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Phase transition, longitudinal spin fluctuations, and scaling in a two-layer antiferromagnet

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We consider a two-layer Heisenberg antiferromagnet which can be either in the Néel-ordered or in the disordered phase at $T = 0$, depending on the ratio of the intralayer and interlayer exchange constants. We reduce the problem to an interacting Bose gas and study the sublattice magnetization and the transverse susceptibility in the ordered phase, and the spectrum of quasiparticle excitations in both phases. We compare the results with spin-wave theory and argue that the longitudinal spin fluctuations, which are not included in the spin-wave description, are small at vanishing coupling between the layers, but increase as the system approaches the transition point. We also compute the uniform susceptibility at the critical point to order $O(T^2)$, and show that the corrections to scaling are numerically small, and the linear behavior of χ_u extends to high temperatures. This is consistent with the results of the recent Monte Carlo simulations by Sandvik and Scalapino.

I. INTRODUCTION

In the past few years, there has been a significant interest in the physics of quantum phase transitions in two-dimensional (2D) spin systems.[1–7] The purpose of the present paper is to study in detail the disordering transition in a two-layer $S = 1/2$ Heisenberg antiferromagnet described by

$$H = J_1 \sum_{\langle i,j\rangle,\alpha} \vec{S}_{\alpha,i}\vec{S}_{\alpha,j} + J_2 \sum_i \vec{S}_{1,i}\vec{S}_{2,i} \quad . \tag{1}$$

Here $\alpha = 1, 2$, the first sum runs over nearest neighbors, and the exchange couplings are assumed to be positive (see Fig. 1).

For small J_2/J_1, the model describes two weakly interacting 2D Heisenberg antiferromagnets. Each of them is ordered at $T = 0$ and possesses Goldstone excitations related to a spontaneous breakdown of a rotational symmetry. In the opposite limit, $J_2/J_1 \gg 1$, pairs of adjacent spins from different layers form spin singlets separated from triplet states by a gap, $\sim J_2$. The presence of a gap implies that the rotational symmetry is not broken. Thus one should expect a disordering phase transition at some critical ratio of J_2/J_1.

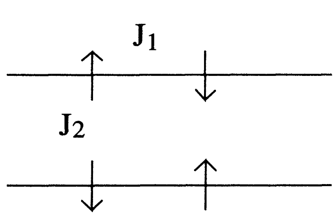

FIG. 1. The system under consideration is a two layer antiferromagnet with intralayer exchange coupling J_1 and interlayer exchange coupling J_2.

The two-layer Heisenberg model has attracted a lot of interest in the last few years.[8–16] This interest was stimulated in part by the experimental observation that some of the high-T_c superconductors contain pairs of CuO_2 layers which are separated from other layers by a charge reservoir.[8,9] In addition, a two-layer antiferromagnet is probably the simplest *nonfrustrated* spin system which displays a quantum disordering transition of the O(3) universality class. Several quantitative predictions about the behavior of observables near such a transition have been made recently,[3] and a two-layer antiferromagnet is an ideal candidate to test these predictions.

The phase diagram of Eq. (1) has been studied numerically, by quantum Monte Carlo,[14] series expansion,[12] and exact diagonalization[16] techniques, and analytically, using spin-wave[9–11] and mean-field Schwinger-boson theory.[13] There are several issues which emerged from these studies. Some of them are related to the universal ratios of various observables and are discussed elsewhere.[17] Here we will focus on the properties of the system at $T = 0$, and on the corrections to scaling at finite T. The key issue we want to address at $T = 0$ is the applicability of perturbative and self-consistent spin-wave approaches (the latter is very similar to the Schwinger-boson mean-field theory). It is well known that spin-wave expansion works extremely well for a single-layer $S = 1/2$ antiferromagnet. At the same time, for a two-layer system, spin-wave and Schwinger-boson theories yield results which are inconsistent with numerical simulations. In particular, the Schwinger-boson mean-field theory yields a critical value of the interlayer coupling of $(J_2/J_1)_{\rm cr} \approx 4.5$,[13] which is nearly 2 times larger than $(J_2/J_1)_{\rm cr} \approx 2.55$ obtained in series expansion[12] and quantum Monte Carlo[14] studies. A self-consistent spin-wave theory (see Ref. 11 and Sec. I A) also predicts a very large value of $(J_2/J_1)_{\rm cr} \approx 4.3$. The predicted value of the spin-wave velocity at the critical point, $c_{\rm sw} \approx 2J_1$, is also somewhat larger than the Monte Carlo result $c_{\rm sw} \approx (1.7 - 1.8)J_1$ (where we set the lattice constant a_0 equal to unity). We will argue that the discrepancies between the spin-wave results and the numerical simulations have a physical origin and are related to the fact that in the spin-wave approach one neglects longitudinal spin fluctuations. Our analytical approach to the problem is based on the introduction of a triplet of $S = 1$ bosons for a pair of $S = 1/2$ spins [see Eq. (7) below]. In the disordered phase, this triplet of bosons describes the excitations above the singlet ground state of a pair, while in the ordered phase, where we introduce a condensate for one type of boson, the excitations are split into two transverse and one longitudinal magnon modes. We will show that the contributions from longitudinal fluctuations to $J_2^{\rm cr}$ and $c_{\rm sw}$ are substantial, which makes the $1/S$ expansion inapplicable. However, we will also show that as J_2 decreases, the spin-wave approximation becomes more and more reliable, and at vanishing J_2, longitudinal spin fluctuations do not contribute to the sublattice magnetization and susceptibility.

Furthermore, we will discuss the temperature dependence of the uniform susceptibility χ_u at the transition point. Monte Carlo simulations have shown that the universal, linear behavior of χ_u at $J_2 = J_2^{\rm cr}$ extends up to very high $T \sim J_1$. For comparison, in a single-layer antiferromagnet, the deviations from linearity become substantial already at $T \sim 0.6J$.[18] To understand this result, we will compute the leading nonuniversal $O(T^2)$ correction to the susceptibility and show that it is numerically quite small for all $T < J_1$.

We start in the next subsection with the spin-wave calculations for Eq. (1). In Sec. II, we will introduce the transformation to bosons and consider in a systematic way the excitations in the disordered phase, the critical value of J_2, and the spin-wave velocity at the critical point. In Sec. III, we extend the approach to the ordered state by introducing a condensate for one of the bosonic fields. We will show how the triplet of excitations splits into two gapless transverse modes and a longitudinal mode with a finite gap. We will obtain the $T = 0$ sublattice magnetization and the uniform susceptibility at arbitrary J_2 and show how they deviate from spin-wave results for increasing J_2. Finally, in Sec. IV, we will compute the uniform susceptibility $\chi_u(T)$ at the critical point and show that the lattice-dependent $O(T^2)$ corrections to the scaling form of χ_u remain small up to $T = J_1$. Our conclusions are stated in Sec.V.

Spin-wave calculations

We start our considerations with a brief review of the spin-wave calculations. At small J_2, the spins are ordered antiferromagnetically in the layers and also between the layers. Introducing bosons via the Holstein-Primakoff transformation, and performing standard manipulations, we obtain two branches of spin-wave excitations with the dispersion $\epsilon_1(k) = \epsilon_2(k+\pi) = \epsilon_k$, where, to order $1/S$,[9,10]

$$\epsilon_k = 4\bar{J}_1 S[(1-\nu_k^2) + (\bar{J}_2/2\bar{J}_1)(1-\nu_k)]^{1/2}, \qquad (2)$$

and $\nu_k = (\cos k_x + \cos k_y)/2$. It is not difficult to show that the fluctuations near $k = (\pi,\pi)$ are in-phase fluctuations of the spins in the two layers, while those near $k = 0$ correspond to out-of-phase fluctuations. There is indeed a Goldstone mode in ϵ_k at $k = (\pi,\pi)$ because of a spontaneous symmetry breaking. The renormalized $\bar{J}_1$ and $\bar{J}_2$ differ from the couplings in (1) due to the $1/S$ corrections:[11]

$$\bar{J}_1 = J_1\left(1 - \frac{\delta_1+\delta_2}{S}\right), \quad \bar{J}_2 = J_2\left(1 - \frac{\delta_1+\delta_3}{S}\right), \qquad (3)$$

where

$$\delta_1 = \frac{1}{N}\sum_k \frac{4\bar{J}_1 S + \bar{J}_2 S}{2\epsilon_k} - \frac{1}{2}, \quad \delta_2 = -\frac{1}{N}\sum_k \frac{(4\bar{J}_1 S\nu_k + \bar{J}_2 S)\nu_k}{2\epsilon_k}, \quad \delta_3 = -\frac{1}{N}\sum_k \frac{4\bar{J}_1 S\nu_k + \bar{J}_2 S}{2\epsilon_k}. \qquad (4)$$

