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Effect of interlayer coupling in a layered antiferromagnet

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Abstract. The effect of interlayer coupling on the magnetic properties of layered antiferromagnets is studied by the use of non-linear spin-wave theory. The sublattice magnetization, internal energy, specific heat and magnetic susceptibilities are calculated for different interlayer coupling strengths over the whole range of temperatures, and the asymptotic expressions for these quantities are given in two low-temperature regimes distinguished by a characteristic reduced temperature Θ_0 which reflects the character of the layered structure. It is shown that the temperature dependences of the physical quantities have a crossover from three-dimensional to two-dimensional behaviour with increase in the reduced temperature from one regime ($\Theta \ll \Theta_0 < \Theta_1$) to another ($\Theta_0 \ll \Theta \ll \Theta_1$) for small interlayer coupling strengths. The correction due to spin-wave interactions is also discussed.

1. Introduction

Motivated by the discovery of almost two-dimensional (2D) antiferromagnetism in the insulating phase of high-T_c materials, there have been several theoretical studies of low-dimensional magnetism in an effort to understand the nature of the superconductivity [1]. Many theoretical models are based on a simple 2D square lattice instead of the quasi-2D system in realistic materials. However, the 2D Heisenberg system does not achieve long-range order at finite temperatures [2]: a quasi-2D system can achieve it, with the interlayer coupling reducing spin fluctuations. Therefore, the interlayer coupling should be considered when the homogeneous 2D Heisenberg model is used to investigate the magnetic properties of high-T_c cuprate superconductors in the normal state.

In fact, layered magnetic systems have been investigated for a long time [3], and the Heisenberg model is usually used to describe them. Several methods have been developed and many results have been obtained. Berezinsky and Blank [4] studied the low-temperature properties of layered magnets with a very weak interlayer coupling and gave the different temperature behaviours of physical quantities at low temperatures according to the suprressing effect of interlayer coupling on the 2D spin thermal excitations. Recently, the work of Singh *et al* [5] has also shown that the temperature dependence of sublattice magnetization in La_2CuO_4 has a crossover from three-dimensional (3D) behaviour to quasi-2D behaviour, and Kopietz [6] argued that the quasi-2D behaviour ($T \ln T$) of sublattice magnetization exists only in the low-temperature region ($T \ll T_N$). Liu [7] gave an asymptotic expression for sublattice magnetization at low temperatures, which actually expresses the quasi-3D behaviour,

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and that of specific heat without a linear temperature term in the pure 2D case. Except for Kopietz who uses the Schwinger boson approach, previous workers have all used the linear spin-wave theory, which is believed to be a useful method at low temperatures [8]. In addition, Soukoulis *et al* [9] also used the spin-wave theory to study the effect of interlayer coupling on the sublattice magnetization, internal energy and perpendicular susceptibility at zero temperature in a layered antiferromagnet, giving the relations between each of the quantities and the Néel temperature obtained by a double-time–temperature spin Green function method.

In this paper we report a systematic study aimed at understanding the effect of interlayer coupling on the magnetic properties of a layered antiferromagnet by employing the non-linear spin-wave theory developed by Liu [10]. Because the spin-wave interactions are considered in this method, the temperature regime for which it is suitable is much wider than that for which the linear spin-wave theory is used, and this method makes the perpendicular susceptibility which is a constant in the linear spin-wave theory dependent on temperature. We start with an anisotropic antiferromagnetic Heisenberg model in section 2 and then calculate numerically and analytically the sublattice magnetization, internal energy, specific heat and magnetic susceptibilities of the system as functions of temperature and interlayer coupling strength in section 3; finally we give our conclusion in section 4.

