Phase Transition, Longitudinal Spin Fluctuations and Scaling in a Two-Layer Antiferromagnet

Andrey V. Chubukov* and Dirk K. Morr

Department of Physics, University of Wisconsin-Madison, 1150 University ave., Madison, WI 53706

* P.L. Kapitza Institute for Physical Problems, Moscow, Russia

(today)

Abstract

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 intra- 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 the 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 $\chi_u$ 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 2D spin systems \[1\]–\[7\]. The purpose of the present communication is to study in detail the disordered transition in a two-layer $S = 1/2$ Heisenberg antiferromagnet described by

$$H = J_1 \sum_{\langle i,j\rangle,\alpha} \vec{S}_{\alpha,i} \vec{S}_{\alpha,j} + J_2 \sum_i \vec{S}_{1,i} \vec{S}_{2,i}.$$ \hspace{1cm} (1)

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

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 disordered phase transition at some critical ratio of $J_2/J_1$.

The two-layer Heisenberg model has attracted a lot of interest in the last few years \[8\]–\[13\]. 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 disordered 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 \[12\] and series expansion \[10\] techniques, and analytically, using spin-wave \[3\] and mean-field Schwinger-boson theory \[11\]. 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 [14]. 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 $(J_2/J_1)_{cr} \approx 4.5$ [11], which is nearly two times larger than $(J_2/J_1)_{cr} \approx 2.5$ obtained in series expansion [10] ($J_2^{cr} = 2.56$) and Quantum Monte-Carlo [12] ($J_2^{cr} = 2.51$) studies. A self-consistent spin-wave theory (see Sec I A) also predicts a very large value of $(J_2/J_1)_{cr} \approx 4.3$. The spin-wave velocity at the critical point, $c_{sw} \approx 2J_1$ is also inconsistent with the Monte-Carlo data which yield $c_{sw} \approx 1.7 - 1.8J_1$ (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 $J_2^{cr}$ and $c_{sw}$ 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, $\chi_u$, at the transition point. Monte-Carlo simulations have shown that the universal, linear behavior of $\chi_u$ at $J_2 = J_2^{cr}$ extends up to very high $T \sim J_1$. For comparison, in a single-layer antiferromagnet, the deviations from linearity become substantial already at $T \sim 0.6J$ [13].
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. (I). 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 \(\chi_u\) remain small up to \(T = J_1\). Our conclusions are stated in Sec V.

A. Spin-wave calculations

We start our considerations with a brief discussion 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 \(1/S\),

\[
\epsilon_k = 4\tilde{J}_1S[(1 - \nu_k^2) + (\tilde{J}_2/2\tilde{J}_1)(1 - \nu_k)]^{1/2},
\]

and \(\nu_k = (\cos k_x + \cos k_y)/2\). It is not difficult to show that the fluctuations near \(k = \pi\) 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 \(\epsilon_k\) at \(k = (\pi, \pi)\) because of a spontaneous symmetry breaking. The renormalized \(\tilde{J}_1\) and \(\tilde{J}_2\) differ from the couplings in (I) due to the \(1/S\) corrections:
\[ \bar{J}_1 = J_1 \left(1 - \frac{\delta_1 + \delta_2}{S}\right); \quad \bar{J}_2 = J_2 \left(1 - \frac{\delta_1 + \delta_3}{S}\right), \]  

(3)

where

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

(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 \(\delta_1\) with bare couplings \(J_{1,2}\), as it is required in the \(1/S\) expansion, we obtain that \(\delta_1\) 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 \(J_{2}^{cr}\) can be obtained if one formally considers the expressions for the renormalized couplings as self-consistent equations, and solve them for \(S = 1/2\). This procedure is similar to the mean-field Schwinger-boson theory, and the results we obtained are similar to those of Millis and Monien [11]: 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 \(J_{2}^{cr} \approx 4.36J_1\). Still, the critical \(J_2\) is much larger than \(J_{2}^{cr} \approx 2.5J_1\) obtained in numerical simulations. We also computed the spin-wave velocity to second order in \(1/S\), and obtained after straightforward but somewhat tedious calculations \[18\]

\[ c_{sw} = 2\sqrt{2S}\bar{J}_1 \sqrt{1 + \frac{\bar{J}_2}{4J_1} \left(1 + \frac{Q}{4S^2}\right)} \]  

