On the self-consistent spin-wave theory of frustrated Heisenberg antiferromagnets

1992 J. Phys.: Condens. Matter 4 5227

(http://iopscience.iop.org/0953-8984/4/22/019)

J. Phys.: Condens. Matter 4 (1992) 5227–5237. Printed in the UK

On the self-consistent spin-wave theory of frustrated Heisenberg antiferromagnets

V Yu Irkhin, A A Katanin and M I Katsnelson
Institute of Metal Physics, 620219 Ekaterinburg, Russia

Received 15 July 1991, in final form 8 January 1992

Abstract. The phase diagrams of Heisenberg antiferromagnets with frustrated exchange interactions are obtained by using the self-consistent spin-wave approximation. The square, simple-cubic and quasi-1D antiferromagnets are considered with different values of spin S. An important role of spin-wave renormalizations of exchange parameters is demonstrated. The temperature dependences of the correlation length and spin-wave damping are calculated. It is shown that a wide temperature region above T_N with a strong short-range order exists in frustrated 3D systems.

1. Introduction

Recently, interest has grown in the problem of the ground state of frustrated two-dimensional (2D) spin systems [1–8]. This is connected mainly with the discovery of quasi-2D antiferromagnetism in La_2CuO_4 and $YBa_2Cu_3O_6$. It was supposed that the destruction of long-range magnetic order by current carriers in these compounds on doping is related to the nature of high-T_c superconductivity and to normal-phase anomalous properties of such systems [9]. The question about the possibility of imitation of frustrations via current carriers by 'competing' exchange interactions in the simple Heisenberg model is not trivial. However, the treatment of the latter model is in any case of interest from both a theoretical and an experimental point of view. Of great importance is the problem of the formation of an RVB-type state with long-range order (LRO) suppressed and unusual order parameters. This problem is actual for some three-dimensional (3D) systems which demonstrate frustrated antiferromagnetism and a large linear term in the specific heat. An analysis of corresponding experimental data for the system $Y_{1-x}Sc_xMn_2$, for heavy-electron compounds as well as for some systems with charge (pseudospin) degrees of freedom (e.g. Sm_3Se_4 and Fe_3O_4) was made in [10, 11].

Quantitative treatment of the phase diagrams of low-dimensional magnetic systems is possible within the self-consistent spin-wave theory (SSWT) [12, 13], which is widely exploited now. (Earlier versions of the SSWT have been proposed in [14, 15].) The consideration of the square lattice in the next-nearest-neighbour approximation was carried out at $T = 0$ in [5–8]. The aim of the present work is to investigate the phase diagram and magnetic properties for 2D and 3D cases both in the ground state and for finite T.

The plan of the paper is as follows. In section 2 we consider the spin-wave correction to the sublattice magnetization of an antiferromagnet and the equations of the SSWT. In section 3 we investigate the phase diagram of the square lattice in the ground state for different values of spin S and calculate the temperature dependences of the correlation length and magnon damping near the frustration point. In section 4 we treat the ground-state phase diagram of the simple-cubic lattice in the next-nearest-neighbour approximation. In section 5 we discuss the short-range order (SRO) above the Néel temperature T_N in the 3D case.

2. Spin-wave corrections to the sublattice magnetization in frustrated systems and self-consistent equations

We consider the Heisenberg Hamiltonian

$$H = \sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j = \sum_q J_q \boldsymbol{S}_q \cdot \boldsymbol{S}_{-q} \tag{1}$$

with J_q the Fourier transforms of the exchange parameters. The suppression of long-range antiferromagnetic ordering owing to frustrations may be demonstrated by a simple spin-wave treatment. The correction to the sublattice magnetization due to zero-point oscillations has the form

$$\delta\bar{S} = -\sum_q v_q^2 \tag{2}$$

$$v_q^2 = \tfrac{1}{4}S(2J_q + J_{Q+q} + J_{Q-q} - 4J_Q)/\omega_q - \tfrac{1}{2}$$

where Q is the wavevector of the AFM structure ($J_Q = J_{\min}$) and ω_q is the magnon frequency given by

$$\omega_q^2 = 2S^2(J_Q - J_q)(2J_Q - J_{Q+q} - J_{Q-q}). \tag{3}$$

Consider the 2D case and assume that, at $q \to 0$,

$$J_{Q+q} + J_{Q-q} - 2J_Q = \tfrac{1}{2}\alpha q^2 + \tfrac{1}{2}\beta q^4 f(\varphi)$$

where $\beta > 0$ and $f(\varphi) \sim 1$ is a positive function of the polar angle of the vector q. The frustration situation corresponds to $\alpha \to 0$. Then we have