2. Effective Hamiltonian

Consider a 3D simple-cubic lattice system with intralayer and interlayer lattice parameters of a, a and c, respectively. The model Hamiltonian is given by

$$H = \sum_{\langle ij \rangle} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1}$$

where J_{ij} is the antiferromagnetic interaction between two nearest-neighbour spins; we define it by

$$J_{ij} = \begin{cases} J & \text{if } i \text{ and } j \text{ lie in the same layer} \\ J_\perp & \text{if } i \text{ and } j \text{ lie in two nearest-neighbour layers.} \end{cases} \tag{2}$$

In order to discuss the antiferromagnetic properties of the system, we assume that the lattice is bipartite and divided into sublattices 1 and 2. Introducing spin deviation operators for the two sublattices and performing a Fourier transform on them as done by Liu [10], we obtain the effective Hamiltonian in terms of spin-wave operators $c_{\boldsymbol{k}}(c_{\boldsymbol{k}}^+)$ and $d_{\boldsymbol{k}}(d_{\boldsymbol{k}}^+)$:

$$\begin{aligned} H = -\frac{NAS}{2} &+ A\sum_{\boldsymbol{k}}[c_{\boldsymbol{k}}^+ c_{\boldsymbol{k}} + d_{\boldsymbol{k}}^+ d_{\boldsymbol{k}} + \eta(\boldsymbol{k})(c_{\boldsymbol{k}} d_{\boldsymbol{k}} + d_{\boldsymbol{k}}^+ c_{\boldsymbol{k}}^+)] \\ &- \frac{A}{2NS}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}}[4\eta(\boldsymbol{k}-\boldsymbol{k}')c_{\boldsymbol{k}}^+ c_{\boldsymbol{k}'} d_{\boldsymbol{k}+\boldsymbol{q}}^+ d_{\boldsymbol{k}'+\boldsymbol{q}} + \eta(\boldsymbol{k}+\boldsymbol{q})c_{\boldsymbol{k}'}^+ c_{\boldsymbol{k}} c_{\boldsymbol{k}'+\boldsymbol{q}} d_{\boldsymbol{k}+\boldsymbol{q}} \\ &+ \eta(\boldsymbol{k})c_{\boldsymbol{k}}^+ d_{\boldsymbol{k}+\boldsymbol{q}}^+ d_{\boldsymbol{k}'-\boldsymbol{q}}^+ d_{\boldsymbol{k}'} + \eta(\boldsymbol{k}+\boldsymbol{q})c_{\boldsymbol{k}'+\boldsymbol{q}}^+ c_{\boldsymbol{k}}^+ c_{\boldsymbol{k}'} d_{\boldsymbol{k}+\boldsymbol{q}}^+ \\ &+ \eta(\boldsymbol{k})c_{\boldsymbol{k}} d_{\boldsymbol{k}'}^+ d_{\boldsymbol{k}+\boldsymbol{q}} d_{\boldsymbol{k}'-\boldsymbol{q}}] \end{aligned} \tag{3}$$

where A is the exchange field and

$$A = 4J(2+\delta)S \tag{4}$$

$$\eta(k) = [\cos(k_x a) + \cos(k_y a) + \delta\cos(k_z c)]/(2+\delta) \tag{5}$$

$$\delta = J_\perp / J \tag{6}$$

The last two terms in the second square brackets in equation (3) come from the requirement that the total Hamiltonian must be Hermitian.

3. Calculation of physical quantities and discussion

In a different way from Liu [10], we define the following retarded matrix Green function:

$$\hat{\mathbf{G}}(k,\tau) = \begin{bmatrix} G_{11}(k,\tau) & G_{12}(k,\tau) \\ G_{21}(k,\tau) & G_{22}(k,\tau) \end{bmatrix} \tag{7}$$

where

$$\begin{aligned} G_{11}(k,\tau) &= \langle\langle c_k(\tau), c_k^+(0)\rangle\rangle \\ G_{12}(k,\tau) &= \langle\langle c_k(\tau), d_k(0)\rangle\rangle \\ G_{21}(k,\tau) &= \langle\langle d_k^+(\tau), c_k^+(0)\rangle\rangle \\ G_{22}(k,\tau) &= \langle\langle d_k^+(\tau), d_k(0)\rangle\rangle. \end{aligned} \tag{8}$$