(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 \((J_2/J_1)_{cr}\) suggested by numerical simulations. Assuming for definiteness that \(J_{2}^{cr} = 2.55J_1\), we obtained \(Q \approx 0.044\). Evaluating then \(\bar{J}_{1,2}\) and substituting them into (4), we find \(c_{sw} \sim 3.62J_1S(1 + 0.094/2S + 0.026/(2S^2))\). Observe that the \(1/S^2\) correction is very small. For \(S = 1/2\), we obtain \(c_{sw} \sim 2.03J_1\). As we mentioned earlier, this value is somewhat larger than \(c_{sw} \sim 1.7 - 1.8J_1\)
extracted from the fit of the Monte-Carlo data for the uniform susceptibility \[12\] to the scaling formula.

The main weakness of the spin-wave theory is that it assumes that the 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 three-fold 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

\[
\vec{M}_i = \vec{S}_{1,i} + \vec{S}_{2,i}, \quad \vec{L}_i = \vec{S}_{1,i} - \vec{S}_{2,i},
\]

and three bosonic fields as

\[
M_i^z = a_i^+ a_i - b_i^+ b_i, \quad L_i^z = -(c_i^+ U_i + U_i c_i),
\]

\[
M_i^+ = \sqrt{2} (a_i^+ c_i - c_i^+ b_i), \quad L_i^+ = \sqrt{2} (a_i^+ U_i + U_i b_i),
\]

\[
M_i^- = \sqrt{2} (c_i^+ a_i - b_i^+ c_i), \quad L_i^- = \sqrt{2} (b_i^+ U_i + U_i a_i).
\]

where \( U_i = \sqrt{1 - a_i^+ a_i - b_i^+ b_i - c_i^+ c_i} \). 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: \([M^\alpha, M^\beta] = i \epsilon_{\alpha \beta \gamma} M^\gamma; \ [L^\alpha, L^\beta] = i \epsilon_{\alpha \beta \gamma} L^\gamma; \ [M^\alpha, L^\beta] = i \epsilon_{\alpha \beta \gamma} L^\gamma.\) 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 $U_i = \sqrt{1 - \lambda (a_i^+ a_i + b_i^+ b_i + c_i^+ c_i)}$, 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 $\lambda$. The physical results, however, correspond only to $\lambda = 1$.

Eq. (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 [17], and also the dimerization transition in a $S = 1$ chain [19]. 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 three-fold degenerate.

We now substitute (6) and (7) into the Hamiltonian. To leading order in $\lambda$, the interaction between bosons can be neglected, and diagonalizing the quadratic form in bosons, we obtain a three-fold degenerate excitation spectrum with the dispersion

$$\epsilon_k = \sqrt{A_k^2 - B_k^2}, \quad (8)$$

where $A_k = J_2 + 2J_1^* \nu_k$, and $B_k = 2J_1^* \nu_k$, and $J_1^* = J_1/\lambda$. 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 \( O(\lambda^2) \):

\[
J_2^{cr} = 4J_1^* \left( 1 - 0.665\lambda + \frac{1}{\pi^2} \lambda^2 \log 1/\lambda + O(\lambda^2) \right)
\]

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 1.34\( J_1 \) and 2.4\( J_1 \), 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 [29], and we cannot obtain the precise value of \( J_2^{cr} \) to order \( \lambda^2 \). 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 \( J_2^{cr} \) can be obtained approaching the transition from the ordered phase, and will be discussed in appendix A. Notice, however, that the first-order estimate of \( J_2^{cr} \) is already closer to the numerical result than \( J_2^{cr} \sim 4.3J_1 \) 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

\[
c_{sw} = 2J_1^* \left( 1 - 0.256\lambda \right)
\]

For the physical case of \( \lambda = 1 \), this gives \( c_{sw} \) between 1.49\( J_1 \) and 1.59\( J_1 \) 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 \( \lambda^2 \log 1/\lambda \) which prevents us from obtaining the precise value of \( c_{sw} \) to order \( O(\lambda^2) \). Alternatively however, we can reexpress \( c_{sw} \) in terms of the critical value of \( J_2 \). Doing this, we find that to order \( \lambda \), \( c_{sw} = 0.5J_2^{cr} \left( 1 + 0.409\lambda + \ldots \right) \).
For $\lambda = 1$, this yields $c_{sw} = 0.705 J_2^{cr}$. Using then the numerical result $J_2^{cr} = 2.55 J_1$, we obtain $c_{sw} \sim 1.80 J_1$ which is consistent with $c_{sw} = 1.7 - 1.8 J_1$, 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 $J_2 < J_2^{cr}$ 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 $N_0 \equiv N_0^r$ implies that there is a single-particle condensate of the $c$-quanta with momentum $\pi = (\pi, \pi)$: $<c_{\pi}> = \alpha$. 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 $\lambda$, but keeping $\beta$ fixed), we find

