Ground States of a Frustrated Quantum Spin Chain with Long-Range Interactions

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The ground state of a spin-1/2 Heisenberg chain with both frustration and long-range interactions is studied using Lanczos exact diagonalization. The evolution of the well-known dimerization transition of the system with short-range frustrated interactions (the J_1-J_2 chain) is investigated in the presence of additional unfrustrated interactions decaying with distance as $1/r^\alpha$. It is shown that the continuous (infinite-order) dimerization transition develops into a first-order transition between a long-range ordered antiferromagnetic state and a state with coexisting dimerization and critical spin correlations at wave number $k = \pi/2$. The relevance of the model to real systems is discussed.

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One-dimensional spin systems have played an important role in quantum many-body physics since the early days of quantum mechanics [1,2]. Several different types of ordered and disordered ground states can be realized, depending on the individual spin magnitude S and the form of the spin-spin interactions [3–6]. For $S = 1/2$, the prototypical Heisenberg chain with antiferromagnetic nearest-neighbor interactions (coupling constant $J_1 > 0$) has a quasiordered (critical) ground state, with spin correlations decaying with distance r as $\sqrt{\ln(r)}/r$ [6]. Including a next-nearest-neighbor coupling $J_2 > 0$ (the J_1-J_2 chain [3]) leads to a quantum phase transition into a doubly degenerate dimerized state (a valence-bond-solid; VBS) at coupling ratio $g = J_2/J_1 \approx 0.2411$. In the effective field theory for the $S = 1/2$ chain [5], the VBS transition is related to a sign change of a marginal operator. It has been investigated in great detail numerically, using, e.g., exact diagonalization [7,8] and the density-matrix renormalization-group (DMRG) method [9].

While long-range spin ordering is rigorously ruled out in one-dimensional systems with finite-range rotationally invariant interactions, long-range interactions make magnetic order possible at zero temperature. The transition between a long-range ordered antiferromagnet (AFM) and the quasi-long-range ordered (QLRO) ground state was recently investigated in a Heisenberg chain with interactions of the form $J_r \propto (-1)^{r-1}/r^\alpha$ [10]. Here, the signs correspond to no magnetic frustration, thus favoring AFM ordering. For $\alpha < \alpha_c$, the ground state possesses true AFM long-range order, while for $\alpha > \alpha_c$, the system is in a QLRO phase, with the same critical form of the spin correlations as in the standard Heisenberg chain. The critical value α_c depends on details of the couplings (e.g., on J_1 when all other J_r are fixed) and the exponents are continuously varying. Another example of long-range interactions is the celebrated Haldane-Shastry chain [11], with frustrated interactions $J_r = 1/r^2$. This system has a critical ground state similar to that of the standard Heisenberg chain, but the marginal operator vanishes [12], and it is, thus, a system right at the dimerization transition.

A natural question arising from previous work is how the combined effects of frustration and long-range interactions could lead to other phases and quantum phase transitions. In particular, is it possible to realize a direct transition between the AFM state and a VBS? In this Letter, the evolution of the standard dimerization transition into an AFM-VBS transition is explored by considering a frustrated J_1-J_2 chain with additional *nonfrustrated* long-range interactions. The Hamiltonian for a finite periodic chain with N spins $S = 1/2$ is given by

$$H = \sum_{r=1}^{N/2} J_r \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+r}, \tag{1}$$

where the couplings are given by

$$J_2 = g, \qquad J_{r\neq 2} = \frac{(-1)^{r-1}}{r^\alpha}\left(1 + \sum_{r=3}^{N/2} \frac{1}{r^\alpha}\right)^{-1}. \tag{2}$$

Here, the normalization is chosen such that the sum of all nonfrustrated interactions $|J_r|$ equals 1 [13] (and J_1 is also given by the $J_{r\neq 2}$ expression).