Using the technique of the equation of motion for the Green function $\hat{\mathbf{G}}$ and decoupling to higher-order Green functions, under the condition of weak interlayer coupling and $\delta = 1$, we obtain $\hat{\mathbf{G}}$ in terms of Fourier transforms:

$$\hat{\mathbf{G}}(k,\omega) = \frac{1}{\omega^2 - \omega_k^2} \begin{bmatrix} \omega + A(1+\alpha) & -A(1+\alpha)\eta(k) \\ -A(1+\alpha)\eta(k) & -\omega + A(1+\alpha) \end{bmatrix} \tag{9}$$

where ω_k is the energy of the spin wave ($\hbar \equiv 1$) given by

$$\omega_k = A(1+\alpha)\{1 - [\eta(k)]^2\}^{1/2} \tag{10}$$

$$\alpha = -\frac{2}{NS}\sum_k [n_k + \eta(k)\xi_k] \tag{11}$$

with

$$n_k = \langle c_k^+ c_k\rangle = \langle d_k^+ d_k\rangle \tag{12}$$

$$\xi_k = \langle c_k d_k\rangle = \langle d_k^+ c_k^+\rangle. \tag{13}$$

Using the spectral theorem and equation (9) and substituting equations (12) and (13) into equation (11) thus results in

$$\alpha = \alpha_0 - \frac{2}{NS}\sum_k \{1 - [\eta(k]^2\}^{1/2}[\exp(\beta\omega_k) - 1]^{-1} \tag{14}$$

with

$$\alpha_0 = \frac{1}{2S}\left(1 - \frac{2}{N}\sum_{k}\{1 - [\eta(k)]^2\}^{1/2}\right) = \frac{C_1}{2S} \tag{15}$$

where $\beta = 1/k_B T$.

The quantity C_1 has been calculated in [11], and the results are 0.097 and 0.158 for the isotropic simple-cubic ($\delta = 1$) and pure 2D ($\delta = 0$) cases, respectively. From equation (10), we see that the renormalization factor α as a function of temperature and δ (equation (14)) appears in the spin-wave energy; so we must first solve equation (14) in order to calculate the correlation functions and related physical quantities. We find that the equation for α has two roots for a given reduced temperature ($\Theta < \Theta_{max}$) and has no solution above a certain reduced temperature $\Theta_{max} = k_B T_{max}/6J$. Θ_{max} decreases with decreasing δ. Liu [10] and Bloch [12] found that Θ_{max} is very close to the Néel reduced temperature Θ_N for an isotropic system ($\delta = 1$); however, Θ_{max} has nothing to do with the transition temperature Θ_N but is rather a consequence of some approximations [10]. The approximation includes three aspects: firstly, the Hermitian conjugate relation between the spin operators S^+ and S^- is destroyed when introducing spin deviation operators; secondly, the kinematic interaction which demands that the spin deviation does not exceed $2S$ is not taken into account; thirdly there is a decoupling approximation for higher-order Green functions. These approximations introduce some unphysical states in the vicinity of Θ_{max}; so the non-linear spin-wave theory is not suitable in this temperature regime.

In order to discuss the effect of interlayer coupling on the properties of the system at low temperatures ($\Theta \ll \Theta_1 = (2+\delta)/3$), we define a characteristic reduced temperature $\Theta_0 = [2\delta(2+\delta)]^{1/2}/3$ which distinguishes the quasi-2D from the 3D case according to the values of δ. The 3D case holds for $\Theta \ll \Theta_0 < \Theta_1$, and the quasi-2D case for $\Theta_0 \ll \Theta \ll \Theta_1$. In the low-temperature regime, $\alpha - \alpha_0$ is a small quantity and α may be solved by iteration.

When $\Theta \ll \Theta_0 < \Theta_1$, using the long-wavelength approximation in all directions of k, we obtain

$$\begin{aligned}\alpha = \alpha_0 &- [(2\pi)^2/30\delta^{1/2}(2+\delta)^{5/2}(1+\alpha_0)^4](3\Theta)^4 \\ &- [(2\pi)^4/225\delta(2+\delta)^5(1+\alpha_0)^9](3\Theta)^8.\end{aligned} \tag{16}$$

When $\Theta_0 \ll \Theta \ll \Theta_1$, using the long-wavelength approximation only in the x–y plane of k and integrating directly [5], we obtain

$$\begin{aligned}\alpha = \alpha_0 &- [4\zeta(3)/\pi(2+\delta)^2(1+\alpha_0)^3](3\Theta)^3 \\ &- \{48[\zeta(3)]^2/\pi^2(2+\delta)^4(1+\alpha_0)^7\}(3\Theta)^6\end{aligned} \tag{17}$$

where $\zeta(3) = 1.202$ is the Riemann zeta function.

