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LETTER TO THE EDITOR

Itinerant electron metamagnetism at finite temperature

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Abstract. An itinerant electron metamagnetism at finite temperature is discussed by taking into account the effect of spin fluctuations. The metamagnetic transition from the paramagnetic to ferromagnetic state is qualitatively shown to occur only below a critical temperature, which is lower than that at which the paramagnetic susceptibility shows a maximum in its temperature dependence. Moreover, a condition for the first-order transition, induced by the spin fluctuations, in the temperature dependence of the spontaneous magnetization is found, connecting with the Landau–Belov expansion coefficients.

The intermetallic compounds $ScCo_2$, YCo_2 and $LuCo_2$ with the cubic Laves phase structure are known to be strongly exchange-enhanced paramagnets. A maximum in the temperature dependence of the susceptibility, $\chi(T)$, of these compounds was observed at room temperature (Ishiyama *et al* 1984, Lemaire 1966, Burzo 1972, Bloch *et al* 1971, Ikeda *et al* 1984) and a metamagnetic transition (MT) from the paramagnetic to ferromagnetic state has recently been observed for an extremely high magnetic field of about 100 T for YCo_2 and $LuCo_2$ (Goto *et al* 1989, 1990). These anomalous magnetic properties have theoretically been shown to be related to a sharp peak of the density-of-states curve near the Fermi level (Yamada 1988). It is noted that the present MT is associated with the change in the electronic structures of d-electrons under the magnetic field; it is then called the itinerant electron metamagnetism, to distinguish it from the classical one in the localized electron model.

On the other hand, spin fluctuations (SF) play an important role in the magnetic properties at finite temperature. The Curie–Weiss law for the paramagnetic susceptibility observed in weakly ferromagnetic metals is attributed to the thermal excitations of the SF (Moriya and Kawabata 1973). Any magnetic property at finite temperature is, more or less, affected by the SF. The aim of the present letter is to study the effect of the SF on the MT. By using the Landau–Belov theory, Shimizu (1981) discussed the effect of the SF on the magnetic properties of metals by using classical Gaussian statistics, extending the phenomenological theory by Murata and Doniach (1972). We start from his theory, including the effect of external magnetic field.

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The equation of state in the magnetic system with magnetic moment M and external magnetic field H at temperature T is given by

$$H = A(T)M + B(T)M^3 + C(T)M^5 + \dots \tag{1}$$

where $A(T)$, $B(T)$ and $C(T)$ are given in terms of the Landau–Belov expansion coefficients, a, b and c, of the magnetic free energy with respect to the square of the magnetization density (Shimizu 1984) as

$$A(T) = a + b[3\langle(\delta m_\parallel)^2\rangle + 2\langle(\delta m_\perp)^2\rangle] + c[15\langle(\delta m_\parallel)^2\rangle + 12\langle(\delta m_\parallel)^2\rangle \times \langle(\delta m_\perp)^2\rangle + 8\langle(\delta m_\perp)^2\rangle] + \dots \tag{2}$$

$$B(T) = b + 2c[5\langle(\delta m_\parallel)^2\rangle + 2\langle(\delta m_\perp)^2\rangle] + \dots \tag{3}$$

$$C(T) = c + \dots . \tag{4}$$

Here $\langle(\delta m_\parallel)^2\rangle$ and $\langle(\delta m_\perp)^2\rangle$ are thermal averages of the square of the longitudinal and transverse components of the fluctuating magnetic moments, respectively.

The temperature dependences of $A(T)$, $B(T)$ and $C(T)$ given by equations (2)–(4) come not only from $\langle(\delta m_\parallel)^2\rangle$ and $\langle(\delta m_\perp)^2\rangle$, but also from the coefficients a, b and c through the Fermi distribution functions involved in the respective expressions (Shimizu 1981). The effect on the MT of the temperature dependences of a, b and c themselves has been discussed in detail (Yamada and Shimizu 1990). In the present paper, only the effect of the SF on the MT will be discussed.