$$\delta\bar{S} = -a \ln\left(\frac{\beta}{\alpha}\right) \qquad a = \frac{1}{4\pi^2}\int_0^{2\pi} \frac{d\varphi}{[\beta f(\varphi)]^{1/2}} \tag{4}$$

which yields $\bar{S} = 0$ in some region $|\alpha| < \beta \exp(-S/a)$. A scaling consideration [1] shows that this result is valid to the leading order in the quasi-classical parameter $1/S$ which plays the role of a coupling constant. For the square lattice in the next-nearest-neighbour approximation we have

$$J_q = 2I(\cos q_x + \cos q_y) + 4I' \cos q_x \cos q_y \qquad \alpha = I - 2I'. \tag{5}$$

A formally similar situation occurs for a quasi-1D antiferromagnet with a weak 2D or 3D exchange interaction, where

$$J_q = 2I \cos q_x + 2\tilde{I} \cos q_y \tag{6}$$

and

$$J_q = 2\tilde{I}(\cos q_x + \cos q_y) + 2I \cos q_z \tag{7}$$

respectively; $\tilde{I} \ll I$. Then we obtain

$$\delta\bar{S} = -(1/2\pi)\ln(I/\tilde{I}) \tag{8}$$

which results in $\bar{S} = 0$ at $\tilde{I} < I \exp(-2\pi S)$.

To treat the two-sublattice antiferromagnet in the quantum case we apply the self-consistent modified spin-wave theory [13]. Using the Dyson–Maleev representation

$$\begin{array}{llll} S_l^- = a_l^+ & S_l^+ = (2S - a_l^+ a_l)a_l & S_l^z = S - a_l^+ a_l & l \in A \\ S_m^- = -b_m & S_m^+ = b_m^+(2S - b_m^+ b_m) & S_m^z = b_m^+ b_m - S & m \in B \end{array} \tag{9}$$

and introducing the 'renormalized' exchange interactions

$$\gamma_q = 2\sum_p J_{q-p}\langle a_p^+ b_{-p}^+\rangle \qquad \gamma'_q = 2\sum_p J'_{q-p}\langle a_p^+ a_p\rangle \tag{10}$$

we obtain the equations of the SSWT in the form

$$S + \tfrac{1}{2} = \sum_k{}' \frac{\lambda_k}{E_k}\coth\left(\frac{E_k}{2T}\right) + \bar{S} \tag{11}$$

$$\gamma_q = \sum_k{}' J_{q-k}\frac{\gamma_k}{E_k}\coth\left(\frac{E_k}{2T}\right) + \bar{S}J_q \tag{12}$$

$$\gamma'_q = \sum_k{}' J'_{q-k}\frac{\lambda_k}{E_k}\coth\left(\frac{E_k}{2T}\right) + \bar{S}J'_q \tag{13}$$

where

$$\lambda_p = \gamma_0 + \gamma'_p - \gamma'_0 - \mu \qquad E_p = (\lambda_p^2 - \gamma_p^2)^{1/2} \tag{14}$$

$\bar{S}$ is the staggered magnetization (the terms with $\bar{S}$ correspond to picking out the contribution with $\boldsymbol{k} = 0$ and describe the boson condensate), Σ' stands for the sum over $\boldsymbol{k} \neq 0$, and μ is the chemical potential of the bosons.

One can see that the SSWT yields the gap in the magnon (spin-wave) spectrum for the state without LRO. This circumstance is not quite satisfactory, e.g. in the case of the linear chain with a half-integer spin, where elementary excitations are known to be gapless, despite the fact there is no LRO in the ground state. It should be noted that the gap, which occurs in the SSWT, is proportional to $\exp(-\pi S)$ and is numerically small even for $S = \frac{1}{2}$. On the other hand, the SSWT (bosonic mean-field theory) is in a fairly good agreement with the scaling consideration [16] and, as noted in [12], works well for systems with LRO in the ground state, which are mainly treated in the present paper. As regards the gap, which arises at finite temperatures, it turns out to be smeared by the spin-wave damping (see below in sections 3 and 5).

