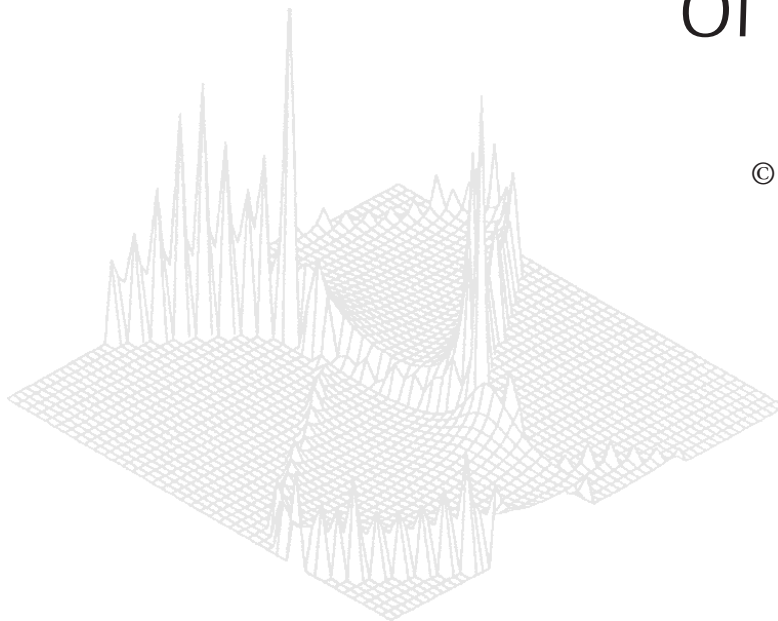

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Spin-wave Gap Critical Index for the Quantum Two-layer Heisenberg Antiferromagnet at $T = 0^*$

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Abstract

The two-layer Heisenberg antiferromagnet exhibits a zero temperature quantum phase transition from a disordered dimer phase to a collinear Neel phase, with long range order in the ground state. The spin-wave gap vanishes as $\Delta \propto (J_{\perp} - J_{\perp c})^{\nu}$ approaching the transition point. To account for strong correlations, the $S = 1$ elementary excitations triplets are described as a dilute Bose gas with infinite on-site repulsion. We apply the Brueckner diagram approach which gives the critical index $\nu \approx 0.5$. We demonstrate also that the linearised in density Brueckner equations give the mean field result $\nu = 1$. Finally, an expansion of the Brueckner equations in powers of the density, combined with the scaling hypothesis, gives $\nu \approx 0.67$. This value agrees reasonably with that of the nonlinear $O(3)$ σ model. Our approach demonstrates that for other quantum spin models the critical index can be different from that in the nonlinear σ model. We discuss the conditions for this to occur.

The physics of quantum phase transitions in $S = \frac{1}{2}$ two-dimensional (2D) Heisenberg models has recently become a subject of considerable interest in connection with the high- T_c cuprate superconductors. Haldane (1983) and Chakravarty *et al.* (1988) have argued that the phase transition is described by the (2+1)-dimensional nonlinear $O(3)$ σ model which predicts that as the transition point is approached the spin-wave gap vanishes as $\Delta \sim (J_{\perp} - J_{\perp c})^{\nu}$ with critical index $\nu \approx 0.7$. The universal dynamic and static properties of 2D antiferromagnets in the vicinity of a zero-temperature phase transition have been studied in detail by assuming the σ -model description (Sachdev and Ye 1992; Chubukov *et al.* 1994). However, mapping of the Heisenberg model to the σ model has been proven only for the one-layer square lattice antiferromagnet which itself does not exhibit a zero temperature quantum phase transition.

In this paper we consider the two-layer $S = \frac{1}{2}$ Heisenberg antiferromagnet described by

$$H = J \sum_{\langle i,j \rangle} (\mathbf{S}_{1i} \mathbf{S}_{1j} + \mathbf{S}_{2i} \mathbf{S}_{2j}) + J_{\perp} \sum_i \mathbf{S}_{1i} \mathbf{S}_{2i}. \quad (1)$$