With the above equations, we may calculate and discuss the physical quantities of the system.

3.1. Sublattice magnetization per site

This is given by

$$m = m_0 - \frac{2}{N}\sum_{k}\{1 - [\eta(k)]^2\}^{-1/2}[\exp(\beta\omega_k) - 1]^{-1} \tag{18}$$

where m_0 is the magnetization per site at zero temperature, and the units of m and m_0 are taken as $g\mu_B$:

$$m_0 = S + \frac{1}{2} - \frac{1}{N}\sum_{k}\{1 - [\eta(k)]^2\}^{-1/2} = S - \tfrac{1}{2}(C_2 - 1). \qquad (19)$$

$(C_2 - 1)/2$ is the zero-point correction to the sublattice magnetization due to the zero-point quantum spin fluctuations. C_2 is a monotonically decreasing function of δ, and it is 1.393 for the pure 2D ($\delta = 0$) case and 1.156 for the isotropic simple-cubic ($\delta = 1$) case [11]; accordingly m_0 is a monotonically increasing function of δ. The numerical result for m_0 as a function of $\delta^{1/2}$ for $S = \frac{1}{2}$ is plotted in figure 1, which is in agreement with [13]. When interlayer coupling is weak, equations (10), (14) and (18) are almost the same as those of Kopietz [6] who uses the Schwinger boson approach within the mean-field approximation.

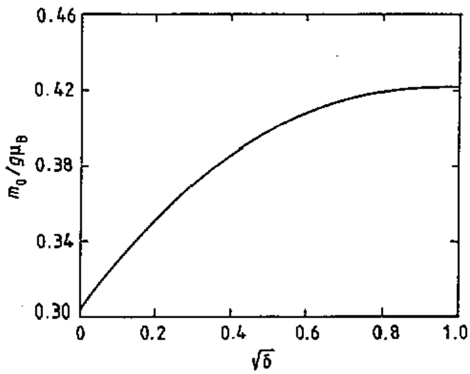

Figure 1. The sublattice magnetization m_0 at zero temperature as a function of the square root of δ with $S = \frac{1}{2}$.

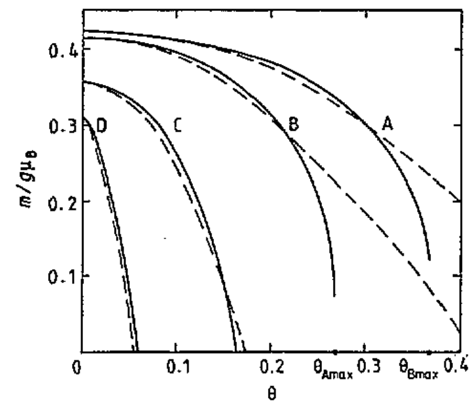

Figure 2. The sublattice magnetization m as a function of reduced temperature Θ with $S = \frac{1}{2}$. The values of δ corresponding to curves A, B, C and D are 1.0, 0.5, 0.05 and 0.0005, respectively. The broken curves correspond to the results of linear spin-wave theory.

The second term in equation (18) is the additional reduction in the sublattice magnetization at finite temperatures arising from spin-wave thermal excitations and interactions. At low temperatures ($\Theta \ll \Theta_1$), we may treat this term in the same way as above; the final results for m in the two low-temperature regimes are

$$m = m_0 - \{1/6[\delta(2+\delta)]^{1/2}(1+\alpha_0)^2\}(3\Theta)^2 - [(2\pi)^2/90\delta(2+\delta)^3(1+\alpha_0)^7](3\Theta)^6 \qquad (\Theta \ll \Theta_0 < \Theta_1) \qquad (20)$$

$$m = m_0 - [3\Theta/\pi(1+\alpha_0)] \times \ln\{3\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}\} - [\![[4\zeta(3)/\pi^2(2+\delta)^2(1+\alpha_0)^5](3\Theta)^4 + \{24[\zeta(3)]^2/\pi^3(2+\delta)^4(1+\alpha_0)^9\}(3\Theta)^7]\!] \times \ln\{3e\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}\} \qquad (\Theta_0 \ll \Theta \ll \Theta_1). \qquad (21)$$

