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Susceptibilities and spin gaps of weakly-coupled spin ladders

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We calculate the uniform and staggered susceptibilities of two-chain spin-$\frac{1}{2}$ Heisenberg ladders using Monte-Carlo simulations. We show that the gap extracted from the uniform susceptibility and the saturation value of the staggered susceptibility are independent of the sign of the inter-chain coupling $J_\perp$ in the asymptotic limit $|J_\perp|/J \to 0$. Furthermore, we examine the existence of logarithmic corrections to the linear scaling of the gap with $|J_\perp|$.

Spin ladders are arrays of coupled spin chains and exhibit structures that interpolate between a single one-dimensional chain and the two-dimensional square lattice. Their properties are peculiar as the magnetic spectrum is gapless only in the case of non-integer-spin ladders formed of an even number of chains.[1,2] Spin-$\frac{1}{2}$ ladders are thus closely related to spin-S chains for which the excitations are gapped for integer spins and gapless otherwise.[3] An important question is the understanding of the transition between the gapless chain and the gapped ladder (the Haldane phase). That issue has been studied both analytically[4,5] and numerically.[6,7]

In this paper, we report results of Monte-Carlo simulations on two-chain spin-$\frac{1}{2}$ ladders with antiferromagnetic coupling along the chain direction and ferromagnetic or antiferromagnetic coupling across the rungs. We calculate the uniform and staggered susceptibilities and show that, in the asymptotically weak rung-coupling regime, these thermodynamic quantities are independent of the sign of the rung coupling. In this regime, our results for the spin gap are consistent with the theoretically-predicted existence of logarithmic corrections to the linear behavior $\Delta \sim |J_\perp|$.

The spin-$\frac{1}{2}$ Heisenberg ladder magnet is described by the following Hamiltonian:

$$H = J\sum_{i=1}^{N}\sum_{n=1}^{2}\mathbf{S}_{i,n}\cdot\mathbf{S}_{i+1,n} + J_\perp\sum_{i=1}^{N}\mathbf{S}_{i,1}\cdot\mathbf{S}_{i,2} \qquad (1)$$

where i runs along the chains, N is the length of the chains, J is the antiferromagnetic coupling along the chain direction and $J_\perp$ is the coupling between the two chains (the rungs of the ladder). We consider both antiferromagnetic ($J_\perp > 0$) and ferromagnetic ($J_\perp < 0$) rung couplings. The Hamiltonian Eq. (1) is investigated with the loop cluster algorithm with a discrete Euclidean time grid.[6,8] Periodic boundary conditions are used along the chain direction as well as in the Euclidean time direction. The chain length is kept larger than six times the spin-spin correlation length[9]. The Trotter number, which defines the discretization of the Euclidean time axis, is kept larger or equal to $20/T$ where T is the temperature. We calculate the uniform and staggered susceptibilities,

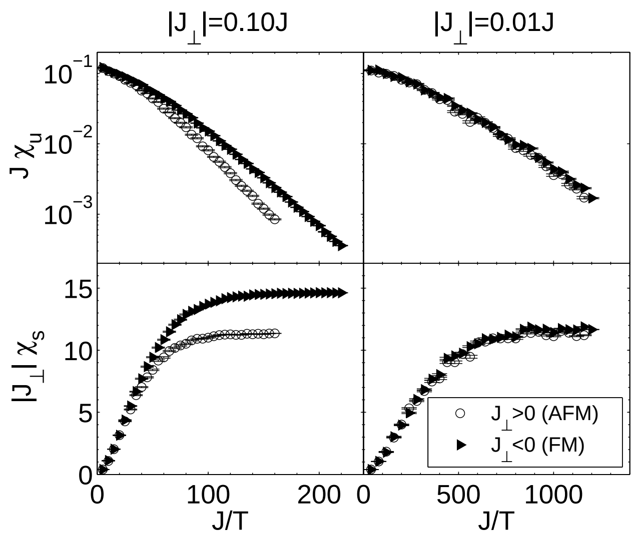

FIG. 1: Uniform (top) and staggered (bottom) susceptibilities as function of the inverse temperature for the spin-$\frac{1}{2}$ ladder. Left (right) panels are for rung couplings $|J_\perp| = 0.10J$ ($|J_\perp| = 0.01J$).

