# Néel and valence-bond crystal phases of frustrated two-dimensional Heisenberg models

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I use an improved version of the two-step density-matrix renormalization group method to study ground-state properties of the two-dimensional (2D) Heisenberg model on the checkerboard lattice. In this version, the Hamiltonian is projected on a tensor product of two-leg ladders instead of chains. This allows investigations of 2D isotropic models. I show that this method can describe both the magnetically disordered and ordered phases. The ground-state phases of the checkerboard model as $J_2$ increases are (i) Néel with $Q=(\pi,\pi)$, (ii) a valence-bond crystal (VBC) of plaquettes, (iii) Néel with $Q=(\pi/2,\pi)$, and (iv) a VBC of crossed dimers. In agreement with previous results, I find that at the isotropic point $J_2=J_1$, the ground state is made of weakly interacting plaquettes with a large gap $\Delta \approx 0.67 J_1$ to triplet excitations. The same approach is also applied to the $J_1$-$J_2$ model. There is no evidence of a columnar dimer phase in the highly frustrated regime.

Frustration-induced magnetically disordered phases in two dimensions have recently attracted substantial interest.[1] Frustrated magnets are known to display unconventional ground states with, in some cases, a large set of low-lying degenerate singlet excitations that are still not well understood. Among models of frustrated systems, the Heisenberg model on the checkerboard lattice (HMCL) has recently been intensively studied by various techniques.[2–8] This model is seen as a first step in the investigation of the three-dimensional pyrochlore model. The emerging picture is that at the isotropic point ($J_1=J_2$), the HMCL spontaneously breaks the lattice's translational symmetry. The ground state is a singlet made of a collection of weakly coupled plaquettes with a large gap, $\Delta \approx 0.7 J_1$, to triplet excitations. Away from the isotropic point, the situation is less clear. There is no single method which can capture the full phase diagram. Another important model which has remained so far very controversial is the $J_1$-$J_2$ model.[1]

In this Brief Report, I introduce an improved version of the two-step density-matrix renormalization group[9,10] (TSDMRG) which, as I will show, is very convenient in the study of the HMCL and other two-dimensional (2D) frustrated models. This version is based on using the two-leg ladder, instead of chains, as the starting point to build the 2D lattice. The main insight in using the two-leg ladder to construct the 2D lattice comes from large $N$ predictions[11] that frustration often induces ground states in which the translational symmetry is broken. In the strong-coupling regime of the disordered phase of $S=1/2$ systems, the system is made of a collection of singlets or plaquettes. This strong coupling regime cannot be described starting from independent chains which are gapless. Starting from a single chain, small transverse perturbations can yield a gap within the TSDMRG, but this gap is often small and it is difficult to obtain reliable extrapolations. The two-leg ladder does not present this problem. It does already present a large gap $\Delta \approx 0.5$ even in the absence of frustration. Coupled ladders naturally evolve toward the 2D Néel state as the number of legs increases. Hence, in principle, disordered and ordered phases could be described within a two-leg ladder version of the TSDMRG.

This suggests that the two-leg ladder is a more natural starting point to describe ground-state phases of 2D antiferromagnets than the single chain.

Additional insights into this idea came from my comparative study of coupled chains with half-integer and integer spins.[12] In Ref. 12, when starting from single chains, I found that although chains with $S=1$ display the Haldane gap, $\Delta \approx 0.4$, they converge much faster to the Néel state than those with $S=1/2$. Furthermore, when a frustration-induced disordered phase is present, it can be much more easily found in the case $S=1$. Hence, following the equivalence between the two-leg ladder and the Haldane spin chain, suggested by the Affleck-Kennedy-Lieb-Tasaki construction,[13] it would be better to adopt the two-leg ladder as the building block for two-dimensional lattices.

I will now illustrate this idea in the cases of the HMCL and the $J_1$-$J_2$ model. Following the usual notation, the Hamiltonian for these models is given by

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

where $\langle i,j \rangle$ represents nearest-neighbor sites and $[i,j]$ stand for next-nearest neighbors on every other plaquette for the HMCL and on every plaquette for the $J_1$-$J_2$ model. $J_1$ is set as the unit energy.