The model is here studied using Lanczos exact diagonalization. A semiquantitative phase diagram based on these calculations in the plane (g, α^{-1}) is shown in Fig. 1. The J_1-J_2 chain corresponds to the horizontal axis ($\alpha^{-1} = 0$). The QLRO phase is here denoted QLRO(π), with π indicating the wave number of the dominant spin correlations. The phase boundaries are approximate, resulting primarily from studies of level crossings, as will be discussed below. The main focus of this initial study of the model will be on the evolution of the QLRO(π)-VBS (dimerization) transition with decreasing α. It will be shown that this continuous transition persists until $\alpha \approx 2$, while for smaller α, it evolves into a first-order transition (of the avoided level-crossing type) between the AFM state and a state with coexisting VBS order and critical spin

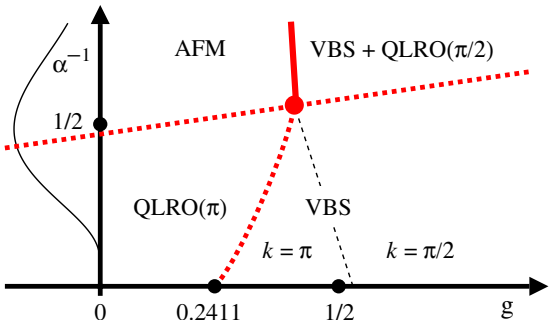

FIG. 1 (color online). Approximate phase diagram as a function of the frustration strength g and the inverse of the long-range exponent α. The dashed curves indicate continuous phase transitions, whereas the thick solid curve represents a first-order transition. The curve for $g < 0$ corresponds to the interaction studied in [10]. At $\alpha^{-1} = 0$, the dominant spin correlations in the VBS state change from $k = \pi$ to $\pi/2$ at $g \approx 0.52$ [9]. This transition (or cross over) evolves to the point where all the phase boundaries come together.

correlations at wave-number $k = \pi/2$, denoted in the phase diagram as VBS + QLRO($\pi/2$).

The coexistence state is not purely of theoretical interest. Recent *ab initio* calculations for metallic chains show unfrustrated spin couplings decaying as $\approx 1/r^2$, with J_2 in some cases frustrating (e.g., Mn) [14]. In the quasiclassical (large-S) limit, spiral states with continuously varying periodicity can arise in such a system. The present study suggests a more exotic scenario in the extreme quantum limit of $S = 1/2$ (and perhaps also for other small S).

Solving the model (1) numerically poses significant technical challenges. Efficient quantum Monte Carlo techniques can be applied to systems with long-range interactions [10,15], but with the frustrating J_2 term, this is no longer possible due to the sign problem [16]. The DMRG method [17,18], on the other hand, can handle frustration but not easily long-range interactions. Here, periodic chains up to size $N = 32$ are solved using Lanczos exact diagonalization (in the standard way, exploiting lattice symmetries and spin-inversion for block-diagonalization in the magnetization $m_z = 0$ sector). This is sufficient for roughly extracting the phase boundaries using level-crossing methods (which in the case of the dimerization transition is a well established technique [7], extended here using different levels to detect other transitions).

The QLRO(π)-VBS transition in the J_1-J_2 chain is of infinite order, i.e., the singlet-triplet gap of the VBS is exponentially small for $g \to g_c$ [5]. It is therefore difficult to locate the transition based on the order parameter for small N. However, g_c can be determined accurately from excited states. The lowest excitation of a chain with even N is a triplet for $g < g_c$ and a singlet for $g > g_c$. The crossing point of these levels is a rapidly converging finite-N definition of g_c [7,8]. The same physics can be expected also in the presence of the long-range interaction, if α is sufficiently large. This is shown for a 16-spin chain at $\alpha = 4$ in the upper panel of Fig. 2. Singlets with momenta $k = 0$ and $k = \pi$ (out of which symmetry-broken dimerized states can be formed) should be degenerate in the VBS phase. For finite N, this degeneracy is not exact (except in the J_1-J_2 chain at the special point $g = 1/2$), but a region of very near degeneracy for $g > 1/2$ can be seen in the figure. The region of approximate degeneracy, which is not easy to demarcate precisely, expands very slowly toward smaller g with increasing N. In contrast, the singlet-triplet crossing point is well defined and converges rapidly. Extrapolating the crossing point to $N = \infty$ for different α, as illustrated in Fig. 3, can reliably give the QLRO(π)-VBS phase boundary $g_c(\alpha)$ for $\alpha \gtrsim 2$.