The summation in (4) is over the whole Brillouin zone. The sublattice magnetization to order $1/S$ is given by $N_0 = S - \delta_1$. Evaluating δ_1 with bare couplings $J_{1,2}$, as is required in the $1/S$ expansion, we obtain that δ_1 reaches a value of $S = 1/2$ only at a very large $J_2/J_1 \approx 13.6$. A somewhat better, though less justified estimate of $J_2^{\rm cr}$ can be obtained if one formally considers the expressions for the renormalized couplings as self-consistent equations, and solve them for $S = 1/2$. These calculations have been performed by Hida,[11] who found that the sublattice magnetization first increases with J_2, passes through a maximum, and then decreases (see Fig. 2). There is a weak first-order disordering transition at $J_2^{\rm cr} \approx 4.36J_1$. Similar results were obtained in the mean-field Schwinger-boson approach by Millis and Monien.[13] Still, the critical J_2 is much larger than $J_2^{\rm cr} \approx 2.55J_1$ obtained in numerical simulations.

In the $1/S$ expansion, one also can compute the spin-wave velocity. We performed calculations to *second* order in $1/S$, and after straightforward but somewhat tedious calculations obtained[19]

$$c_{\rm sw} = 2\sqrt{2}S\bar{J}_1\sqrt{1 + \frac{\bar{J}_2}{4\bar{J}_1}}\left(1 + \frac{Q}{4S^2}\right), \qquad (5)$$

where now $\bar{J}_{1,2}$ are the solutions of (3) and (4) to order $1/S^2$, and Q is a cumbersome function of J_2/J_1 whose explicit form we do not present. At $J_2 = 0$, we obtained $Q \approx 0.022$ which completely agrees with the results of other studies.[20] The spin-wave velocity remains finite at the critical point, and it is therefore reasonable to compute it at $(J_2/J_1)_{\rm cr} \approx 2.55$ which is suggested by numerical simulations. For this ratio of the couplings, we obtained $Q \approx 0.044$. Evaluating then $\bar{J}_{1,2}$ and substituting them into (5), we find $c_{sw} \sim 3.62 J_1 S[1+0.094/2S+0.026/(2S)^2]$. Observe that the $1/S^2$ correction is very small. For $S = 1/2$, we obtain $c_{sw} \sim 2.03\ J_1$. As we mentioned earlier, this value is somewhat larger than $c_{sw} \sim (1.7 - 1.8)J_1$ extracted from the fit of the Monte Carlo data for the uniform susceptibility[14] to the scaling formula.

The main weakness of the spin-wave theory is that it assumes that long-range order is well established, and only includes transverse spin fluctuations. However, at the critical point, transverse and longitudinal fluctuations become indistinguishable and should be treated on equal ground. We therefore proceed now to perturbative calculations which explicitly take the longitudinal spin fluctuations into account.

II. DISORDERED PHASE

The key starting point of our consideration is an observation that for sufficiently large J_2, pairs of adjacent spins from the two planes form spin singlets. The excited state of a given pair is a threefold-degenerate triplet state. It is then natural to introduce a triplet of bosons for any given pair. Each boson describes the transformation from a singlet state to one of the states with $S = 1$. Specifically, we introduce

$$\vec{M}_i = \vec{S}_{1,i} + \vec{S}_{2,i}, \qquad \vec{L}_i = \vec{S}_{1,i} - \vec{S}_{2,i}, \tag{6}$$

and three bosonic fields as

$$\begin{aligned} M_i^z &= a_i^\dagger a_i - b_i^\dagger b_i, \quad L_i^z = -(c_i^\dagger U_i + U_i c_i), \\ M_i^+ &= \sqrt{2}(a_i^\dagger c_i - c_i^\dagger b_i), \quad L_i^+ = \sqrt{2}(a_i^\dagger U_i + U_i b_i), \\ M_i^- &= \sqrt{2}(c_i^\dagger a_i - b_i^\dagger c_i), \quad L_i^- = \sqrt{2}(b_i^\dagger U_i + U_i a_i), \end{aligned} \tag{7}$$

where $U_i = \sqrt{1 - a_i^\dagger a_i - b_i^\dagger b_i - c_i^\dagger c_i}$. It is easy to check that the commutation relations for $\vec{M}$ and $\vec{L}$ are the same as for a vector and a generator of rotations: $[M^\alpha, M^\beta] = i\epsilon_{\alpha\beta\gamma} M^\gamma$, $[L^\alpha, L^\beta] = i\epsilon_{\alpha\beta\gamma} M^\gamma$, $[M^\alpha, L^\beta] = i\epsilon_{\alpha\beta\gamma} L^\gamma$. This in turn implies that the spin commutation relations for S_1 and S_2 are satisfied. The U term, however, imposes the constraint that only one boson can be excited at each lattice site. This indeed follows from the fact that there are only four physical states for a given pair of spins. For the physical states, we have $S_i^2 = 3/4$ as it should be. Notice that a similar restriction on the number of bosons holds also for the conventional Holstein-Primakoff transformation for $S = 1/2$. In this sense, the transformation above can be viewed as an extension of the Holstein-Primakoff transformation to nonmagnetic states. One can also introduce an analog to the Dyson-Maleev transformation, but we found that the latter is less convenient for practical purposes.

Furthermore, a conventional way to perform spin-wave calculations for a Néel-ordered state of a $S = 1/2$ system is to extend a model to large S, perform $1/S$ expansion, and set $S = 1/2$ at the very end of the calculations. We will now do the same for a disordered state. To this end, we modify the transformation to bosons by introducing a factor $\lambda \ll 1$ into the square root as $U_i = \sqrt{1 - \lambda(a_i^\dagger a_i + b_i^\dagger b_i + c_i^\dagger c_i)}$, and simultaneously introducing an overall factor $1/\sqrt{\lambda}$ into all three components of $\vec{L}_i$. It is not difficult to check that the commutation relations between $\vec{L}$ and $\vec{M}$ (and, hence, the spin algebra) do not change under this transformation; however, the value of the spin on each site in the ground state is now $O(1/\lambda) \gg 1$. Below, we perform a systematic perturbative expansion in λ which is similar in spirit to the $1/S$ expansion in conventional spin-wave theory. The physical results indeed correspond only to $\lambda = 1$, but we will see that the first two terms in the expansion already yield results consistent with the Monte Carlo data.

Equation (7) has been applied before to study the dimerization in the $S = 1/2$ Heisenberg model on a square lattice with an interaction between first and second neighbors,[21] and also the dimerization transition in a $S = 1$ chain.[22] We believe that this approach has some advantages over the mean-field Schwinger-boson theory. For example, it correctly reproduces the fact that at the critical point and in the disordered phase, the magnon excitation spectrum is threefold degenerate.

We now substitute (6) and (7) into the Hamiltonian. To leading order in λ, the interaction between bosons can be neglected, and diagonalizing the quadratic form in bosons, we obtain a threefold-degenerate excitation spectrum with the dispersion (cf. Ref. 16)

$$\epsilon_k = \{J_2 [J_2 - 4J_1^* + 4J_1^*(1 + \nu_k)]\}^{1/2}, \tag{8}$$

where $J_1^* = J_1/\lambda$. For sufficiently large J_2, the excitation energy is real (which indicates a stability), and there is a finite gap in the spectrum whose minimum is at $k = \pi$. This gap vanishes at $J_2 = J_2^{cr} = 4J_1^*$. Below this point, the excitations near $k = \pi$ are purely imaginary which signals an instability and implies a need for a change of the ground state.

