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Magnetic properties of weak itinerant electron ferromagnets below the Curie temperature

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Abstract. We discuss how to treat the magnetic properties of the ordered phase of the weak itinerant electron ferromagnets using a method based on solving a differential equation for the transverse component of the magnetic susceptibility. We show that the simple analytic continuation of the paramagnetic solution does not give the stable solution in the ordered phase below T_c. The low-temperature solutions have an ambiguity corresponding to various choices of initial conditions. We discuss how to choose the unique stable solution at a finite temperature below T_c.

1. Introduction

The self-consistently renormalized spin fluctuation (SCR) theory has been quite successful in explaining and predicting many magnetic properties of weak itinerant electron magnets (Moriya 1985). Experimental investigations have made it possible to test the theory and as a result the quantitative validity of the theory has now been well established. In the ordered phase, however, there remains a difficulty. Because of the presence of the static uniform magnetization, the spin fluctuation spectrum becomes anisotropic. Therefore we have to treat both the fluctuations simultaneously maintaining the restriction coming from the rotational invariance. A naive treatment sometimes leads to the fictitious first-order transition (see, e.g., Murata and Doniach 1972). In the framework of the SCR theory, a straightforward way is to introduce two coupled equations for longitudinal and transverse spin fluctuations. However, one has to solve complicated integro-differential equations (Moriya 1985, Lonzarich and Taillefer 1985). It is, however, not easy to handle them and to see the behaviour of the solution in some limiting cases. This is the reason why the external field dependences have not yet been fully discussed.

In order to derive the equations of the SCR theory, the present author introduced an interesting idea, i.e. that the total spin fluctuation amplitude remains constant (Takahashi 1986). The spin fluctuation amplitude consists of the sum of the thermal and zero-point spin fluctuation amplitudes. In this treatment the effect of the temperature dependence of the zero-point spin fluctuations, which had been previously neglected, were taken into account. Not only was this equation derived for the SCR theory, but various interesting relations, which are satisfied by parameters characterizing the nature of spin fluctuations, were also calculated. These consequences were supported by later experimental investigations (Yoshimura *et al* 1987, Shimizu *et al* 1990).

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In the same paper, a method to treat the ordered phase properties was proposed. It was noticed that the longitudinal and transverse components of the magnetic susceptibility are related to each other by differentiation with respect to the magnetization. It was proposed that the basic equation should be regarded as an ordinary differential equation for the static transverse magnetic susceptibility. The approach is conceptually simple and practically very easy since one needs only to treat a single equation and both the transverse and longitudinal susceptibilities are automatically determined by solving the differential equation. As an application, it was possible to derive analytically the interesting magnetization process of weak itinerant ferromagnets at the critical point:

$$H \propto M^5 \tag{1.1}$$

where H and M are the external magnetic field and saturation magnetization, respectively. However there still remains a difficulty in the ordered phase concerning the ambiguity of the initial condition. In the previous work, an artificial assumption was used in order to define the fluctuation amplitude for negative values of the susceptibility and to solve the equation starting from the fictitious non-magnetic state (Takahashi 1986, Nakayama and Moriya 1987).

The purpose of the present paper is to give a possible solution to this difficulty. We first try to solve the problem by analytic continuation of the paramagnetic solution with respect to the temperature below T_c. It seems natural to assume that the static susceptibility is analytic with respect to the temperature T in the presence of the external magnetic field. We will, however, see that the solution thus obtained does not give a reasonable stable state. This unexpected result seems to have an interesting consequence. As another approach, we note that each solution corresponding to the various initial conditions results in a different form for the free energy as a function of the uniform magnetization. This enables us to choose the initial condition by imposing a condition on the behaviour of the free energy.

In the next section we briefly review the framework of the spin fluctuation theory. In section 3, we discuss a method of analytic continuation of the paramagnetic solution. In section 4, we show how to deal with the initial value problem of our basic differential equation. The conclusions and implications of this study are presented in the final section, section 5.

2. Theoretical framework

In the following, we briefly review our theoretical framework for the description of the magnetic properties of itinerant electron ferromagnets (Takahashi 1986). We start with the assumption that the amplitude of the local spin fluctuation amplitude, $\langle S^2 \rangle$, remains almost constant with increasing temperature or an externally applied magnetic field. In the case of the single band Hubbard model, $\langle S^2 \rangle$ can be expressed in terms of the charge density correlation function whose temperature dependence is characterized by the ratio $k_B T/U$ or $k_B T/W$, where U and W are the intra-atomic Coulomb interaction and the bandwidth, respectively. Because the temperature range of interest is of the order of T_c, the temperature dependence of $\langle S^2 \rangle$ can be practically neglected. Analogous arguments will be applied in more general cases with band

degeneracy. The mean square spin fluctuation amplitude consists of the sum of contributions from the thermal, zero-point and saturation moments:

$$\langle S^2 \rangle = \langle S^2 \rangle_{zp} + \langle S^2 \rangle_{th} + m^2/4 \tag{2.1}$$

where m represents the saturation magnetic moment per magnetic atom in units of $g\mu_B$. From the fluctuation–dissipation theorem, the thermal and zero-point components, $\langle S^2 \rangle_{th}$ and $\langle S^2 \rangle_{zp}$, are related to the dynamical magnetic susceptibilities of the longitudinal and transverse components as follows:

$$\langle S^2 \rangle_{th} = \frac{2}{N_0^2} \sum_q \int_0^\infty \frac{d\omega}{\pi} n(\omega)[\mathrm{Im}\,\chi^{zz}(q,\omega) + 2\,\mathrm{Im}\,\chi^{\perp}(q,\omega)]$$

$$\langle S^2 \rangle_{zp} = \frac{1}{N_0^2} \sum_q \int_0^\infty \frac{d\omega}{\pi} [\mathrm{Im}\,\chi^{zz}(q,\omega) + 2\,\mathrm{Im}\,\chi^{\perp}(q,\omega)]. \tag{2.2}$$

In weak itinerant ferromagnets, the spin fluctuation spectrum in the small q,ω space is well represented by the following form:

$$\mathrm{Im}\,\chi^{zz}(q,\omega) = \frac{\chi_0^{zz}}{1 + q^2/\kappa_z^2} \frac{\omega\Gamma_z(q)}{\omega^2 + \Gamma_z(q)^2}$$

$$\mathrm{Im}\,\chi^{\perp}(q,\omega) = \frac{\chi_0^{\perp}}{1 + q^2/\kappa_\perp^2} \frac{\omega\Gamma_\perp(q)}{\omega^2 + \Gamma_\perp(q)^2} \tag{2.3}$$

with

$$\Gamma_{zz}(q) = \Gamma_0 q(q^2 + \kappa_z^2) \qquad \Gamma_\perp(q) = \Gamma_0 q(q^2 + \kappa_\perp^2)$$

$$\chi_0^{zz} = N_0/2\bar{A}\kappa_z^2 \qquad \chi_0^{\perp} = N_0/2\bar{A}\kappa_\perp^2$$

where χ_0^{zz} and $\chi_0^{\perp}$ are the longitudinal and transverse static magnetic susceptibilities, Γ_0 and $\bar{A}$ are parameters which characterize the spin fluctuation spectrum and N_0 is the number of magnetic ions in the crystal. Since spin waves are limited to the very small wavevector region and its phase volume is very small, we can neglect their contributions. We here introduce two characteristic energy scales T_0 and T_A by

$$T_0 = \Gamma_0 q_B^3/2\pi \qquad T_A = \bar{A}q_B^2 \qquad (q_B = (6\pi^2/v_0)^{1/3}) \tag{2.4}$$

where q_B is the zone boundary vector for the unit volume v_0 per magnetic ion. The temperatures T_0 and T_A give the measure of the distribution of the spin fluctuation spectrum in the energy space and the wavevector space, respectively, which correspond to the exchange constant in insulator magnets. The zero-point and thermal fluctuation amplitudes can be written in the following form:

$$\langle S^2 \rangle_{zp} = \langle S^2 \rangle_{zp}(T_c) - \frac{3T_0}{2T_A}\{Z(y_z) + 2Z(y)\}$$

$$\langle S^2 \rangle_{th} = \frac{3T_0}{T_A}\{T(y_z) + 2T(y)\} \tag{2.5}$$

with

$$Z(y) = y - y^2 \ln(1 + 1/y)/2 + \ln(1 + y)/2 - y/2$$

$$T(y) = \eta^4 \int_0^{\eta^{-1}} dz\, z^3[\ln u - \tfrac{1}{2}u - \psi(u)] \qquad u = z(y/\eta^2 + z^2)/t$$

$$\eta^3 = T_c/T_0 \qquad t = T/T_c \tag{2.6}$$

where $\psi(u)$ is the digamma function and t is the reduced temperature. We introduced in equations (2.5) and (2.6) the reduced reciprocal static magnetic susceptibilities of the transverse and longitudinal components, y and y_z, by

$$y = \kappa_\perp^2/q_B^2 \qquad y_z = \kappa_z^2/q_B^2.$$

From the rotational invariance of the system, y and y_z can be expressed in terms of m and h (an external magnetic field, i.e. $h = g\mu_B H$):

$$y = \frac{1}{k_B T_A}\frac{h}{m} \qquad y_z = \frac{1}{k_B T_A}\frac{\partial h}{\partial m}. \tag{2.7}$$

Now by imposing the conditions, $y = 0$ and $y_z = 0$ at $T = T_c$ ($t = 1$), we can determine the constant term, $\langle S^2\rangle_{zp}(T_c)$, in equation (2.5):

$$\langle S^2\rangle - \langle S^2\rangle_{zp}(T_c) = \frac{9T_0}{T_A}c(\eta^*)^4 = \frac{9T_0}{T_A}\eta^4 \int_0^{\eta^{-1}} dz\, z^3\{\ln z^3 - \tfrac{1}{2}z^3 - \psi(z^3)\}$$

$$c = \frac{1}{3^{3/2}(2\pi)^{1/3}}\Gamma(4/3)\zeta(4/3) = 0.335\,363\,0\ldots \tag{2.8}$$

where $\Gamma(x)$ and $\zeta(x)$ are the gamma and zeta functions, respectively. Now with the use of equations (2.5) and (2.8), our basic assumption (2.1) is finally written in the form:

$$\tfrac{1}{2}\{Z(y_z) + 2Z(y)\} - \{T(y_z) + 2T(y)\} + c(\eta^*)^4\{3 - 5\sigma^2\} = 0$$

$$y_z = \sigma\frac{\partial y}{\partial \sigma} + y. \tag{2.9}$$

The second line of equation (2.9) is easily derived from the definition (2.7). We introduced the relative saturation magnetization σ by m/m_s and m_s by

$$\frac{m_s^2}{4} = \frac{15T_0}{T_A}c(\eta^*)^4 \tag{2.10}$$

which gives the saturation magnetization in the ground state as shown later. Our proposal is to regard equation (2.9) as an ordinary differential equation for y with respect to σ. In the paramagnetic phase ($t \geqslant 1$), we have a well defined limit, i.e. $y_z = y$ for $\sigma = 0$, and we can determine the initial value of y at $\sigma = 0$ by solving

$$Z(y)/2 - T(y) + c(\eta^*)^4 = 0. \tag{2.11}$$

Starting from this solution, we can determine $y(\sigma, t)$ and $y_z(\sigma, t)$ as a function of σ for any finite value of σ. On the other hand, in the ordered phase a difficulty arises because we do not have such a well defined limit. The values of y and y_z are, in general, different for finite σ, but a single equation cannot determine both of them simultaneously. For example, when we choose $y = 0$, we can only determine $\sigma\partial y/\partial\sigma$ as a function of σ with the use of equation (2.9). But we can fix neither σ nor $\sigma\partial y/\partial\sigma$ uniquely.

3. Analytic continuation of the paramagnetic solution

In order to overcome this difficulty of the initial value problem, we try, at first, to assume that $y(\sigma,t)$ is analytic with respect to the temperature t for a finite value of σ. In the presence of the finite static magnetization, physical properties will vary smoothly with temperature and no singularities as a function of the temperature will appear. Therefore it seems to be natural to assume the analyticity of $y(\sigma,t)$ and to consider that the solution for $t<1$ can be simply obtained by the direct continuation of the paramagnetic solution below T_c. We then need derivatives, $y^{(1)}=\partial y/\partial t,\ldots,y^{(n)}=\partial^n y/\partial t^n,\ldots$ of $y(\sigma,t_0)$ around a fixed temperature t_0 under the presence of finite σ. Although we can choose any temperature t_0 as a reference, $t_0=1$ will be the most appropriate one for the reason of fast convergence. Then we can construct the value of $y(\sigma,t)$ for $t<1$ by the following Taylor expansion around $t=1$:

$$y(\sigma,t)=\sum_0^\infty \frac{(t-1)^n}{n!}y^{(n)}(\sigma,1). \tag{3.1}$$

Any higher derivatives of $y(\sigma,t)$ at finite σ are, in principle, evaluated by solving differential equations derived by differentiating equation (2.9) with respect to t. For example the first and second derivatives, $y^{(1)}$ and $y^{(2)}$, are determined by solving

$$\begin{aligned}
&\left(\frac{1}{2}Z'(y_z)-\frac{\partial T(y_z)}{\partial y_z}\right)\left(\sigma\frac{\partial y^{(1)}}{\partial\sigma}\right)+\left\{\frac{1}{2}Z'(y_z)+Z'(y)-\frac{\partial T(y_z)}{\partial y_z}-2\frac{\partial T(y)}{\partial y}\right\}\\
&\qquad\times y^{(1)}=\frac{\partial T(y_z)}{\partial t}+2\frac{\partial T(y)}{\partial t}\\
&\left(\frac{1}{2}Z'(y_z)-\frac{\partial T(y_z)}{\partial y_z}\right)\left(\sigma\frac{\partial y^{(2)}}{\partial\sigma}\right)+\left(\frac{1}{2}Z''(y_z)-\frac{\partial^2 T(y_z)}{\partial y_z^2}\right)\left(\sigma\frac{\partial y^{(1)}}{\partial\sigma}+y^{(1)}\right)^2\\
&\qquad+\left\{\frac{1}{2}Z'(y_z)+Z'(y)-\frac{\partial T(y_z)}{\partial y_z}-2\frac{\partial T(y)}{\partial y}\right\}y^{(2)}\\
&\qquad+\left(Z''(y)-\frac{\partial^2 T(y)}{\partial y^2}\right)(y^{(1)})^2\\
&\quad=\frac{\partial^2 T(y_z)}{\partial t^2}+2\frac{\partial^2 T(y)}{\partial t^2}+2\frac{\partial^2 T(y_z)}{\partial y_z\partial t}\left(\sigma\frac{\partial y^{(1)}}{\partial\sigma}+y^{(1)}\right)+4\frac{\partial^2 T(y)}{\partial y\partial t}y^{(1)}.
\end{aligned} \tag{3.2}$$