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The spins \mathbf{S}_1 and \mathbf{S}_2 represent two planes coupled by J_\perp . Both couplings are antiferromagnetic ($J, J_\perp > 0$) and the first sum runs over nearest neighbours on a square lattice. The system has a zero temperature quantum phase transition from a disordered dimer phase to a collinear Neel phase as the dimerisation decreases. For this model the numerical results of Singh *et al.* (1988) and Weihong (1997) obtained by series expansions, as well as Monte Carlo calculations performed by Sandvik and Scalapino (1994), demonstrate reasonable consistency of the critical index with that in the σ model. At the same time, Sandvik and Vekic (1995) using quantum Monte Carlo simulations have shown that for some other 2D antiferromagnetic models (dimers arranged in ladders and dimers in a staggered pattern) the critical exponents are different from the nonlinear σ model prediction. In this situation it is very important to analyse the behaviour near the critical points by an independent analytical method. Such a method, based on the Brueckner perturbation theory, has been developed by Kotov *et al.* (1998). In the present work we apply it for the calculation of the spin-wave gap critical index in the two-layer Heisenberg antiferromagnet. This method gives an independent calculation of the index for this model, and additionally it allows us to formulate the conditions when one could expect deviations from the σ model behaviour.

Considering the ‘ J terms’ in equation (1) as a perturbation, one can introduce the bond operator representation (Chubukov 1989; Sachdev and Batt 1990) and *exactly* map the Hamiltonian (1) to the effective Hamiltonian (Kotov *et al.* 1998):

$$H_{\text{eff}} = H_2 + H_4 + H_U, \quad (2)$$

$$H_2 = \sum_{\mathbf{k}, \alpha} A_{\mathbf{k}} t_{\mathbf{k}, \alpha}^\dagger t_{\mathbf{k}, \alpha} + \frac{B_{\mathbf{k}}}{2} (t_{\mathbf{k}, \alpha}^\dagger, t_{-\mathbf{k}, \alpha}^\dagger + \text{h.c.}), \quad (3)$$

$$H_4 = \frac{J}{2} \sum_{\langle i, j \rangle, \alpha\beta} \{t_{\alpha i}^\dagger t_{\beta j}^\dagger t_{\beta i} t_{\alpha j} - t_{\alpha i}^\dagger t_{\alpha j}^\dagger t_{\beta i} t_{\beta j}\}, \quad (4)$$

$$H_U = U \sum_{i, \alpha\beta} t_{\alpha i}^\dagger t_{\beta i}^\dagger t_{\beta i} t_{\alpha i}, U \rightarrow \infty, \quad (5)$$

where $t_{\alpha i}^\dagger$ is the creation operator of the triplet at the bond i and $\alpha = x, y, z$ is the polarisation of the triplet. The operator $t_{\mathbf{k}, \alpha}^\dagger$ is the Fourier transform of $t_{\alpha i}^\dagger$: $t_{\mathbf{k}, \alpha}^\dagger = (1/\sqrt{N}) \sum_{\mathbf{r}} t_{\mathbf{r}, \alpha} e^{i(\mathbf{k} + \mathbf{k}_0)\mathbf{r}}$. As usual the momentum takes values inside the Brillouin zone $-\pi < k_x \leq \pi$, $-\pi < k_y \leq \pi$, but we shift the argument in the Fourier transform by $\mathbf{k}_0 = (\pi, \pi)$. In this notation the minimum of the spin-wave dispersion is at $\mathbf{k} = 0$. The coefficients are of the form $A_{\mathbf{k}} = J_\perp + 2J\xi_{\mathbf{k}}$, $B_{\mathbf{k}} = 2J\xi_{\mathbf{k}}$, with $\xi_{\mathbf{k}} = -\frac{1}{2}(\cos k_x + \cos k_y)$. An infinite on-site repulsion between triplets H_U is introduced to take into account the hard-core constraint $t_{\alpha i}^\dagger t_{\beta i}^\dagger = 0$ (only one triplet can be excited on a bond). The interaction H_U gives the dominant contribution to the renormalisation of the spin-wave spectrum. It has been

demonstrated (Kotov *et al.* 1998) that in the Brueckner approximation this renormalisation is described by the self-energy operator

$$\Sigma(\mathbf{k}, \omega) = \frac{4}{N} \sum_{\mathbf{q}} Z_{\mathbf{q}} v_{\mathbf{q}}^2 \Gamma(\mathbf{k} + \mathbf{q}, \omega - \omega_{\mathbf{q}}), \quad (6)$$

where the scattering amplitude is

$$\Gamma(\mathbf{q}, \omega) = - \left(\frac{1}{N} \sum_{\mathbf{p}} \frac{Z_{\mathbf{p}} Z_{\mathbf{q}-\mathbf{p}} u_{\mathbf{p}}^2 u_{\mathbf{q}-\mathbf{p}}^2}{\omega - \omega_{\mathbf{p}} - \omega_{\mathbf{q}-\mathbf{p}}} \right)^{-1}, \quad (7)$$