To obtain a better estimate for the critical value of J_2, we included anharmonic terms into consideration, computed the self-energy terms by usual means, and obtained to order $O(\lambda^2)$

$$J_2^{cr} = 4J_1^* \left(1 - 0.665\lambda + \frac{1}{\pi^2}\ \lambda^2 \ln(1/\lambda) + O(\lambda^2)\right) . \tag{9}$$

We see that the first-order correction shifts the transition towards smaller J_2. If we had restricted the calculation to include only this term, we would obtain J_2^{cr} in a range between $1.34J_1$ and $2.4J_1$, depending on whether we leave the correction in the numerator or put it into the denominator. The second-order correction is *positive* and partly compensates the downshift renormalization due to the first-order term. Unfortunately, the second-order correction is logarithmically divergent at the transition,[23] and we cannot obtain the precise value of J_2^{cr} to order λ^2. We therefore can only argue that the actual value of J_2^{cr} is in between our zero-order and first-order results.

A somewhat better estimate of $J_2^{\rm cr}$ can be obtained approaching the transition from the ordered phase, and will be discussed in the Appendix. Notice, however, that the first-order estimate of $J_2^{\rm cr}$ is already closer to the numerical result than $J_2^{\rm cr} \sim 4.3 J_1$ which was obtained in a self-consistent spin-wave approach.

We also computed the spin-wave velocity at the critical point. To order $O(\lambda)$, we obtained

$$c_{\rm sw} = 2J_1^* \,(1 - 0.256\lambda) \ . \tag{10}$$

For the physical case of $\lambda = 1$, this gives $c_{\rm sw}$ between $1.49J_1$ and $1.59J_1$ again depending on whether we keep the correction in the numerator or put it into the denominator. The second-order correction to the spin-wave velocity is again positive and partly compensates the $O(\lambda)$ contribution, but it is again of the form $\lambda^2 \ln(1/\lambda)$ which prevents us from obtaining the precise value of $c_{\rm sw}$ to order $O(\lambda^2)$. Alternatively, however, we can reexpress $c_{\rm sw}$ in terms of the critical value of J_2. Doing this, we find that to order λ, $c_{\rm sw} = 0.5J_2^{\rm cr}(1 + 0.409\lambda + \cdots)$. For $\lambda = 1$, this yields $c_{\rm sw} = 0.705 J_2^{\rm cr}$. Using then the numerical result $J_2^{\rm cr} = 2.55J_1$, we obtain $c_{\rm sw} \sim 1.80J_1$ which is consistent with $c_{\rm sw} = (1.7 - 1.8)J_1$, extracted from the Monte Carlo data. In any case, the velocity we found is smaller than that obtained in the spin-wave theory.

III. ORDERED PHASE

We now consider the case $J_2 < J_2^{\rm cr}$ when the system possesses a Néel order. We assume that the sublattice magnetization N_0 is directed along the z axis. In our approach, a nonzero $N_0 \equiv N_0^z$ implies that there is a single particle condensate of the c quanta with momentum $\pi \equiv (\pi, \pi)$: $\langle c_\pi \rangle = \alpha$. In a mean-field approximation, we then have $N_0 = \lambda^{-1}\sqrt{\beta(1-\beta)}$, where $\beta = \lambda\alpha^2$. Introducing the condensate into the Hamiltonian and evaluating the ground state energy E_0 in the mean-field approximation (i.e., to leading order in λ, but keeping β fixed), we find

$$\lambda E_0 = J_2\beta - 4J_1^*\beta(1-\beta) \ . \tag{11}$$

Minimizing the energy, we obtain $\beta = \beta_0 = (4J_1^* - J_2)/8J_1^*$. For $J_2 = 0$, we have $\beta_0 = 1/2$, and hence $N_0 = 1/(2\lambda)$ as it should be. We then performed the standard computations for a Bose gas with a condensate and obtained the quasiparticle spectrum. It now contains two different branches of quasiparticle excitations. The excitation spectrum for fluctuations in the direction perpendicular to the condensate (i.e., for a- and b-type bosons) is doubly degenerate. For these excitations, we obtained to leading order in λ

$$\epsilon_\perp(k) = 4J_1^* \,(1-\beta)\, \left[(1+\nu_k)\, \left(1 - \frac{\beta}{1-\beta}\,\nu_k\right)\right]^{1/2} \ . \tag{12}$$

We see that the transverse fluctuations are gapless as they indeed should be. For the spin-wave velocity near $k = \pi$ we have

$$c_{\rm sw} = 2J_1^* \,(1-\beta)^{1/2} \ . \tag{13}$$

Observe that for $J_2 = 0$ we recover the mean-field dispersion for the Heisenberg antiferromagnet: $\epsilon_\perp = 2J_1^*(1 - \nu_k^2)^{1/2}$.

For the dispersion relation of the fluctuations along the direction of the condensate (i.e., for c-type bosons), we found

$$\epsilon_\parallel(k) = 4J_1^* \,\left[1 + (1-2\beta)^2\nu_k\right]^{1/2} \ . \tag{14}$$

We see that the longitudinal fluctuations in the ordered phase have a finite gap at the antiferromagnetic momentum, $\epsilon_\parallel(\pi) = 8J_1^*\,[\beta\,(1-\beta)]^{1/2}$. Also observe that at $J_2 = 0$, the longitudinal mode becomes dispersionless: $\epsilon_\parallel(k) = 4J_1^*$. However, we do not know whether this result survives beyond the leading order in λ. The actual dispersion for a c boson may also contain some finite imaginary part (due to higher-order terms in λ) which can be substantial at small J_2.

The computations which lead to Eq. (14) require some care. The important point is that since $\alpha \sim \lambda^{-1/2}$, there is a cancellation of the overall factor λ^n in the nth term in the expansion over density in U, and all terms in the series are in fact relevant. In practice, this implies that evaluating the contribution to the longitudinal dispersion from L_zL_z, one has to examine each term in the series, put all c bosons except for two into a condensate, compute the numerical combinatoric factor, and explicitly sum the resulting series.

We then used the results for the quasiparticle spectra and computed the sublattice magnetization and the uniform spin susceptibility beyond the mean-field level, to order $O(\lambda)$. The computations and the procedure of extending the first-order results to $\lambda = 1$ are discussed at some length in the Appendix. The results are presented in Fig. 2 and Fig. 3. For comparison, in Fig. 2, we also plotted the self-consistent spin-wave result for the magnetization. It is essential that at $J_2 = 0$, both our results are *exactly* the same as obtained in the first-order $1/S$ expansion. In other words, for a single-layer antiferromagnet, there are no independent contributions from longitudinal fluctuations. This result provides a qualitative explanation of why the $1/S$ expansion works so well for a single-layer antiferromagnet. Indeed, in our approach, we treat longitudinal fluctuation as a separate bosonic mode. At the same time, in the $1/S$ expansion, the longitudinal mode appears as a pole in the two-particle Green function. To obtain this pole, one has to sum an infinite number of the $1/S$ terms. Then, roughly speaking, the contribution from the longitudinal mode represents the contributions from high-order terms in the $1/S$ expansion. The absence of the longitudinal correction in our effective "spin-wave theory" therefore implies that the series in $1/S$ converges rapidly, and the dominant contribution comes from the first-order term.