Moriya and Kawabata (1973) and Lonzarich and Taillefer (1985) have discussed the SF from the microscopic point of view. $\langle(\delta m_\parallel)^2\rangle$ and $\langle(\delta m_\perp)^2\rangle$ have been shown to be written in terms of the longitudinal and transverse components of the dynamical spin susceptibilities. The problem is how to get these susceptibilities. The expression obtained in the simple random phase approximation cannot be relied upon to describe the SF accurately. Moriya (1985) has proposed the self-consistent renormalization theory. Lonzarich and Taillefer (1985) have also given a simple model for the dynamical spin susceptibilities. The dynamical spin susceptibilities in any model depend on the magnetic moment, M, and so $\langle(\delta m_\parallel)^2\rangle$ and $\langle(\delta m_\perp)^2\rangle$ in the ferromagnetic state also depend on M.

These thermal averages are, however, finite even in the paramagnetic state, and can be written for the weak ferromagnet as

$$\left.\begin{array}{l}\langle(\delta m_\parallel)^2\rangle \\ \langle(\delta m_\perp)^2\rangle\end{array}\right\} = \tfrac{1}{3}\xi_{\mathrm{p}}(T)^2 + \mathrm{O}(M^2) \tag{5}$$

where $\xi_{\mathrm{p}}(T)^2$ is the thermal average of the square of the fluctuating magnetic moments in the paramagnetic state. Here, the coefficient of M^2 in the right-hand side of equation (5) should be negative to represent a decrease of the SF with increasing M (Wagner and Wohlfarth 1986, Mohn and Wohlfarth 1987). In this letter, we do not give the explicit expression of $\xi_{\mathrm{p}}(T)$. Nevertheless, we can discuss the dependence of the MT on T through $\xi_{\mathrm{p}}(T)$, as $\xi_{\mathrm{p}}(T)$ is a monotonically increasing function of T (Moriya 1985, Shimizu 1981, Lonzarich and Taillefer 1985).

Neglecting the dependence on M of $\langle(\delta m_\parallel)^2\rangle$ and $\langle(\delta m_\perp)^2\rangle$ in equation (5), $A(T)$, $B(T)$ and $C(T)$ given by equations (2)–(4) are approximately written as

$$A(T) = a + \tfrac{5}{3}b\xi_{\mathrm{p}}(T)^2 + \tfrac{35}{9}c\xi_{\mathrm{p}}(T)^4 \tag{6}$$

$$B(T) = b + \tfrac{14}{3}c\xi_{\mathrm{p}}(T)^2 \tag{7}$$

$$C(T) = c. \tag{8}$$

As mentioned above, $\xi_p(T)$ in equations (6)–(8) is the monotonically increasing function of T. Thus the temperature T_{max}, where $\chi(T)^{-1}$ reaches a minimum, is given by $\partial A(T)/\partial\xi_p(T) = 0$, as $\chi(T)^{-1} = A(T)$. We get

$$\xi_p(T_{max})^2 = -\tfrac{3}{14}b/c \tag{9}$$

and

$$\chi(T_{max}) = (a - \tfrac{5}{28}b^2/c)^{-1}. \tag{10}$$

It is noted here that T_{max} given by equation (9) is also the temperature at which $B(T) = 0$.

From equations (9) and (10), the following conditions among a, b and c are obtained for the appearance of a maximum in $\chi(T)$ as

$$a > 0 \qquad b < 0 \qquad c > 0 \tag{11}$$

and

$$ac/b^2 > 5/28 \tag{12}$$

where the sign of c is assumed to be positive to keep $\xi_p(T)^2$ finite.