3. Phase diagram of the square lattice and the correlation length

Consider the two-dimensional case (5). At small I'/I the AFM ordering with $\boldsymbol{Q} = (\pi, \pi)$ is realized and the solution has the form

$$\gamma_p = \tfrac{1}{2}\gamma(\cos p_x + \cos p_y) \qquad \gamma'_p = \gamma' \cos p_x \cos p_y. \tag{15}$$

Substiututing (15) into (12)–(14) we derive ($T = 0$)

$$\lambda_p = \gamma + \gamma'(\cos p_x \cos p_y - 1) \tag{16}$$

$$\frac{\gamma}{I} = \sum_p{}' \frac{\gamma}{E_p}(\cos p_x + \cos p_y)^2 + 4\bar{S} \tag{17}$$

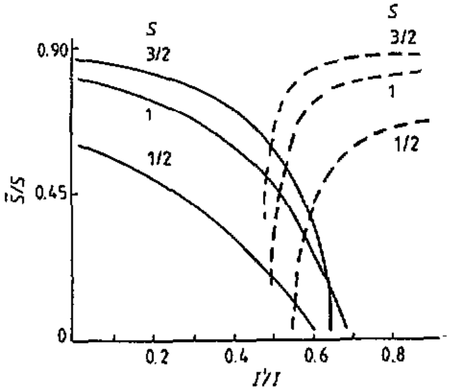

Figure 1. Values of $\bar{S}$ for the phases with $Q = (\pi, \pi)$ (——) and $Q = (\pi, 0)$ (- - -) for different S.

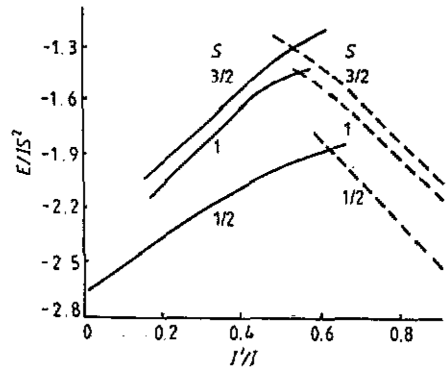

Figure 2. The total energy of the $Q = (\pi, \pi)$ (——) and $Q = (\pi, 0)$ (- - -) for different S.

$$\frac{\gamma'}{I'} = 4\sum_p{}' \frac{\lambda_p}{E_p} \cos p_x \cos p_y + 4\bar{S}. \tag{18}$$

Besides the phase with $Q = (\pi, \pi)$ we have to take into account the AFM phase with $Q = (\pi, 0)$ which corresponds to large I'/I. The corresponding solution may be represented as

$$\gamma_p = \gamma_x \cos p_x + \gamma' \cos p_x \cos p_y \qquad \gamma'_p = \gamma' \cos p_x \cos p_y \tag{19}$$

and equations (12)–(14) take the form

$$\begin{aligned}
\lambda_p &= \gamma_x + \gamma' + \gamma_y(\cos p_y - 1) \\
\frac{\gamma_x}{I} &= 2\sum_p{}' \frac{\gamma_p}{E_p} \cos p_x + 2\bar{S} \\
\frac{\gamma_y}{I} &= 2\sum_p{}' \frac{\lambda_p}{E_p} \cos p_y + 2\bar{S} \\
\frac{\gamma'}{I'} &= 4\sum_p{}' \frac{\gamma_p}{E_p} \cos p_x \cos p_y + 4\bar{S}.
\end{aligned} \tag{20}$$

The results of numerical solution of equations (11), (17), (18) and (20) for different S are given in figures 1 and 2. One can see that $\bar{S}$, corresponding to the phase with $Q = (\pi, \pi)$, vanishes for $I'/I > \frac{1}{2}$ (in particular for $S = \frac{1}{2}$ the critical value $p_c = (I'/I)_c = 0.61$ [5–8]). This seems to contradict the above scaling consideration since the point $I'/I = \frac{1}{2}$ corresponds to the absolute instability of the (π, π) structure. Besides this, the dependence of p_c versus S turns out to be non-monotonic. So, $p_c(S = 1) = 0.69$ and $p_c(\frac{3}{2}) = 0.65$. Even for $S = 10$, p_c turns out to be far from the classical value of $\frac{1}{2}$. These paradoxes may be resolved if we plot the phase diagram versus the ratio of 'renormalized' exchange parameters γ' and γ rather than the ratio of the bare parameters (figure 3). Then the critical value of γ'/γ increases monotonically with increasing S, and the point $\gamma'/\gamma = 0.5$ is unreachable. Thus the renormalization of exchange parameters turns out to play an important role in the phase diagram. As follows from figure 1, the solution corresponding to $Q = (\pi, 0)$ arises before the instability point of the $Q = (\pi, \pi)$ phase

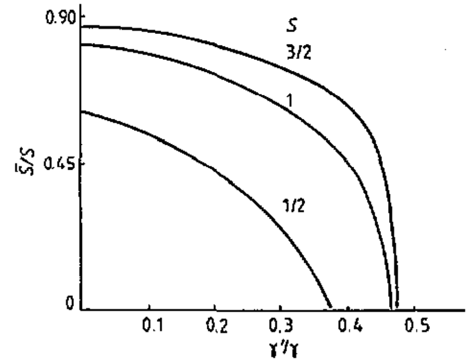

Figure 3. Values of $\bar{S}$ for $Q = (\pi, \pi)$ versus ratio of the renormalized exchange parameters γ'/γ.