We emphasize, however, that the longitudinal fluctuations can be neglected only for $J_2/J_1 \ll 1$. As J_2 increases, the deviation of our result for N_0 from the self-consistent spin-wave result becomes more and more substantial as seen in Fig. 2. Near the disordering transition, longitudinal and transverse fluctuations have nearly

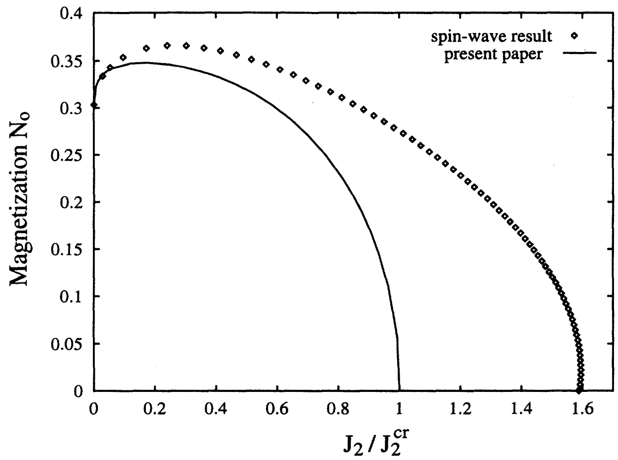

FIG. 2. Sublattice magnetization as a function of J_2/J_1. Points, the self-consistent spin-wave result; solid line, the result of our present calculations which take longitudinal spin fluctuations into account. The critical value of interlayer exchange is $J_2^{\rm cr} = 2.73 J_1$ (see the Appendix). Note that the self-consistent spin-wave theory predicts a weak first-order transition at $J_2^{\rm cr} = 4.36 J_1$ which is probably an artifact of the approximation.

equal strength, and the actual behavior of sublattice magnetization and uniform susceptibility differs in an essential way from the prediction based on the spin-wave theory.

Notice that in some range of small J_2, both the sublattice magnetization and the uniform susceptibility are larger than for a single layer; i.e., the system first becomes more "classical," and only then, at larger J_2, do quantum fluctuations push the system towards the disordering transition. The region of more "classical" behavior at intermediate J_2 has been observed in the mean-field Schwinger-boson approach;[13] it is also present in the self-consistent spin-wave analysis (see Fig. 2).

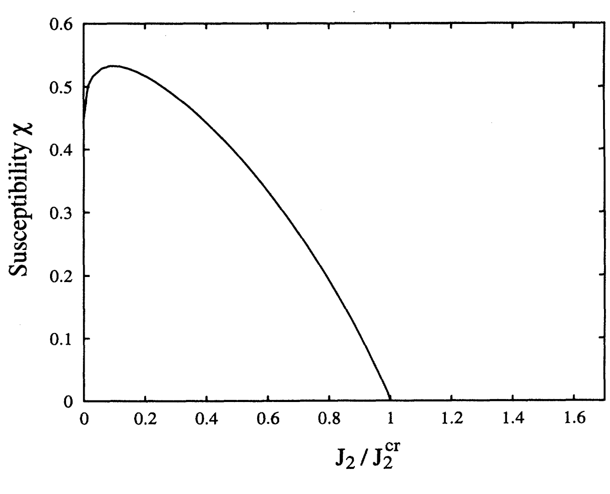

FIG. 3. Transverse susceptibility in the ordered phase as a function of J_2/J_1. The critical value of J_2 is the same as in Fig. 2.

Near the transition point, we obtained

$$N_0 = \frac{Z_N}{\lambda}\sqrt{\beta}, \qquad \chi_\perp = A(Z_\chi/4J_1)\,(\beta/\lambda^2)^{1/(1+\eta)}, \quad (15)$$

where $Z_N = 1 - 0.163\lambda$, $Z_\chi = 1 + 0.255\lambda$, and $\eta \approx 0.03$ is the critical exponent for spin correlations at criticality. The factor A cannot be obtained within the present approach because of the divergence of the Gaussian corrections near the transition point in $2+1$ dimensions. Our estimates in the Appendix place A to be roughly equal to 2. The ratio $N_0^2/[2\pi(\rho_s)^{1/(1+\eta)}]$ is an overall factor for the dynamical spin susceptibility. Using (15) and the result for the spin-wave velocity at the transition point, we obtain $N_0^2/[2\pi(\rho_s)^{1+\eta}] = B/J_1^{1+\eta}$, where $B = (1-0.06\lambda)/(2\pi A^{1+\eta})$. Three different numerical estimates of B all yield $B = 0.063$.[17] This is roughly consistent with our estimate $B = 0.149/A$, though we only approximately know that $A \sim 2$.

We also computed the quasiparticle dispersion to order $O(\lambda)$ near the transition, and explicitly obtained the Goldstone mode in the transverse channel. These calculations were performed only to leading order in β, when one can neglect cubic terms. For a general β, the Goldstone modes arise as a result of cancellations between the second-order contributions from the cubic terms and the first-order contributions from the quartic terms. A similar situation is known to exist in frustrated spin systems.[24] We did not perform explicit calculations of the spin-wave spectrum at arbitrary β and therefore cannot make a definite prediction about how longitudinal fluctuations influence the spin-wave velocity at small J_2. However, given the good agreement between our result and the spin-wave result for the susceptibility in a single-layer antiferromagnet, and the consistency between the spin-wave result for the spin stiffness, $\rho_s = c_{\rm sw}^2\chi_\perp$, and the numerical data,[25] we expect the corrections due to longitudinal fluctuations to be zero or at least small at vanishing J_2. However, near the transition point, we have already shown that the corrections to the spin-wave velocity cannot be reduced to only those due to transverse fluctuations. Thus the spin-wave result for $c_{\rm sw}$, which neglects longitudinal contributions, is most probably not quite accurate even though the velocity remains finite at the transition point, and the $O(1/S^2)$ correction to $c_{\rm sw}$ is much smaller than the $O(1/S)$ correction (see Sec. I A). In other words, we argue that near the transition, the series of $1/S$ terms is *not* rapidly convergent even if the first few terms in the series seem to indicate the contrary.

IV. UNIFORM SUSCEPTIBILITY AT THE CRITICAL POINT

In a single-layer Heisenberg antiferromagnet, the linear temperature dependence of the uniform susceptibility associated with quantum-critical behavior has been observed in the temperature range $0.35J_1 < T < 0.6J_1$. At lower temperatures, there is a crossover to another linear behavior associated with the renormalized-classical regime (which, however, has not yet been observed), while at higher temperatures, χ_u flattens and has a broad maximum at $T \sim J_1$.[18,26] How far the linear dependence extends at high T depends on the lattice-dependent corrections to scaling. The Monte Carlo results for a two-layer antiferromagnet at the critical J_2 have shown that the linearity extends to sufficiently high temperatures, $T \sim J_1$; i.e., the corrections to scaling at $J_2 = J_2^{\rm cr}$ are smaller than those of a single-layer antiferromagnet. Below we will compute these corrections perturbatively. But first we consider the σ-model description of a two-layer system, from which one can obtain the leading, universal, linear in T term in the uniform susceptibility.

A. σ-model analysis

A simple way to obtain a σ-model description of a spin-S quantum antiferromagnet, which we will follow, was suggested by Affleck.[27] In application to our system, one has to double a unit cell in each of the two layers and introduce $\vec{n}_{\alpha,i} = (\vec{S}_{\alpha,i} - \vec{S}_{\alpha,i+1})/2S$, $\vec{l}_{\alpha,i} = (\vec{S}_{\alpha,i} + \vec{S}_{\alpha,i+1})/2S$. At large S, $\vec{n}$ becomes a classical unit field with commuting components, while the commutation relations between $\vec{n}$ and $\vec{l}$ are the same as for a vector and a generator of rotations. Introducing $\vec{n}_\alpha$ and $\vec{l}_\alpha$ into the Heisenberg Hamiltonian and making a transformation from the Hamiltonian to the corresponding action which contains only the derivatives of $\vec{n}_\alpha$, we obtain the action of two interacting $O(3)$ σ models. In terms of $\vec{n}$ and $\vec{l}$, the interaction term has the form $\Xi^2(\vec{n}_1\vec{n}_2 - \vec{l}_1\vec{l}_2)$, where $\Xi^2 \propto J_2$. The generator of rotations itself contains a derivative of $\vec{n}$, $\vec{l} \sim \vec{n} \times \frac{\partial \vec{n}}{\partial \tau}$, and the $\vec{l}_1\vec{l}_2$ term thus only leads to a velocity renormalization. Neglecting this term, and also introducing the magnetic field into the action for susceptibility calculations, we obtain

