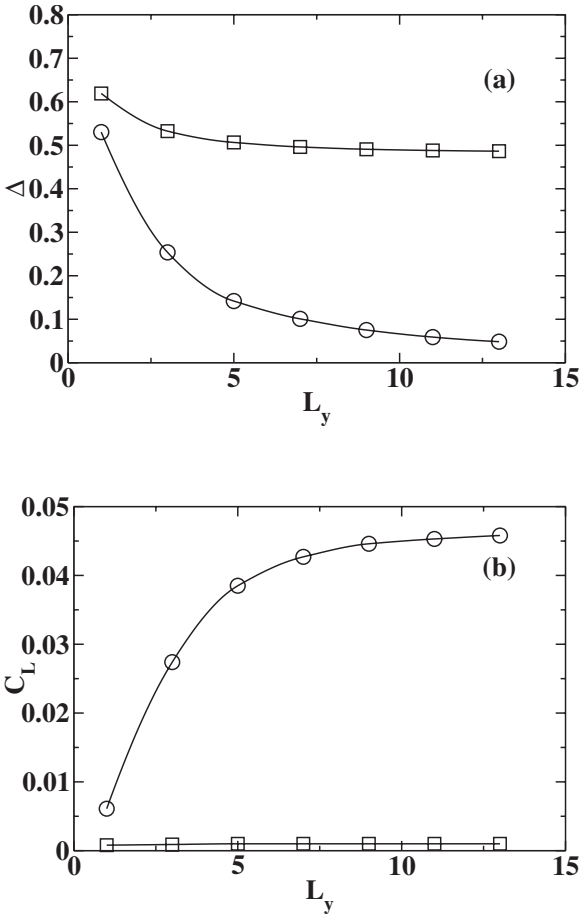

FIG. 5. Irrelevant (squares, $J_2=1.3J_1$) and relevant (circles, $J_2=0$) flows from the single ladder as a function of L_y (a) for the spin gap and (b) for the center-to-edge correlation function.

action is given by $|C_{l_d}|$. It is not negligible as in the checkerboard ladder.[19] It is about one-third of the intraplaquette interaction in the Shastry-Sutherland ladder, while it is only 5% of the intraplaquette in the checkerboard ladder at the isotropic point $J_2=J_1$. This is also seen in the ground-state energy E_g of the ladders shown in Fig. 4. In the checkerboard ladder, there is a relatively small renormalization of $E_g=-0.5086J_1$, which is not very far from $E_g=-0.5000J_1$ of an isolated plaquette. The renormalization is more important in the Shastry-Sutherland ladder where $E_g=-0.5263J_1$. Nevertheless, the value of C_{l_d} shows that even the SSM is in the weak-coupling regime of plaquette-plaquette interaction.

The second step of the two-step DMRG consists in projecting Hamiltonian (1) onto the basis states of the tensor product of Φ_{ladder}'s and solving the resulting effective Hamiltonian, which is one dimension (in the transverse direction) with the usual DMRG. Strictly speaking, this can only rigorously be justified if the interladder coupling is small. Apparently this is not the case for Hamiltonian (1) since neither J_1 nor J_2 is always small. But as seen above, effective small interactions can be generated by the inherent competition between J_1 and J_2. The coupling between ladders in the SSM is also given by $|C_{l_d}|$, as can be seen in Fig. 1. In Ref. 16, it has been shown that when the ratio, $\rho=\delta E/J_{\text{eff}}$ between the bandwidths of the states kept, and the effective transverse coupling, which is $J_{\text{eff}}\approx|C_{l_d}|J_1$, is large ($\rho\gtrsim 4$), the two-step DMRG yields results which are comparable to those of QMC. Typical values of ρ for the largest systems studied are 5 for $J_2=1.3J_1$ and 2 for $J_2=0$. This justifies the isolated ladder starting point for $J_2=1.3J_1$. I study lattices with $L_x\times L_y=L\times(L+1)=8\times 9$ to 24×25. Analysis of the performance of this approach has been discussed in previous publications.[15,19] When the interladder is turned on, the flows as the function of the number of ladders of Δ and C_L for $J_2=0$ and $J_2=1.3J_1$, shown in Fig. 5 for $L\times(L+1)=24\times 25$, are very different.

For $J_2=0$, as expected from the existence of long-range order, Δ decays rapidly as L_y increases. $\Delta=0$ in the thermodynamic limit as seen in Fig. 2. At the same time, C_L grows away from its small value found in the two-leg ladder. C_L becomes finite in the thermodynamic limit. The extrapolated order parameter $M=\sqrt{C_\infty}$ is found to be $M=0.1738$. This is somewhat lower than the QMC results,[23] $M=0.3070$. Part of this discrepancy is due to the use of open boundary conditions which yield an undervaluated C_L. Better extrapolations can be obtained if the lattice sizes are reduced and if periodic boundary condition is used. This relatively poor performance of the DMRG deep in the magnetically ordered phase is a

consequence of the fundamental limitations of the DMRG when faced with an exponentially dense low energy spectrum, as discussed previously. Nevertheless, this result shows that the approximation by $\tilde{\Psi}$ of the exact wave function retains the correct qualitative behavior. Hence the DMRG could still be very useful in the magnetic regime as well.

However, when $J_2=1.3J_1$, the interladder coupling does not qualitatively affect the physics of a single ladder which is itself that of nearly isolated plaquettes as seen above. The irrelevant flows for Δ and C_L with the number of ladders are shown in Fig. 5. Δ for the two-dimensional system is renormalized by about 20% from its single ladder value. The extrapolated gap $\Delta=0.4758J_1$ is lower than $\Delta=0.67J_1$ found in the checkerboard model at the isotropic point.[19] This is consistent with the fact that interplaquette interactions are more important in the SSM. For large lattices, C_L for the two-dimensional systems is practically identical to its ladder value. This suggests that the correlation length is very short. In this regime short-ranged plaquettes are dominant in the exact wave function; hence $\tilde{\Psi}$ is an excellent variational approximation.

Recently in a variational wave function based on doping an orthogonal dimer wave function has been used to explore the nature of an eventual superconductive state in $SrCu_2(BO_3)_2$.[12] The estimated values of the couplings in this compound are $J_1\approx 85$ K and $J_2=54$ K.[24] This places it at the boundary of the orthogonal dimer phase, not very far for the plaquette phase. Given the possible incertitude in this estimation and the fact that these values may be affected by doping, it is worth exploring the superconductivity upon doping the plaquette ground state as well.

To summarize, I have argued that the DMRG technique is a natural approach to study spin-Peierls phases that spontaneously arise in frustrated quantum antiferromagnets. I have used the two-step DMRG to confirm the nature of the controversial phase between the Néel and dimer phases. The phase diagram of the SSM bears some similarity to that of the checkerboard model.[19] In the checkerboard model, an additional Néel phase was recently found between the plaquette and the crossed dimer phases.[19,25] It is quite possible that this additional phase exists in the SSM in the vicinity of $J_2\approx 1.5J_1$. Unfortunately, in the SSM, unlike the checkerboard model, the starting ladder does not have the full symmetry of the bond pattern of the 2D lattice. As the dimer phase is approached, the variational wave function used in this study is not optimal, as it leaves half of the spins unpaired in the orthogonal dimer phase. It will be more advantageous to start with the orthogonal dimer pattern shown in Fig. 1.

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*Present address: The Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel.

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