$$\lambda E_0 = J_2 \beta - 4 J_1^* \beta (1 - \beta) \quad (11)$$

Minimizing the energy, we obtain $\beta = \beta_0 = (4 J_1^* - J_2)/8 J_1^*$. 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 $\lambda$

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

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

$$
c_{sw} = 2 J_1^* (1 - \beta)^{1/2} \quad (13)
$$
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

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

We see that the longitudinal fluctuations in the ordered phase have a finite gap at the antiferromagnetic momentum, \( \epsilon_\parallel(\pi) = 8J_1^* \left[ \beta (1 - \beta) \right]^{1/2} \). 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 \( \lambda \). The actual dispersion for a \( c \)-boson may also contain some finite imaginary part (due to higher-order terms in \( \lambda \)) 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 \( \lambda^n \) in the \( n \)-th 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 \( L_z L_z \), 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 disordered transition, longitudinal and transverse fluctuations have nearly 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 disordered transition. The region of more “classical” behavior at intermediate \( J_2 \) has been observed in the mean-field Schwinger-boson approach [11]; it is also present in the self-consistent spin-wave analysis (see Fig. 2).

Near the transition point, we obtained

\[
N_0 = \frac{Z_N}{\lambda} \sqrt{\beta}, \quad \chi_\perp = A(Z_X/4J_1) (\beta/\lambda^2)^{1/(1+\eta)},
\]

where \( Z_N = 1 - 0.163\lambda, \ Z_X = 1 + 0.255\lambda, \) 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 $B = 0.063$. 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 $\beta$, when one can neglect cubic terms. For a general $\beta$, the Goldstone modes arise as a result of cancellations between the 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 $[22]$. We did not perform explicit calculations of the spin-wave spectrum at arbitrary $\beta$ 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, $\rho_s = c_{sw}^2 \chi_\perp$, and the numerical data $[30]$, 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 $c_{sw}$, 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 $c_{sw}$ 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, $\chi_u$ flattens and has a broad maximum at $T \sim J_1$ \cite{15,24}. 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 $J_2 = J_2^{cr}$ are smaller than those of a single-layer antiferromagnet. Below we will compute these corrections perturbatively. But first we consider the sigma-model description of a two-layer system, from which one can obtain the leading, universal, linear in $T$ term in the uniform susceptibility.

A. Sigma-model analysis

A simple way to obtain a sigma-model description of a spin-$S$ quantum antiferromagnet, which we will follow, was suggested by Affleck \cite{24}. 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 $O(3)$ sigma-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

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

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 sigma-model action as
The constraints on the \(\sigma\)-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 [3], we obtain

\[
\chi_u = \left(\chi_1 + \chi_2\right)/2,
\]

where \(\chi_u\) is a susceptibility per spin, and \(\chi_{1,2}\) are the mean-field susceptibilities for the two sigma-fields

\[
\chi_{1,2} = \frac{T}{\pi c_{sw}} \left[ \frac{\epsilon_{cswm_{1,2}}}{T} - \frac{e^{\epsilon_{cswm_{1,2}}/T}}{e^{\epsilon_{cswm_{1,2}}/T} - 1} \right],
\]

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 \([26]\) \(\Theta = 2\log((\sqrt{5} + 1)/2)\). At low \(T \ll \Xi\), \(\chi_1\) is exponentially small in \(T\) and can be neglected compared to \(\chi_2\). It is not difficult to show that the contributions related to the fluctuations of \(\sigma_1\) 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 \(\sigma_2\), and \(\chi_u\) is precisely half of that in a single-layer model.