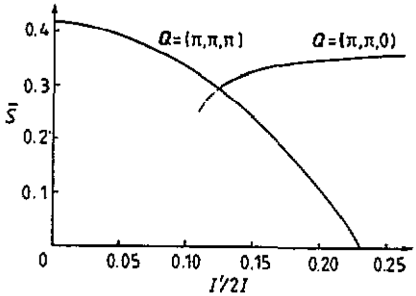

Figure 4. Values of $\bar{S}$ for the $Q = (\pi, \pi, \pi)$ and $Q = (\pi, \pi, 0)$ phases for the simple-cubic lattice, $S = \frac{1}{2}$.

for any S. Thus the non-magnetic spin-liquid state does not occur in the approximation under consideration. However, quantum effects may be important in the region of coexistence of the magnetic phases and change the situation.

Now we consider the behaviour of a 2D frustrated antiferromagnet at finite T. For $T \ll I$ the LRO is absent, but pronounced SRO with a large correlation length ξ exists. The latter quantity determines the gap in the spectrum of the bosons E_k.

Expanding E_k in k, $\xi^{-1} = (2/\gamma\delta)^{1/2}\Delta$ (where $\Delta = (\lambda_0^2 - \gamma_0^2)^{1/2}$ is the gap in the spectrum, and $\delta = \gamma - 2\gamma'$ is small near the frustration point) we obtain

$$E_k^2 = \gamma\delta(k_x^2 + k_y^2)/2 + \gamma\gamma' k_x^2 k_y^2/2 + \gamma\delta/2\xi^2. \tag{21}$$

For $\bar{S} = 0$, equation (11) gives

$$\int_0^\gamma \frac{dE}{E}\,\nu(E)\coth\left(\frac{E}{2T}\right) = 2S + 1 \qquad \nu(E) = 2\sum_p \delta(E - E_p). \tag{22}$$

Then we obtain

$$\bar{S}(0) - (1/\pi)(\gamma/2\delta)^{1/2}\xi^{-1}(0) = -(2T/\pi\delta)\ln\{2\sinh[(1/2T\xi)(\gamma\delta/2)^{1/2}]\}. \tag{23}$$

The second term on the left-hand side of (23) is absent if the ground state possesses LRO ($\bar{S}(0) \neq 0$). Later we consider this case. Then we obtain

$$\xi^{-1} = \begin{cases} 2T(2/\gamma\delta)^{1/2}\exp[-\pi\bar{S}(0)\delta/2T] & T \ll \bar{S}(0)\delta \\ 2T(2/\gamma\delta)^{1/2}\ln(1 + 2^{1/2}) & (\gamma\delta)^{1/2} \gg T \gg \bar{S}(0)\delta. \end{cases} \tag{24}$$

(Note that, in the classical limit $S \to \infty$, we have $\gamma = 2(2S+1)I$ and $\gamma' = 2(2S+1)I'$.) Thus at $J \gg T \gg \delta$ the correlation length demonstrates non-exponential behaviour. Generally speaking, our approximation, corresponding to the one-loop approximation [16], does not yield correctly the pre-exponential factor in $\xi(T)$. However, the weakening of the T-dependence of ξ seems to be reasonable.

To clarify the physical meaning of the gap Δ we calculate the magnon damping which arises on considering corrections to the mean-field theory. Using, similar to [17], the diagram technique approach we derive for the damping

$$\Gamma_k = \frac{\pi}{4} J_0^2 \left[1 - \exp\left(\frac{-E_k}{T}\right)\right] \sum_{pq} n_p (1 + n_{k+p-q})(1 + n_q)$$
$$\delta(E_k + E_p - E_{k+p-q} - E_q) M_{22}(k, p, q, k + p - q) \tag{25}$$

where

$$M_{22}(k, p, q, r) = (1/\varepsilon_k \varepsilon_p \varepsilon_r \varepsilon_q)[(2\alpha r \cdot q - \varepsilon_r \varepsilon_q)(2\alpha k \cdot p - \varepsilon_k \varepsilon_p)$$
$$+ (2\alpha p \cdot r - \varepsilon_p \varepsilon_r)(2\alpha k \cdot q - \varepsilon_k \varepsilon_q) + (2\alpha p \cdot q - \varepsilon_p \varepsilon_q)(2\alpha k \cdot r - \varepsilon_k \varepsilon_r)]$$