On the other hand, the condition for the appearance of the MT at finite temperature is obtained by the equation of state (1) as,

$$A(T) > 0 \qquad B(T) < 0 \qquad C(T) > 0 \tag{13}$$

and

$$3/16 < A(T)C(T)/B(T)^2 < 9/20 \tag{14}$$

which has already been obtained by Shimizu (1982), where $A(T)$, $B(T)$ and $C(T)$ are replaced by a_1', a_3 and a_5, corresponding to a, b and c in our letter, respectively. On the other hand, the ferromagnetic state becomes stable even at $H = 0$ when the following condition is satisfied:

$$A(T)C(T)/B(T)^2 < 3/16. \tag{15}$$

Substituting equations (6)–(8) into (14), we get a critical temperature T_0, where the MT disappears, as

$$\xi_p(T_0)^2 = (|b|/c)(3/14 - \sqrt{45/266}\sqrt{ac/b^2 - 5/28}) \tag{16}$$

which is positive when $ac/b^2 < 9/20$. As seen from equations (9) and (16), $\xi_p(T_0)^2$ is smaller than $\xi_p(T_{max})^2$. T_0 is then found to be always lower than T_{max}, as $\xi_p(T)$ is the monotonically increasing function of T. This critical temperature, T_0, has actually been observed to be about 65 K in $Lu(Co, Al)_2$ (Iijima *et al* 1990), which is rather lower than $T_{max} \sim 350$ K observed by Bloch *et al* (1971). Thus the observed results in the $Lu(Co, Al)_2$ system are consistent with the present theory.

On the other hand, when equation (15) is satisfied, the system becomes ferromagnetic at $H = 0$. Substituting equations (6)–(8) into (15), we get a critical temperature T_1, at which the ferromagnetic state becomes unstable and the first-order transition in the temperature dependence of M occurs at $H = 0$, as

$$\xi_p(T_1)^2 = (|b|/c)(3/14 - \sqrt{36/7}\sqrt{ac/b^2 - 5/28}) \tag{17}$$

which is positive when $ac/b^2 < 3/16$. As seen from equations (16) and (17), T_1 is found to be lower than T_0, as $\xi_p(T)$ is the monotonically increasing function of T. Then, in the case of $5/28 < ac/b^2 < 3/16$, the system becomes the metamagnetic state at $T_1 < T < T_0$, after the first-order transition of M occurs at $T = T_1$. A maximum of $\chi(T)$ then appears at $T = T_{max} > T_0$. The present first-order transition at $T = T_1$ is different from that discussed by Yamada (1975), when the case of $a < 0$ and $b > 0$ was considered.

Under the conditions (11) and (12) for the appearance of a maximum of $\chi(T)$, we have thus obtained the following results:

(i) When $ac/b^2 > 9/20$, a maximum of $\chi(T)$ appears but the MT does not occur.

(ii) When $9/20 > ac/b^2 > 3/16$, both a maximum of $\chi(T)$ and the MT occur but the ferromagnetic state does not appear at $H = 0$.

(iii) When $3/16 > ac/b^2 > 5/28$, the ferromagnetic state becomes stable below T_1, the MT occurs at $T_1 < T < T_0$ and a maximum of $\chi(T)$ appears at T_{max}.

As mentioned at the beginning of this letter, $\chi(T)$ in $ScCo_2$, YCo_2 and $LuCo_2$ shows a maximum and the MT is also observed, however the ferromagnetic state is not observed at $T = H = 0$. Therefore, these compounds correspond to case (ii) above.

In the present letter, the MT at finite temperature has been discussed by taking into account the effect of the SF. When the conditions (11) and (12) are satisfied, the value of $A(T)$ or the inverse of $\chi(T)$ has been found to show a minimum at $T = T_{max}$. At the same time, the absolute value of $B(T)$ has also been shown to decrease with increasing T, as $\xi_p(T)$ is the monotonically increasing function of T and the MT has been shown to occur only below T_0 which is lower than T_{max}. In this way, two curious magnetic properties, the MT and the appearance of a maximum in $\chi(T)$, have been shown to be closely connected with each other through the SF at finite temperature. Furthermore, the condition for the first-order transition induced by the SF in the temperature dependence of M has been found. This means that there may exist magnetic materials that show three curious magnetic properties together, i.e., a first-order transition of M, an MT and a maximum in $\chi(T)$.

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