Upon decreasing α below ≈ 2, the broad maximum in the ground state energy versus g becomes increasingly sharp. As seen in the lower panel of Fig. 2, at $\alpha = 1$, it has developed into a sharp tip due to an avoided level crossing with the second singlet at $k = 0$. The real singlet-triplet crossing has moved to the same region. An avoided level crossing leading to a discontinuity in the derivative of the ground state energy with respect to g for $N \to \infty$ is the hallmark of a first-order transition. The nature of the phases at this transition will be discussed below. First, let us investigate how the transition evolves from continuous to first order.

Figure 3 shows the size dependence of the level-crossing point g_{cross} and the location g_{peak} of the maximum in the ground state energy. In the J_1-J_2 chain, the size correction to the crossing point is $\propto 1/N^2$, which also can be seen for large α. For smaller α, the corrections instead seem to be $\propto 1/N$, but a crossover to $1/N^2$ for large N seems likely as

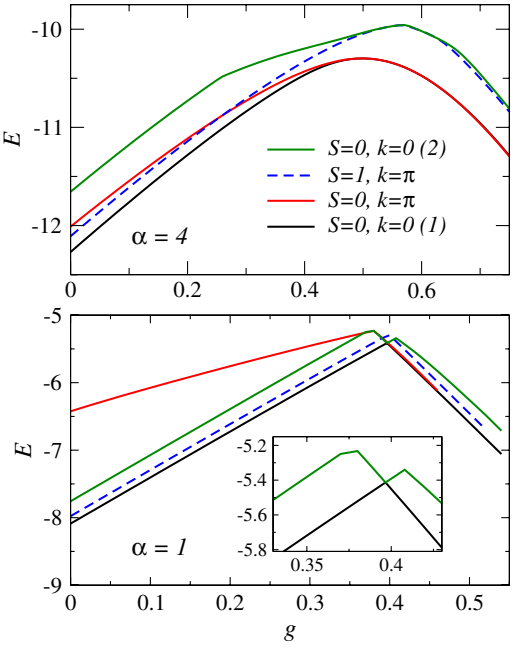

FIG. 2 (color online). Low-energy levels of a 16-spin system at $\alpha = 4$ (upper panel) and $\alpha = 1$ (lower panel). The spin S and the momentum k of the states are indicated in the upper panel. The inset in the lower panel shows the avoided level crossing of the two $k = 0$ singlets in greater detail.

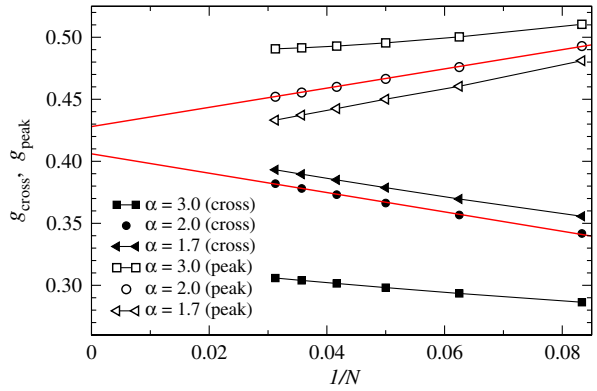

FIG. 3 (color online). Dependence on the inverse chain length of the singlet-triplet crossing point g_{cross} and the location g_{peak} of the ground state energy maximum for different long-range interaction exponents α. The two lines show extrapolations of the $g = 2.0$ numerical data to $N = \infty$.

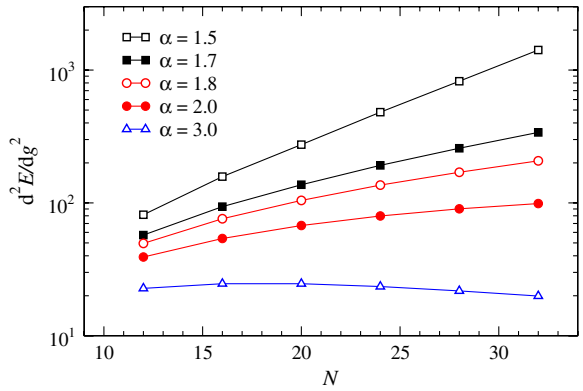

FIG. 4 (color online). Size dependence of the second derivative of the ground state energy with respect to the frustration parameter g at the point g_{peak} where the ground state energy takes its maximum value.

long as the transition remains continuous. The peak location moves in the opposite direction. For some α and $N \to \infty$, g_{cross} and g_{peak} should coincide. The results indicate that both g_{cross} and g_{peak} have dominant $1/N$ corrections at this point. Fitted lines are shown in Fig. 3 at $\alpha = 2$, where there is still a small gap between the two extrapolated values. For $\alpha = 1.7$, where the transition is first order, they should coincide (and then the asymptotic size correction should be exponential).