is the magnon–magnon scattering amplitude,

$$\alpha = -[(1/2J_q)(\partial^2 J_q / \partial q_x^2)]_{q=0} \qquad \varepsilon_k = E_k / \lambda_k$$

and $n_k = n(E_k)$ is the Bose distribution function. For $k \gg \Delta/(\gamma\delta)^{1/2}$, the renormalization of the spectrum E_k and the presence of the energy gap are not important, and we reproduce the results of [17]. However, at $k \to 0$ the damping in SSWT remains finite;

$$\Gamma_0 \sim (T/S\delta)^2 \Delta. \tag{26}$$

At $T \ll S\delta$, both Δ and Γ_0 are exponentially small. At $T > S\delta$ the gap is completely smeared by the damping.

It should be noted that similar results may be obtained in the quasi-1D case. The solution to equations (11) and (12) corresponding to (6) has the form

$$\gamma_p = \gamma \cos p_x + \tilde{\gamma} \cos p_y$$

and we obtain for the correlation length

$$\bar{S}(0) - \bar{\tilde{\gamma}}[2\pi(\gamma\tilde{\gamma})^{1/2}\xi(0)]^{-1} = -(T/\pi)(\gamma\tilde{\gamma})^{-1/2} \ln[2\sinh(\bar{\tilde{\gamma}}/2\xi T)]$$
$$\bar{\tilde{\gamma}} = [\gamma(\gamma + \tilde{\gamma})]^{1/2}. \tag{27}$$

Since, in the SSWT, ξ is large even in the ground state of the linear chain with $S = \frac{1}{2}$ ($\xi^{-1}(0) \simeq 0.17$), the approximation (27) is satisfactory for arbitrary $\tilde{I}/I < 1$.

4. Ground state of the simple-cubic lattice in the next-nearest-neighbour approximation

It is instructive to investigate, within the self-consistent theory, frustrated 3D systems. As an example we consider the simple-cubic lattice in the next-nearest-neighbour approximation where

$$J_q = 2I(\cos q_x + \cos q_y + \cos q_z)$$
$$+ 4I'(\cos q_x \cos q_y + \cos q_y \cos q_z + \cos q_z \cos q_x). \tag{28}$$

We treat the case of antiferromagnetic exchange interactions $I > 0$, $I' > 0$. In the classical limit the minimum of the exchange energy is realized for the AFM structure with $Q = (\pi, \pi, \pi)$ at $I' < I/4$ and with $Q = (\pi, \pi, 0)$ (and with cyclic permutations) at $I' > I/4$, so that the frustration means competition of these structures at $I \simeq 4I'$. We do not

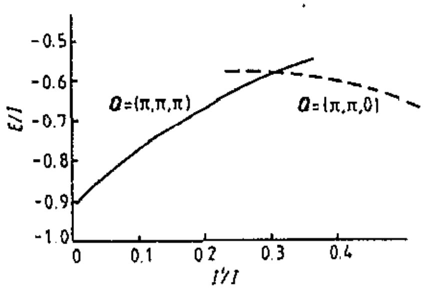

Figure 5. Total energies corresponding to figure 4.

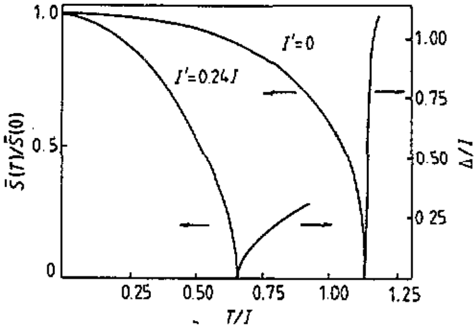

Figure 6. Temperature dependences of the sublattice magnetization ($T < T_N$) and the gap in the excitation spectrum ($T > T_N$) in the frustrated and non-frustrated cubic lattice, $S = \frac{1}{2}$.

discuss here the case when $I' < 0$ where the instability with respect to the spiral structure with

$$Q_x = Q_y = Q_z = \cos^{-1}(I/4|I'|)$$

takes place. This case will be considered elsewhere.

As follows from the expression for the spin-wave spectrum (3), terms, linear in q, are cancelled in ω_q at $I' \to I/4$, similar to the 2D case at $I' \to I/2$. However, unlike the 2D case, we do not have in 3D 'dangerous' divergent corrections to the sublattice magnetization. Nevertheless, one can assume that the spin-wave corrections with the 'soft' spectrum ω_q in the frustrated case are more important than in the case $I' = 0$.

