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A model for the heavy-fermion behaviour of YMn_2: influence of frustration on the spin fluctuation spectrum

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Abstract. We show that the magnetic properties of frustrated itinerant systems can be described by a peculiar shape of the q-dependent susceptibility. We justify the fact that the spin fluctuation spectrum is especially broad in this case. This spectrum is used to calculate the spin fluctuation contribution to the specific heat; we show that this contribution can be very large close to a magnetic–non-magnetic instability. Comparison with recent experimental results on YMn_2 is made and the similarities of this compound with the 4f heavy-fermion compounds are emphasized.

1. Introduction

Frustration is present in many magnetic systems and it can lead to several original behaviours (for a review see [1]): incommensurate magnetic structures, absence of long-range ordering, order by disorder, spin liquid states, etc. Frustration can be due either to the existence of competing interactions as in the ANNI model or to the crystallographic structure itself as in the triangular, Kagomé or pyrochlore lattices.

In metallic magnetic systems we have shown recently that new ground states can be stabilized in strongly frustrated crystallographic structures, when the itinerant electrons are close to the magnetic–non-magnetic instability [2]. Typical examples of frustrated itinerant systems are the RMn_2 Laves phase compounds in which the Mn sublattice presents several kinds of ordering, depending on the Mn–Mn distance [3]; with a heavy rare earth, Mn is non-magnetic (or has a small moment induced by the R–Mn interactions) whereas, with a light rare earth, complicated antiferromagnetic structures are obtained; with R $\equiv$ Dy or Th, both magnetic and non-magnetic Mn sites are present in the ordered state. We have shown that these new magnetic structures are stabilized in frustrated lattices because it is the best way of reducing frustration close to a magnetic–non-magnetic instability [2].

More recently the paramagnetic phase of RMn_2 has also been found to exhibit peculiar behaviours. The most striking compound is YMn_2 which has a complicated antiferromagnetic structure, but magnetic order is rapidly suppressed under hydrostatic [4] or chemical pressure induced by a small substitution of Sc [5]. At the same time, strong spin fluctuations are observed and the electronic contribution to the specific heat becomes very large; γ is of the order of 180 mJ K^{-2} mol^{-1} in YMn_2 under pressure and reaches 200 mJ K^{-2} mol^{-1} in $Y(Sc)Mn_2$ [6]; these are the highest values measured in 3d systems. Large values of the resistivity coefficient A (where $\rho = \rho_0 + AT^2$) are also observed [7]

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and the ratio A/γ^2 is very close to the value found in 4f or 5f heavy-fermion compounds [8]: $A/\gamma^2 \simeq 10^{-5}$ $\mu\Omega$ cm mJ^{-2} mol^2. Thus YMn_2 exhibits heavy-fermion-like behaviour, although it is a good example of a 3d itinerant antiferromagnet. The existence of strong spin fluctuations in $Y(Sc)Mn_2$ has been interpreted by Shiga *et al* [9] as a proof of the existence of a quantum spin liquid state in this compound, this quantum spin liquid state being stabilized through frustration. However, in this interpretation, only transverse spin fluctuations are considered and it is not easy to understand the effect of pressure on YMn_2; if the absence of ordering in $Y(Sc)Mn_2$ is due only to the strong frustration in the Laves phase structure (which is similar to the pyrochlore structure), why should YMn_2 become ordered at zero pressure? On the other hand, this explanation does not take into account the large-amplitude fluctuations of the Mn magnetic moments observed in magnetovolume measurements [3] and polarized-neutron experiments [10]. In this paper we present a different point of view: the heavy-fermion behaviour of YMn_2 results from the proximity of the magnetic–non-magnetic transition in this compound which induces large-amplitude spin fluctuations and from the effect of strong frustration on the spin fluctuation spectrum.

In the next section we propose a modelization of the dynamical susceptibility $\chi(q,\omega)$ in order to take into account frustration effects. Then this susceptibility is used to calculate the contribution of spin fluctuations to the specific heat close to the magnetic–non-magnetic instability; we show that large values of γ can be obtained close to the antiferromagnetic–paramagnetic instability. Finally we show that spin fluctuations strongly reduce the Néel temperature.