The last term in each equation is the correction due to the spin-wave interactions, and the second term with the temperature dependence reflects 3D behaviour in equation (20) and quasi-2D behaviour in equation (21). It is found that, in the pure 2D ($\delta = 0$) case, the last two terms in equation (21) diverge logarithmically at finite temperatures, indicating that the antiferromagnetic Heisenberg model achieves long-range order only at zero temperature which is in agreement with [2]. Therefore the interlayer coupling strength is essential to keep 3D antiferromagnetic ordering at finite temperatures, no matter how small it is, which is in agreement with the work of Huang and Manousakis [14]. Because the spin-wave interactions are considered, there is a renormalization factor α_0 appearing in the above equations. When we assume α_0 to be zero, the leading terms in equations (20) and (21) are very similar but not equal to the results of [5], for [5] neglects a factor $[2/(2+\delta)]^{1/2}$ in taking the long-wavelength approximation for the spin-wave energy Ω_k. Kopietz [6] not only obtains similar formulae for the sublattice magnetization but also gives its critical behaviour when the temperature approaches the Néel point.

We also calculate the sublattice magnetization per site as a function of temperature and δ for $S = \frac{1}{2}$ by the numerical method over the whole range of temperatures; the results for several values of δ are plotted in figure 2. Here and hereafter, the values of δ corresponding to curves A, B, C and D are 1.0, 0.5, 0.05 and 0.0005, respectively. In contrast, the results of the linear spin-wave theory are also plotted in the same figure using broken curves. Curves A and B do not intersect the temperature axis, because the equation for α has no solution for $\Theta > \Theta_{max}$. When $\delta \leqslant 0.2$, $\Theta_N \leqslant \Theta_{max}$; thus the magnetization curves intersect the temperature axis (see curves C and D). From figure 2 we see that the spin-wave interaction correction to the sublattice magnetization becomes small as the interlayer coupling becomes weak. For given T_N and J in [6] for La_2CuO_4, the estimated value of δ is about 8×10^{-5}.

3.2. Internal energy and specific heat per site

From the definition $E = \langle H \rangle / N$, the internal energy per site may be obtained after a lengthy calculation:

$$E = -(SA/2)(1+\alpha)^2. \tag{22}$$

Similar to α, E is a function of temperature and δ.

At low temperatures ($\Theta \ll \Theta_1$), the asymptotic expressions for E in the two temperature regimes are given by

$$E = E_0 + [(2\pi)^2 J/30\delta^{1/2}(2+\delta)^{3/2}(1+\alpha_0)^3](3\Theta)^4 + [14\pi^4 J/225\delta(2+\delta)^4(1+\alpha_0)^8](3\Theta)^8 \qquad (\Theta \ll \Theta_0 < \Theta_1) \tag{23}$$

and

$$E = E_0 + [4\zeta(3) J/\pi(2+\delta)(1+\alpha_0)^2](3\Theta)^3 + \{40[\zeta(3)]^2 J/\pi^2(2+\delta)^3(1+\alpha_0)^6\}(3\Theta)^6 \qquad (\Theta_0 \ll \Theta \ll \Theta_1) \tag{24}$$

where E_0 is the ground-state energy:

$$E_0 = -2JS^2(2+\delta)(1+\alpha_0)^2 = -2JS(2+\delta)[S + C_1 + C_1^2/4S] \tag{25}$$

which is in agreement with [15] for the isotropic simple-cubic lattice ($\delta = 1$). When $\delta = 1$, equations (16), (20) and (23) are simply the results of Liu [10]; when $\delta \ll 1$, the second temperature regime $\Theta_0 \ll \Theta \ll \Theta_1$ exists; equations (17), (21) and (24) reflect the low-temperature properties of the quasi-2D system. The leading terms of equations (21), (23) and (24) are in agreement with [4] in which the linear spin-wave theory is used to study the low-temperature properties of layered magnets; however, the corresponding coefficients are not the same, for $z = 4$ is used instead of our $z = 2(2 + \delta)$ for $\delta \ll 1$; an approximate relation $\alpha \ln x = x^\alpha - 1$ ($\alpha \ll 1$; $x > 0$) is also used so that the logarithmic form does not appear in the final formulae in [4].