and the spin-wave spectrum $\omega_{\mathbf{k}}$, quasiparticle residue $Z_{\mathbf{k}}$ and Bogoliubov parameters $u_{\mathbf{k}}$, $v_{\mathbf{k}}$ are given by the formulas:

$$\omega_{\mathbf{k}} = Z_{\mathbf{k}} \sqrt{\tilde{A}_{\mathbf{k}}^2 - \tilde{B}_{\mathbf{k}}^2}, \quad (8)$$

$$\begin{aligned} \tilde{A}_{\mathbf{k}} &= J_{\perp} + 2J\xi_{\mathbf{k}} + \Sigma(\mathbf{k}, 0) + 4J\xi_{\mathbf{k}} \sum_{\mathbf{q}} \xi_{\mathbf{q}} Z_{\mathbf{q}} v_{\mathbf{q}}^2, \\ \tilde{B}_{\mathbf{k}} &= 2J\xi_{\mathbf{k}} - 4J\xi_{\mathbf{k}} \sum_{\mathbf{q}} \xi_{\mathbf{q}} Z_{\mathbf{q}} u_{\mathbf{q}} v_{\mathbf{q}}, \end{aligned} \quad (9)$$

$$Z_{\mathbf{k}} = \left(1 - \left. \frac{\partial \Sigma}{\partial \omega} \right|_{\omega=0} \right)^{-1}, \quad u_{\mathbf{k}}^2, v_{\mathbf{k}}^2 = \frac{Z_{\mathbf{k}} \tilde{A}_{\mathbf{k}}}{2\omega_{\mathbf{k}}} \pm \frac{1}{2}. \quad (10)$$

These equations also take into account the quartic interaction (4) in the one-loop approximation. In order to find spectrum, equations (6)–(10) have to be solved self-consistently for $\Sigma(\mathbf{k}, 0)$ and $Z_{\mathbf{k}}$. The plot of the spin-wave gap Δ versus J_{\perp}/J is presented in Fig. 1. In the same figure we present results from the papers by Weihong (1997) and Kotov *et al.* (1998) obtained by the dimer series expansions.

Close to the critical point ($\Delta \ll J$) and for small momenta ($k \ll 1$), the dispersion can be represented as

$$\omega_{\mathbf{k}} \approx \sqrt{\Delta^2 + c^2 k^2}, \quad (11)$$

where $c = 1.85J$ is the spin-wave velocity (Weihong 1997; Kotov *et al.* 1998; Gelfand 1996). To find the critical index let us write equation (8) at the point $\mathbf{k} = 0$ as

$$\Delta^2 = Z_0^2 (\tilde{A}_0^2 - \tilde{B}_0^2). \quad (12)$$

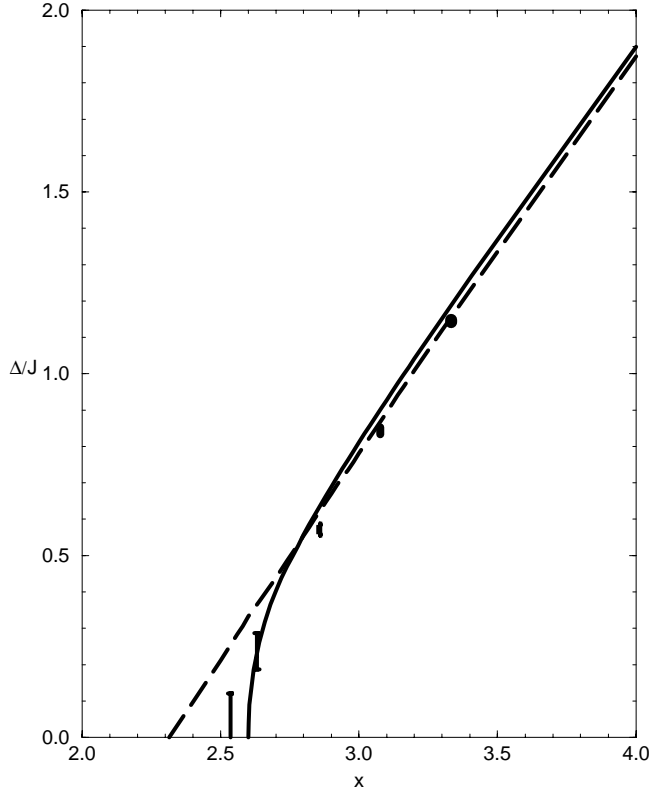


Fig. 1. Triplet gap Δ/J as a function of $x = J_{\perp}/J$. Solid and dashed lines are the results of the self-consistent solution using the Bruekner approach and the Bruekner equations linearised in density respectively. The dots (with error bars) are estimates obtained by dimer series expansions.