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

The sigma-model approach gives us the leading, universal, temperature dependence of the uniform susceptibility. Now we compute the leading nonuniversal correction to \(\chi_u\). 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 \(\lambda\) 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, 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 \[27\]. However, we found it more convenient to use a similar but slightly different form of the transformation to bosons, introduced by Bhatt and Sachdev \[28\]. In their approach, one introduces an extra bosonic field instead of a $U-$ term in (7):

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

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 $a_i^+ a_i + b_i^+ b_i + c_i^+ c_i + s_i^+ s_i = 1$. 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 ($<s> = s_0$), 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 $\lambda$. In the disordered phase, we indeed again find the three-fold 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 $J_2^{cr} = 4J_1 s_0^2 \approx 3.2J_1$, and the $T = 0$ spin-wave velocity at criticality is $c_{sw} = 2J_1 s_0 \approx 1.8J_1$.

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 $k = \pi$, $\epsilon_k^2 = c_{sw}^2 (k^2 + m^2)$. Substituting the full expressions for $A_k$ and $\epsilon_k$ into a self-consistency equation at finite $T$, expanding in $T$ and evaluating the lattice sums, we obtain

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

(20)
Here $\Theta$ is the same as in the sigma-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

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

(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% [23]). 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 [12].

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 intra- 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 $\chi_u$ extends to sufficiently high temperatures $T \sim J_1$ and flattens only at even higher temperatures.

It is our pleasure to thank A. Millis, H. Monien, S. Sachdev, A. Sandvik and A. Sokol for useful conversations.

VI. APPENDIX

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

A. Sublattice magnetization

Our point of departure is the expression for $L_z$, eq. (7), extended to $\lambda \ll 1$. In the ordered phase, $N_0 = \langle L_z \rangle / 2 = \langle c^+ U \rangle / \sqrt{\lambda}$, 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, $\alpha$ 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

$$N_0 = \frac{\sqrt{\beta(1 - \beta)}}{\lambda} \left[ 1 - \lambda (Z_1(\beta) + Z_2(\beta) + Z_3(\beta) + Z_4(\beta)) \right]$$  (22)

17
where, we recall, $\beta = \lambda \alpha^2$, and

$$Z_1(\beta) = \frac{\beta}{8(1 - \beta)^2}$$

$$Z_2(\beta) = -\frac{2 - \beta}{4(1 - \beta)^2} \frac{1}{N} \sum_k \frac{B_{\parallel}(k)}{2\epsilon_{\parallel}(k)}$$

$$Z_3(\beta) = \frac{4 - 3\beta}{4(1 - \beta)^2} \frac{1}{N} \sum_k \left( -\frac{1}{2} + \frac{A_{\parallel}(k)}{2\epsilon_{\parallel}(k)} \right)$$

$$Z_4(\beta) = \frac{1}{1 - \beta} \frac{1}{N} \sum_k \left( -\frac{1}{2} + \frac{A_{\perp}(k)}{2\epsilon_{\perp}(k)} \right).$$

(23)

Here

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

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

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

(24)

$J_1^* = J_1/\lambda$, 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 $\beta$ 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

$$\lambda E_0 = J_2\beta - 4J_1^*\beta[(1 - \beta) - 2\lambda(1 - \beta) Z_1(\beta)]$$

$$-\lambda \sum_k [A_{\perp}(k) - \epsilon_{\perp}(k)] - \frac{\lambda}{2} \sum_k [A_{\parallel}(k) - \epsilon_{\parallel}(k)]$$

(25)

Minimization with respect to $\beta$ then yields

$$\beta = \beta_0 - \lambda (Z_5(\beta_0) + Z_6(\beta_0) + Z_7(\beta_0) + Z_8(\beta_0))$$

(26)

where

$$Z_5(\beta_0) = \frac{1}{N} \sum_k (1 - \nu_k) \left( -\frac{1}{2} + \frac{A_{\perp}(k)}{2\epsilon_{\perp}(k)} \right)$$

$$Z_6(\beta_0) = \frac{1}{4N(1 - \beta)^2} \sum_k \left( 4 - 6\beta + 3\beta^2 + (-3 + 8\beta - 4\beta^2)\nu_k \right) \left( -\frac{1}{2} + \frac{A_{\parallel}(k)}{2\epsilon_{\parallel}(k)} \right)$$
$$Z_7(\beta_0) = -\frac{1}{4N} \frac{1}{(1-\beta)^2} \sum_k \left(2 - 2\beta + \beta^2 + (-3 + 8\beta - 4\beta^2)\nu_k \right) \frac{B_{\parallel}(k)}{2\epsilon_{\parallel}(k)}$$

$$Z_8(\beta_0) = \frac{\beta(2-\beta)}{8\beta(1-\beta)^2}$$

(27)

