Quantum Phase Transition in Coupled Spin Ladders

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The ground state of an array of coupled, spin-half, antiferromagnetic ladders is studied using quantum wave theory, exact diagonalization (up to 36 sites) and quantum Monte Carlo techniques (up to 256 sites). Our results clearly indicate the occurrence of a zero-temperature phase transition between a Néel ordered and a non-magnetic phase at a finite value of the inter-ladder coupling ($\alpha_c \simeq 0.3$). This transition is marked by remarkable changes in the structure of the excitation spectrum.

Ground-state (GS) correlations in a quantum antiferromagnet are closely related to the nature of low-energy excitations. This is deeply connected to the mechanism of spontaneously symmetry breaking and turns out clearly whenever competing GS’s give rise to a quantum phase transition, leading in general to remarkable changes of the excitation spectrum at the critical point. A simple model system experiencing such changes in the structure of low-energy excitations in correspondence of a quantum phase transition is the spin-half Heisenberg antiferromagnet on a two-dimensional array of coupled ladders:

$$\hat{H} = J \sum_r \hat{S}_r \cdot \hat{S}_{r+x} + \sum_r J_\alpha \hat{S}_r \cdot \hat{S}_{r+y},$$

where $\hat{S}_r = (\hat{S}^x_r, \hat{S}^y_r, \hat{S}^z_r)$ are $s = 1/2$ operators on the sites $r = (r_x, r_y)$ of a $L \times L$ lattice with periodic boundary conditions; $\hat{y} = (1, 0)$, $\hat{y} = (0, 1)$, $J_r = J$ or $J_r = \alpha J$ ($J > 0$), depending on the parity of $r_y$, and $\alpha$ is the inter-ladder coupling (see Fig. 1). Such Hamiltonian interpolates between the Heisenberg model on the square lattice ($\alpha = 1$) and a system of $L/2$ decoupled two-leg ladders ($\alpha = 0$). In the square lattice limit, the GS has Néel long-range order, with a gapless excitation spectrum and a sizable value of the antiferromagnetic order parameter. The two-leg ladder, instead, has a finite triplet gap in the thermodynamic limit and no long-range antiferromagnetic order. As a result a quantum critical point between a gapless, magnetically ordered phase and a non-magnetic GS of purely quantum mechanical nature is expected at a critical value of the inter-ladder coupling, $\alpha_c$. Besides its intrinsic theoretical interest, this model has been recently studied due to the discovery of several compounds, such as SrCu$_2$O$_3$ and (VO)$_2$P$_2$O$_7$, displaying clear signatures of a finite gap ($\sim J/2$) in the excitation spectrum related to the underlying ladder structure. In addition, the coupled-ladder Hamiltonian has been also considered as a simplified model for the magnetism of the striped phase in CuO$_2$ planes of hole-doped high-–$T_c$ copper-oxides.

In this paper, by means of spin-wave (SW) theory, exact diagonalization by the Lanczos method and zero-temperature quantum Monte Carlo techniques, including variational and Green function Monte Carlo techniques (GFMC), we focus on the GS and the low-energy excitations of the coupled spin-ladder model. In particular, by means of a systematic size-scaling analysis, we will show how the structure of low-energy excitation spectrum provides very clear indications of the changes of the GS state correlations occurring at a critical point, thus allowing us to put on firmer grounds the existence of a quantum phase transition at $\alpha_c \simeq 0.3$.

The simplest approach to the study the effects of zero-point fluctuations on the GS correlations of a quantum magnet is SW theory. This has turned out to be a very reliable approximation of the GS of spin-half systems whenever it has long-range antiferromagnetic order even in presence of strong quantum fluctuations. By the use of the standard Holstein-Primakoff representation of the spin operators we can compute the fluctuations over the classical solution at the leading order in $1/\beta$. In contrast to the Heisenberg model on the square lattice, the reduced translation symmetry along the $y$ direction, implies the existence of two inequivalent branches of SW excitations, and the energy of such SW modes, $\omega^{\pm}_k$, reads

$$\omega^{\pm}_k = \left[2D^2 - (\gamma^2_k + \gamma^2_k) - 2\delta^2_k \pm 2F_k \right]^{1/2},$$

with $F_k = \left[(\gamma^2_k - \gamma^2_k)^2 + 4\delta^2_k (\gamma_k + \gamma^2_k)^2 \right]^{1/2}$, $\gamma_k = (\cos k_x + \cos k_y)/2$, $\delta_k = (1 - \alpha)/(2 + (1 + \alpha) \sin k_y)$, $k = k + (0, \pi)$, $D = (1 + \beta)/2$, and $\beta = 2/(1 + \alpha)$. The dispersion relation of the two SW modes is plotted in Fig. 3. Notice that...
for $\alpha < 1$ a finite gap develops between the optical and the acoustical branch of the SW dispersion along the $y$-direction due to the reduced translation symmetry. The acoustical branch remains always gapless at $k = (0, 0)$ and $k = (\pi, 0)$, corresponding to the Goldstone modes (in a reduced-zone scheme) associated with the SU(2) symmetry-breaking assumption.