The TSDMRG with ladders is similar to the method with chains. So I refer the reader to Refs. 9 and 10 for a complete exposition of the algorithm. Here, I will discuss only briefly the main points of the algorithm. I start by dividing the 2D lattice into two-leg ladders; the Hamiltonian (1) is written as

$$H = \sum_{ladders} H_{ladder} + H_{int}, \qquad (2)$$

where $H_{ladder}$ is the Hamiltonian of a single two-leg ladder, and $H_{int}$ contains the interladder part. In the first step of the method, the usual density-matrix renormalization group (DMRG) method is applied to generate a low-energy Hamiltonian of an isolated ladder of $N_x$ sites, keeping $m_1$ states. Then $m_2$ low-lying states of the superblock states, the corre-

sponding energies, and all the local spin operators are retained. These energies represent the renormalized low-energy Hamiltonian of a single ladder. The Hamiltonian (2) is then projected onto the tensor product basis of independent ladders, $\Psi = \Pi_{ladders}\Phi_{ladder}$, where $\Phi_{ladder}$ is an eigenfunction of $H_{ladder}$. This yields an effective Hamiltonian, $H_{eff}=H_0+\tilde{H}_{int}$, where $H_0$ is diagonal and its eigenfunction are the $\Psi$'s.

The resulting effective coupled ladder problem, which is one-dimensional (1D), is studied again by the DMRG method in the transverse direction. The TSDMRG, like the original DMRG method, is variational. The subspace spanned by the wave functions of the form $\Psi$ is a subspace of the full Hilbert space of Hamiltonian (1). Its convergence depends on $m_1$ and $m_2$, and 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. $m_2$ fixes the energy bandwidth $\delta E$. The method is accurate only when the interladder couplings are small with respect to $\delta E$. In the present simulations, $\delta E \approx 4$. Since for the HMCL the interladder and intraladder are of the same magnitude, in principle, this approach would be plagued by the same deficiencies as the block renormalization group method. However, if the starting point is chosen so that the essential physics is already contained at the level of the ladder, the effective strength of the interladder couplings will be small even if the bare couplings are not. This is particularly the case with frustrated models in which the competing interactions largely cancel each other in the strong frustration regime, yielding weakly coupled subclusters.

I start by the analysis of the HMCL. The ground-state properties of an isolated ladder can readily be obtained. I keep up to $m_1=128$ and $N_x=16$, and I target spin sectors from $S_z=0$ to $S_z=\pm 4$ and I use open boundary conditions (OBCs). The maximum error is $\rho_1=1\times 10^{-4}$. There is a gap $\Delta$ for all values of $J_2$ investigated between 0 and 2. The finite size behavior of gaps for some typical values of $J_2$ are shown in Fig. 1. The case $J_2=0$ reduces to the usual two-leg ladder which has been widely studied in the literature.[14] For $J_2=0$, $\Delta \approx 0.5$. As $J_2$ increases, $\Delta$ has a nonmonotonous behavior. This suggests a rich structure which is revealed more clearly by the analysis of the correlation functions. I computed the following short-range correlation functions: the bond strength along a leg $C_{l_{u,c}}=\langle \mathbf{S}_{i,1}\mathbf{S}_{i+1,1}\rangle_{u,c}$ for uncrossed (u) and crossed (c) plaquettes, the diagonal correlation $C_{d_{u,c}}=\langle \mathbf{S}_{i,1}\mathbf{S}_{i+1,2}\rangle_{u,c}$, and bond strength along the rungs $C_r=\langle \mathbf{S}_{i,1}\mathbf{S}_{i,2}\rangle$. Note that I have introduced a second index to the local spin. These correlations are shown in Fig. 2. Four regions can be identified: (i) Region I (rung dimers): $0 \lesssim J_2 \lesssim 0.6$, $C_{l_{u,c}}<0$, $C_{l_u}\approx C_{l_c}$, $C_{d_{u,c}}>0$, $C_r<0$, and $|C_r|>|C_{l_u}|$; the dominant spin-spin correlations are along the rungs. The ground-state properties of the ladder in this region are identical to those of the unfrustrated ladder ($J_2=0$). (ii) Region II (plaquettes I): $0.6 \lesssim J_2 \lesssim 1$, $C_{l_{u,c}}<0$, $|C_{l_u}|>|C_{l_c}|$, $C_{d_{u,c}}>0$, $C_r<0$, and $|C_r|<|C_{l_u}|$; the physics is dominated by that of the isotropic point. At this point, the ground state is a collection of weakly interacting uncrossed plaquettes. Both $C_{d_c}$ and $C_{l_c}$ vanish at $J_2=1$. In this region, the local spin configuration is the same on all the uncrossed plaquettes as shown in Fig. 3(b) (iii) Region III (plaquettes II):
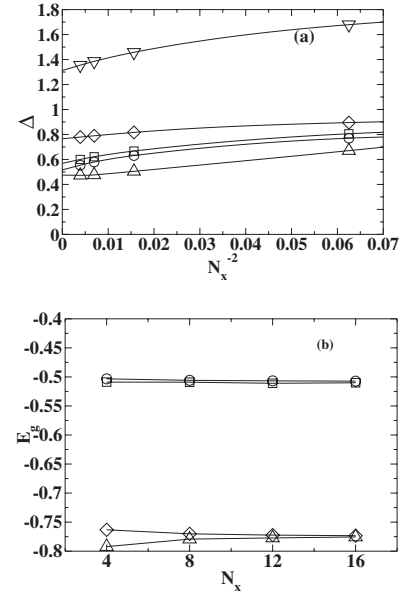