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 (26) into (22), we obtain, to order $O(\lambda)$

$$N_0 = \left(\frac{\lambda}{1-\lambda Z_a/\beta_0}\right)^{1/2} (1-\lambda Z_a)$$

(28)

where

$$Z_a = Z_1(\beta_0) + Z_2(\beta_0) + Z_3(\beta_0) + Z_4(\beta_0)$$

$$Z_b = Z_5(\beta_0) + Z_6(\beta_0) + Z_7(\beta_0) + Z_8(\beta_0)$$

At $J_2 = 0$, $\beta_0 = 1/2$, and evaluating the lattice sums, we obtain $N_0 = (1/2\lambda) - n_0$, where $n_0 = N^{-1} \sum_k ((1 - \nu_k^n)^{-1/2} - 1)/2 = 0.197$ 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 $\lambda$. 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 disordered 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

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

(30)

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

$$8J_1\beta(1 - (3/\pi) \lambda/\sqrt{\beta_0} + ...) = J_2^c - J_2,$$

(31)

where $J_2^c = 4J_1^*(1 - 0.665\lambda + ...)$ is the same as we obtained approaching the critical point from the disordered phase. We have checked that the two analytical expressions for $J_2^c$ are
indeed also identical. The subleading term in (31) 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 $\beta$ rather than $\beta_0$. The correction term then diverges as one approaches $J^r_2$ as it indeed should in 2+1 dimensions. Due to this divergence, the self-consistent approach is valid only at $J^r_2 - J_2 > \lambda^2$. In the opposite limit $J^r_2 - J_2 \ll \lambda^2$, scaling considerations predict that the sublattice magnetization should behave as $N_0 \sim (J^r_2 - J_2)^{\bar{\beta}}$, 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 $\beta$ 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 $J^r_2$ on both sides of the transition, one has to perform calculations self-consistently, i.e., evaluate the subleading terms in (26) with the fully renormalized $\beta$. To first order in $\lambda$, both procedures are indeed equivalent. However, the extension to $\lambda = 1$ yields different results in the two cases. The self-consistent solution of (26) for $\lambda = 1$ is plotted in Fig. 4. We see that there is a substantial downturn renormalization of $\beta$ in the region $J^r_2 - J_2 \ll \lambda^2$, where the self-consistent solution is in fact invalid. If instead, we approximate the critical value of $J_2$ from the region of intermediate $\beta$ (see Fig. 4), we obtain the larger $J^r_2 \sim 2.3$, which is in better agreement with numerical results. On the other hand, the perturbative solution (with $\beta_0$ 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 $J^r_2 \sim 2.73J_1$, which is reasonably close to the numerical result. For all these reasons, we plotted the perturbative solution for $N_0$ in Fig. 2.

**B. 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:

$$s_i = \frac{a_i + b_i}{\sqrt{2}} \quad p_i = \frac{a_i - b_i}{\sqrt{2}}$$  \hfill (32)

In terms of these new operators, the transformation to bosons, extended to large $\lambda$, is

$$M_i^x = s_i^+ p_i + p_i^+ s_i, \quad L_i^x = -\lambda^{-1/2}(c_i^+ U_i + U_i c_i),$$

$$M_i^y = c_i^+ p_i^+ c_i, \quad L_i^y = -i\lambda^{-1/2}(p_i^+ U_i - U_i p_i),$$

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

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 $\pi$.

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

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

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 $\gamma_0$ and substituting the result into $M_\perp$, we obtain

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

To obtain the susceptibility, we need $M_\perp$ only at vanishing magnetic field. Substituting $\beta_0 = (4J_1^* - J_2)/8J_1^*$ into (35), we find

$$\chi_\perp = \frac{1}{4J_1^*} \frac{4J_1^* - J_2}{8J_1^*}$$

(36)
Observe that at $J_2 = 0$, we recover the classical spin-wave result $\chi_\perp = 1/8 J_1$. For the spin-stiffness we obtain using (33)

$$\rho_s = \frac{J_1}{4\lambda^2} \frac{16(J_1^*)^2 - J_2^2}{16(J_1^*)^2}$$  \hfill (37)

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 $N_0^2/\rho_s$ 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 (33) we have $M_\perp = \lambda^{-1}\sqrt{\beta \gamma} + \Delta M_\perp$, where $\Delta M_\perp = N^{-1} \sum_{k \neq \pi} < c_k^\dagger p_k >$. To compute $\gamma$ and $\Delta M$ to first order in $\lambda$, 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 (33), keeping in mind that both $\gamma$ and $\beta$ are not small in $\lambda$.