The specific heat per site is easily obtained from $C_m = \partial E/\partial T$. From equations (22) and (14), we have

$$C_m/k_B = S[\beta A(1+\alpha)]^2 C_3/(4S - A\beta C_3) \tag{26}$$

where

$$C_3 = \frac{2}{N}\sum_{k} \frac{1-[\eta(k)]^2}{[\sinh(\beta\omega_k/2)]^2}. \tag{27}$$

In the two low-temperature regimes, asymptotic expressions for the specific heat may be obtained from equations (23) and (24) as follows:

$$C_m/k_B = [(2\pi)^2/15\delta^{1/2}(2+\delta)^{3/2}(1+\alpha_0)^3](3\Theta)^3 + [56\pi^4/225\delta(2+\delta)^4(1+\alpha_0)^8](3\Theta)^7 \qquad (\Theta_0 \ll \Theta < \Theta_1) \tag{28}$$

and

$$C_m/k_B = [6\zeta(3)/\pi(2+\delta)(1+\alpha_0)^2](3\Theta)^2 + \{120[\zeta(3)]^2/\pi^2(2+\delta)^3(1+\alpha_0)^6\}(3\Theta)^5 \qquad (\Theta_0 \ll \Theta \ll \Theta_1). \tag{29}$$

The last term in each equation is the correction due to the spin-wave interactions. From the first term in each equation, we find the dependence of the specific heat on the temperature crossovers from the 3D behaviour (T^3) to the quasi-2D behaviour (T^2) with increase in temperature. There is no linear term in the quasi-2D case, which is in complete agreement with the experimental data [16] for $La_{2-x}Ba_xCuO_4$. In the pure 2D ($\delta = 0$) case, the coefficient of the leading term in equation (29) is different from that in [7], because there is always a correction factor α_0 for the non-linear spin-wave theory [10] in internal energy (specific heat) and it modifies the results of the linear spin-wave theory. The numerical results of the specific heat ($S = \frac{1}{2}$) for the linear and non-linear spin-wave theories are plotted in figure 3. The correction for spin-wave interactions to the specific heat is similar to that for sublattice magnetization.

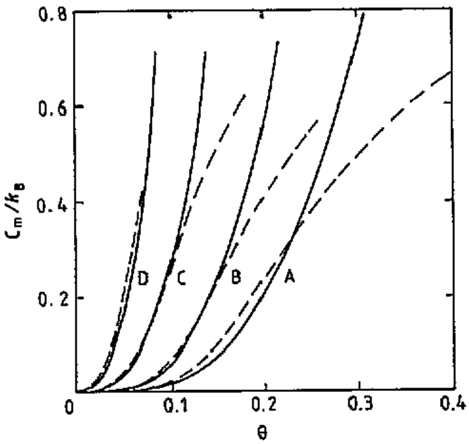

Figure 3. The specific heat C_m as a function of reduced temperature Θ with $S = \frac{1}{2}$. Curves A, B, C and D and the broken curves have the same meanings as in figure 2.

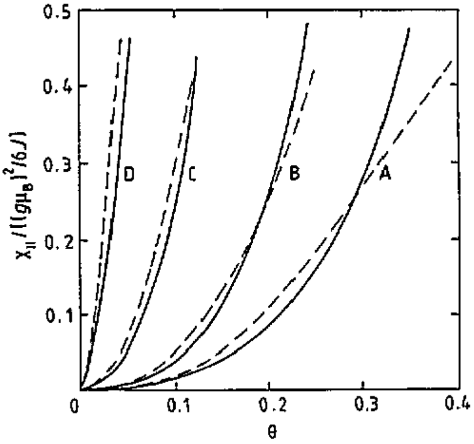

Figure 4. The parallel susceptibility $\chi_{\|}$ as a function of reduced temperature Θ with $S = \frac{1}{2}$. Curves A, B, C and D and the broken curves have the same meanings as in figure 2.