To verify an avoided level crossing with a discontinuous energy derivative for $\alpha \lesssim 1.8$, the second derivative of the ground state energy at its maximum is graphed on a lin-log scale in Fig. 4. It grows exponentially with N for $\alpha = 1.5$, showing that the slope of the energy curve indeed changes discontinuously for an infinite chain. In contrast, at $\alpha = 3$, the second derivative decreases for large N. For $\alpha = 2$, convergence to a finite value also seems plausible, whereas $\alpha = 1.7$ and 1.8 appear to be close to a separatrix (where the form of the divergence is consistent with a power law) between the two different behaviors.

This analysis suggests that the continuous dimerization transition changes smoothly into a first-order transition at ($g_m \approx 0.41$, $\alpha_m \approx 1.8$). The singlet-triplet crossing moves toward the ground state energy maximum and coincides with it at the multicritical point (g_m, α_m), beyond which it develops into a first-order singularity. Note that the rounded energy maximum in the VBS phase for large α has no special significance (except at $\alpha^{-1} = 0$ where it corresponds to the exact singlet-product ground state). It is only when it develops into the sharp avoided level crossing that it is associated with a phase transition.

To discuss the states involved in the first-order transition, consider the spin and bond correlation functions,

$$C(r) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle, \tag{3}$$

$$D(r) = \langle (\mathbf{S}_i \cdot \mathbf{S}_{i+1})(\mathbf{S}_{i+r} \cdot \mathbf{S}_{i+r+1}) \rangle. \tag{4}$$

In Fig. 5, these are graphed for two g values, at either side of the transition for $\alpha = 1$. At $g < g_c$, the dominant spin correlation $C(k)$ in Fourier space is at wave number $k = \pi$, and finite-size scaling shows that the sublattice magnetization remains nonzero for $N \to \infty$. There is no structure in $D(r)$, i.e., there is no VBS order. This is thus an AFM phase, the continuation of the AFM state studied in [10], as indicated in Fig. 1. For $g > g_c$, there is VBS order. Interestingly, in this phase, there are also strong spin correlations at $k = \pi/2$, which can be seen clearly as a real space period-four oscillation in Fig. 5. Finite-size scaling indicates that there is no long-range spin order, but the correlations appear to decay as $1/r^{\gamma}$ with $\gamma \approx 1$; thus, this state is denoted as QLRO($\pi/2$).

Examining the correlations as a function of g, discontinuities (increasingly sharp jumps with increasing N) develop for $\alpha < 1.5$. This should persist until the multicritical point at $\alpha_m \approx 1.8$, but larger systems are needed to observe the discontinuity very close to this point.

The VBS + QLRO($\pi/2$) state should have gapless spin excitations. The lowest triplet has $k = \pi/2$. It is, however, difficult to demonstrate the gaplessness based on data for small systems because the size-dependence of the gaps (and other quantities) for $N = 4n$ exhibit even-odd oscillations in n. In the VBS phase, the lowest triplet is at $k = \pi$, even when the spin correlations (exponentially decaying) are peaked at $k = \pi/2$. The level crossing between the lowest $k = \pi$ and $k = \pi/2$ triplets can be used to extract the boundary between the VBS and VBS + QLRO($\pi/2$) phases. The size dependence of the crossing point is not smooth, however, and cannot be extrapolated very reliably. The boundary between dominant $k = \pi$ and $k = \pi/2$ spin correlations in the VBS phase has also not been extracted accurately.