2. Spin fluctuation spectrum in a strongly frustrated system

A common property to all frustrated systems (ordered or disordered) is the existence of several degenerate or nearly degenerate states; for example in the case of the ANNI model, this quasi-degeneracy gives rise to the devil's staircase [11]; in the case of the Heisenberg model for the Kagomé lattice this degeneracy can be lifted by the fluctuations ('order by disorder') [12]. Spin-glass systems also have degenerate ground states. This degeneracy has a strong influence on the susceptibility both in localized (Heisenberg or XY models) and in itinerant models; in the Hartree–Fock approximation the ordering is determined by the Q-value which maximizes the susceptibility $\chi(q,\omega)$ and this Q-value is usually unique (if the symmetries of the Brillouin zone are correctly taken into account). In itinerant systems, $\chi(q,\omega)$ is related to the non-interacting band susceptibility and, in the RPA, one has

$$\chi(q,\omega) = \frac{\chi^0(q,\omega)}{1 - U\chi^0(q,\omega)} \tag{1}$$

where

$$\chi^0(q,\omega) = \sum_k \frac{f(\epsilon_k) - f(\epsilon_{k+q})}{-\omega - \epsilon_k + \epsilon_{k+q}}.$$

However it was pointed out [13] that close to the magnetic–non-magnetic instability, it is necessary to include vertex corrections which can be of the same order of magnitude as the RPA contribution. Then equation (1) should be replaced by

$$\chi(q,\omega) = \frac{\chi^0(q,\omega)}{1 - U\chi^0(q,\omega)} + \frac{U^3[\chi^0(q,\omega)]^4}{1 - [U\chi^0(q,\omega)]^2}. \tag{2}$$

Close to the instability the vertex corrections become one half of the RPA term. Thus it is equivalent to introducing a factor $\frac{3}{2}$ in front of the RPA expression (equation (1)).

The spin fluctuation spectrum in a paramagnetic system is completely determined by the dynamical susceptibility $\chi(q,\omega)$ and, as can be seen from equation (2), it depends only on the band structure ϵ_k. Usually one needs only to expand $\chi(q,\omega)$ (or $\chi^0(q,\omega)$) around its maximum; in ferromagnetic (or nearly ferromagnetic) systems, one takes the standard form [14]

$$\chi^0(q,\omega) = \chi_0[1 - aq^2 - b(\omega/q)^2 + \mathrm{i}c\omega/q] \qquad \text{with } q \ll 1, \omega \ll 1 \quad (3)$$

where the coefficients $\chi_0 = \chi^0(0,0)$, a, b and c depend on the band structure ϵ_k. In antiferromagnetic or nearly antiferromagnetic systems the expansion is slightly different [14]; if $\chi^0(q,\omega)$ is maximum at $q = Q$, the expansion around Q can be written

$$\chi^0(Q+q,\omega) = \chi_Q(1 - aq^2 - b\omega^2 + \mathrm{i}c\omega) \qquad \text{with } q \ll Q, \omega \ll 1 \quad (4)$$

where $\chi_Q = \chi^0(Q,0)$, a, b and c depend on the band structure.

In the frustrated case the susceptibility $\chi^0(q,\omega)$ will be affected by the existence of several nearly degenerate states. Two cases can be considered.

(i) *Discrete degeneracy.* The susceptibility has two degenerate (or nearly degenerate) maxima at Q_1 and Q_2; this situation has been studied by Moriya and Usami [15] for the special case $Q_1 = 0$ (coexistence of ferromagnetism and antiferromagnetism). This form of $\chi^0(q,\omega)$ can lead to complex ordered states but we have verified that in the paramagnetic phase the spin fluctuation contribution is not much enhanced; thus this case will not be discussed further.

(ii) *Continuous degeneracy.* The susceptibility has a broad maximum around $q = Q$. This can be described by introducing q^4 term in the expansion; equation (4) is then replaced by

$$\chi^0(Q+q,\omega) = \chi_Q(1 - aq^2 - a'q^4 - b\omega^2 + \mathrm{i}c\omega). \qquad \text{with } q \ll Q, \omega \ll 1 \quad (5)$$

and, for the case of continuous degeneracy, one has $a \ll a'$.