The expansion of the staggered magnetization at the first order in $1/\alpha$ provides accurate estimates of the GS energy only in the regime of large inter-ladder coupling ($\alpha \gtrsim 0.6$) thus suggesting that the SW approach underestimates the actual effect of quantum fluctuations and, therefore, the critical value of the inter-ladder coupling.

By means of the SW analysis it is also possible to derive a variational wave function providing a good representation of the GS and low-lying excited states at least for $\alpha \to 1$, when long-range antiferromagnetic correlations are expected. This wave function, which is also easily computable when used for importance sampling in a GFMC calculation to reduce the numerical effort \cite{1}, can be obtained starting from a Néel ordered state and including Gaussian fluctuations by means of a Jastrow factor \cite{1}:

$$|AF\rangle = \mathcal{P}_S \sum_x S_M(x) \exp \left\{ \frac{1}{2} \sum_{r, r'} v(r - r') S^z_r S^z_{r'} \right\} |x\rangle .$$

Here $|x\rangle$ is an Ising spin configuration specified by assigning the value of $S^z$ for each site, $\mathcal{P}_S$ is the projector onto the subspace with $S^z_{tot} = \sum_r S^z_r = S$, and $S_M(x) = (-1)^N_1(x)$ is the Marshall sign, reproducing exactly the phases of the GS \cite{2}. For the two-body Jastrow potential, the simple form, based on the consistency with linear SW theory in the square lattice case \cite{1}, $v(r) = (\eta/L^2) \sum_{k \neq 0} e^{-ik \cdot r} v_k$, with $v_k = 1 - \sqrt{(1 + \Gamma_k)/(1 - \Gamma_k)}$, $\Gamma_k = (\cos k_x + \cos k_y)/2$, and $\eta$ variational parameter, provides good variational estimates only for values of $\alpha$ very close to 1 (see Fig. 3-b), as it is expected since the modulation of the exchange interaction weakens the antiferromagnetic ordering and enhances spin fluctuations.

![FIG. 2. Linear SW dispersion relation for $\alpha = 1.0$ (continuous line), $\alpha = 0.8$ (short dashes), and $\alpha = 0.6$ (long dashes).](image)

![FIG. 3. (a): $\alpha$-dependence of the exact GS energy per site for $L = 4$ (triangles), 6 (squares), 10 (pentagons), and 12 (circles). Stars and continuous line are bulk-limit extrapolations and the dashed line is the linear SW prediction. (b): accuracy of the variational energy of the SW-like wave function of Eq. (4) with the isotropic Jastrow potential of Ref. \cite{1} (empty symbols) and with its generalization to coupled ladders (full symbols). 6 $\times$ 6: squares; 12 $\times$ 12: circles.](image)
Useful indications on the nature of the thermodynamic GS can be obtained numerically by studying the finite-size scaling of the GS energy, which is deeply connected to the nature of the excitation spectrum and therefore to possible thermodynamic broken symmetries [13]. In fact, in presence of Néel long-range order, being the spectrum gapless and the magnon dispersion relation linear in the wave vector $k$, the leading finite-size correction to the GS energy per site, $e_0(L) = E_0(L)/L^2$, is $O(L^{-3})$ [14]. Instead, in presence of a finite correlation length, a finite gap in the spin excitation spectrum and an exponential asymptotic dependence is expected. Here we have assumed a size dependence of the form

$$e_0(L) = e_0(\infty) + e_0 \exp(-L/L_0)/L^2,$$

which has been employed in Ref. [15] for the two-leg ladder. As it is shown in Fig. 4, the size-scaling law predicted for a long-range ordered GS is fulfilled for values of $\alpha$ close enough to 1 while for small value of $\alpha$ a clear deviation from this behavior is observed and the exponential law (5) is instead satisfied. This provides another numerical evidence of the melting of the antiferromagnetic long-range order due to the transition to the ladder-like regime.

The occurrence of a quantum phase transition to a non-magnetic GS is clearly confirmed by the study of the spin gap shown in Fig. 3. This physical quantity can be measured straightforwardly with GFMC by performing two different simulations in the $S_{\text{ladder}}^z = 0$ and $S_{\text{ladder}}^z = 1$ subspaces. In contrast to finite-temperature algorithms, the calculation of the spin gap within GFMC does not involve any fitting procedure of low-temperature data and it is exact within statistical error. As shown in the left panel of Fig. 5 the triplet gap, $\Delta = E_1 - E_0$, is a decreasing function of the inter-ladder coupling even if, on finite-sizes, this quantity is always non-zero for any value of $\alpha$. However, the size scaling of the spin gap, shown in the right panel of the same figure, indicates a clear deviation from the size dependence expected in presence of long-range Néel order [14].