The solutions to the equations of the SSWT (11)–(13) have the form

$$\begin{aligned}\lambda_q &= \gamma + \tfrac{1}{3}\gamma'(\cos q_x \cos q_y + \cos q_z \cos q_x + \cos q_y \cos q_z) - \mu \\ \gamma_q &= \tfrac{1}{3}\gamma(\cos q_x + \cos q_y + \cos q_z)\end{aligned} \tag{29}$$

for the phase with $\boldsymbol{Q} = (\pi, \pi, \pi)$ and

$$\begin{aligned}\lambda_q &= \gamma_{xy} + \gamma'_{xy} + \gamma_z(\cos q_z - 1) + \gamma'_z(\cos q_y \cos q_x - 1) - \mu \\ \gamma_q &= \tfrac{1}{2}(\cos q_x + \cos q_y)(\gamma_{xy} + \gamma'_{xy}\cos q_z)\end{aligned} \tag{30}$$

for the phase with $\boldsymbol{Q} = (\pi, \pi, 0)$. Results of the numerical calculations of the ground-state sublattice magnetization and total energy (for $S = \frac{1}{2}$, when the spin-wave corrections are most important) are presented in figures 4 and 5, respectively. One can see that the point of the transition between the structures $I'/I = 0.30$ differs weakly from the classical value at 0.25. The value of staggered magnetization at this point, namely $\bar{S}(0) \simeq 0.27$, is appreciably smaller than that for $I' = 0$, namely $\bar{S} \simeq 0.42$. The ranges of existence of the phases with $\boldsymbol{Q} = (\pi, \pi, \pi)$ and $(\pi, \pi, 0)$ overlap in a broad interval, so that the non-magnetic phase does not arise, as also in the 2D case.

As follows from the sum rule

$$S(S+1) = \bar{S}^2 + \sum_q \langle \delta S_{-q} \cdot \delta S_q \rangle$$

the smallness of $\bar{S}(0)$ means inevitably the existence of developed spin fluctuations.

Table 1. Temperature dependence of the sublattice magnetization $\bar{S}$ ($T < T_N$), chemical potential μ ($T > T_N$) and short-range order parameters γ and γ' for $S = \frac{1}{2}$ and $I' = 0.24I$.

T/I	$\bar{S}$	γ/I	γ'/I
0.00	0.30	3.20	1.13
0.10	0.29	3.20	1.13
0.20	0.28	3.19	1.12
0.30	0.25	3.16	1.10
0.40	0.21	3.07	1.06
0.50	0.15	2.93	0.97
0.60	0.09	2.70	0.85
0.70	0.00	2.36	0.66
T/I	μ/I	γ/I	γ'/I
0.75	−0.00	2.11	0.53
0.85	−0.09	1.96	0.44
0.95	−0.18	1.31	0.17
1.05	−0.49	0.95	0.06
1.15	−0.83	0.37	0.02
1.25	−1.08	0.22	0.00
1.35	−1.24	0.06	−0.02

Therefore one can expect that the frustrated 3D systems may exhibit, despite the presence of LRO at finite T, some features of a spin liquid. In the next section we investigate the SRO above T_N.

5. Simple-cubic lattice at finite temperatures

We consider the AFM structure with $Q = (\pi, \pi, \pi)$ near the point of instability putting $I' = 0.24I$. Temperature dependences of the staggered magnetization at $T < T_N$ and of the gap in the spin-wave spectrum $\Delta = (\lambda_0^2 - \gamma_0^2)^{1/2}$ at $T > T_N$, calculated from (11)–(14) are shown in figure 6. Compared with the case $I' = 0$, T_N/I decreases from 1.13 to 0.70 at $S = \frac{1}{2}$ and from 5.9 to 3.4 at $S = \frac{3}{2}$. The temperature dependences of γ and γ' are presented in tables 1 and 2. At $T > T_N$, these quantities are characteristics of SRO. The phase transition with vanishing of $\gamma(T)$ and $\gamma'(T)$ at high T is an artefact of the mean-field approximation; strictly speaking, a local SRO parameter does not exist and is removed by fluctuations [12] (cf also the $1/N$-expansion for the Kondo problem [18]). Thus at small γ and γ', our approach is inadequate. Therefore, we determine the temperature interval with strong SRO as the region between T_N and the temperature of rapid decrease in $\gamma(T)$. The parameter γ' characterizes the SRO corresponding to the $(\pi, \pi, 0)$ structure. One can see that $\gamma'(T)$ decreases more rapidly than $\gamma(T)$, and $\gamma'/\gamma \ll I'/I$ at $T > T_N$, so that the 'foreign' SRO is suppressed.