In the case of localized models, frustration can also induce a quasi-degeneracy associated with a broad maximum in the spin fluctuation spectrum; as already mentioned in the introduction, the classical Heisenberg model does not become ordered for the Kagomé and pyrochlore lattices and this is associated in the Hartree–Fock approximation with the existence of flat modes (independent of q) in the spin-wave spectrum [16, 17], at least in some directions of reciprocal space. It has been shown further that, if the calculation is made beyond the harmonic approximation, the spin-wave excitations on the Kagomé lattice have a quadratic q-dependence [18]. Similarly, for the frustrated square lattice, the spin-wave spectrum of the Heisenberg model has to be expanded up to fourth order in q because the second-order term vanishes in the strongly frustrated case [19].

Recent inelastic neutron experiments on $Y(Sc)Mn_2$ also suggest a peculiar behaviour of the spin fluctuation spectrum in this compound [20]; a flat maximum around $Q = 1.5$ Å^{-1} has been observed. However, the experimental results also indicate that the susceptibility $\chi(Q+q,\omega)$ is strongly anisotropic; it is dispersionless only along particular symmetry directions. Consequently we have considered two other possible expansions of $\chi^0(Q+q, \omega)$, besides equation (5):

$$\chi^0(Q+q, \omega) = \chi_Q[1 - a_1(q_x^2 + q_y^2) - a_1' q_z^4 - b\omega^2 + \mathrm{i}c\omega] \tag{6}$$

and

$$\chi^0(Q+q, \omega) = \chi_Q[1 - a_2 q_z^2 - a_2'(q_x^4 + q_y^4) - b\omega^2 + \mathrm{i}c\omega]. \tag{7}$$

Equation (6) describes a spin fluctuation spectrum elongated only along the z direction, while equation (7) describes a spectrum which is almost flat in the x–y plane. Experimental results indicate that $Y(Sc)Mn_2$ is better described by equation (6) than by equation (5) [20] with $Q = (5\pi/2, 5\pi/2, 0)$ and the spectrum is very broad along the [001] axis.

3. Specific heat for nearly magnetic frustrated compounds

On the assumption of one of the equations (equation (5), (6) or (7)) for $\chi^0(Q+q,\omega)$ it is easy to calculate the contribution of the spin fluctuations to the free energy [14] in the paramagnetic phase:

$$\Delta F = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega \coth\left(\frac{\omega}{2T}\right)\sum_q \int_0^U \mathrm{d}U \,\mathrm{Im}[\chi(q,\omega)] \tag{8}$$

where $\chi(q,\omega)$ is given by equation (2) (or (1) in the RPA). In the following it will be assumed that the system is paramagnetic at $T = 0$ K, but very near to the anitferro–paramagnetic instability, i.e. $U\chi_Q$ is close to 1. We define $\alpha_Q = U\chi_Q$. Then the contribution of spin fluctuations to the specific heat can easily be obtained from equation (8) by derivation. This contribution can be expanded at low temperatures as $C_v = \gamma T + \beta T^3$ (or $T^3 \ln T$ in nearly ferromagnetic systems).

In the non-frustrated case a completely different behaviour is obtained for the nearly ferromagnetic and antiferromagnetic cases corresponding to equations (3) and (4) [14].

(i) For the nearly ferromagnetic case the paramagnon contribution gives a logarithmic contribution to the coefficient γ, which diverges at the paramagnetic–ferromagnetic transition [21]; including the vertex corrections, γ is given by

$$\gamma \approx \frac{3\pi}{2q_c^3}\frac{c}{a}\ln\left(1 + \frac{a\alpha_0 q_c^2}{1-\alpha_0}\right) \qquad \text{with } \alpha_0 = U\chi_0 \tag{9}$$

where q_c is determined by the volume of the unit cell: $q_c = (6\pi^2)^{1/3}$.

(ii) For the nearly antiferromagnetic case, γ remains finite at the paramagnetic–antiferromagnetic instability [22] and one obtains

$$\gamma \approx \frac{3\pi}{q_c^2}\frac{c}{a}\left[\frac{4}{3} - \frac{\kappa}{q_c}\tan^{-1}\left(\frac{q_c}{\kappa}\right)\right] \qquad \text{with } \kappa = \left(\frac{1-\alpha_Q}{a\alpha_Q}\right)^{1/2}. \tag{10}$$

Equation (10) indicates that γ is limited by the ratio c/a, which depends only on the characteristics of the band. On the other hand, we show in the following that γ can be divergent in the nearly antiferromagnetic case if $\chi^0(Q+q,\omega)$ takes one of the forms given by equation (5), (6) or (7), as expected in presence of frustration.