defined as:

$$\chi_u(T) = \frac{1}{2NT}\left\langle\left(\sum_{i=1}^{N}\sum_{n=1}^{2}S^z_{i,n}\right)^2\right\rangle \qquad (2)$$

$$\chi_s(T) = \frac{1}{2NT}\left\langle\left(\sum_{i=1}^{N}\sum_{n=1}^{2}(-sgn(J))^i(-sgn(J_\perp))^n S^z_{i,n}\right)^2\right\rangle \qquad (3)$$

Studies at intermediate and large couplings show that finite-size effects, both in the Euclidean time direction and in the chain direction, are smaller than the statistical uncertainties for the two observables when the lattice dimensions were kept larger than the previously defined limits. The same relations for the required system size were assumed to apply in the small coupling regime.

Figure 1 shows examples of the uniform susceptibility and staggered susceptibility for ferromagnetic and antiferromagnetic $J_\perp$. For $|J_\perp| = 0.01J$ we find that the

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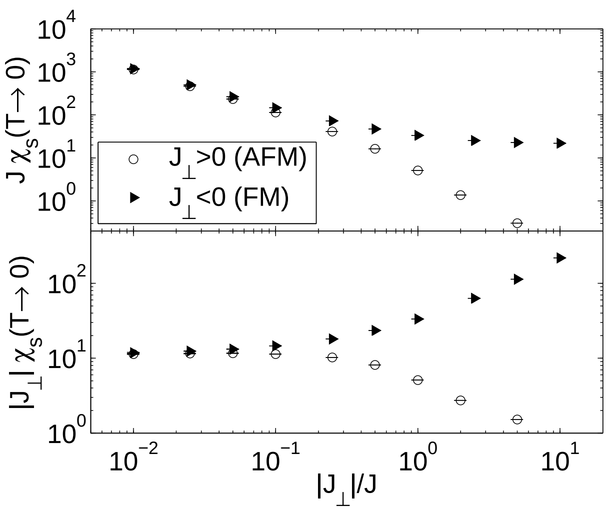

FIG. 2: Low-temperature staggered susceptibility as a function of the rung coupling.

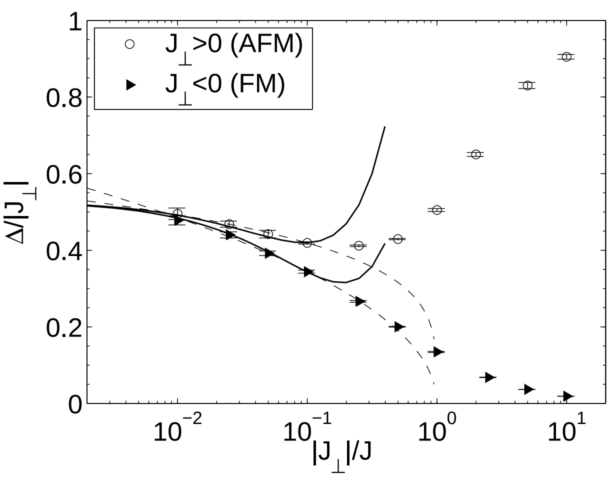

FIG. 3: Spin gap as function of the rung coupling for both ferromagnetic and antiferromagnetic rung couplings. The dashed lines are fits to $D\,[ln(|J_\perp|/J)]^E$ with exponent E of 0.5 and 0.23 for, respectively, for ferromagnetic and antiferromagnetic rung coupling (Eq. (6) and Eq. (7), respectively). The continuous lines are fits to Eq. (5), with coefficients $A = 0.53(2)$, $B = 2.2(5)$, as well as $C = 3.9(5)$ ($C = 2.0(6)$) in the antiferromagnetic (ferromagnetic) case.

susceptibilities become independent of the sign of $J_\perp$, consistent with theoretical expectations for two weakly-coupled Heisenberg chains.[5]

Figure 2 shows the dependence of the extrapolated zero-temperature staggered susceptibility on $J_\perp/J$. In the weak-rung-coupling regime, $\chi_s(0)$ varies linearly with $|J/J_\perp|$, as can be seen in the bottom panel of Fig. 2. We find that $|J_\perp|\chi_s(0) = 11.5(5)$ for $|J_\perp|/J \to 0$.

