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Frustration effects in quantum spin-S chains

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In 1969, Majumdar and Ghosh [1] showed that the $J_1 - J_2$ spin-1/2 Heisenberg chain has an exactly dimerized ground state if the next-nearest neighbor exchange interaction J_2 is half the nearest neighbor one J_1. For larger spin, this model has two natural generalizations: the $J_1 - J_2$ model, and a model where the next-nearest neighbor interaction J_2 is replaced by a three-site term $J_3 \sum_i \, [(\vec{S}_i.\vec{S}_{i+1})(\vec{S}_{i+1}.\vec{S}_{i+2}) + H.c.]$. This term reduces to a next-nearest neighbor interaction of magnitude $J_2 = J_3/2$ for spin 1/2, but it is a different interaction for larger spin. A few years ago, it has been shown [2] that the $J_1 - J_3$ model has an exactly dimerized ground state for $J_3/J_1 = 1/[4S(S+1) - 2]$ whatever the value S of the spin, while the spin-1 $J_1 - J_2$ model has a first-order transition to a next-nearest neighbor Haldane phase.

In this talk, I will discuss the effect of these interactions for spin-*S* in the context of the Hamiltonian

$$H_{J_1-J_2-J_3} = J_1 \sum_i \vec{S}_i.\vec{S}_{i+1} + J_2 \sum_i \vec{S}_i.\vec{S}_{i+2} + J_3 \sum_i \, [(\vec{S}_i.\vec{S}_{i+1})(\vec{S}_{i+1}.\vec{S}_{i+2}) + H.c.]$$

Using extensive Density Matrix Renormalization Group simulations, we have derived the phase diagram of Fig. 1 for S=1. It consists of three phases [3]: a Haldane phase for small J_2 and J_3, a dimerized phase for large enough J_3, and a next-nearest neighbour (NNN) Haldane phase for large enough J_2. One remarkable aspect of this phase diagram is the nature of the phase transitions. The phase transition between the Haldane phase and the dimerized phase is continuous in the Wess-Zumino-Witten (WZW) $SU(2)_2$ universality class for small J_2, and first order for larger J_2. The transition between the Haldane phase and the NNN Haldane phase is first order. It is a topological phase transition between a topologically non-trivial phase with edge states, the Haldane phase, and a topologically trivial phase with no edge states, the NNN Haldane phase. Finally, and quite unexpectedly for an SU(2) invariant model, there is an Ising transition between the NNN Haldane phase and the dimerized phase. The continuous WZW $SU(2)_2$ and Ising transitions have been fully characterized by their central charge, their critical exponent, and their conformal tower of states. The towers of states were obtained thanks to an extension of the DMRG algorithm that allows one, in certain cases including that of critical systems, to access several excited states at almost no additional cost [4].

Inside these phases, which are all gapped, there are regions where the short-range correlations are incommensurate [5,6]. In particular, for $J_3 = 0$, i.e. for the $J_1 - J_2$ model, the correlations become incommensurate for $J_2/J_1 \approx 0.28$, still in the Haldane phase and long before the first-order transition into the NNN Haldane phase at $J_2/J_1 \approx 0.75$. These incommensurate correlations have a remarkable consequence on the edge states of the Haldane phase. In the standard Haldane phase, the ground state of an open chain is a singlet with a low-lying triplet (the Kennedy triplet [7]) if the number of sites is even, while it is a triplet with a low-lying singlet if the number of sites is odd. This means that the coupling between the emergent spin-1/2 at the edges is antiferromagnetic or ferromagnetic depending on whether the number of sites is even or odd. If, as a function of J_2, the correlations become incommensurate with a J_2-dependent wave vector, one can expect the effective coupling to oscillate between antiferromagnetic and ferromagnetic, leading in particular to zero modes where the singlet and the triplet are strictly degenerate, an expectation that is fully confirmed by DMRG calculations on finite chains [8].

Finally, similar phase diagrams with competing dimerized and Haldane phases are also realized for larger spins. DMRG results for spin 3/2 and spin 2 will be briefly discussed.

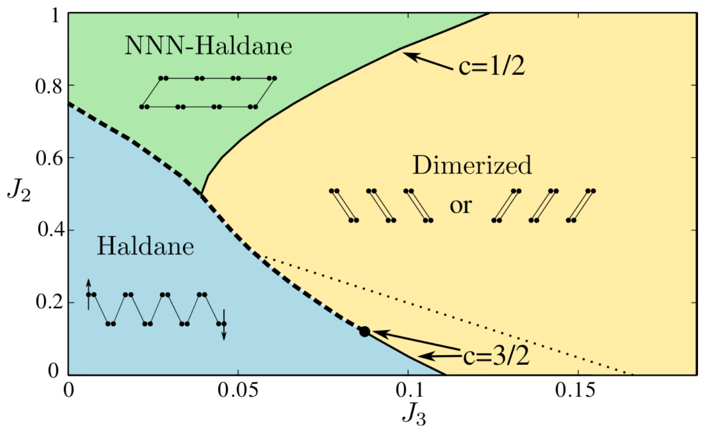

Fig. 1: Phase diagram of the spin-1 $J_1 - J_2 - J_3$ model. The sketches are illustrations of the valence-bond configurations inside each phase. Continuous lines stand for continous transitions, while the dashed line stand for first-order transitions. The dotted line is a line where the ground state is exactly dimerized.

References

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