$$\mathcal{S} = \frac{1}{2g}\left[(\nabla\vec{n}_1)^2 + (\nabla\vec{n}_2)^2 + \Xi^2\vec{n}_1\vec{n}_2 + \frac{1}{c_{\rm sw}^2}\left(\frac{\partial\vec{n}_1}{\partial\tau} - i\vec{H}\times\vec{n}_1\right)^2 + \frac{1}{c_{\rm sw}^2}\left(\frac{\partial\vec{n}_2}{\partial\tau} - i\vec{H}\times\vec{n}_2\right)^2\right], \tag{16}$$

where g is a coupling constant which depends on the ratio J_2/J_1, and H is measured in units of $g\mu_B/\hbar$. Introducing $\vec{\sigma}_{1,2} = (\vec{n}_1 \pm \vec{n}_2)/\sqrt{2}$, we can rewrite the σ-model action as

$$\mathcal{S} = \frac{1}{2g}\left[(\nabla\vec{\sigma}_1)^2 + (\nabla\vec{\sigma}_2)^2 + \Xi^2\vec{\sigma}_1^2 + \frac{1}{c_{\rm sw}^2}\left(\frac{\partial\vec{\sigma}_1}{\partial\tau} - i\vec{H}\times\vec{\sigma}_1\right)^2 + \frac{1}{c_{\rm sw}^2}\left(\frac{\partial\vec{\sigma}_2}{\partial\tau} - i\vec{H}\times\vec{\sigma}_2\right)^2\right]. \tag{17}$$

The constraints on the σ fields are $\vec{\sigma}_1\vec{\sigma}_2 = 0$, $\vec{\sigma}_1^2 + \vec{\sigma}_2^2 = 2$.

The evaluation of the susceptibility at the mean-field ($N = \infty$) level is straightforward. Using the results of Ref. 3, we obtain $\chi_u = (\chi_1 + \chi_2)/2$, where χ_u is a susceptibility *per spin*, and $\chi_{1,2}$ are the mean-field susceptibilities for the two σ fields,

$$\chi_{1,2} = \frac{T}{\pi c_{\rm sw}^2}\left[\frac{c_{\rm sw}m_{1,2}}{T}\,\frac{e^{c_{\rm sw}m_{1,2}/T}}{e^{c_{\rm sw}m_{1,2}/T} - 1} - \ln\left(e^{c_{\rm sw}m_{1,2}/T} - 1\right)\right] \tag{18}$$

where $m_1 = \sqrt{\Xi^2 + m^2}$, and $m_2 = m$, where m is the mass obtained from the second constraint equation. At $g = g_c = 8\pi(\Lambda + \sqrt{\Lambda^2 + \Xi^2} - |\Xi|)^{-1}$ where $\Lambda \sim J$ is the upper cutoff, we have $m = \Theta T + O(T^2)$, where[28] $\Theta = 2\ln[(\sqrt{5}+1)/2]$. At low $T \ll \Xi$, χ_1 is exponentially small in T and can be neglected compared to χ_2. It is not difficult to show that the contributions related to the fluctuations of σ_1 are exponentially small and persist even beyond the mean-field level. As a result, the universal term in the uniform susceptibility is solely due to σ_2, and χ_u is precisely *half* of that in a single-layer model.

B. Computation of the subleading term in $\chi_u(T)$

The σ-model approach gives us the leading, universal, temperature dependence of the uniform susceptibility. Now we compute the leading nonuniversal correction to χ_u. We will again use a microscopic approach based on a transformation to bosons. However, this approach clearly has to be modified compared to what we did before at $T = 0$ because the quasiparticle densities (both normal and anomalous) diverge at finite temperature, and the expansion in λ is no longer valid. For this reason, we will perform a self-consistent, mean-field calculation of the susceptibility: We first assume that anharmonic contributions to the quasiparticle spectrum produce a T-dependent gap which eliminates divergencies of quasiparticle densities at the transition point, and then we evaluate the quasiparticle densities with the renormalized spectrum and solve the self-consistent equations for the gap. In principle, one can perform these calculations using the same transformation to bosons as before. This procedure is then equivalent to self-consistent $1/S$ calculations in 2D.[29] However, we found it more convenient to use a similar but slightly different form of the transformation to bosons, introduced by Sachdev and Bhatt.[30] In their approach, one introduces an extra bosonic field instead of a U term in (7):

$$L_i^z = -(c_i^\dagger s_i + s_i^\dagger c_i), \quad L_i^+ = \sqrt{2}(a_i^\dagger s_i + s_i^\dagger b_i), \quad L_i^- = \sqrt{2}(b_i^\dagger s_i + s_i^\dagger a_i). \tag{19}$$

The expressions for $\vec{M}$ are the same as before. The commutation algebra for spins is again satisfied, while the constraint on the length of the spin now reduces to $a_i^\dagger a_i + b_i^\dagger b_i + c_i^\dagger c_i + s_i^\dagger s_i = 1$. The advantage of this transformation is that one no longer needs to assume that the density of excitations is small. However, we did not use this transformation for our $T = 0$ calculations above because we found it difficult to perform a systematic expansion about the mean-field solution. However, the mean-field calculation is straightforward: One has to put the s field into a condensate ($\langle s \rangle = s_0$), neglect fluctuations of s, and reduce the on-site constraint to a constraint imposed on average quantities. We first list the $T = 0$ results which are similar (but not identical) to the results we obtained to the zeroth order in λ. In the disordered phase, we indeed again find the threefold-degenerate quasiparticle spectrum with $\epsilon_k = \sqrt{A_k^2 - B_k^2}$, where $A_k = J_2 + 2J_1 s_0^2 \nu_k$, $B_k = 2J_1 s_0^2 \nu_k$, and the self-consistent equation for s_0 follows from the constraint on the length of the spin: $s_0^2 = 1 - (3/N)\sum_k (A_k - \epsilon_k)/2\epsilon_k$. At the transition point, we obtained $s_0 \approx 0.9$. The critical value of J_2 is then $J_2^{\rm cr} = 4J_1 s_0^2 \approx 3.2J_1$, and the $T = 0$ spin-wave velocity at criticality is $c_{\rm sw} = 2J_1 s_0 \approx 1.8J_1$.

We now consider finite temperatures. Assume that the condensate of the s field has a form $s_0^2 = (s_0^2)_{T=0}\ (1 - m^2/4)$, such that at the critical point and near $k = \pi$, $\epsilon_k^2 = c_{\rm sw}^2 (k^2 + m^2)$. Substituting the full expressions for A_k and ϵ_k into a self-consistency equation at finite T, expanding in T, and evaluating the lattice sums, we obtain

$$\frac{c_{\rm sw} m}{T} = \Theta\left(1 + \mu\, \frac{T}{J_1} + O(T^2)\right) . \tag{20}$$

Here Θ is the same as in the σ-model calculations, and the second term is a lattice-dependent correction which we found to be $\mu = -0.061$. Furthermore, we have checked that the mean-field formula for the uniform susceptibility is given precisely by Eq. (18) with no extra lattice-dependent corrections (we applied a magnetic field, rediagonalized the quadratic form in bosons, and computed the magnetization along the field). Substituting then the result for the mass m to order T^2 into (18), we obtained

$$\chi_u = Q\, \frac{T}{c_{\rm sw}^2} \left[1 - \left(\frac{2\Theta\mu}{\sqrt{5}}\right) \frac{T}{J_1} + O(T^2)\right], \tag{21}$$

where $Q = \sqrt{5}\Theta/4\pi$ in the mean-field approximation [the $1/N$ correction extended to a physical case of $N = 3$ reduces this value by about 20% (Ref. 31)]. We see that the numerical factor in the subleading term in the susceptibility is very small, and, e.g., at $T = J_1$, constitutes only 5% of the mean-field value. Indeed, at $T \sim J_1$, higher-order corrections in T/J_1 could also be relevant, but the fact that the leading correction to the scaling result is small is at least an indication that the universal linear dependence of the uniform susceptibility extends to sufficiently high $T \sim J_1$. As we already discussed, this is consistent with the Monte Carlo data.[14]

V. CONCLUSIONS

In this paper, we considered a two-layer Heisenberg antiferromagnet which can either be in the Néel-ordered or in the disordered phase at $T = 0$ depending on the ratio of the intralayer and interlayer exchange constants. We applied a transformation to bosons which is suitable for a singlet configuration of a pair of spins, and considered in a systematic expansion the quasiparticle excitations in the disordered phase, and the critical value of the interlayer coupling. We then extended the approach to the ordered phase by introducing a single-particle condensate of one of the Bose fields and computed the mean-field quasiparticle dispersion, the sublattice magnetization, and the transverse susceptibility at arbitrary J_2. We then computed one-loop corrections to the sublattice magnetization and the susceptibility, and considered the relative strength of the longitudinal spin fluctuations. We found that the contributions of these fluctuations are zero in a single-layer antiferromagnet, but are quite substantial near the transition point, where the transverse and the longitudinal fluctuations are equally important. The results of our $T = 0$ calculations are in a reasonable agreement with the Monte Carlo and series expansion data. We also computed the temperature dependence of the uniform susceptibility at the critical point, and found that the lattice-dependent corrections to the universal scaling behavior $\chi_u \propto T$ are small for all $T \leq J_1$. This is again consistent with the Monte Carlo data which show that the linear behavior of χ_u extends to sufficiently high temperatures $T \sim J_1$ and flattens only at even higher temperatures.