The spin gap is extracted from the uniform susceptibility using the following low temperature form:[4]

$$J\chi_u(J_\perp, T) \sim T^{-1/2} e^{-\Delta(J_\perp)/T} \tag{4}$$

where Δ is the gap. This limit is derived from a non-interacting magnon model with a quadratic band dispersion. The fits are performed for $T \lessapprox \Delta/3$, and the results are shown in Fig. 3. The data for antiferromagnetic rung couplings ($J_\perp > 0$) agree well with previously reported results.[6] In the weak coupling limit, the gap deviates from a linear dependence on $J_\perp$. For the ferromagnetic rung coupling, values of the gap at intermediate rung couplings ($0.1 \le |J_\perp|/J < 1$) are in agreement with previous reports[10,11,12].

At very large ferromagnetic rung coupling, the spin-$\frac{1}{2}$ ladder is equivalent to a spin-1 chain with coupling $J/2$. The gap for the spin-1 chain was calculated to be $\Delta = 0.41050(2)J$[13] or $\Delta = 0.4107(1)J$[14] by the density matrix renormalization group (DMRG) technique. In the present investigation, the spin-1 chain gap was estimated at $0.406(3)J$, which agrees reasonably well with the DMRG value. At finite ferromagnetic coupling $J_\perp$, the ratio $\Delta/J_\perp$ increases with decreasing value of $J_\perp$. At small rung coupling, the data for the antiferromagnetic and ferromagnetic rung coupling exhibit a similar trend. Together with the behavior of the staggered susceptibility, this seems to confirm the assertion[5,15] that the properties of a two-chain spin-1/2 spin ladder are independent of the sign of $J_\perp$ in the weak coupling limit.

In the weak-coupling regime, the gap has a nearly linear dependence on the rung coupling $J_\perp$. Logarithmic corrections have been proposed to this linear dependence based on field theoretical considerations. Shelton, Nersesyan and Tsvelik[5] concluded that the gap follows the form:

$$\Delta = A|J_\perp|\left(1 + BJ_\perp ln\left(C\frac{|J_\perp|}{J}\right)\right) \tag{5}$$

where A, B and C are unknown constants. Totsuka and Suzuki[16], on the other hand, suggested that the gap be described by

$$\Delta = D|J_\perp|\sqrt{ln\left(\frac{|J_\perp|}{J}\right)} \tag{6}$$

For $|J_\perp|/J \le 0.1$, Eq. (5) describes the gap well for both antiferromagnetic and ferromagnetic rung couplings, while Eq. (6) satisfactorily describes only the ferromagnetic result. A modified form of Eq. (6) is necessary to obtain an acceptable description for antiferromagnetic rung couplings:

$$\Delta = 0.344(4)|J_\perp|\left(ln\left(\frac{|J_\perp|}{J}\right)\right)^{0.23(2)} \tag{7}$$

Although Eq. (5) describes both results well below $|J_\perp| = 10^{-1}J$, it would be necessary to know the gap at rung couplings well below $|J_\perp| = 10^{-2}J$ in order to conclusively establish that this form is asymptotically correct in the limit $|J_\perp|/J \to 0$.

In conclusion, we have calculated the uniform and staggered susceptibilities for the spin-$\frac{1}{2}$ two-chain Heisenberg ladder. We establish that the susceptibilities are independent of the sign of $J_\perp$ in the weak-coupling regime $|J_\perp|/J \ll 1$. In that regime, the staggered susceptibility is linear in $J/|J_\perp|$, while the excitation gap is described by a logarithmic correction to the linear dependence on $|J_\perp|$.

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