The correlation length may be estimated as $\xi \sim I/\Delta(T)$. As follows from figure 6, the region with appreciable SRO ($\xi > 1$) is about 40% of T_N for $S = \frac{1}{2}$. Thus, similar to the quasi-2D systems [19], the width of the region with strong SRO in the frustrated 3D systems is large in comparison with that in the case $I' = 0$ where it makes up about 1% of T_N (figure 6).

Table 2. Temperature dependence of the sublattice magnetization $\bar{S}$ ($T < T_N$), chemical potential μ ($T > T_N$) and short-range order parameters γ and γ' for $S = \frac{5}{2}$ and $I' = 0.24I$.

T/I	$\bar{S}$	γ/I	γ'/I
0.00	1.25	9.07	3.85
0.40	1.17	9.05	3.83
0.80	1.10	8.98	3.80
1.20	0.99	8.75	3.64
1.60	0.84	8.36	3.39
2.00	0.67	7.88	3.09
2.40	0.53	7.37	2.79
2.80	0.29	6.56	2.30
3.20	0.04	5.49	1.69
3.60	0.00	4.70	1.30
T/I	μ/I	γ/I	γ'/I
4.00	−0.56	1.95	0.18
4.40	−1.58	0.65	0.01
4.80	−2.25	0.09	−0.03

To understand the peculiar features of the 3D situation we treat analytically the case where $\gamma = 2\gamma'$ (an analogue of the classical case $I' = I/4$; in the classical limit, $\gamma = 3I(2S+1)$ and $\gamma' = 6I'(2S+1)$). Then the spin-wave spectrum at $q \to 0$ is given by

$$E_q^2 = \tfrac{1}{12}\gamma^2(q_x^2 q_y^2 + q_y^2 q_z^2 + q_x^2 q_z^2 + 1/\xi^4). \tag{31}$$

As follows from the calculation of the spin-correlation function $\langle S_R \cdot S_0 \rangle$ in the SSWT [13] by the multi-dimensional saddle-point method, the quantity $\xi = (\gamma\gamma'/6\Delta^2)^{1/4}$ is simply the correlation length, which is divergent at $T = T_N$ (in our case, $T_N \sim \delta = \gamma - 2\gamma' \to 0$). Calculating the integral in (11) at $\bar{S} = 0$ we obtain

$$\int_0^\gamma \frac{dE}{E}\,\bar{\nu}(E)\coth\left(\frac{E}{2T}\right) = \frac{12T}{\pi^3\gamma'\xi} I_1 I_2 I_3 \qquad \bar{\nu}(E) = 2\sum_p \delta(E - E_p)\lambda_p \tag{32}$$

$$I_1 = \int_0^1 \frac{dx}{(1-x^4)^{3/4}} = 1.855 \qquad I_2 = \int_0^1 \frac{dx}{(1-x^4)^{1/2}} = 1.311$$

$$I_3 = \int_1^\infty \frac{dx}{x(x^2-1)^{1/2}} = 2.119.$$

Then the correlation length is expressed as

$$\xi = (\pi^3/24 I_1 I_2 I_3)[\gamma(2S+1)/T] \simeq \gamma(2S+1)/4T. \tag{33}$$

Thus the limiting case considered demonstrates the peculiar features of the frustrated 3D state: a small value of T_N and a large width of the region with strong SRO ($\xi \gg 1$ at $T \ll \gamma$). Unlike the 2D case, $\xi(T)$ demonstrates power-law rather than exponential behaviour. Estimate of the ‘spin-wave’ damping at $k \to 0$ ($k \ll T/I$) from (25) for the spectrum (31) yields

$$\Gamma \sim T^2/\gamma S \sim \Delta = (\gamma\gamma')^{1/2}/\xi^2. \tag{34}$$

Thus the gap is smeared in the frustrated 3D case as well as in the frustrated 2D case.

6. Discussion

In the present paper we have applied the SSWT [13] to investigate the properties of frustrated 2D and 3D systems both in the ground state and at finite temperatures. Our calculations demonstrate that the spin-liquid state with zero staggered magnetization does not form within the approach used. The question of the role of quantum effects and collective excitations remains open.

At the same time, for finite T the behaviour of frustrated system is reminiscent of a spin-liquid (RVB-type) state. To describe systems exhibiting spin-liquid-type properties with pseudospin degrees of freedom [10], a treatment of anisotropic spin Hamiltonians would be useful. However, this seems to be a difficult mathematical problem.