Let us briefly return to Fig. 2 for another interesting feature of the level spectrum: The lowest singlet excitation for small g has momentum $k = \pi$ for $\alpha = 4$ but $k = 0$ for $\alpha = 1$. The switching of the order of these levels as a function of α for $g < g_c$ is associated with the QLRO(π)-AFM transition. The level crossings can be

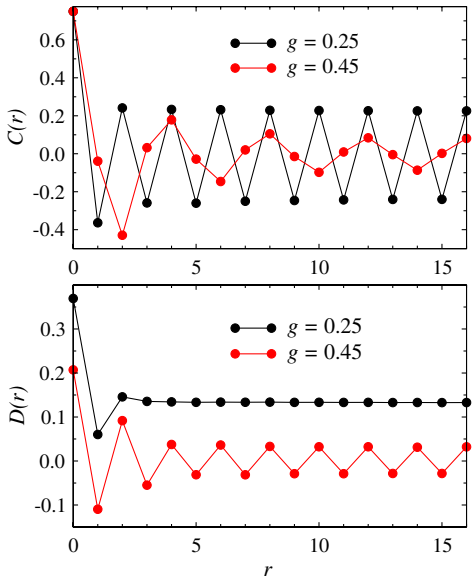

FIG. 5 (color online). Spin (upper panel) and dimer (lower panel) correlations in a 32-spin chain at $\alpha = 1$. At $g = 0.25$ and 0.45, the system is in the AFM and VBS-QLRO($\pi/2$) phases, respectively. A first-order transition between these states occurs at $g \approx 0.39$.

used to extract this phase boundary very accurately up to $g \approx 0.25$ (while for higher g the $N \to \infty$ extrapolations become difficult); a more detailed discussion of this issue is given as a footnote [19]. As indicated in Fig. 1, α_c depends only weakly on g. The results are consistent with the location quoted above for the multicritical point.

In summary, the combination of short-range frustration and long-range unfrustrated interactions in one dimension has been shown to lead to a first-order transition between a Néel state and a VBS with coexisting critical $k = \pi/2$ spin correlations. It should be noted that the system sizes studied here are small, and it cannot be excluded that the spin correlations could become incommensurate, as they do in the J_1-J_2 chain for $J_2/J_1 > 1$ [20]. Hopefully, field theories that very successfully describe the standard dimerization transition [5], and recently also the transition between the critical spin state and the Néel state [10], could be generalized to the coexistence state as well.

Recent calculations [14] for metallic chains have shown that interactions of the type used here are realistic, but in these systems, $S > 1/2$. Although one cannot describe these systems completely using a spin-only model, it would still be interesting to repeat the calculations discussed here for larger S. This is much more challenging, however, because of the rapidly growing size of the Hilbert space with S. Although the DMRG method [17,18] is not ideally suited for systems with long-range interactions, it may still be possible to use it to study lattice sizes beyond the limits of Lanczos calculations.

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[19] In the QLRO(π) phase, the low-energy excitations arise from two deconfined spinons. The lowest (for $N = 4n$) is a triplet at $k = \pi$. The lowest singlet is also at $k = \pi$, with a small finite-size gap to the triplet due to weak spinon-spinon interactions. In the AFM phase, the spinons are no longer deconfined and the $k = \pi$ singlet energy is higher. The Lanczos calculations show that the lowest singlet is at $k = 0$. In [10], the QLRO(π)-AF transition in a model with $J_1 = 1$ and $J_{r>1} = \lambda(-1)^{r-1}/r^{\alpha}$ was located using quantum Monte Carlo data for the order parameter, which gave $\alpha_c = 2.225 \pm 0.025$ at $\lambda = 1$ using N up to 4096. Extrapolating the $k = 0$, π singlet crossing points (which have size corrections $\propto 1/N^{\beta}$, with $\beta \approx 1.50$) for $N \leq 32$ gives a marginally higher value: $\alpha_c = 2.262 \pm 0.001$. Analyzing the singlet and triplet gaps at the crossings, assuming $\Delta \sim N^{-z}$, gives the dynamic exponent $z = 0.764 \pm 0.005$, in very good agreement with [10]. For the frustrated model (1) on the QLRO(π)-AFM boundary, $z \approx 0.75$ for g up ≈ 0.25, while for larger g, it is not possible to reliably extract α_c and z this way, because of large scaling corrections and the absence of level crossings for increasingly large systems as the multicritical point ($g_m \approx 0.41$, $\alpha_m \approx 1.8$) is approached (for reference $\alpha_c = 2.220 \pm 0.005$ for $g = 0$ and 2.170 ± 0.01 for $g = 0.2$). At the multicritical point, z can be extracted using gaps at the singlet-triplet crossing point and the ground state energy maximum, giving $z \approx 0.8$.
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