The initial conditions of $\partial y/\partial t$, and $\partial^2 y/\partial t^2$ at $\sigma=0$ are obtained by the solutions of the equations:

$$\begin{aligned}
&\left(\frac{1}{2}Z'(y)-\frac{\partial T(y)}{\partial y}\right)\frac{\partial y}{\partial t}-\frac{\partial T(y)}{\partial t}=0\\
&\left(\frac{1}{2}Z'(y)-\frac{\partial T(y)}{\partial y}\right)\frac{\partial^2 y}{\partial t^2}+\left(\frac{1}{2}Z''(y)-\frac{\partial^2 T(y)}{\partial y^2}\right)\left(\frac{\partial y}{\partial t}\right)^2\\
&\qquad=\frac{\partial^2 T(y)}{\partial t^2}+2\frac{\partial^2 T(y)}{\partial y\partial t}\left(\frac{\partial y}{\partial t}\right).
\end{aligned} \tag{3.3}$$

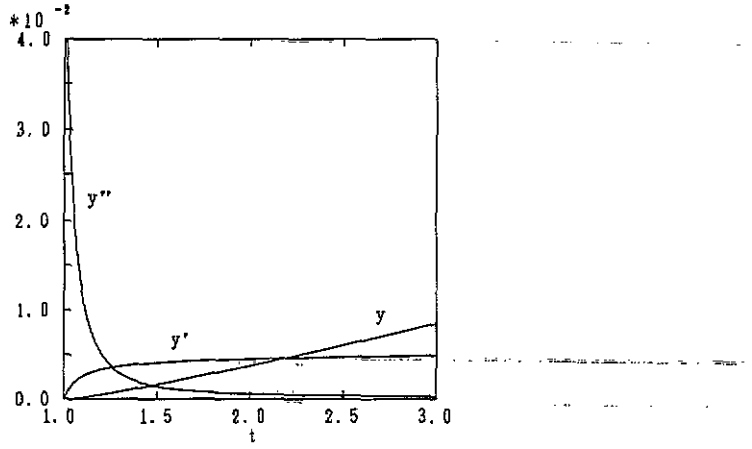

Figure 1. Temperature dependence of the reciprocal magnetic susceptibility y and its derivatives, $y' = \partial y/\partial t$, and $y'' = \partial^2 y/\partial t^2$ in the paramagnetic phase for $\eta = 0.3$.

Temperature dependencies of y, $\partial y/\partial t$ and $\partial^2 y/\partial t^2$ at $\sigma = 0$ numerically determined by equations (2.11) and (3.3) are shown in figure 1 for $\eta = 0.3$. Near the critical temperature, we see that the higher derivatives $y^{(n)}$ for $n \geqslant 2$ become very large. With increasing t they rapidly decrease. In the previous expressions, derivatives of $T(y)$ were calculated by

$$\frac{\partial T(y)}{\partial y} = \frac{\eta^2}{t} I_4^{(1)}(y) \qquad \frac{\partial T(y)}{\partial t} = -\frac{\eta^2}{t^2}\{y I_4^{(1)}(y) + \eta^2 I_6^{(1)}(y)\}$$

$$\frac{\partial^2 T(y)}{\partial y^2} = \frac{1}{t^2} I_5^{(2)}(y) \qquad \frac{\partial^2 T(y)}{\partial y \partial t} = -\frac{1}{t}\frac{\partial T(y)}{\partial y} - \frac{1}{t^3}\{y I_5^{(2)}(y) + \eta^2 I_7^{(2)}(y)\}$$

$$\frac{\partial^2 T(y)}{\partial t^2} = -\frac{2}{t}\left(\frac{\partial T(y)}{\partial t} + y\frac{\partial^2 T(y)}{\partial y \partial t} + \frac{y}{t}\frac{\partial T(y)}{\partial y}\right) - \frac{y^2}{t^2}\frac{\partial^2 T(y)}{\partial y^2} + \frac{\eta^4}{t^4} I_9^{(2)}(y) \qquad (3.4)$$

where we defined $I_n^{(m)}(y)$ by

$$I_n^{(1)}(y) = \int_0^{\eta^{-1}} \mathrm{d}z\, z^n \left\{\frac{1}{u} + \frac{1}{2u^2} - \psi'(u)\right\}$$

$$I_n^{(2)}(y) = \int_0^{\eta^{-1}} \mathrm{d}z\, z^n \left\{-\frac{1}{u^2} - \frac{1}{u^3} - \psi''(u)\right\}$$

$$u = z(y/\eta^2 + z^2)/t. \qquad (3.5)$$

At the critical point ($t = 1$), for small values of σ these functions behave as follows:

$$y = A\sigma^4 \qquad y^{(1)} = B\sigma^2 \qquad y^{(2)} = y_0^{(2)} + C\sigma^2 \qquad (3.6)$$

with

$$A = \left[\frac{5c(\eta^*)^4}{C_1(2+\sqrt{5})}\right]^2 \qquad B = \frac{10\sqrt{5}c(\eta^*)^4}{(16+7\sqrt{5})C_1^2}\left[-3\eta^4 I_6^{(1)}(0)\right]$$

$$y_0^{(2)} = \frac{9+2\sqrt{5}}{1+2\sqrt{5}}\frac{B^2}{10A} \qquad C = \frac{6\sqrt{5}}{(3+2\sqrt{5})C_1}\left[\eta^4\{2I_6^{(1)}(0) + I_9^{(2)}(0)\} - 2B\right]$$

$$C_1 = \pi\eta^3/4.$$

For finite σ, we have numerically solved equations (2.9) and (3.2) for several values of temperatures starting from the initial values determined by equation (3.3). Higher order derivatives $y^{(n)}$ $(n \geqslant 3)$ can be evaluated in the same manner. In this paper we estimated $y^{(n)}(\sigma, 1)$ up to $n = 5$ by numerical differentiation from a knowledge of $y(\sigma, t)$, $y'(\sigma, t)$, and $y''(\sigma, t)$ for several values of t (see the appendix for details).