FIG. 1. (a) Spin gap of the HMCL two-leg ladder for $J_2=0$ (circles), 0.5 (squares), 1 (diamonds), 1.1 (triangles up), and 2 (triangles down). (b) Ground-state energies as function of the system size for a two-leg ladder for $J_2=1$ (circles) and $J_2=2$ (diamonds), and for the 2D lattice for $J_2=1$ (squares) and $J_2=2$ (triangle up).

$1 \lesssim J_2 \lesssim 1.3$, $C_{l_u}<0$, $C_{l_c}>0$, $C_{d_u}>0$, $C_{d_c}<0$, $C_r<0$, and $|C_r|<|C_{l_u}|$; in this region, the ground state is again dominated by uncrossed plaquettes, but now the local spin configurations on two consecutive uncrossed plaquettes are images of one another by reflection with respect to a plane passing through the middle of the crossed plaquette between them. Region IV (crossed dimers): $1.3 \lesssim J_2$, $C_{l_u}<0$, $C_{d_c}<0$, $C_{l_c}=C_r=C_{d_u}\approx 0$, and $|C_r|<|C_{l_u}|$; the ground state is domi-
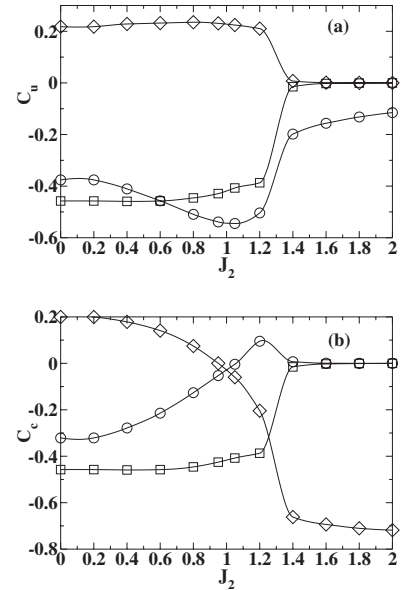


FIG. 2. Short-range correlations of the HMCL $C_l$ (circles), $C_r$ (squares), and $C_d$ (diamonds) for the two-leg ladder for (a) uncrossed and (b) crossed plaquettes as function of $J_2$.

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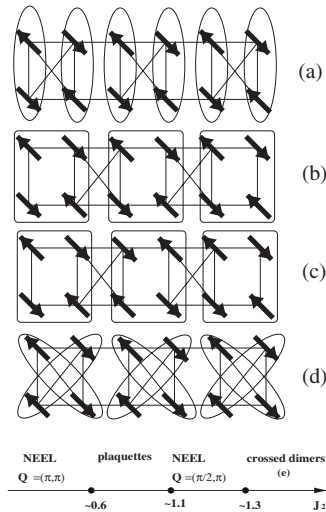PHYSICAL REVIEW B **77**, 052408 (2008)



FIG. 3. The four phases of the HMCL two-leg ladder: (a) rung dimers, (b) plaquette I, (c) plaquette II, and (d) crossed dimers. Ground-state phases of the 2D checkerboard model as function of $J_2$. Note that the phase boundaries are rough estimates taken from the phases of the two-leg ladder (e).



FIG. 4. (a) 2D gaps of the HMCL as function of the system size $J_2=0$ (circles), 0.5 (squares), 1 (diamonds), 1.1 (triangles up), and 2 (triangles down). (b) Correlation function along the legs as function of the distance for $J_2=1.25$.

nated by the crossed dimers on crossed plaquettes as shown in Fig. 3(d). The sketch of the spin structure corresponding to each region is summarized in Fig. 3. Since I applied OBC, for a given size, there are two possible ground states depending on the plaquette pattern: (a) $ucu\ldots ucu$ or (b) $cuc\ldots cuc$. In region I, the configurations (a) and (b) have nearly the same energy. This is consistent with the fact that the translational symmetry is not broken. However, in regions II and III, (a) has the lowest energy, since it has a larger number of uncrossed plaquettes. By contrast, in region IV where dimer order is dominant, it is (b) that has the lowest energy.

