Quantum phase transitions beyond the dilute Bose gas limit

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Abstract

We study a Heisenberg $S=1/2$ ring-exchange antiferromagnet which exhibits a quantum phase transition from a spontaneously dimerized (valence bond solid) phase to a magnetically ordered (Néel) phase. We argue that the quantum transition is of unconventional nature; both singlet and triplet modes of high density condense as the transition is approached from the dimer side, signaling restoration of lattice symmetry. These features are consistent with "deconfined quantum criticality", of which the present model is believed to be the only example so far.

Key words: Quantum phase transitions, Quantum antiferromagnets, Deconfined criticality

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Recent work on quantum critical phenomena has revealed the fascinating possibility of "deconfined criticality", where spinon deconfinement occurs at a quantum critical point (QCP) separating a valence bond solid (VBS) and magnetically ordered (Néel) phase \[1\]. In order for this exotic scenario to take place, the magnetic and VBS orders must not coexist; otherwise the spinons remain permanently “paired” in $S=1$ quasiparticles \[1,2\]. The intense search for a microscopic Heisenberg model that exhibits this novel criticality has led to a solid possibility: a $S=1/2$ model with four-spin ring exchanges \[3\]. The Hamiltonian of this two-dimensional, square-lattice model reads

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j - K \sum_{i,j,k,l} (S_i \cdot S_j)(S_k \cdot S_l),$$

(1)

where the couplings are antiferromagnetic, $J, K > 0$. The four-spin term acts on a given plaquette as $-K \{(S_1 \cdot S_2)(S_3 \cdot S_4) + (S_2 \cdot S_3)(S_1 \cdot S_4)\}$, where the spins are numbered as in Fig. 1(b). Summation is performed over all plaquettes, so that $H$ does not break the square lattices symmetries. The quantum Monte Carlo study of Ref. \[3\] found a critical coupling $(K/J)c \approx 2$, separating a VBS phase ($K > K_c$) and a Néel phase ($K < K_c$). The spontaneous dimerization in the VBS state was suggested to be of the columnar dimer type, as in Fig. 1(b).

In the present work we study the model \(\text{[1]}\) by approaching the QCP from the dimerized phase. In this case it is natural to represent the spins in terms of “bond triplons” \(t^\dagger_{\alpha} \), $\alpha = x, y, z$ \[4\] which create $S=1$ triplet excitations on a given dimer $i$ (see Fig. 1(b)). These quasiparticles are hard-core, meaning that two triplons cannot be created on the same site (dimer). The analysis of the effective Hamiltonian $H_{\text{eff}}[t_\alpha]$, written in terms of the triplon operators, leads to the spectrum $\omega(k)$ which determines the location of the QCP where the magnetically ordered state emerges.

Even though the representation of the original spin Hamiltonian in terms of $H_{\text{eff}}[t_\alpha]$ is exact, in practice one has to deal with the various interactions between the triplons in an approximate way. These interactions include both the kinematic hard-core constraint and the various dynamic triplon-triplon scattering vertices. For the model \(\text{[1]}\) up to 8-point vertices appear. The success of perturbation theory in treating such interactions is determined by the quasiparticle density $n$ which it typically low (microscopically the density is related to the quantum fluctuations). In quantum spin models involving explicit dimerization, i.e. situations where some of the exchange coupling are stronger than the others (such as spin ladders, coupled ladders, bilayer models, etc.), calculations based on the triplon representation are reliable even at the mean-field level \[4\]. Improvements beyond mean-field theory can be made by resummation of selected diagrams (at lowest order in the density) as typically done in the case of a dilute Bose gas \[5\]. This leads to accuracy within 10 percent, corresponding roughly to the low quasiparticle density $n \lesssim 0.1$.

It is clear that since for the model \(\text{[1]}\) the VBS order is spontaneous and is expected to disappear at the QCP, the triplons are not necessarily in the dilute limit, especially around the QCP. This makes the analysis quite involved.
and the results somewhat dependent on the level of approximation. Moreover, the destruction of the dimer order at the QCP is expected to lead to vanishing of a singlet energy scale $E_s$ (in addition to the vanishing of the triplon gap). Here we present our main results while the technical details will be available elsewhere [6].

We have found that the quantum fluctuations in the dimer background are strong, which is evident from the fact that the four-spin $K$ term in (1) favors equally “vertical” dimer ladders (as in Fig. 1(b)) and horizontal ones, obtained by a 90 degree rotation. Since the triplons are constructed on a fixed dimer pattern, such a tendency towards restoration of rotational symmetry is related to the tendency of the triplons to form “pairs” with total spin $S=0$, in essence reflecting “plaquetization”. Within our approach this is a non-perturbative effect. We denote the energy of such a two-triplon singlet excited state by $E_s$ (it is easy to see that the lowest singlet branch also carries zero total momentum), and its wave-function is of the form $|\Psi\rangle = \sum_\alpha, q \Psi(q) t_\alpha^\dagger t_\alpha |0\rangle$. The pairing involving four triplons is energetically much less favorable. The excitation energy $\omega(k)$ of the one-triplon $(t_{\alpha, k}^\dagger |0\rangle)$ spin $S=1$ state has a minimum at the Néel ordering wave-vector $k_{AF} \equiv (\pi, \pi)$: we define the gap as $\Delta \equiv \omega(k_{AF})$. The evolution of $\Delta$ and $E_s$ as a function of the coupling $K/J$ is shown in Figure 1(a). We find that the quantum phase transition to the Néel phase takes place at $(K/J)_c \approx 2.16$, where $\Delta \rightarrow 0$, in good agreement with the Monte Carlo result [3]. In addition, the singlet energy scale $E_s$ also vanishes at the QCP, reflecting the destruction of the dimer order. The direct evaluation of the two dimer order parameters $D_x = |\langle S_3 \cdot S_i \rangle - |\langle S_5 \cdot S_i \rangle|$ and $D_y = |\langle S_3 \cdot S_i \rangle - |\langle S_1 \cdot S_i \rangle|$, where spins are numbered as in Fig. 1(b), indeed shows that they exhibit a tendency to vanish at the QCP. $D_x, D_y$ are plotted in Figure 1(c).

The unconventional merger of singlet and triplet modes at the QCP is accompanied however by an increase of the triplon quasiparticle density $n$. (c.) Dimer order parameters.

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Fig. 1. (a.) Lowest triplet ($\Delta$) and singlet ($E_s$) energy gaps near the QCP. The singlet binding energy $\epsilon = 2\Delta - E_s$. (b.) Triplon quasiparticle density $n$. (c.) Dimer order parameters.