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SPIN FLUCTUATIONS IN WEAKLY ITINERANT SYSTEMS

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Abstract. – A simple new approach to the spin fluctuation problem is presented. Its basis is that the fluctuating moments may themselves be expressed in terms of the bulk magnetisation. On this basis magnetic and magnetoelastic properties are calculated. The Curie temperatures obtained for a wide variety of materials agree well with experiment.

1. Introduction

At finite temperatures it has become clear that spin fluctuation effects persist side by side with single particle excitations but that it is difficult to describe these theoretically for realistic models of metals [1-5]. Hence we have developed a very much simpler new approach to the problem of spin fluctuations. This retains the Stoner model in its equivalent expression as a Landau theory of phase transitions but takes account of the influence of spin fluctuations by appropriately renormalizing the Landau coefficients [4, 6].

For small values of the bulk magnetisation M of a magnetic material the free energy expression takes the usual form in Stoner theory

$$F = 1/2AM^2 + 1/4BM^4 - H.M. \quad (1)$$

Here the coefficients A and B are given by

$$A = - (1 - T^2/T_c^2) / 2\chi_0, \quad B = 1/2\chi_0 M_0^2 \quad (2)$$

for the weak itinerant ferromagnets. Also M_0 is the value of M at $T = 0$, χ_0 is the ferromagnetic susceptibility at $T = 0$, T_c^2 is the Curie temperature given by Stoner theory and H is the applied field.

A simple theory of magnetoelastic phenomena can be established by renormalising $A \Rightarrow A'$ and $B \Rightarrow B'$ where

$$A' = A + 2\kappa CP, \quad B' = B - 2\kappa C^2. \quad (3)$$

Here κ is the compressibility, C the magnetoelastic coupling constant and $P = -\omega/\kappa$ the externally applied volume strain. A similar idea is now applied to the theory of spin fluctuations where a Landau-Ginzburg theory [3] leads to isotherms in the form

$$\frac{H}{M} = A + BM^2 + 3B \langle m_{\parallel}^2 \rangle + 2B \langle m_{\perp}^2 \rangle, \quad (4)$$

where the additional terms are the mean values of the parallel and transverse local spin fluctuations. It was noted that these terms should increase as the bulk magnetisation increases. Hence it was proposed to expand these terms in even powers of the bulk magnetisation as

$$3B \langle m_{\parallel}^2 \rangle + 2B \langle m_{\perp}^2 \rangle = a_1 - a_2 M^2 + a_3 M^4 + \dots$$

where a_1, a_2, a_3 are all positive. Hence once again the Landau coefficients have been renormalised, to give

$$A' = A + a_1, \quad B' = B - a_2. \quad (6)$$

2. Results

The analogy between (3) and (6) implies that spin fluctuations act as if they exerted an effective magnetic pressure $P_m(T)$ given by

$$a_1(T) = 2\kappa CP_m(T). \quad (7)$$

Assuming a linear dependence of $a_1(T)$ on the temperature we get from the condition that A' must vanish at $T = T_c$

$$P_m(T) = P_c (1 - t_c^2) T/T_c. \quad (8)$$

Here $t_c = T_c/T_c^s$ and $P_c = 1/4C\chi_0$ is the critical pressure for the disappearance of ferromagnetism. The quantity t_c was found to be a very useful measure for the characterisation of the importance of spin fluctuations. For $t_c = 0$ spin fluctuations overwhelm single particle excitations and the reverse is the case for $t_c = 1$. Generally a value of $t_c = 0.5$ gives the borderline between the relative importance of the two elementary excitations involved. If both externally applied and effective magnetic pressures due to spin fluctuations are present then the pressure dependence of T_c is found to be given by [6]

$$t_c^2 \tau^2 + (1 - t_c^2) \tau + p - 1 = 0, \quad (9)$$

where

$$\tau = T_c(P)/T_c(0), \quad p = P/P_c.$$

Relation (9) interpolates between a linear and a quadratic $T_c(P)$ dependence in the limits $t_c = 0$ and 1. As shown in (6) the present approach also leads to an expression for the magnetic volume strain in the form

$$\omega_m(T) = \kappa P_c [b \{ 1 - t_c^2 (T/T_c)^2 \} - (1 - t_c^2) (T/T_c)], \quad (10)$$

where $b = \Delta B/B$ is the bulk modulus anomaly at T_c . Relation (10) recalls the well known Pettifor pressure formula [7].