3.1. Isotropic frustrated case

In the extreme case where the spin fluctuation spectrum is completely independent of $q(a = a' = 0)$, equation (8) gives the following expression for γ close to the instability:

$$\gamma \approx \pi c \frac{\alpha_Q}{1-\alpha_Q}. \tag{11}$$

Thus, in that case, γ diverges at the antiferromagnetic–paramagnetic transition. Such a q-independent spectrum describes localized fluctuations. In fact in frustrated systems the flat maximum of $\chi^0(Q+q,\omega)$ can also be interpreted as due to quasi-localized fluctuations; for example in the Kagomé lattice, it has been shown that spin fluctuations with vanishing excitation energy are localized on the hexagons [1], and these localized excitations are at the origin of most of the peculiar properties of this lattice.

If now we consider a strongly frustrated system with an isotropic susceptibility (equation (5) with $a \ll a'$), the coefficient γ can be calculated using equation (8) and we give below the expressions for the most divergent contributions.

(i) Close to the instability, i.e. when $1-\alpha_Q \ll a$, we obtain

$$\gamma \approx \frac{c}{\sqrt{a}}\left(\frac{1}{\sqrt{a'}} - \frac{\sqrt{1-\alpha_Q}}{a}\right). \tag{12}$$

In this case, γ remains finite at the antiferromagnetic–paramagnetic transition, but it can become very large if the system is strongly frustrated (i.e. if $a \ll a'$).

(ii) In an almost fully frustrated system ($a \ll 1-\alpha_Q$),

$$\gamma \approx \frac{c}{a'^{3/4}}\left(\frac{1}{(1-\alpha_Q)^{1/4}} - \frac{a}{\sqrt{a'}(1-\alpha_Q)^{3/4}}\right). \tag{13}$$

In the peculiar case of fully frustrated system ($a = 0$), γ diverges at the instability as (figure 1): $\gamma \propto 1/(1-\alpha_Q)^{1/4}$.

3.2. Anisotropic frustrated cases

In the anisotropic frustrated case, which is 'less' frustrated than the isotropic case because the spin fluctuation spectrum is flat only along some directions of the reciprocal space, γ does not always diverge close to the paramagnetic–antiferromagnetic instability. Calculations in that case have been performed numerically for values of the susceptibility coefficients of the order of those of the simple-cubic lattice (see appendix).

If the spin fluctuation spectrum is flat in the x–y plane (equation (7)), γ diverges close to the instability, but less strongly than in the isotropic case (equations (11), (12) and (13)). From figures 2 and 3, one can deduce that

$$\gamma \approx \frac{-\ln(1-\alpha_Q)}{\sqrt{a_2'}}. \tag{14}$$

On the other hand, if the spin fluctuation spectrum is elongated only along the z direction (equation (6)), as is the case in YMn_2, γ remains finite close to the instability (figure 4).

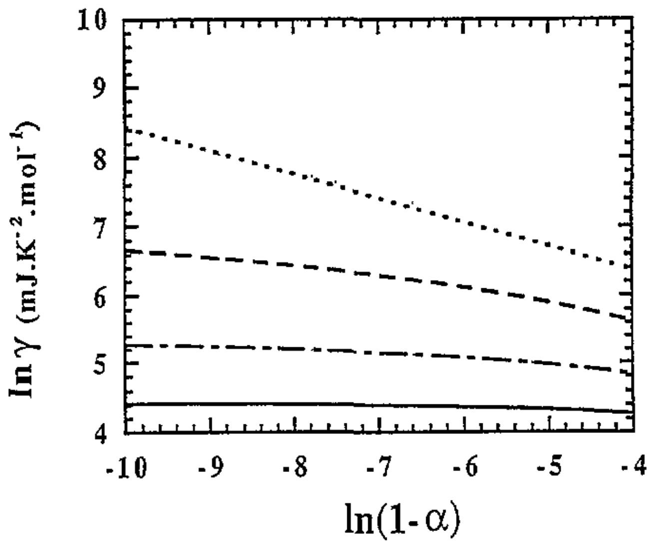

Figure 1. $\ln\gamma$ as a function of $\ln(1-\alpha)$ close to the instability for a frustrated system with isotropic degeneracy (equation (5) for $a = 0$ and $a' = 42.5$ Å^4) (· · · · · ·) and with anisotropic degeneracy (equation (6) (— · —) and equation (7) (– – –) for $a_1 = a_2 = 170$ Å^2 and $a'_1 = a'_2 = 42.5$ Å^4) and for a nearly antiferromagnetic system (equation (4) with $a = 170$ Å^2) (——). See the appendix for the other parameters.