It is convenient to introduce the values of \tilde{A}_0 and \tilde{B}_0 at the critical point: $\tilde{A}_{0c} = -\tilde{B}_{0c}$. Let us vary J_{\perp} keeping J fixed, and let us introduce the deviation from the critical point $\delta J_{\perp} = J_{\perp} - J_{\perp c}$. Considering δJ_{\perp} and Δ as independent variables and using equations (9)–(11), we find the variations of \tilde{A}_0 and \tilde{B}_0 :

$$\begin{aligned}\tilde{A}_0 &= \tilde{A}_{0c} + \delta J_{\perp} + \delta\Sigma(0,0) - \frac{Z_0 J \tilde{A}_{0c}}{\pi c^2} \Delta, \\ \tilde{B}_0 &= \tilde{B}_{0c} + \frac{Z_0 J \tilde{A}_{0c}}{\pi c^2} \Delta.\end{aligned}\quad (13)$$

To find the variation of the self-energy notice that, according to equation (7), $\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) \propto q$ at $\Delta/c \sim q \ll 1$. Therefore from (6) we find

$$\delta\Sigma(0,0) \propto \sum_{\mathbf{q}} q \delta v_{\mathbf{q}}^2 \propto \Delta^2 \ln \frac{J}{\Delta}.\quad (14)$$

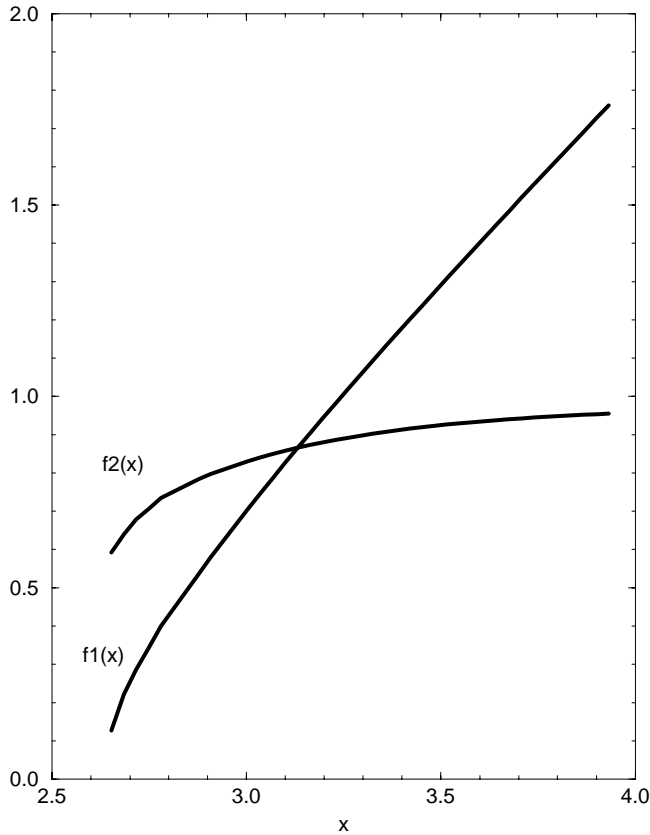


Fig. 2. Functions $f_1(x) = [(d \ln(\Delta/J)/dx)]^{-1}$ and $f_2(x) = -[d \ln(\Delta/J)/dx]^2 / d^2 \ln(\Delta/J)/dx^2$ versus $x = J_{\perp}/J$ (see text).

Terms linear in Δ are cancelled out after substitution of (13) and (14) into equation (12) and, neglecting logarithmic dependence, we find that

$$\Delta \propto \sqrt{\delta J_{\perp}}. \quad (15)$$

Thus, the critical index in the Brueckner approximation is $\nu = 0.5$. It is known from nuclear and atomic physics (Dzuba *et al.* 1989) that the Brueckner approximation usually works quite well even in systems with high density, but parametrically it is justified only at the low density limit. In essence it is the dilute gas approximation. It has been demonstrated (Kotov *et al.* 1998) that for the model under consideration the actual small parameter is $n_b \ln(J/\Delta)$, where $n_b \approx 0.1$ is the density of the triplet excitations. It is clear that when the gap is very small this parameter becomes large and the gas approximation can fail. To analyse the situation numerically we plot in Fig. 2 the functions