Assembling the contributions from all terms in the series, we obtain

$$\mathcal{H} = E_0 + \sum_k A_s(k) s_k^\dagger s_k + \frac{B_s(k)}{2} (s_k^\dagger s_{-k}^\dagger + s_k s_{-k}) + A_p(k) p_k^\dagger p_k + \frac{B_p(k)}{2} (p_k^\dagger p_{-k}^\dagger + p_k p_{-k}) + A_c(k) c_k^\dagger c_k + \frac{B_c(k)}{2} (c_k^\dagger c_{-k}^\dagger + c_k c_{-k}) + C(k)(c_k^\dagger p_k + p_k^\dagger c_k) + D(k)(p_k^\dagger c_{-k}^\dagger + p_k c_{-k})$$  \hfill (38)

where

$$\lambda E_0 = J_2(\beta + \gamma) - 4J_1^*\beta(1 - \beta)[1 - 2\lambda Z_1(\beta)] - 2H_x\sqrt{\beta \gamma} + 8J_1^* \beta \gamma(1 + \lambda/(8(1 - \beta)^2)$$  \hfill (39)

and

$$A_s(k) = J_2 + 2J_1^* (2\beta + \nu_k(1 - 2\beta - 2\gamma)) , \quad B_s(k) = 2J_1^* \nu_k(1 - 2\gamma)$$

$$A_p(k) = J_2 + 2J_1^* \left( 2\beta + \frac{\beta \gamma}{1 - \beta} + \nu_k \left( 1 - 2\beta - \gamma + \frac{\beta \gamma}{1 - \beta} \right) \right) ,$$

$$B_p(k) = 2J_1^* \left( \frac{\beta \gamma}{1 - \beta} - \nu_k \left( 1 - \gamma - \frac{\beta \gamma}{1 - \beta} \right) \right)$$
we obtain to order $H_x$ state energy. Collecting the zero-point contributions, which appear after diagonalization, a gapless excitation is a direct consequence of the Goldstone theorem. Furthermore, we found after a diagonalization that one of the two coupled modes of the $c-$ and $p-$bosons remain 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 $H_x^2$

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

where $E_0$ is given by (39), $i = s, p$ 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

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

Evaluating $\gamma \propto \beta H_x^2$ from $\partial E_{tot}/\partial \gamma = 0$ and using (26) and (42), 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, 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

$$\Delta M_\perp = \frac{H_x \beta}{12 \pi \lambda J_1} \left( \frac{\lambda^2}{\beta} \right)^{1/2} \left( 1 + O(\beta) \right)$$

where $Z_\gamma = N^{-1} \sum_k \nu_k / \sqrt{1 + \nu_k} = -0.328$, $J_2^r$ is given by (9), and we keep $\beta$ rather than $\beta_0$ in the $O(\lambda)$ terms. Collecting the two contributions to $M_\perp$, we obtain

$$\chi_\perp = \frac{Z_\chi}{4J_1} \beta \left( 1 + \frac{1}{3\pi} \left( \frac{\lambda^2}{\beta} \right)^{1/2} + O \left( \frac{\lambda^2}{\beta} \right) + \ldots \right)$$

with $Z_\chi = 1 + 0.255\lambda$. The subleading term is a Gaussian correction. Its divergence again implies that the self-consistent approach only works for $\beta > \lambda^2$ [29]. In the opposite limit, $\lambda^2 \gg \beta$, a self-consistent theory is inapplicable. Scaling considerations [3] predict that in this limit $\chi_\perp = A(Z_\chi/4J_1a_0^2)(\beta/\lambda^2)^{1/(1+\eta)}$, 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 $\rho_s = \chi_\perp c_{sw}^2 = AJ_1 Z_\rho (\beta/\lambda^2)^{1/(1+\eta)}$, where $Z_\rho = 1 - 0.257\lambda$.