The formalism can also be used to compute the Curie temperature T_c , which is given by the equation

$$\frac{T_c^2}{T_c^s} + \frac{T_c}{T_{SF}} - 1 = 0, \quad (11)$$

where

$$T_{SF} = M_0^2/10k_B\chi_0 \quad (12)$$

is the spin fluctuation temperature [4] giving a measure of these effects. This formula interpolates again between two limits. For $t_c = T_c/T_c^s = 0$, T_c is given entirely by spin fluctuation effects, i.e. by T_{SF} . As seen in (12), however, this temperature is given exclusively by the entities M_0 , the saturation magnetisation, and χ_0 , the ferromagnetic susceptibility, both at $T = 0$ and thus given by Stoner theory. For $t_c = 1$, T_c is itself determined by this theory. The formula for T_{SF} is based on a calculation of the mean value of fluctuating magnetisation in the long wave length limit giving

$$\langle m^2 \rangle = 3k_B T / |A|, \quad (13)$$

with A as being defined by (2). Figure 1 gives a plot of T_c/T_{SF} vs. T_c^s/T_{SF} given by (11). The experimental values were obtained from measurements of T_c for a wide variety of materials and computations of T_{SF} and T_c^s based on the band structure and the Stoner param-

eter. The detailed results for most of the materials are given in reference [4], results for $ZnZn_2$ and Ni_3Al are from reference [5], those of the borides are from [8], those of $MnSi$ are from reference [9].

In figure 1, materials close to the horizontal asymptote $T_c=T_{SF}$ have properties governed by spin fluctuations and those close to the tangent $T_c/T_{SF}=T_c^s/T_{SF}$ properties governed by Stoner excitations. The relative importance of these two influences is determined by the band structure and the interactions. The agreement shown in figure 1 is very satisfactory in view of the simplicity of our approach. Some materials with very low Curie points would deviate from our graph by straight forwardly applying equation (11). To account for this result we have considered, using the example $ZrZn_2$ and Ni_3Al [5], that the linear dependence of the locally fluctuating moments on T must break down if the moments are small and χ_0 is high.

In this extreme explicit case the moments were shown to saturate well below T_c so that the behaviour of $ZnZn_2$ around T_c is of Stoner behaviour and the value of the Curie temperature thus calculated agrees well with experiment. It also appears that Ni_3Al has properties between the linear and saturating regimes but that spin fluctuation effects are still overwhelming, in agreement with [3].

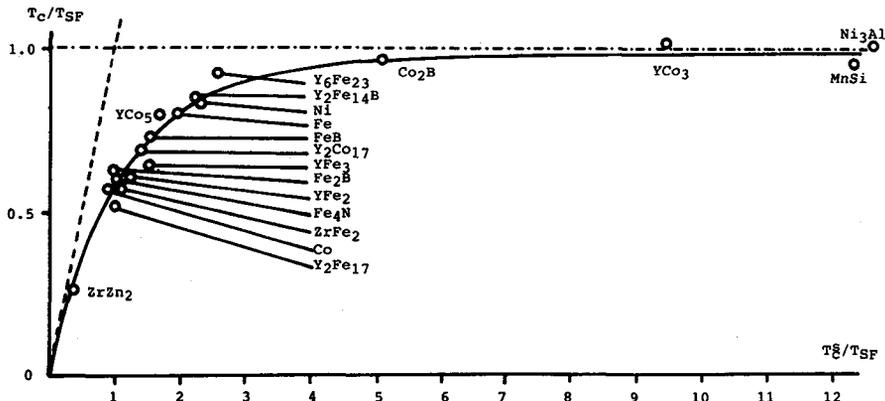


Fig. 1. - Comparison between theory (full curve) given by equation (11) the experimental Curie temperatures for various systems. The broken lines refer to the two extreme cases; the asymptote for pure fluctuation behaviour ($T_c/T_{SF} = 1$) and the tangent for pure Stoner behaviour ($T_c = T_c^s$).

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