With the use of these derivatives $y^{(n)}(\sigma, 1)$ we can now extend our solutions below T_c. Our results suggest that even and odd higher derivatives have negative and positive signs, respectively. It then follows that higher order terms in equation (3.1) for $t > 1$ cancel with each other and the convergence is good. In contrast, for $t < 1$, all the higher order terms contribute additively and the convergence of equation (3.1) is comparatively slow, especially as we approach the ground state. To see the behaviour of $y(\sigma, t)$ for $t < 1$, we evaluate equation (3.1) up to the fifth order for $\eta = 0.3$. As long as y is very small, we found that it is already a very good approximation. We show in figure 2, the t-dependence of $y(\sigma, t)$ for several values of $x = \sigma^2$. From the figure, we see a clear upturn in behaviour as t decreases.

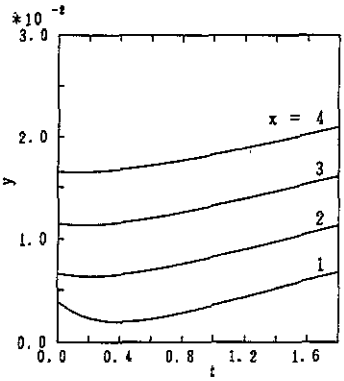

Figure 2. Temperature dependence of $y(\sigma, t)$ below T_c extrapolated from the paramagnetic solutions for several values of σ^2 and $\eta = 0.3$.

As for the ground state ($t = 0$), the general solution of equation (2.9) is simply obtained as follows if we assume $Z(y) = y$ justified for small y (hereafter we assume this relation for the ease of comparison with the analytic expression):

$$y = 2c(\eta^*)^4\{\sigma^2 - 1\} + \xi\sigma^{-3} \tag{3.7}$$

where ξ is an arbitrary constant determined from the initial condition. In our preceding paper (Takahashi 1986), we assumed $\xi = 0$ considering that otherwise equation (3.7) will give a divergent y as $\sigma \to 0$. Equation (3.7) then gives the solution $\sigma = 1$ at $T = 0$ K, which justifies equation (2.10) for the saturation magnetization in the ground state. It is easy to see that a free energy corresponding to the negative ξ is higher than the free energy with $\xi = 0$. On the other hand, although positive ξ gives the lower free energy, it does not give a stable minimum value. In figure 3, $y(\sigma, t)$ plotted against x in the ground state is shown. The figure shows the upward deviation of calculated $y(\sigma, 0)$ from $y_0(\sigma, 0) = 2c(\eta^*)^4(x - 1)$, showing ξ of the solution constructed by equation (3.1) is finite. We further found that we can fit the calculated $y(\sigma, 0)$ with equation (3.7) by assuming $\xi = 4c(\eta^*)^4/3$ (see figure 3).

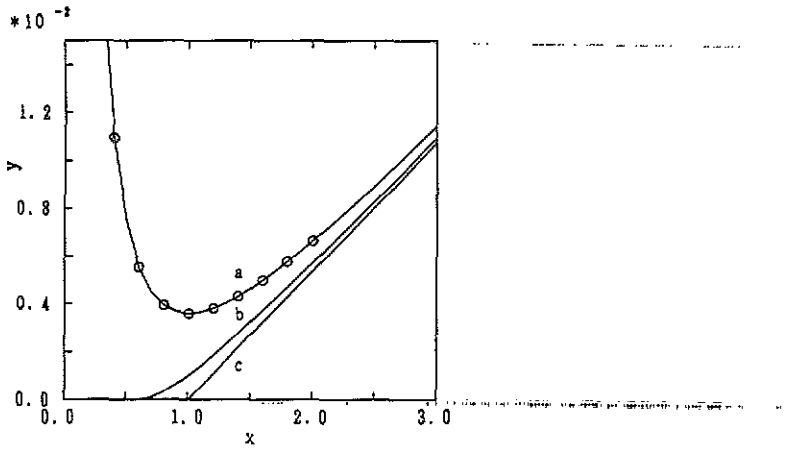

Figure 3. σ^2-dependence of the ground-state solution, $y(\sigma,0)$ for $\eta = 0.3$: a, with $\xi = 4c(\eta^*)^4/3$; b, with $\xi = (3/5)^{2.5}4c(\eta^*)^4/3$; and c, with $\xi = 0$. Open circles are evaluated by equation (3.1) up to the fifth order from the paramagnetic solutions.

This value of ξ is very large and we cannot satisfy the condition $y(\sigma,0) = 0$ for any finite value of σ. It corresponds to the condition $y = y_z$ at $t = 0$ and $\sigma = 1$.