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APPENDIX

In this appendix, we compute the sublattice magnetization, the transverse susceptibility, and the spin stiffness in the Néel phase to order λ. We start with the calculations of the magnetization.

Sublattice magnetization

Our point of departure is the expression for L_z, Eq. (7), extended to $\lambda \ll 1$. In the ordered phase, $N_0 =$

$\langle L_z\rangle/2 = \langle c^\dagger U\rangle\sqrt{\lambda}$, where the averaging is over the exact ground state. The mean-field calculations in the ordered state were presented in Sec. III. In these calculations, we considered only the condensate piece of the c field, $\langle c\rangle = \alpha$. Here we will need both α and the fluctuating component of c. Substituting $c_k = \alpha\delta_{k,\pi} + \tilde{c}_k$, into N_0, expanding in U up to an infinite order, and collecting all terms which contain at most one pair product of fluctuating fields, we obtain after some simple combinatorics

$$N_0 = \frac{\sqrt{\beta(1-\beta)}}{\lambda}\,\{1-\lambda[Z_1(\beta)+Z_2(\beta)+Z_3(\beta) +Z_4(\beta)]\}\ , \tag{A1}$$

where, we recall, $\beta = \lambda\alpha^2$, and

$$\begin{aligned} Z_1(\beta) &= \frac{\beta}{8(1-\beta)^2}\ , \\ Z_2(\beta) &= -\frac{2-\beta}{4(1-\beta)^2}\,\frac{1}{N}\sum_k \frac{B_\parallel(k)}{2\epsilon_\parallel(k)}\ , \\ Z_3(\beta) &= \frac{4-3\beta}{4(1-\beta)^2}\,\frac{1}{N}\sum_k\left(-\frac{1}{2}+\frac{A_\parallel(k)}{2\epsilon_\parallel(k)}\right)\ , \\ Z_4(\beta) &= \frac{1}{1-\beta}\,\frac{1}{N}\sum_k\left(-\frac{1}{2}+\frac{A_\perp(k)}{2\epsilon_\perp(k)}\right). \end{aligned} \tag{A2}$$

Here

$$A_\parallel(k) = J_2 + \frac{2J_1^*}{1-\beta}\,\left[\beta(4-3\beta)+\nu_k(1-2\beta)^2\right]\ ,$$

$$B_\parallel(k) = \frac{2J_1^*}{1-\beta}\,\left[\beta(2-\beta)+\nu_k(1-2\beta)^2\right]\ ,$$

$$A_\perp(k) = J_2 + 2J_1^*\nu_k + 4J_1^*\beta(1-\nu_k), \tag{A3}$$

$J_1^* = J_1/\lambda$, and the dispersions for transverse and longitudinal fluctuations are given by (12) and (14). Observe that near the critical point, $N_0 \propto \sqrt{\beta}$. The next step is to express β in terms of J_1 and J_2. To this end, we compute the ground state energy E_0 with the $O(\lambda)$ corrections which come from noninteracting spin waves *and* from the normal ordering of c operators in the expansion of U. Combining the two contributions, we obtain

$$\lambda E_0 = J_2\beta - 4J_1^*\beta[(1-\beta) - 2\lambda(1-\beta)\,Z_1(\beta)] - \lambda\,\sum_k[A_\perp(k)-\epsilon_\perp(k)] - \frac{\lambda}{2}\,\sum_k[A_\parallel(k)-\epsilon_\parallel(k)]\ . \tag{A4}$$

Minimization with respect to β then yields

$$\beta = \beta_0 - \lambda\,[Z_5(\beta_0)+Z_6(\beta_0)+Z_7(\beta_0)+Z_8(\beta_0)]\ , \tag{A5}$$

where

$$\begin{aligned} Z_5(\beta) &= \frac{1}{N}\sum_k\,(1-\nu_k)\left(-\frac{1}{2}+\frac{A_\perp(k)}{2\epsilon_\perp(k)}\right)\ , \\ Z_6(\beta) &= \frac{1}{4N}\frac{1}{(1-\beta)^2}\sum_k\,\left[4-6\beta+3\beta^2+(-3+8\beta-4\beta^2)\nu_k\right]\left(-\frac{1}{2}+\frac{A_\parallel(k)}{2\epsilon_\parallel(k)}\right)\ , \\ Z_7(\beta) &= -\frac{1}{4N}\frac{1}{(1-\beta)^2}\sum_k\,\left[2-2\beta+\beta^2+(-3+8\beta-4\beta^2)\nu_k\right]\frac{B_\parallel(k)}{2\epsilon_\parallel(k)}\ , \\ Z_8(\beta) &= \frac{\beta(2-\beta)}{8\,(1-\beta)^2}\ . \end{aligned} \tag{A6}$$

Notice that the correction terms Z_1, Z_2, Z_3, Z_6, Z_7, and Z_8 are due to fluctuations in the direction of the condensate, while the terms Z_4 and Z_5 come from transverse fluctuations.

Substituting (A5) into (A1), we obtain, to order $O(\lambda)$,

$$N_0 = \frac{\sqrt{\beta_0(1-\beta_0)}}{\lambda}\,\left[\frac{1-\lambda\,Z_b/\beta_0}{1-\lambda\,Z_b/(1-\beta_0)}\right]^{1/2}\,(1-\lambda Z_a)\ , \tag{A7}$$

where

$$\begin{aligned} Z_a &= Z_1(\beta_0)+Z_2(\beta_0)+Z_3(\beta_0)+Z_4(\beta_0)\ , \\ Z_b &= Z_5(\beta_0)+Z_6(\beta_0)+Z_7(\beta_0)+Z_8(\beta_0)\ . \end{aligned} \tag{A8}$$

At $J_2 = 0$, $\beta_0 = 1/2$, and evaluating the lattice sums, we obtain $N_0 = (1/2\lambda) - n_0$, where $n_0 = N^{-1}\sum_k[(1-\nu_k^2)^{-1/2}-1]/2 = 0.197$ is the density of transverse fluctuations (spin waves).[20] This result is equivalent to the first-order spin-wave result; i.e., longitudinal fluctuations do not contribute to sublattice magnetization to first order in λ. This is a direct consequence of the fact that the longitudinal mode is dispersionless at $J_2 = 0$, and hence the c bosons on adjacent sites do not interact with each other. It is essential, however, that the longitudinal fluctuations are small only for $J_2/J_1 \ll 1$. Near the disordering transition, longitudinal and transverse fluctuations have nearly equal strength, and the actual behavior of magnetization differs in an essential way from the prediction based on the spin-wave theory. In this limit, we obtained

$$N_0 = \frac{Z_N}{\lambda} \sqrt{\beta}, \tag{A9}$$

where $Z_N = 1 - 0.163\lambda$, and the fully renormalized β satisfies the equation

$$8J_1\beta[1 - (3/\pi)\ \lambda/\sqrt{\beta_0} + \cdots] = J_2^{\rm cr} - J_2, \tag{A10}$$

where $J_2^{\rm cr} = 4J_1^*(1 - 0.665\lambda + \cdots)$ is the same as we obtained approaching the critical point from the disordered phase. We have checked that the two analytical expressions for $J_2^{\rm cr}$ are indeed also identical. The subleading term in (A10) is a Gaussian correction to the sublattice magnetization. In the theory of phase transitions, it is usually assumed that the Gaussian term is in fact expressed in terms of fully renormalized β rather than β_0. The correction term then diverges as one approaches $J_2^{\rm cr}$ as it indeed should in 2+1 dimensions. Due to this divergence, the self-consistent approach is valid only at $J_2^{\rm cr} - J_2 > \lambda^2$. In the opposite limit $J_2^{\rm cr} - J_2 \ll \lambda^2$, scaling considerations predict that the sublattice magnetization should behave as $N_0 \sim (J_2^{\rm cr} - J_2)^{\bar{\beta}}$, where $\bar{\beta} \sim 0.35$.