3.3. Parallel and perpendicular susceptibilities per site

Using the Kubo [17] method for the linear response function, the parallel and perpendicular susceptibilities of the system can be expressed as [10]

$$\chi_{\|} = \beta \frac{2}{N} \sum_{k} \exp(\beta\omega_k)\,[\exp(\beta\omega_k) - 1]^{-2} \tag{30}$$

and

$$\chi_{\perp} = m/2A(1+\alpha) \tag{31}$$

where m is the sublattice magnetization per site, and the units of $\chi_{\|}$ and $\chi_{\perp}$ are $(g\mu_B)^2$. In the linear spin-wave approximation, we cannot obtain the perpendicular susceptibility in the form of equation (31); instead $\chi_{\perp} = S/2A$, a function depending only on the interlayer coupling strength δ, and so it is necessary to take into account spin-wave interactions to calculate the perpendicular susceptibility of an antiferromagnet, although the spin-wave interaction corrections to the other physical quantities are small at low temperatures.

In the two low-temperature regimes, the asymptotic expressions for the parallel susceptibility are given by

$$\chi_{\|} = [1/6J(2+\delta)][\![\{1/[\delta(2+\delta)]^{1/2}(1+\alpha_0)^3\}(3\Theta)^2 + [2/5\delta(2+\delta)^3(1+\alpha_0)^8](3\Theta)^6]\!] \qquad (\Theta \ll \Theta_0 < \Theta_1) \tag{32}$$

and

$$\begin{aligned}\chi_{\|} = {} & [1/2J(2+\delta)]([3\Theta/\pi(1+\alpha_0)^2]\ln\{3e\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}\} \\ & + [\![[8\zeta(3)/\pi^2(2+\delta)^2(1+\alpha_0)^6](3\Theta)^4 \\ & + \{48[\zeta(3)]^2/\pi^3(2+\delta)^4(1+\alpha_0)^{10}\}(3\Theta)^7]\!] \\ & \times \ln[3e^{3/2}\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}]) \qquad (\Theta_0 \ll \Theta \ll \Theta_1).\end{aligned} \tag{33}$$

The terms can be understood as mentioned above. Similarly, $\chi_\parallel$ diverges logarithmically for the pure 2D ($\delta = 0$) case; as a consequence, there is no antiferromagnetic long-range ordering at finite temperatures.

The numerical results for $\chi_\parallel$ and $\chi_\perp$ as functions of reduced temperature and δ for $S = \frac{1}{2}$ over the whole range of temperatures based on equations (30) and (31) are shown in figures 4 and 5, respectively. From figure 5, we find that the region of magnetic ordering is reduced as δ decreases and disappears completely when δ equals zero. However, the perpendicular susceptibility at zero temperature is not a monotonic function of interlayer coupling strength; this result seems to be different from that in [9] but, in fact, they are in agreement with each other for [9] takes $z = 4 + 2\delta$ (γ in [9] is equivalent to our δ) as a renormalization parameter. In the same way, we may give the asymptotic expressions for $\chi_\perp$ in the two low-temperature regimes as

$$\begin{aligned}\chi_\perp = [1/4J(2+\delta)][\![m_0/(1+\alpha_0) - \{1/6[\delta(2+\delta)]^{1/2}(1+\alpha_0)^3\}(3\Theta)^2 \\ + [(2\pi)^2 m_0/30\delta^{1/2}(2+\delta)^{5/2}(1+\alpha_0)^6](3\Theta)^4 \\ - [\pi^2/15\delta(2+\delta)^3(1+\alpha_0)^8](3\Theta)^6]\!] \qquad (\Theta \ll \Theta_0 < \Theta_1)\end{aligned} \tag{34}$$

and

$$\begin{aligned}\chi_\perp = [1/4J(2+\delta)][\![m_0/(1+\alpha_0) - [3\Theta/\pi(1+\alpha_0)^2] \\ \times \ln\{3\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}\} + [4m_0\zeta(3)/\pi(2+\delta)^2(1+\alpha_0)^5](3\Theta)^3 \\ - [8\zeta(3)(3\Theta)^4/\pi^2(2+\delta)^2(1+\alpha_0)^6] \\ \times \ln\{3e^{1/2}\Theta/(1+\alpha_0)[\delta(2+\delta)]^{1/2}\}]\!] \qquad (\Theta_0 \ll \Theta \ll \Theta_1).\end{aligned} \tag{35}$$

In the linear spin-wave approximation, [4] gives a uniform susceptibility as a function of temperature and interlayer coupling strength; the results are the linear combination of $\chi_\parallel$ and $\chi_\perp$ obtained in the linear spin-wave theory in a definite form.