4. Magnetization below T_c

The general solution of our first-order differential equation contains a parameter which generally depends on temperature. We have so far implicitly assumed that this constant is analytic with respect to the finite reduced temperature t. Therefore the parameter ξ in equation (3.7) in the ground state, for example, would be uniquely determined. However what we found in section 3 is simple analytic continuation of the paramagnetic solutions with respect to the temperature at finite σ does not lead to a favourable solution at low temperature. This finding is very interesting but our problem still remains unsolved. From the stability condition of the free energy, we can anyway restrict the range of σ. For example, in the ground state, by differentiating equation (3.7) with respect to σ, we find the minimum value of $y(\sigma,0)$ for a given positive value of ξ:

$$y_{\min} = 2c(\eta^*)^4\left\{\frac{5}{3}\left(\frac{3\xi}{4c(\eta^*)^4}\right)^{2/5} - 1\right\} \qquad \text{at } \sigma = \left(\frac{3\xi}{4c(\eta^*)^4}\right)^{1/5}. \tag{4.1}$$

In order to satisfy $y = 0$, we must have $y_{\min} \leqslant 0$, and we obtain the condition:

$$\xi \leqslant \left(\frac{3}{5}\right)^{5/2}\frac{4c(\eta^*)^4}{3} \qquad \sigma \geqslant \left(\frac{3}{5}\right)^{1/2} = 0.774\,59\ldots. \tag{4.2}$$

This condition can be easily generalized for the case of finite temperatures. We see that condition (4.2) corresponds to the free-energy stability requirement, the positive curvature of the free energy. In other words, we have the following condition:

$\partial y/\partial x > 0$ for $y = 0$, or from equation (2.9) we have

$$\sigma^*(t) < \sigma \qquad \text{at } y = 0$$

$$\sigma^*(t)^2 = \frac{3}{5}\left(1 - \frac{T(0)}{c(\eta^*)^4}\right) = \frac{3}{5}\{1 - t^{4/3} - (\eta/\eta^*)^4 t^{4/3} c_1\}$$

$$c_1 = \int_{1/\eta}^{1/\eta t^{1/3}} \mathrm{d}z\, z^3\{\log z^3 - \tfrac{1}{2}z^3 - \psi(z^3)\}. \tag{4.3}$$

In order to determine the unique solution, we particularly note the fact that if we know the σ-dependence of $y(\sigma, t)$, we can construct free energy as a function of σ by using the relation $y = h/\sigma$ and integrating h with respect to σ. For each initial condition, we can thus find the corresponding free energy as a function of σ. If we assume $y = y_0$ at $x = x_0$, we can, in principle, evaluate any higher derivatives $\partial^n y/\partial x^n$ $(x = \sigma^2)$ with the use of equation (2.9). From the thermodynamic relation of the normalized free energy $\partial f(\sigma, t)/\partial\sigma = h$, we see that $f(\sigma, t)$ is related to y by

$$\frac{1}{\sigma}\frac{\partial f(\sigma, t)}{\partial \sigma} = y. \tag{4.4}$$

Let the σ dependence of $f(\sigma, t)$ be expanded around $\sigma = \sigma_0 = \sqrt{x_0}$:

$$f(\sigma, t) = f_0 + f_1(\sigma - \sigma_0) + \frac{f_2}{2}(\sigma - \sigma_0)^2 + \frac{f_3}{3}(\sigma - \sigma_0)^3 + \cdots \tag{4.5}$$

then coefficients f_n are given by

$$f_1 = \sqrt{x_0}\, y_0 \qquad f_2 = 2x_0\frac{\partial y}{\partial x} + y_0 \qquad f_3 = \sqrt{x_0}\left(2x_0\frac{\partial^2 y}{\partial x^2} + 3\frac{\partial y}{\partial x}\right)$$

$$f_4 = \frac{4}{3}x_0^2\frac{\partial^3 y}{\partial x^3} + 4x_0\frac{\partial^2 y}{\partial x^2} + \frac{\partial y}{\partial x}. \tag{4.6}$$

In these expressions, $\partial^n y/\partial x^n$ stands for the derivative of y at $x = x_0$. We cannot solve equation (2.9) beyond the stable solution with $y \geqslant 0$ since we have to deal with the fluctuation amplitudes for negative y. However, from equation (4.5) we can analytically extend our solution to the unstable region. In order to determine x_0, we now assume $\partial f/\partial\sigma = 0$ at the origin $\sigma = 0$, expecting the σ^2-dependence of the free energy there. Then by introducing $g(x_0, t)$ by

$$g(x_0, t) = \frac{1}{\sigma_0}\frac{\partial f}{\partial \sigma}\bigg|_{\sigma=0} = y_0 - f_2 + f_3\sqrt{x_0} - f_4 x_0 + \cdots \tag{4.7}$$

it follows that the zero of $g(x, t)$ determines x_0. Up to the fourth derivative of $f(\sigma, t)$, g is explicitly given by

$$g(x, t) = -2x^2\frac{\partial^2 y}{\partial x^2} - \frac{4}{3}x^3\frac{\partial^3 y}{\partial x^3}. \tag{4.8}$$