The above considerations are also relevant as to how one should extend the perturbative result for N_0 at arbitrary β to $\lambda = 1$. We have seen that near $J_2 = 0$, one should keep $\beta = \beta_0$ in the $O(\lambda)$ terms. At the same time, it is not difficult to make sure that in order to obtain the same $J_2^{\rm cr}$ on both sides of the transition, one has to perform calculations self-consistently, i.e., evaluate the subleading terms in (A5) with the fully renormalized β. To first order in λ, both procedures are indeed equivalent. However, the extension to $\lambda = 1$ yields different results in the two cases. The self-consistent solution of (A5) for $\lambda = 1$ is plotted in Fig. 4. We see that there is a substantial downturn renormalization of β in the region $J_2^{\rm cr} - J_2 \ll \lambda^2$, where the self-consistent solution is in fact invalid. If instead, we approximate the critical value of J_2 from the region of intermediate β (see Fig. 4), we obtain the larger $J_2^{\rm cr} \sim 2.3$, which is in better agreement with numerical results. On the other hand, the perturbative solution (with β_0 in the subleading terms) gives a correct description of the sublattice magnetization at small J_2, shows no unphysical downturn renormalization near the transition, and yields $J_2^{\rm cr} \sim 2.73J_1$, which is reasonably close to the numerical result. For all these reasons, we plotted the perturbative solution for N_0 in Fig. 2.

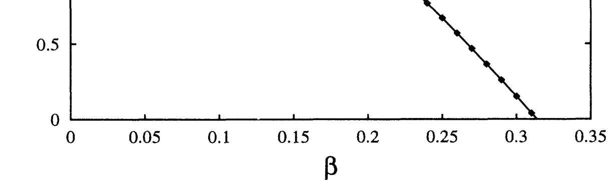

FIG. 4. The solution of the self-consistent equation for the fully renormalized value of the single-particle condensate, $\beta = \langle c_\pi \rangle^2$. Points are the results of the self-consistent calculations extended to the physical case of $\lambda = 1$. The downturn renormalization at small β is due to divergent Gaussian fluctuations, and is probably unphysical. The solid line is the extrapolation of the self-consistent formula at intermediate β to $\beta = 0$.

Transverse susceptibility

We will use a direct way to obtain the transverse susceptibility in the ordered phase; that is, we will apply a homogeneous transverse magnetic field and compute the induced magnetization. For definiteness, we will assume that N_0 is directed along the z axis, and apply a magnetic field in the x direction.

For the calculations of the transverse magnetization, we found it convenient to introduce new Bose operators as linear combinations of the original a and b bosons:

$$s_i = \frac{a_i + b_i}{\sqrt{2}}, \qquad p_i = \frac{a_i - b_i}{\sqrt{2}}\ . \tag{A11}$$

In terms of these new operators, the transformation to bosons, extended to large λ, is

$$\begin{aligned} M_i^z &= s_i^\dagger p_i + p_i^\dagger s_i, \quad L_i^z = -\lambda^{-1/2}(c_i^\dagger U_i + U_i c_i), \\ M_i^x &= p_i^\dagger c_i + c_i^\dagger p_i, \quad L_i^x = \lambda^{-1/2}(s_i^\dagger U_i + U_i s_i), \\ M_i^y &= -i(s_i^\dagger c_i - c_i^\dagger s_i), \quad L_i^y = -i\lambda^{-1/2}(p_i^\dagger U_i - U_i p_i), \end{aligned} \tag{A12}$$

where $U_i = [1 - \lambda(s_i^\dagger s_i + p_i^\dagger p_i + c_i^\dagger c_i)]^{1/2}$.

The advantage of using this new form of the transformation is that a magnetic field applied along x only introduces a condensate of the p field. As the expectation value of M_x is obviously site independent, the c- and p-field condensates should have the same momentum; i.e., the condensate of p should also have a momentum π.

Let us first discuss the mean-field results. In the mean-field approximation, the transverse magnetization per spin is $M_\perp = M_x/2 = \langle p \rangle \cdot \langle c \rangle = \lambda^{-1}\ (\gamma_0\beta_0)^{1/2}$, where we have introduced $\gamma = \lambda \langle p \rangle^2$, and $\gamma = \gamma_0$ at the mean-field level. The mean-field ground state energy depends on both β_0 and γ_0 and is given by

$$\begin{aligned} \lambda E_0 = {} & J_2(\beta_0 + \gamma_0) - 4J_1^*\beta_0(1 - \beta_0) + 8J_1^*\ \beta_0\gamma_0 \\ & -2H_x\ (\gamma_0\ \beta_0)^{1/2}, \end{aligned} \tag{A13}$$

where E_0 is the energy per a pair of spins, and, as before, the magnetic field is measured in units of $g\mu_B/\hbar$. Differentiating over γ_0 and substituting the result into $M_\perp$, we obtain

$$M_\perp = \frac{(\gamma_0\ \beta_0)^{1/2}}{\lambda} = \frac{1}{\lambda}\ \frac{\beta_0 H_x}{J_2 + 8J_1^*\beta_0}\ . \qquad \text{(A14)}$$

To obtain the susceptibility, we need $M_\perp$ only at vanishing magnetic field. Substituting $\beta_0 = (4J_1^* - J_2)/8J_1^*$ into (A14), we find

$$\chi_\perp = \frac{1}{4J_1}\ \frac{4J_1^* - J_2}{8J_1^*}\ . \qquad \text{(A15)}$$

Observe that at $J_2 = 0$, we recover the classical spin-wave result $\chi_\perp = 1/8J_1$. For the spin-stiffness we obtain using (13)

$$\rho_s = \frac{J_1}{4\lambda^2}\ \frac{16(J_1^*)^2 - J_2^2}{16(J_1^*)^2}\ . \qquad \text{(A16)}$$

For $J_2 = 0$, we again recover the classical spin-wave result. In the opposite limit, $J_2 \approx 4J_1$, $\rho_s = (J_1/\lambda^2)\ [(4J_1^* - J_2)/8J_1]$. Finally, for the ratio N_0^2/ρ_s we have $N_0^2/\rho_s = 1/J_1$ independent of J_2.