$$f_1(x) = \left(\frac{d \ln(\Delta/J)}{dx} \right)^{-1}, \quad f_2(x) = - \left(\frac{d \ln(\Delta/J)}{dx} \right)^2 \bigg/ \frac{d^2 \ln(\Delta/J)}{dx^2}, \quad (16)$$

where $x = J_{\perp}/J$ and Δ is found from equations (6)–(10). For pure scaling behaviour [$\Delta \propto (\delta J_{\perp})^{\nu}$] the function $f_1(x)$ is linear and the function f_2 gives the index: $f_2(x) = \nu$. Keeping in mind that when the gap is small [$\ln(J/\Delta) \gg 1$] our approximation is not justified, we conclude from the plot of f_2 that the estimate of the critical index is $\nu \in [0.6, 0.75]$ or

$$\nu \approx 0.67 \pm 0.07. \quad (17)$$

Another way to look at the critical index is to expand the Brueckner equations in powers of the density n_b . In the leading approximation $Z_{\mathbf{q}} = u_{\mathbf{q}} = 1$ and therefore the vertex (7) takes the form

$$\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \left(\int \frac{d^2\mathbf{p}}{(2\pi)^2} \frac{1}{\omega_{\mathbf{q}} + \omega_{\mathbf{p}} + \omega_{\mathbf{p}-\mathbf{q}}} \right)^{-1}. \quad (18)$$

In contrast to (7) it does not vanish at $q \rightarrow 0$. Let us denote $\Gamma(0,0) = \Gamma_c$. The last terms in equations (13) are due to the quartic interaction H_4 (4). This interaction is relatively small and therefore we neglect these terms. Below we prove that they are really small. So instead of equations (13) we have

$$\begin{aligned} \tilde{A}_0 &= \tilde{A}_{0c} + \delta J_{\perp} + \delta\Sigma(0,0) \\ \tilde{B}_0 &= \tilde{B}_{0c}. \end{aligned} \quad (19)$$

If we substitute this into (12) and neglect terms quadratic in Δ we find that variation of \tilde{A}_0 must vanish:

$$\delta\tilde{A}_0 = \delta J_{\perp} + \delta\Sigma(0,0) = 0. \quad (20)$$

The variation of the self-energy should be found from equation (6):

$$\delta\Sigma(0,0) = 4 \int \frac{d^2\mathbf{q}}{(2\pi)^2} \Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) \delta v_{\mathbf{q}}^2 + 4 \int \frac{d^2\mathbf{q}}{(2\pi)^2} \delta\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) v_{\mathbf{q}}^2. \quad (21)$$

The main contribution to the first integral in this formula comes from small momenta ($q \sim \Delta/c \ll 1$) since

$$\delta v_{\mathbf{q}}^2 = \frac{1}{2} \left\{ \frac{\delta\tilde{A}_{\mathbf{q}}}{\omega_{\mathbf{q}}} + \tilde{A}_{\mathbf{q}} \delta \left(\frac{1}{\omega_{\mathbf{q}}} \right) \right\} \approx -\frac{\tilde{A}_{0c} \Delta^2}{4(\Delta^2 + c^2 q^2)^{\frac{3}{2}}}. \quad (22)$$

The variation of \tilde{A} in this formula vanishes according to (20). Then the integral can be easily evaluated and the result is $-\Gamma_c \tilde{A}_{0c} \Delta / \pi c^2$. The main contribution to the second integral in (21) comes from large momenta ($q \sim 1$), where we can write $\delta\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \Gamma' \delta J_{\perp}$. It is obvious from (18) that at $J_{\perp} \gg J$ the derivative is $\Gamma' = 3$. However, we need this derivative near the critical point where the

numerical calculation shows that $\Gamma' \approx 2.9$ independent of momenta. Altogether the variation (21) can be represented as

$$\delta\Sigma(0,0) \approx -\frac{\Gamma_c \tilde{A}_{0c}}{\pi c^2} \Delta + \frac{4}{3} \Gamma' n_b \delta J_\perp, \quad (23)$$

where $n_b = 3 \sum_{\mathbf{q}} v_{\mathbf{q}}^2 \approx 0.12$ is the density of spin-wave excitations at the critical point. At this step we can check how small the neglected quartic interaction term is in equations (13). The ratio of this term to the ‘ Δ -term’ in (23) is $J/\Gamma_c \approx 0.15$, since $\Gamma_c \approx 6.3J$. After substitution of (23) into (21), we find the relation between the gap and δJ_\perp :

$$\Delta \approx \frac{\pi c^2}{\Gamma_c A_{0c}} \left(1 + \frac{4}{3} \Gamma' n_b\right) (J_\perp - J_{\perp c}) \approx 1.1 (J_\perp - J_{\perp c}). \quad (24)$$