As a simple example, we see from equation (2.9) that $g(x)$ in the ground state ($t = 0$) is given by

$$g(x) = 10\{y_0 - 2c(\eta^*)^4(x-1)\}. \tag{4.9}$$

From equation (4.9), we easily see that the squared magnetization x_0 for finite y_0 is given by $x_0 = 1 + y_0/2c(\eta^*)^4$, which is equivalent to $\xi = 0$ in equation (3.7). For an illustration of this procedure at finite temperature, we plot $g(x,t)$ in equation (4.8) as a function of x for various temperatures t for $\eta = 0.3$ and $y_0/2c(\eta^*)^4 = 0.05$ in figure 4. For a given temperature t, we evaluate x_0 from the zero of $g(x,t)$. The result is shown in figure 5 as curve a. We show t-dependence of σ^2 in figure 6. It should be noted that the finite y_0 is necessary at finite temperatures. If $y = 0$, we cannot define derivatives, $\partial^n y/\partial x^n$, for $n > 1$ because $\partial^n T(y)/\partial y^n$ diverge as $y \to 0$. Care must be taken here that curve a in figures 5 and 6 is the magnetization under the static external magnetic field, and this is the reason curve a exceeds one at low temperature. By solving equation (2.9) starting from x_0 on curve a, we can obtain the squared saturation magnetization x at $y = 0$. The result is shown as curve b in figure 5. The magnetization process for the higher external magnetic field is calculated in the same way.

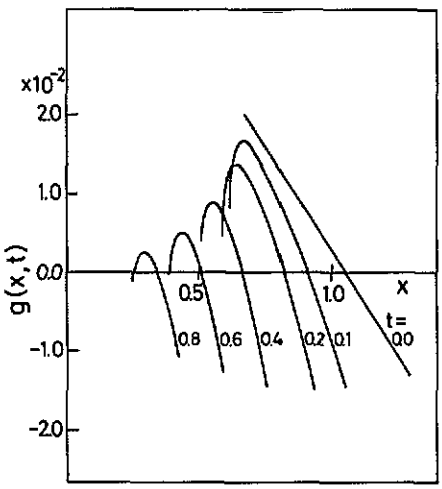

Figure 4. x-dependence of the function $g(x,t)$ defined in equation (4.8) in the text for $y_0 = 0.05 \times 2c(\eta^*)^4$.

Near the critical temperature, it is hard to determine the precise value of the magnetization at $y = 0$ using this method. In our scheme, we first estimate the zero of $g(x,t)$ corresponding to the finite y. Then we solve equation (2.9) to obtain the value of x for $y = 0$. As we approach to the critical point, we need an increasingly more accurate value of x_0 because a slight difference in x for finite y results in a large difference in x as y decreases. This circumstance is clearly seen if we solve equation (2.9) starting from various initial conditions as shown in figure 7 for $t = 0.95$, for example. From the figure we see that solutions starting from different values of x_0 at $y = 0$ rapidly converge to nearly the same value of y as y increases. The reason that the x value for $y = 0$ becomes smaller than the stability limit, $\sigma^*(t)^2$, around $t = 0.93$, as shown in figure 7, seems to come from the fact

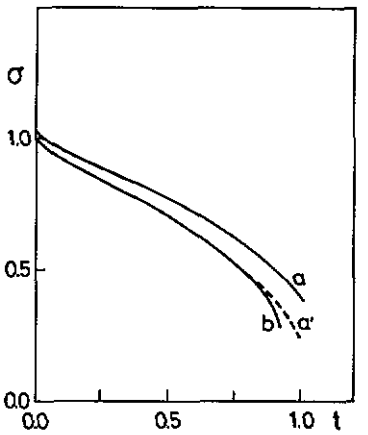

Figure 5. Temperature dependence of the saturation magnetization, σ. The curves a and a' correspond to the zero of $g(x,t)$ for $y_0/2c(\eta^*)^4 = 0.05$ and 0.01, respectively. Curve b is obtained by solving equation (2.9) starting from the point (x_0, y_0) of curve a.

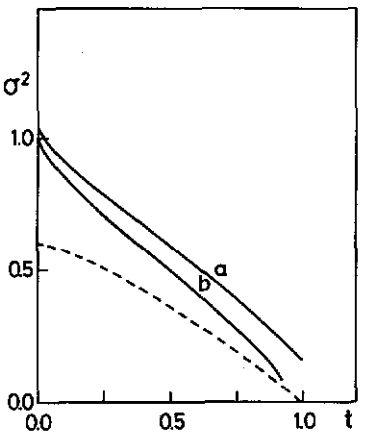

Figure 6. Temperature dependence of the squared saturation magnetization, σ^2. Curves a and b correspond to the zero of $g(x,t)$ for $y_0/2c(\eta^*)^4 = 0.05$ and 0.01, respectively. The broken curve represents the stability condition, $\sigma^*(t)^2$, of the free energy given in equation (4.3).

that the zero of equation (4.8) slightly underestimates the value of x_0. From the behaviour of the ratio, $x_0/\sigma^*(t)^2$, for $t \leqslant 0.9$, we expect the precise value of x_0 to behave as $x_0 \simeq 1.5 \times \sigma^*(t)^2$ for $t \sim 1$.