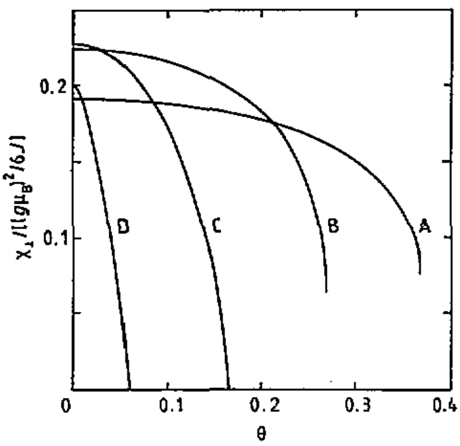

Figure 5. The perpendicular susceptibility $\chi_\perp$ as a function of reduced temperature Θ with $S = \frac{1}{2}$. Curves A, B, C and D have the same meanings as in figure 2.

4. Conclusion

We studied the effect of interlayer coupling on the magnetic and thermodynamic properties of a layered Heisenberg antiferromagnet by the use of the non-linear spin-wave theory. Numerical results show that for a given temperature, when the ratio δ of interlayer coupling strength to intralayer coupling strength $(J_\perp/J)$ increases, the sublattice magnetization increases, but the specific heat and parallel susceptibility decrease. The dependence of the perpendicular susceptibility on the interlayer coupling strength is not a monotonic relation, and it is necessary to take into account the spin-wave interactions to make the perpendicular susceptibility depend on the temperature.

At low temperatures $(T \ll T_1 = 2J(2+\delta)/k_B)$, we have defined a characteristic temperature $T_0 = 2J[2\delta(2+\delta)]^{1/2}/k_B$ which distinguishes the quasi-2D from the quasi-3D case according to the values of δ, given the asymptotic expressions for sublattice magnetization, internal energy, specific heat, parallel and perpendicular susceptibilities in two low-temperature regimes $T \ll T_0 < T_1$ and $T_0 \ll T \ll T_1$. The behaviours with temperature of these physical quantities at low temperatures are in agreement with that of the 3D system for $T \ll T_0 < T_1$. However, for $T_0 \ll T \ll T_1$, the behaviours with T and δ for the sublattice magnetization, parallel and perpendicular susceptibilities are in the forms of $-T \ln T$ and $-\ln\delta$; thus they diverge logarithmically when $\delta = 0$ at finite temperatures. There is no linear term in T in the expressions for specific heat at low temperatures, which is in agreement with experimental data.

References

[1] Anderson P W 1987 *Science* **235** 1196
[2] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[3] De Jongh L J and Miedema A R 1974 *Adv. Phys.* **23** 1
[4] Berezinsky V L and Blank A Ya 1973 *Zh. Eksp. Teor. Fiz.* **64** 725
(Engl. Transl. 1973 *Sov. Phys.–JETP* **37** 369)
[5] Singh A, Tešanovic Z, Tang H, Xiao G, Chien C L and Walker J C 1990 *Phys. Rev. Lett.* **64** 2571
[6] Kopietz P 1992 *Phys. Rev. Lett.* **68** 3480
[7] Liu B G 1990 *Phys. Rev.* B **41** 9563
[8] Dyson F J 1956 *Phys. Rev.* **102** 1217, 1230
[9] Soukoulis C M, Datta S and Lee Y H 1991 *Phys. Rev.* B **44** 446
[10] Liu S H 1966 *Phys. Rev.* **142** 267
[11] Anderson P W 1952 *Phys. Rev.* **86** 694
Kubo R 1952 *Phys. Rev.* **87** 568
[12] Bloch M 1962 *Phys. Rev. Lett.* **9** 286; 1963 *J. Appl. Phys.* **34** 1151
[13] Singh A and Tešanovic Z 1990 *Phys. Rev.* B **41** 11 457
[14] Huang K and Manousakis E 1987 *Phys. Rev.* B **36** 8302
[15] Oguchi T 1960 *Phys. Rev.* **117** 117
[16] Kumagai K, Nakamichi Y, Watanabe I, Nakamura Y, Nakajima H and Waka N 1988 *Phys. Rev. Lett.* **60** 724
[17] Kubo R 1957 *J. Phys. Soc. Japan* **12** 570