The coefficient 1.1 corresponds to $\Gamma_c \approx 6.3J$, $A_{0c} \approx 2.4J$, $c \approx 1.9J$, $\Gamma' \approx 2.9$ and $n_b \approx 0.12$, which have been found by numerical solution of the linearised in density equations (6), (8), (9) and (10). We remind the reader that the linearisation means that the vertex is taken from (18) and the residues in (9) are replaced by unity ($Z_{\mathbf{q}} = 1$). The numerical solution also gives $\Delta(J_\perp)$ shown in Fig. 1. The slope at $J_\perp = J_{\perp c}$ is in perfect agreement with the semianalytical formula (24). Thus the leading term in powers of the density gives the critical exponent $\nu = 1$, the same as the mean field approximation.

Now, consider the first correction due to the triplet density n_b . We keep only those terms which contain additional $\ln q$ or $\ln(\Delta/J)$, so the parameter is $n_b \ln(\Delta/J)$. The $n_b \ln(\Delta/J)$ terms arise only from expansion of the vertex (7). Replacing $u_{\mathbf{p}}^2 u_{\mathbf{q}-\mathbf{p}}^2 = (1 + v_{\mathbf{p}}^2)(1 + v_{\mathbf{q}-\mathbf{p}}^2) \approx 1 + v_{\mathbf{p}}^2 + v_{\mathbf{q}-\mathbf{p}}^2$, we obtain

$$\Gamma(\mathbf{q}, -\omega_{\mathbf{q}}) = \left(\int \frac{d^2 p}{(2\pi)^2} \frac{1 + v_{\mathbf{p}}^2 + v_{\mathbf{q}-\mathbf{p}}^2}{\omega_{\mathbf{q}} + \omega_{\mathbf{p}} + \omega_{\mathbf{q}-\mathbf{p}}} \right)^{-1}. \quad (25)$$

After simple integration one can find that for small q ($q \sim \Delta/c \ll 1$) the vertex is

$$\Gamma(q, -\omega_q) \approx \Gamma_c + \frac{\Gamma_c^2 \tilde{A}}{4\pi c^2} \ln q. \quad (26)$$

Substitution into (21) gives the variation of the self-energy

$$\delta\Sigma(0,0) \approx -\frac{\Gamma_c \tilde{A}_{0c}}{\pi c^2} \Delta \left(1 + \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \ln \frac{\Delta}{J}\right) + \frac{4}{3} \Gamma' n_b \delta J_\perp, \quad (27)$$

which together with equation (20) results in

$$\Delta = \frac{\pi c^2}{\Gamma_c \tilde{A}_{0c}} \left(1 + \frac{4}{3} \Gamma' n_b\right) \delta J_\perp \left(1 - \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \ln \frac{\delta J_\perp}{J}\right). \quad (28)$$

Let us assume the scaling behaviour $\Delta \propto (\delta J_{\perp})^{\nu}$ with $\nu = 1 - \beta$. Expanding this formula in powers of β and comparing with (28), we find

$$\nu = 1 - \frac{\Gamma_c \tilde{A}_{0c}}{4\pi c^2} \approx 0.67 \pm 0.04, \quad (29)$$

which agrees with the estimate (17) and with the result of the σ -model approach $\nu \approx 0.70$ (Ferer and Hamid-Aidinejad 1986).

In conclusion, we have calculated the spin-wave critical index for the zero temperature quantum phase transition in a two-layer Heisenberg antiferromagnet using the Brueckner approach. The result is in agreement with that of the nonlinear $O(3)$ σ model. This agreement is due to the relative smallness of the quartic interaction for the model under consideration. In this situation the hard-core constraint is the most important and it is very natural that the result is similar to that of the σ model. However, this situation is not general. There are many models where the quartic interaction is very important. It can even produce bound states of triplet spin waves (Sushkov and Kotov 1998) which effectively changes the number of relevant degrees of freedom. In this situation one can expect a very substantial deviation from the simple σ model. An important example of such a system is the 2D $J_1 - J_2$ model where the singlet bound state has an extremely low energy (Kotov *et al.* 1999).

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