We now obtain the expression for $\chi_\perp$ to order $O(\lambda)$. From (A12) we have $M_\perp = \lambda^{-1}\sqrt{\beta\gamma} + \Delta M_\perp$, where $\Delta M_\perp = N^{-1}\sum_{k\neq\pi}\langle c_k^\dagger\ p_k\rangle$. To compute γ and ΔM to first order in λ, we will need the excitation spectra of quasiparticles in the presence of the field. To obtain them, we substitute the transformation to bosons into the spin Hamiltonian and restrict our calculations to the terms which are quadratic in bosons. The fluctuations of the s field are decoupled from the other two modes, while the fluctuations of the c and p fields are coupled in the presence of a field. The computation of the quadratic form in the c and p bosons again requires some care as one needs to carefully examine all terms in the expansion of the square root in (A12), keeping in mind that both γ and β are not small in λ. Assembling the contributions from all terms in the series, we obtain

$$\begin{aligned}\mathcal{H} = E_0 + \sum_k A_s(k)\ s_k^\dagger s_k + \frac{B_s(k)}{2}\ (s_k^\dagger s_{-k}^\dagger + s_k s_{-k}) + A_p(k) p_k^\dagger p_k + \frac{B_p(k)}{2}\ (p_k^\dagger p_{-k}^\dagger + p_k p_{-k})\\ + A_c(k)\ c_k^\dagger c_k + \frac{B_c(k)}{2}\ (c_k^\dagger c_{-k}^\dagger + c_k c_{-k}) + C(k)(c_k^\dagger p_k + p_k^\dagger c_k) + D(k)(p_k^\dagger c_{-k}^\dagger + p_k c_{-k})\ ,\end{aligned} \qquad \text{(A17)}$$

where

$$\lambda E_0 = J_2(\beta+\gamma) - 4J_1^*\beta(1-\beta)[1 - 2\lambda Z_1(\beta)] - 2H_x\sqrt{\beta\gamma} + 8J_1^*\beta\gamma[1 + \lambda/(8(1-\beta)^2)] \qquad \text{(A18)}$$

and

$$\begin{aligned}
A_s(k) &= J_2 + 2J_1^*\ [2\beta + \nu_k(1 - 2\beta - 2\gamma)], \quad B_s(k) = 2J_1^*\nu_k(1-2\gamma),\\
A_p(k) &= J_2 + 2J_1^*\left[2\beta + \frac{\beta\gamma}{1-\beta} + \nu_k\left(1 - 2\beta - \gamma + \frac{\beta\gamma}{1-\beta}\right)\right]\ ,\\
B_p(k) &= 2J_1^*\left[\frac{\beta\gamma}{1-\beta} - \nu_k\left(1 - \gamma - \frac{\beta\gamma}{1-\beta}\right)\right]\ ,\\
A_c(k) &= J_2 + 2J_1^*\left[\beta\frac{4-3\beta}{1-\beta} + \frac{\beta^2\gamma}{(1-\beta)^2} + \nu_k\left(\frac{(1-2\beta)^2}{1-\beta} - \gamma\frac{2-4\beta+\beta^2}{(1-\beta)^2}\right)\right],\\
B_c(k) &= 2J_1^*\left[\beta\frac{2-\beta}{1-\beta} + \frac{\beta^2\gamma}{(1-\beta)^2} + \nu_k\left(\frac{(1-2\beta)^2}{1-\beta} - \gamma\frac{2-4\beta+\beta^2}{(1-\beta)^2}\right)\right],\\
C(k) &= -H_x + 2J_1^*\ (\beta\ \gamma)^{1/2}\ \frac{3 - 2\beta - \nu_k(2-3\beta)}{1-\beta}\ ,\\
D(k) &= 2J_1^*\ (\beta\ \gamma)^{1/2}\ \frac{1 - \nu_k(2-3\beta)}{1-\beta}\ .
\end{aligned} \qquad \text{(A19)}$$

Diagonalizing then the 2×2 matrix for s bosons and the 4×4 matrix for coupled c and p bosons by the usual means, we obtain three branches of quasiparticle excitations. The dispersion of the s boson has a gap, $\epsilon_s(\pi,\pi) \equiv H_x$. This result is valid for any J_2 and is indeed the expected result since s quanta describe the fluctuations of the transverse components of $\vec{M}$, and the $k=\pi$ mode of these fluctuations is a homogeneous precession of the magnetization around the direction of the field [we recall that both condensates have momentum π, and hence homogeneous ($k=0$) modes of composite fields M_z and M_x correspond to $k=\pi$ mode of the s boson]. Furthermore, we found after a diagonalization that one of the two coupled modes of the c and p bosons remains gapless at $k=\pi$, while the other has a gap which in the absence of the field is the same as the gap for the c quanta. The presence of a gapless excitation is a direct consequence of the Goldstone theorem.

For the calculation of the transverse magnetization, we actually need only the ground state energy. Collecting the zero-point contributions, which appear after diagonalization, we obtain to order H_x^2

$$E_{\rm tot} = E_0 - \frac{1}{2} \sum_i \sum_k [A_i(k) - \epsilon_i(k)] - \sum_k l_p^2 \, l_c^2 \, \frac{[C(x_p + x_c) + D(1 + x_p x_c)]^2}{\epsilon_p + \epsilon_c} \,, \tag{A20}$$

where E_0 is given by (A18), $i = s, p$ or c, $\epsilon_i = (A_i^2 - B_i^2)^{1/2}$, and $l_i^2 = (A_i + \epsilon_i)/2\epsilon_i$, $x_i = -B_i/(A_i + \epsilon_i)$. Simultaneously, substituting old Bose operators in terms of new ones into $\Delta M_\perp$, we also obtain

$$\Delta M_\perp = -\sum_k l_p^2 l_c^2 (x_p + x_c) \, \frac{C(x_p + x_c) + D(1 + x_p x_c)}{\epsilon_p + \epsilon_c} \,. \tag{A21}$$

Evaluating $\gamma \propto \beta H_x^2$ from $\partial E_{\rm tot}/\partial\gamma = 0$ and using (A5) and (A21), we obtain the result for $\chi_\perp = M_\perp/H_x$ to order $O(\lambda)$. The full expression is, however, too cumbersome to be presented here, and so we analyze only the limiting cases and plot the result for arbitrary J_2 in Fig. 3 (we used the same procedure of extending the result to $\lambda = 1$ as for the sublattice magnetization). Near the critical point, we found

$$\begin{aligned} (\gamma \, \beta)^{1/2} &= \frac{\beta H_x}{J_2^{\rm cr} - 5\lambda J_1^* Z_\gamma} \,, \\ \Delta M_\perp &= \frac{H_x \beta}{12\pi\lambda J_1^*} \left(\frac{\lambda^2}{\beta}\right)^{1/2} [1 + O(\beta)] \,, \end{aligned} \tag{A22}$$

where $Z_\gamma = N^{-1} \sum_k \nu_k/\sqrt{1 + \nu_k} = -0.328$, $J_2^{\rm cr}$ is given by (9), and we keep β rather than β_0 in the $O(\lambda)$ terms. Collecting the two contributions to $M_\perp$, we obtain

$$\chi_\perp = \frac{Z_\chi}{4J_1} \, \beta \left[1 + \frac{1}{3\pi} \left(\frac{\lambda^2}{\beta}\right)^{1/2} + O\left(\frac{\lambda^2}{\beta}\right) + \cdots \right] , \tag{A23}$$

where $Z_\chi = 1 + 0.255\lambda$. The subleading term is a Gaussian correction. Its divergence again implies that the self-consistent approach only works for $\beta > \lambda^2$.[32] In the opposite limit $\lambda^2 \gg \beta$, a self-consistent theory is inapplicable. Scaling considerations[3] predict that in this limit $\chi_\perp = A(Z_\chi/4J_1) \, (\beta/\lambda^2)^{1/(1+\eta)}$, where $\eta \approx 0.03$ is the critical exponent for spin correlations at criticality, and A is a constant whose value cannot be obtained in the present approach. At $\lambda^2 \gg \beta$, we also have $\rho_s = \chi_\perp c_{\rm sw}^2 = AJ_1 Z_\rho \, (\beta/\lambda^2)^{1/(1+\eta)}$, where $Z_\rho = 1 - 0.257\lambda$.

In the opposite limit, $J_2 = 0$, we find

$$\chi_\perp = \frac{Z_\perp}{8J} \,, \tag{A24}$$

where

$$Z_\perp = 1 - \lambda \frac{1}{N} \sum_k \frac{\nu_k^2}{(1 - \nu_k^2)^{1/2}} = 1 - 0.551\lambda \tag{A25}$$

is the contribution from s and p bosons, which is *exactly* the same as in the first-order spin-wave theory. In other words, longitudinal fluctuations do not contribute to the susceptibility of a single-layer antiferromagnet. This is consistent with the fact that the first-order $1/S$ result for $\chi_\perp$ agrees well with the numerical data.[25] However, the longitudinal fluctuations are again small only for $J_2/J_1 \ll 1$. As J_2 increases, our expression for χ_u deviates from the spin-wave result, and eventually turns to zero much earlier than in the self-consistent spin-wave theory.

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