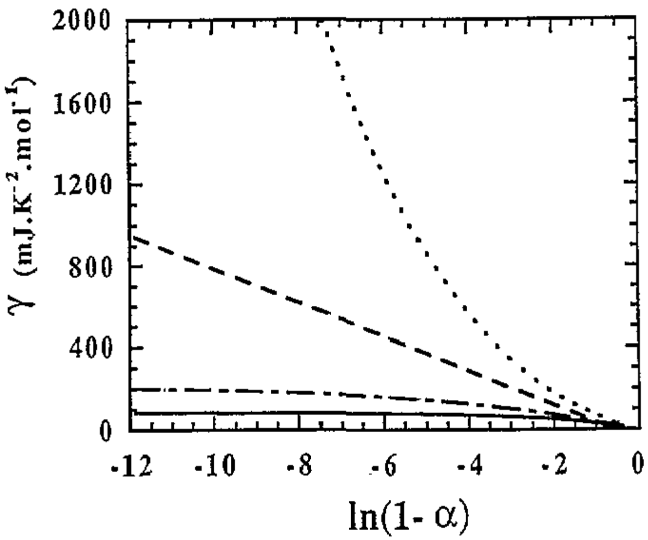

Figure 2. Coefficient γ as a function of $\ln(1-\alpha)$ close to the instability. The symbols have the same meanings as in figure 1.

Nevertheless, if frustration increases, i.e. if the fourth-order coefficient a' decreases, γ can become rather large since for $\alpha_Q = 1$; it varies as (see figure 3)

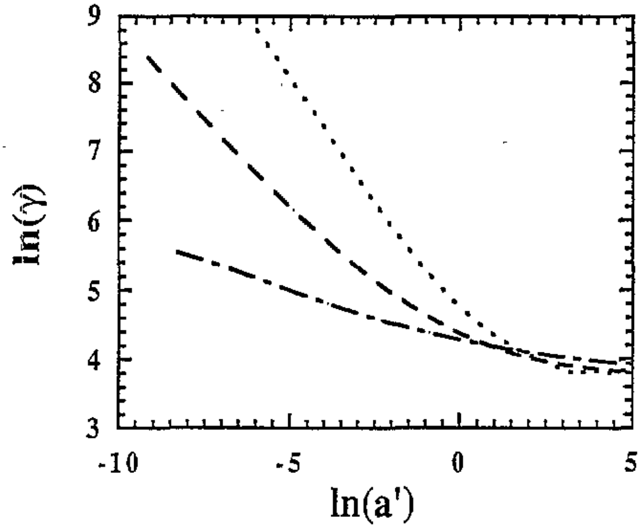

Figure 3. $\ln \gamma$ as a function of $\ln a'$ for $1 - \alpha = 10^{-7}$. The symbols have the same meanings as in figure 1.

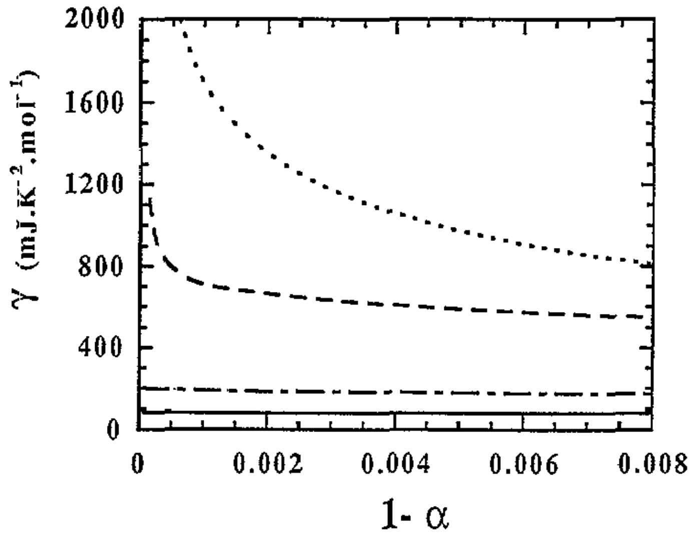

Figure 4. Coefficient γ as a function of $1 - \alpha$ close to the instability. The symbols have the same meanings as in figure 1.