The most important physical result of the paper is the presence in frustrated 3D systems of a wide temperature region above T_N with pronounced SRO. Note that a similar conclusion holds for quasi-2D systems [19]. In this connection, experimental data demonstrating the existence of the SRO above T_N are instructive. For example, strong SRO vanishing sharply at $T \simeq 5T_N$ was observed in MnO and $KMnF_3$ using the electron diffraction technique [20]. As follows from our consideration, Heisenberg systems demonstrating such a behaviour should possess frustrating exchange interactions. The role of frustrations for the strong SRO above T_N was discussed in connection with experimental data on GdB_6 [21] and pyrochlore-structure compounds [22]. SRO above T_N is observed in helicoidal antiferromagnets such as Tb, Dy, Ho [23] and, in particular, $ZnCr_2Se_4$ [24].

For frustrated itinerant-electron systems such as $YMn_{2-x}Sc_x$ [25] the situation may be more complicated because of the non-Heisenberg character of the exchange. Thus, a generalization of our approach to real lattices and various microscopic models would be of interest.

References

[1] Ioffe L B and Larkin A I 1988 *Int. J. Mod. Phys.* B **2** 203
[2] Chandra P and Doucot B 1988 *Phys. Rev.* B **38** 9335
[3] Coleman P 1988 *J. Magn. Magn. Mater.* **82** 159
[4] Chandra P, Coleman P and Larkin A I 1990 *J. Phys.: Condens. Matter* **2** 7933
[5] Xu J H and Ting C S 1990 *Phys. Rev.* B **42** 6861
[6] Barabanov A F and Starykh O A 1990 *Zh. Eksp. Teor. Fiz. Piz. Red.* **51** 271
[7] Oguchi T and Kitatani H 1990 *J. Phys. Soc. Japan* **59** 3322
Nishimori H and Saika Y 1990 *J. Phys. Soc. Japan* **59** 4454
[8] Mila F, Poilblanc D and Bruder C 1991 *Phys. Rev.* B **43** 7891
[9] Anderson P W 1987 *Science* **235** 1196
[10] Irkhin V Yu and Katsnelson M I 1990 *Phys. Lett.* **150A** 47
Vonsovsky S V, Irkhin V Yu and Katsnelson M I 1991 *Physica* B **171** 135
[11] Irkhin V Yu and Katsnelson M I 1991 *Z. Phys.* B **82** 77
[12] Arovas D P and Auerbach A 1988 *Phys. Rev.* B **38** 316

[13] Takahashi M 1989 *Phys. Rev.* B **40** 2494

[14] Loly P 1971 *J. Phys. C: Solid State Phys.* **1** 1365

[15] Rastelli E and Tassi A 1974 *Phys. Lett.* **48A** 119; 1975 *Phys. Rev.* B **11** 4711

[16] Chakravarty S, Halperin B I and Nelson D R 1989 *Phys. Rev.* B **39** 2344

[17] Tyč S and Halperin B I 1990 *Phys. Rev.* B **42** 2096

[18] Coleman P 1987 *Phys. Rev.* B **35** 5072

[19] Irkhin V Yu, Katanin A A and Katsnelson M I 1991 *Phys. Lett.* **157A** 295

[20] Hermsmeier B, Osterwalder J, Friedman D J and Fadley C S 1989 *Phys. Rev. Lett.* **62** 478

[21] Fisk Z, Taylor R H and Coles B P 1971 *J. Phys. C: Solid State Phys.* **4** 129

[22] Reimers J N, Greedman J E, Kremer R K, Gmelin E and Subramanian M A 1991 *Phys. Rev.* B **43** 3387
Reimers J N, Greedman J E, Stager C V, Bjarguinnsen M and Subramanian M A 1991 *Phys. Rev.* B **43** 5692

[23] Mandzhavidze A G and Haradze G A 1969 *Zh. Eksp. Teor. Fiz. Pis. Red.* **10** 68
Amitin E B, Bessergenev V G and Kovalevskaya Yu A 1983 *Zh. Eksp. Teor. Fiz.* **84** 205

[24] Akimitsu J, Siratori K, Shirane G, Iizumi M and Watanabe T 1977 *J. Phys. Soc. Japan* **44** 172

[25] Deportes J, Ouladdiaf B and Ziebeck K R A 1987 *J. Magn. Magn. Mater.* **70** 14
Wada H, Nakamura H, Fukami E, Yoshimura K, Shiga M and Nakamura Y 1987 *J. Magn. Magn. Mater.* **70** 17