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 $1/r^n$. 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 $J_{ij}$. For $S = 1/2$, the prototypical Heisenberg chain with antiferromagnetic nearest-neighbor interactions (coupling constant $J_1 > 0$) has a quasi-ordered (critical) ground state, with spin correlations decaying with distance $r$ as $\sqrt{\ln(r)/r}$ [3]. 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 [3], 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 [3, 4] and the density-matrix renormalization-group (DMRG) method [5, 6].

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 $J_r \propto (-1)^{r-1}/r^\alpha$ [7, 8]. 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 $\alpha_c$ 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 non-frustrated long-range interactions. The hamiltonian for a finite periodic chain with $N$ spins $S = 1/2$ is given by

$$H = \sum_{r=1}^{N/2} J_r \sum_{i=1}^N S_i \cdot S_{i+r},$$

where the couplings are given by

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

Here the normalization is such that the sum of all non-frustrated 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 semi-quantitative phase diagram based on these calculations in the plane $(g, \alpha^{-1})$ 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($\pi$), with $\pi$ 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($\pi$)–VBS (dimerization) transition with decreasing $\alpha$. It will be shown that this continuous transition persists until $\alpha \approx 2$, while for smaller $\alpha$ 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 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 quasi-classical (large-$S$) limit, spiral states with continuously varying periodicity can arise in such a systems. 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, 13], 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($\pi$)–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 $g \rightarrow g_c$ [7]. 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 $\alpha$ 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 $\alpha$, as illustrated in Fig. 3, can reliably give the QLRO($\pi$)–VBS phase boundary $g_c(\alpha)$ for $\alpha \gtrsim 2$.

Upon decreasing $\alpha$ below $\approx 2$, 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 $N \rightarrow \infty$ 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.

Fig. 3 shows the size dependence of the level crossing point $g_c(\alpha)$ 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 $\alpha$. For smaller $\alpha$, the corrections instead seem to be $\propto 1/N$, but a cross-over to $1/N^2$ for large $N$ seems
likely as long as the transition remains continuous. The peak location moves in the opposite direction. For some $\alpha$ and $N \to \infty$, $g_{\text{cross}}$ and $g_{\text{peak}}$ should coincide. The results indicate that both $g_{\text{cross}}$ and $g_{\text{peak}}$ have dominant $1/N$ corrections at this point. Fitted lines are shown in Fig. 3 at $\alpha = 2$, were 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 the ground state energy maximum for different long-range interaction exponents $\alpha$. The two lines show extrapolations of the $g = 2.0$ numerical data to $N = \infty$.

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

$$C(r) = \langle S_i \cdot S_{i+r} \rangle,$$

$$D(r) = \langle (S_i \cdot S_{i+1})(S_{i+r} \cdot S_{i+r+1}) \rangle.$$  

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 non-zero 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 $\alpha$ for $g < g_c$ is associated with the QLRO($\pi$)-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(\(\pi/2\)) phase, 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 \( \alpha_c \) depends only weakly on \( g \). The results are consistent with the location quoted above for the multi-critical point.

In summary, the combination of short-range frustration and long-range frustrated interactions in one dimension has been shown to lead to a first-order transition between a Néel state and a VBS with coexistence state as well. This guarantees a finite energy per spin for \( N \to \infty \) even for \( \alpha < 1 \). Instead of summing \( J_\alpha \) up to \( r = N/2 \), one could also include \( N/2 < r < N \). This should not affect the phase boundaries and critical exponents for \( \alpha > 1 \).

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