$$\gamma \approx \frac{1}{a_1'^{1/6}}. \tag{15}$$

3.3. Comparisons of γ for the different spin fluctuation spectra

Calculations of γ have been performed for different values of the susceptibility coefficients

a and a' (or a_1, a_2, a'_1 and a'_2); results are shown in figures 1–4; the parameters have been estimated for a free-electron band on a cubic lattice, as explained in the appendix.

In figure 4, it appears that, in the anisotropic frustrated case, γ is larger than in the non-frustrated case close to the instability, but smaller than in the isotropic frustrated one; frustration strongly affects the coefficient γ close to the instability.

In the case of the anisotropic spectrum elongated along the z direction, which, among the different models considered in this work, gives a better description of YMn_2, γ is approximately twice that for the nearly antiferromagnetic case at the instability; our results explain qualitatively the experimental results in [4] where it was found that the values of γ in the paramagnetic phase of YMn_2 are one order of magnitude larger than in ordinary 3d metals. We show in section 3.5 that better agreement is found if the parameters a and a' are taken from the experimental results.

3.4. Calculation of the T^3 term

We have also calculated the T^3 contribution of the spin fluctuations to the specific heat using equation (8). Note that the phonon contribution is not taken into account here.

It appears that in all cases, with or without frustration, β diverges and becomes negative at the magnetic–non-magnetic instability. The coefficient β can be calculated and we find that: (i) $\beta \propto -1/(1-\alpha_Q)$ in the nearly antiferromagnetic case (non-frustrated) (equation (4)); (ii) $\beta \propto -1/(1-\alpha_Q)^2$ in the strongly frustrated case with an isotropic susceptibility (equation (5) with $a=0$); (iii) $\beta \propto -1/(1-\alpha_Q)^3$ in the extreme case of a q-independent spectrum.

Negative values of β have never been observed in nearly antiferromagnetic 3d systems. Nevertheless, in connection with large values of γ, negative values of β are observed in many heavy-fermion compounds (e.g. $CeCu_6$ [23]) and more recently in $Y(Sc)Mn_2$ [6]; these are, to our knowledge, the only metallic systems with negative β.

Our values of β very close to the instability are much larger than those measured for $Y(Sc)Mn_2$ [6]. However, better agreement with experiments can be found if the parameters are chosen in such a way that the system is not too close to the instability; for example, for $1-\alpha_Q \simeq 10^{-2}$ we obtain (see appendix for the other parameters) $\beta = -3.04$ mJ K^{-4} mol^{-1} for an antiferromagnetic system (equation (4) with $a = 170$ Å^2), $\beta = -0.1$ mJ K^{-4} mol^{-1} for a frustrated system with isotropic degeneracy (equation (5) with $a = 0$ and $a' = 42.50$ Å^4), $\beta = -0.5$ mJ K^{-4} mol^{-1} for a frustrated system with anisotropic degeneracy (equation (6) with $a_1 = 170$ Å^2 and $a'_1 = 42.50$ Å^4) and $\beta = -4.15$ mJ K^{-4} mol^{-1} for a frustrated system with anisotropic degeneracy (equation (7) with $a_2 = 170$ Å^2 and $a'_2 = 42.50$ Å^4).

In fact, YMn_2 under pressure never reaches $\alpha_Q = 1$ because in this compound the transition between the paramagnetic and antiferromagnetic states is always first order and accompanied by a volume change which implies a discontinuous variation in α_Q at the transition.

In the next section we show that good agreement with the value measured is obtained if a and a' are taken from the neutron experiment.