The 2D systems are obtained by applying the DMRG on $H_{eff}$ in the transverse direction. I studied systems of size $N_x \times N_y = 4 \times 6$, $8 \times 10$, $12 \times 14$, and $16 \times 18$. I kept up to $m_2 = 128$ and used OBC. Interladder interactions will have very different effects depending on whether they correspond to a magnetic regime or a disordered regime. I will first consider their effects on region II, which includes the isotropic point. The interladder interactions do not substantially modify the ground state wave function of decoupled ladders. Figure 1(b) shows that the ground-state energy and Fig. 4(a) $\Delta$ are not very different from that of an isolated plaquette displayed in Fig. 1(a). Thus, in the vicinity of $J_2=1$, interladder interactions do not strongly renormalize the properties of an isolated ladder, which themselves are close to those of an isolated plaquette. The extrapolated gap in Fig. 4(a) is found to be $\Delta=0.67J_1$, which is in good agreement with the prediction from exact diagonalization.[6] The same conclusion is seen in Fig. 1 for region IV, where the crossed-dimer ground state found for the ladder is also the ground state of the 2D lattice. In both cases, the wave function made of the tensor product of the wave function of single two-leg ladders is a good variational wave function for the 2D system. In each case, the ground-state energy of the 2D system remains very close to that of individual plaquettes ($-0.5J_1$) or crossed dimers ($-0.375J_2$). This can be explained as follows: when
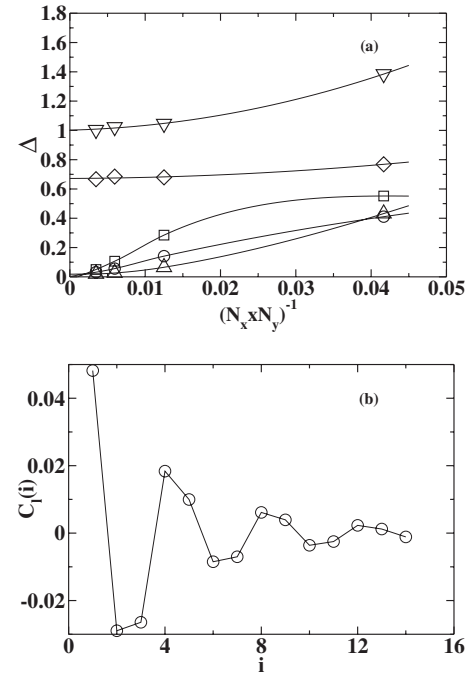
ladders are brought together to build the 2D lattice, the dominant local correlations are $C_{l_u}$ in region II and $C_{d_c}$ in region IV; during this process, magnetic energy cannot be gained efficiently. For region II, this is because the two neighboring plaquettes of an uncrossed plaquette in the direction of the rungs involve frustrated bonds. Hence, the system prefers the original configuration to avoid increasing its energy. For region IV, $C_r$ is very small. The system cannot increase it when the ladders are coupled, because the spins are already involved in strong diagonal dimers. There is, however, the possibility of gaining magnetic energy by forming Néel order along the direction of the diagonal bonds ($J_2$ direction) as suggested in Ref. 8. This is unlikely, however, because once such a phase is reached, I do not see how the system could go to crossed dimers at larger $J_2$. The action of $J_1$, which acts as frustration in this regime, decreases as $J_2$ increases. Hence, once this hypothetical Néel phase along the $J_2$ bonds is reached, there is no obvious mechanism that could destroy it as $J_2$ increases to yield the crossed-dimer phase as suggested in Ref. 8. Such a Néel phase would be favored only when $J_2 \gg J_1$. I made rough calculations with $J_2=4$ and 8, and I found that the system remains in the crossed-dimer phase. The situation is apparently identical to the $J_1$-$J_2$ chain where the independent chains regime is only reached in the infinite $J_2$ limit.