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

$$\chi_\perp = \frac{Z_\perp}{8J}$$

where

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

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 [30]. However, the longitudinal fluctuations are again small only for $J_2/J_1 \ll 1$. As $J_2$ increases, our expression for $\chi_\perp$ deviates from
the spin-wave result, and eventually turns to zero much earlier than in the self-consistent spin-wave theory.
REFERENCES

[1] J.A. Hertz, Phys. Rev. B 14, 525 (1976).

[2] S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. Lett. 60, 1057 (1988); Phys. Rev. B 39, 2344 (1989).

[3] A. V. Chubukov, S. Sachdev, and J. Ye, Phys. Rev. B 49, 11919 (1994).

[4] B. Andraka and A.M. Tsvelik, Phys. Rev. Lett. 67, 2886 (1991); A.M. Tsvelik and M. Reizer, Phys. Rev. B 48, 9887 (1993).

[5] A.J. Millis, Phys. Rev. B 48, 7183 (1993).

[6] A. V. Chubukov, S. Sachdev, and A. Sokol, Phys. Rev. B, to appear.

[7] L.B. Ioffe and A.J. Millis, preprint

[8] T. Siegrist et al, Phys. Rev. B 35, 7137 (1989).

[9] J. M. Tranquada, G. Shirane, B. Keimer, S. Shamoto, and M. Sato, Phys. Rev. B 40, 4503 (1989)

[10] K. Hida, J. Phys. Soc. Jpn. 61, 1013 (1992)

[11] A. J. Millis and H. Monien, Phys. Rev. Lett. 70, 2810 (1993); Phys. Rev. B 50, 16606 (1994).

[12] A. W. Sandvik and D. J. Scalapino, Phys. Rev. Lett. 72, 2777 (1994)

[13] H. Monien and A. W. Sandvik, preprint.

[14] A. W. Sandvik, A.V. Chubukov, S. Sachdev and D. J. Scalapino, in preparation.

[15] H.Q. Ding and M. Makivic, Phys. Rev. B 43, 3662 (1990).

[16] Greven M. et al., Phys. Rev. Lett. 72, 1096 (1994).

[17] A. V. Chubukov and Th. Jolicoeur, Phys. Rev. B 44, 12050 (1991).
These calculations were performed in collaboration with D. Dalidovich.

A. V. Chubukov, Phys. Rev. B 43, 3334 (1991).

C.M. Canali, S.M. Girvin and M. Wallin, Phys. Rev. B 45, 10131 (1992); G.E. Castilia and S. Chakravarty, Phys. Rev. 43, 3334 (1991); J. Igarashi, Phys. Rev. B 46, 10763 (1992).

A similar divergence of a perturbative correction to the critical value of the coupling was earlier found in the $1/S$ expansion for a square-lattice Heisenberg model with the interaction between first and second neighbors [A..V. Chubukov, Phys. Rev. B 43, 362 (1991)].

A.V. Chubukov, Phys. Rev. Lett. 69, 832 (1992); Rastelli E., Reatto R., and Tassi A., Jornal of Physics C 18, 353 (1985); A.V. Chubukov, S. Sachdev and T. Senthil, J. Phys. CM 6, 8891 (1994).

A. V. Chubukov and S. Sachdev, Phys. Rev. Lett. 71, 169 (1993).

D.C. Johnston, Phys. Rev. Lett. 62, 957 (1989).

I. Affleck, Nucl. Phys. B 257, 397 (1985).

S. Sachdev and J. Ye, Phys. Rev. Lett. 69, 2411 (1992).

M. Takahashi, Phys. Rev. B 36, 3791 (1987).

S. Sachdev and R. Bhatt, Phys. Rev. B 41, 9323 (1990).

Notice that the square-root divergence of the Gaussian term is consistent with the Josephson relation $\chi_\perp \sim (\xi_J)^{D-2}$ where $D$ is a spacetime dimension. In the Gaussian approximation, $\xi_J \propto \beta^{1/2}$, i.e., for $D = 3$, $\chi_\perp \propto \beta^{1/2}$ as in [14].

R.R.P. Singh, Phys. Rev. B 39, 9760 (1989).
FIGURES

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

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 $J_2^{c\tau} = 2.73J_1$ (see appendix A).

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.

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 $\beta$ is due to divergent Gaussian fluctuations, and is probably unphysical. The solid line is the extrapolation of the self-consistent formula at intermediate $\beta$ to $\beta = 0$. 
Fig. 1
Fig. 3
Fig. 4