3.5. Estimation of γ and β for $Y(Sc)Mn_2$

The numerical results in the preceding sections have been obtained using a one-band model in a cubic lattice. One can obtain a better estimation of the susceptibility coefficients a and a' directly from the spin fluctuation spectrum obtained by inelastic neutron experiments

[20] on Y(Sc)Mn_2: $a_1 \simeq 11.1$ Å^2; $a_1' \simeq 39.1$ Å^4; $c \simeq 0.12$ meV^{-1} in equation (6). For these values, we obtain

$$\gamma \simeq 195 \text{ mJ K}^{-2} \text{ mol}^{-1}$$

and

$$\beta \simeq \begin{cases} -0.025 \text{ mJ K}^{-4} \text{ mol}^{-1} \\ -2.40 \text{ mJ K}^{-4} \text{ mol}^{-1} \end{cases} \quad \text{for} \quad \begin{cases} 1-\alpha_Q \simeq 10^{-2} \\ 1-\alpha_Q \simeq 10^{-3} \end{cases}.$$

These values are close to those measured on the same sample [6]: $\gamma \simeq 200$ mJ K^{-2} mol^{-1} and $\beta \simeq -1.9$ mJ K^{-4} mol^{-1}. However, in order to compare with the experimental value of β, the phonon contribution has to be estimated from a similar compound; in YCo_2 for example, this contribution is about 0.3 mJ K^{-4} mol^{-1} [24]. Thus the spin fluctuation contribution to the T^3 term in Y(Sc)Mn_2 can be evaluated to be $\beta \simeq -2.2$ mJ K^{-4} mol^{-1}.

Owing to the large number of unknown parameters in the calculation, the very good agreement between experimental and numerical results can be considered as fortuitous. Nevertheless, it shows that Y(Sc)Mn_2 is well described by our model of quasi-degenerate spin fluctuations.

4. Spin fluctuations in the ordered state

The spin fluctuations also influence strongly the properties of the ordered state, especially if the Stoner factor $\alpha_Q = U\chi_Q$ is close to 1. We discuss in this section the effect of spin fluctuations on the staggered magnetization at $T = 0$ K (zero-point spin fluctuations) and on the ordering temperature.

Close to the instability, the spin fluctuations reduce the staggered magnetization $M(T)$. It has been shown by Moriya [14] that the magnetization at temperature T can be calculated as follows:

$$M^2(T) = \frac{1}{4g}\left(2\frac{\alpha_Q - 1}{\chi_Q} - \frac{1}{M}\frac{\partial(\Delta F)}{\partial M}\right) \tag{16}$$

where ΔF is the contribution of the spin fluctuations to the free energy (equation (8)) and g is the mode–mode coupling coefficient which can be calculated used the Hartree–Fock free-energy development close to the instability:

$$F_{\mathrm{HF}}(M,T) = \frac{\alpha_Q - 1}{\chi_Q}M^2(T) + gM^4(T). \tag{17}$$

The correction ΔF due to the transverse spin fluctuations is determined from equation (8) where the RPA susceptibility (equation (1)) is calculated in the ordered phase. The band susceptibility $\chi^0(q,\omega)$ now depends on the staggered magnetization $M(T)$ and, as we are close to instability, M is small and it is justified to use the development of $\chi_M^0(q,\omega)$ for small M:

$$\chi_M^0(q,\omega) = \chi^0(q,\omega) + D\omega M - F\frac{M^2}{2} + \cdots \tag{18}$$

where D and F depend on the band structure.

The correction to $M^2(T)$ (equation (16)) contains a constant term (zero-point fluctuations) and a temperature-dependent term which we have determined numerically. At low temperatures ($T \leqslant 1$ K), it varies as [14]

$$\frac{1}{M}\frac{\partial(\Delta F)}{\partial M} = K_1 + K_2 T^2 \tag{19}$$

where K_1 and K_2 are positive and depend on the band structure.

Equation (16) indicates that the transition at $T = 0$ K then occurs for a critical value of α greater than 1: $\alpha_c = 1 + (\chi_Q/2)K_1$. The transition temperature T_N is given by

$$T_N = \sqrt{\frac{2(\alpha - \alpha_c)}{\chi_Q K_2}}. \tag{20}$$

We have calculated K_1 and K_2 in the isotropic frustrated case (equation (5) with $a = 0$) and in the non-frustrated case (equation (4)), for values of the susceptibility coefficients of the order of those of the simple-cubic lattice (see appendix). At $T = 0$ K, the corrections are very small; we find that $(\chi_Q/2)K_1 \simeq 10^{-3}$. Thus, the zero-point fluctuations do not modify the critical value of α: $\alpha_c \simeq 1$. From equation (16) it can also be shown that the staggered magnetization at $T = 0$ K is reduced by the fluctuations only if the system is close to the instability, i.e. when $\alpha - 1$ is of the order of 10^{-3}.