The situation is very different for regions I and III. In region I, the dominant local correlation is $C_r$; when the ladders are brought together, magnetic energy can be gained by an antiferromagnetic arrangement along the rungs. This enhances the local antiferromagnetic order which exists along the legs and ultimately leads to a Néel order with

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$Q=(\pi,\pi)$. This is seen in the vanishing of the spin gap for $J_2=0$ and $J_2=0.5$ shown in Fig. 4(a). This is in agreement with results for $J_2=0$ from quantum Monte Carlo (QMC) simulations[15] and large $S$ analysis.[4] I find that the TSDMRG ground-state energy $-0.6011$ at $J_2=0$ is not in very good agreement with the QMC result $-0.6699$ of Ref. 15. Despite this discrepancy, the TSDMRG, is nevertheless, able to reproduce the low-energy behavior of the ordered phase. This is not, in fact, surprising. In the resonating, valence-bond picture, the Néel state and its low-energy excitations can be written as a linear combination of a tensor product of dimers. The TSDMRG variational solution of Hamiltonian (1), which is a linear combination of the wave functions $\Psi$, has this form. A similar analysis also applies for region III. $C_{l_u}$ is dominant in region II, but as seen in Fig. 2, $C_{l_u}$ has a minimum at $J_2=1$ and then increases. It becomes very close to $C_r$ when $J_2$ enters region III. Hence, magnetic energy can be gained again through the rungs. Since the structure along the legs is not modified from Fig. 3(d), the resulting wave vector will be $Q=(\pi/2,\pi)$. This is seen in Fig. 4 in the behavior of the spin-spin correlation function $C_l(i)$ along the legs. $C_l(i)$ displays a period of 4. The correlations between the rungs (not shown) oscillate with $q_y=\pi$. The state with $Q=(\pi,\pi/2)$ are degenerate, as are the $(\pi,0)$ and $(0,\pi)$ states in the $J_1$-$J_2$ model. Figure 3 presents a sketch of the different ground-state phases of the HMCL as a function of $J_2$. I note that in Ref. 8, a very similar phase diagram was suggested; the only difference with the TSDMRG phase diagram is the wave vector of the Néel phase between the plaquette and crossed-dimer phases.

I now apply the above analysis to the $J_1$-$J_2$ model. Previous studies[1] have concluded that the model has three phases: a Néel phase with $Q=(\pi,\pi)$ for $J_2\lesssim0.4J_1$, a disordered phase, which is thought to be a columnar dimer phase, for $0.4J_1\lesssim J_2\lesssim0.6$, and a Néel phase with $Q=(\pi,0)$ or $Q=(0,\pi)$ for $J_2\gtrsim0.6J_1$. While the existence of the two magnetic phases is clearly established, there has not been any convincing evidence of a disordered phase between them. Indeed, recent two-step DMRG studies based on weakly coupled chains[9,10] suggest that this disordered phase does not exist. In Fig. 5, I show the short-range spin-spin correlations of the ladder, which show only two phases: the rung-singlet
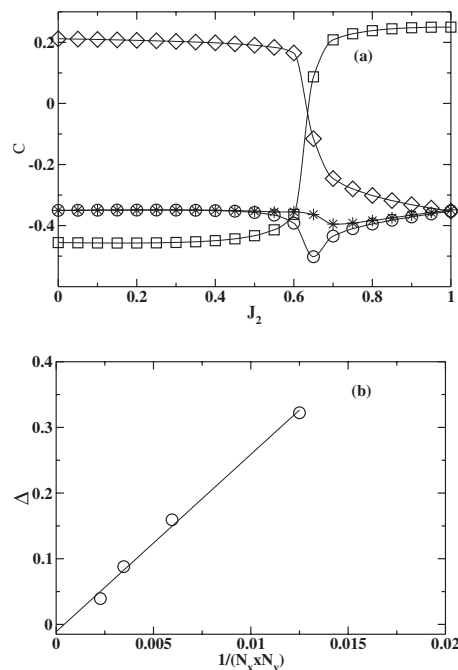


FIG. 5. (a) Short-range correlations in the $J_1$-$J_2$ model $C_l$ for two consecutive bonds (circle and stars), $C_r$ (squares), and $C_d$ (diamonds). (b) 2D gap for $J_2=0.5J_1$.

phase with dominant antiferromagnetic $C_r$ for $J_2\lesssim0.6J_1$, and the haldane phase with dominant $C_d$ and ferromagnetic $C_r$ for $J_2\gtrsim0.6J_1$. These phases naturally evolve respectively to the Néel phases with $Q=(\pi,\pi)$ and $Q=(\pi,0)$ in the 2D systems. There is a small finite size dimerization in the vicinity of the critical point. The maximum of dimerization occurs at the point where $C_r=0$ and the 1D character is enhanced. This is suggestive of a finite size critical behavior, not of a disordered phase. The absence of a disordered phase is supported by the vanishing of $\Delta$ of the 2D system at $J_2=0.5J_1$ as shown in Fig. 5.

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