$$\Delta_L = a/L^2 + b/L^3,$$

and the opening of a finite gap in the thermodynamic excitation spectrum for $\alpha \lesssim 0.35$. In this regime the extrapolation to the bulk limit of the finite-size data can be done using a law of the type [16]:

$$\Delta_L = \Delta + a/L^2 + b/L^4.$$  

An estimate of the critical value of the inter-ladder coupling can be obtained by fitting the extrapolated values of the gap with the scaling law $\Delta \sim (\alpha_c - \alpha)^{\nu}$, with $\nu \approx 0.69$, predicted for a quantum phase transition in (2+1) dimensions [1]. This procedure gives the value $\alpha_c \approx 0.32 \pm 0.03$, in agreement with previous numerical estimates obtained with finite-temperature algorithms [5,7] and the mean-field predictions of Ref. [17] but in contrast with the conclusions of bond-mean-field theory [2] indicating the vanishing of the gap for infinitesimal values $\alpha$. In contrast to frustrated systems like the $J_1-J_2$ model, where the SW theory provides an accurate prediction of the transition to a non-magnetic phase due to competing interactions [18,19], in this case the SW result ($\alpha_c \sim 0.01$) grossly underestimate the exact one. This can be ascribed to the fact that in this model there are no competing GS’s at the classical level, the Néel state being stable up to $\alpha = 0$, and the transition has therefore a pure quantum origin. Within the $1/s$ expansion, instead, the SW velocity remains finite up to $\alpha = 0$ and the reduction of the staggered magnetization is only due to the crossover to the one-dimensional regime in which antiferromagnetic long-range order is unstable.

![FIG. 4. Size scaling of the GS energy per site for $\alpha = 0.1$ and $\alpha = 0.6$. The dashed line is the linear fit of the data for $L \leq 10$ and the continuous line is the fit according to Eq. (5).](image1)

![FIG. 5. Left panel: $\alpha$-dependence of the triplet gap for various lattice sizes. Stars are bulk-limit extrapolations according to Eq. (5) and the dashed line is a fit according to $\Delta \sim (\alpha_c - \alpha)^{0.69}$. Right panel: size scaling of the triplet gap for different values of $\alpha$. Continuous and dashed lines are fits according to Eqs. (6) and (7), respectively.](image2)
E to behave as the spectrum of a free quantum rotator, indications of the opening of a finite spin gap in inter-ladder coupling, our numerical results provide ro-
theory turns out to be reliable only in the regime of weak spin-wave theory and a numerical analysis of the finite-
properties of an array of coupled spin-half ladders using behavior of is evident from Fig. 6 displaying the very different be-
ent zero-temperature phases of the present model, as it excitation spectrum clearly discriminate the two differ-
verges linearly with the volume. These features of the

A major fingerprint of the dramatic changes in the structure of the excitation spectrum occurring in corre-
spondence of the above quantum phase transition can be found in the finite-size behavior of the so called rigid rotator anomaly $\tilde{\chi}^{-1}$, $\alpha < 0.2$, and $\alpha = 0.8$: $L = 6$ (triangles), 8 (squares), 10 (circles). Upper panel: size scaling of $\delta \chi L^2$ for (from the top) $\alpha = 0.2$, 0.25, 0.3, 0.4, and 0.8. Lines are weighted quadratic fits.

where $E_S$ is the energy of the lowest excitation with spin $S$. In fact, in presence of long-range antiferromagnetic order, the low-lying excited states of spin $S$ are predicted to behave as the spectrum of a free quantum rotator, $E_S - E_0 \propto S(S+1)/L^2$, as long as $S \ll L^2$. In contrast, the expected behavior for a spin ladder is $E_S - E_0 \propto S$, as it is easy to understand in a spin-liquid Resonating Valence Bond (RVB) picture $[10]$. As a result, in the gapless phase the rigid rotator anomaly $\delta \chi^{-1}$ has to vanish identically in the thermodynamic limit while in the gapped regime $\delta \chi^{-1}(S) \propto L/(S(S+1) - 1)$ diverges linearly with the volume. These features of the excitation spectrum clearly discriminate the two different zero-temperature phases of the present model, as it is evident from Fig. 6 displaying the very different behavior of $\delta \chi^{-1}$ below and above the critical point.

In summary, we have investigated the ground-state properties of an array of coupled spin-half ladders using spin-wave theory and a numerical analysis of the finite-size low-energy excitation spectrum. While the spin-wave theory turns out to be reliable only in the regime of weak inter-ladder coupling, our numerical results provide robust indications of the opening of a finite spin gap in the thermodynamic limit for $\alpha \lesssim 0.3$, corresponding to a quantum phase transition between a gapless Néel ordered phase and a spin-liquid RVB ground state.

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\[ \frac{1}{2\chi_S} = \frac{L^2 E_S - E_0}{S(S+1)}, \]