On the other hand, the temperature-dependent term is strongly affected by the susceptibility shape close to the instability. In particular, K_2 is one order of magnitude larger in strongly frustrated systems (equation (5)) than in non-frustrated antiferromagnetic systems: $K_2 = 7.7 \times 10^{-6}$ eV K^{-2} in the nearly antiferromagnetic case (equation (4) with $a = 170$ Å^2) and $K_2 = 57.3 \times 10^{-6}$ eV K^{-2} in the strongly frustrated case with an isotropic susceptibility (equation (5) with $a = 0$ and $a' = 4250$ Å^4). See the appendix for the other parameters.

In the intermediate cases of anisotropic susceptibility, we can expect values for K_2 between these two values. Thus we can conclude that frustration reduces the ordering temperature by a factor which is approximately proportional to $K_2^{1/2}$.

5. Conclusions

We have shown in this paper that, even in itinerant systems, frustration strongly modifies the spin fluctuation spectrum. Consequences for the specific heat coefficients have been studied and this allows comparison between YMn_2 and the 4f heavy-fermion compounds; these systems are very often close to a magnetic–non-magnetic instability owing to the competition between the Kondo effect and magnetic interactions. Calculation of the spin fluctuation resistivity would also be interesting since, as mentioned in the introduction, YMn_2 obeys the Kadowaki–Woods [8] relation for the ratio A/γ^2. We can suggest that this relation is associated with the existence of quasi-localized spin fluctuations since it has been shown that this relation is verified if the spectrum is q independent [25]. In heavy-fermion compounds these localized fluctuations are attributed to the Kondo effect, while in our case they are a consequence of the frustration in the Laves phase structure.

Appendix

Except in section 3.5, the numerical calculations have been performed using values of the various coefficients of the order of those of the simple-cubic lattice as given by Hasegawa and Moriya [26] for the free-electron model with Umklapp processes.

In these calculations, the energy unit is taken as $h^2/8ma_0^2$ where a_0 is the lattice parameter. The effective mass m can be estimated for free electrons in a band of width $2W$. The relation between m and W is then $m \simeq h^2(4\pi)^{2/3}/a_0^3 W$. We have taken $a_0 = 5$ Å and $W = 5$ eV, i.e. of the order of the values for transition metals.

The susceptibility coefficients a, a', b, c and F (see equations (5), (6), (7) and (18)) are given in [26] in units of $[\chi_Q(k_F = 1)/2]^{-1}$ where k_F is the Fermi vector. An order of magnitude for $\chi_Q(k_F = 1)$ can also be estimated from $\chi_Q(k_F = 1) \simeq n(\epsilon_F) \simeq 2/\pi W$.

We have considered several values for these coefficients in the calculation of γ, β and magnetization $M(T)$ close to the instability. First, we have checked that variations in the b, c, F and χ_Q parameters are not preponderant; we have thus limited our calculations to

$$b = 0.011 \text{ meV}^{-2} \qquad c = 1.23 \text{ meV}^{-1} \qquad F = 136 \qquad \chi_Q = 0.24 \text{ eV}^{-1}.$$

On the other hand, the values of a and a' play a determining role in these calculations, as expected; a is of the order of 170 Å^2 in [26].

We also need a cut-off wavevector q_c and a cut-off energy ω_c. Following Hasegawa and Moriya we have taken $q_c = 1$ in units of π/a_0. Finally ω_c has been estimated as the width of $\mathrm{Im}[\chi^0(q, \omega)]$ for an isotropic susceptibility (equation (5)), i.e. $\omega_c \approx (aq_c^2 + a'q_c^4)/c$. These parameters do not influence strongly our numerical results; we have thus limited our calculations to

$$q_c = 0.63 \text{ Å}^{-1} \qquad \omega_c = 0.44 \text{ eV}.$$

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