This difficulty around the critical point, however, does not seem to be serious for comparison with experiments from the following reason. Experimentally it is also very difficult to measure the temperature dependence of the saturation magnetization of weak itinerant ferromagnets especially around the critical region. Magnetization at zero-field is determined by extrapolating the Arrott plot (M^2–H/M plot) to the $H/M = 0$ limit. This is only justified when the linearity of the plot is good. However, because we expect the behaviour $y \propto x^2$ near the critical point, we cannot determine the precise magnetization from this extrapolation procedure. The magnetization process around small y and σ region is also very sensitive to the sample

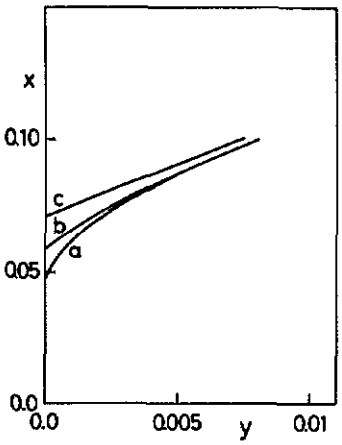

Figure 7. Dependence of the magnetization process on the initial condition for $t = 0.95$. Curves a, b and c represent solutions of equation (2.9) starting from $x/\sigma^*(t)^2 = 1.2$, 1.5 and 1.8, respectively at $y = 0$.

quality. Therefore the reliable quantity to be observed experimentally is the magnetization under the finite external field. If comparison is made at finite y, the problem of the sensitive initial condition is not so serious. Curve a' in figure 5 shows the t-dependence of σ for smaller y value, $y_0/2c(\eta^*)^4 = 0.01$. We can use curve a' as an approximate solution under a finite external field. The solution of equation (2.9) passing through this point does not cross the $y = 0$ line because of the slight relative error of x at finite y.

As shown earlier we can evaluate the magnetization curve starting from various initial conditions. Most of these states are not true stable states, and they realized when various relaxation processes to lower energy states are for some reason prohibited. The effect of the presence of solutions with various initial conditions is particularly conspicuous around the critical region of the appearance of ferromagnetism, where we have $y \sim 0$ around $T = 0$ K and various relaxation processes become ineffective. A slight difference in the initial condition appears in a magnified form at low temperature. All the solutions, however, asymptotically tend to the unique lowest energy solution as we increase the magnetization by applying the external magnetic field. This behaviour is clearly seen in the ground state, equation (3.7): as we increases σ, $y(\sigma, 0)$ approaches the unique solution $y(\sigma, 0) = 2c(\eta^*)^4(\sigma^2 - 1)$ irrespective of our choice of ξ value.

5. Conclusions

In the present paper, we discussed the ordered phase properties of itinerant electron ferromagnets. We first discussed the problem by straightforward analytic continuation of paramagnetic solutions with respect to the temperature. We found that these solutions do not directly continue to the stable solutions below T_c. Based on this fact we pointed out a possibility that solutions with various initial conditions are actually realized in the ordered phase. We then proposed a method by which to find the most stable state among these states. All the other solutions, although they have different

magnetizations for the weak external field, tend to the unique stable solution as we increase the magnetization by applying an external magnetic field.

We emphasize the importance of the degrees of freedom concerning the initial condition. Even if we fix the equation, we are still left with a choice of initial conditions. We would like to point out here a possibility that the existence of solutions with various initial conditions is related to the metamagnetic behaviour associated with the peculiar form of the Arrott plot at low temperature widely observed in nearly ferromagnetic materials around their critical concentration of the occurrence of the ferromagnetism such as $TiBe_2$ (Acker *et al* 1981) and $Y(Co\text{-}Al)_2$ (Sakakibara *et al*). In these compounds the longitudinal magnetic susceptibility shows divergent behaviour at some field strength around the metamagnetic transition. If we solve equation (2.9) starting from a slightly smaller value of x than the precise one towards smaller x, the solution will become unstable (i.e. $y_z = 0$) beyond a certain x value near the critical temperature ($y = 0$). If we interchange x- and y-axes in figure 3, curve a looks like an observed peculiar behaviour. Because we need $y = 0$ around $T = 0$ K from the earlier argument, we only expect metamagnetic behaviour just around the critical concentration of the ferromagnetism.

Our approach shows a clear contrast with conventional approaches based on the expansion in terms of the small magnetization or small spin fluctuation amplitudes. We usually assume the linearity of the Arrott plot as given from the beginning. The slope of the plot is an independent parameter related to the curvature of the electronic density of states at the Fermi level. On the other hand, our approach is based on an equation for the transverse magnetic susceptibility and the Arrott plot is obtained as a consequence of the theory. The slope of the Arrott plot is determined instead from the nature of spin fluctuation spectrum in q, ω space. The spin fluctuation spectrum determines all the magnetic properties. In this sense our approach is more like the situation in the localized moment limit where all the magnetic properties are characterized by the parameter of the spin Hamiltonian. The difference lies in the energy scale of the spin fluctuation spectrum and the existence of the large zero-point spin fluctuation amplitude, which are new characteristic features of itinerant electron magnets.

Appendix. A numerical method to evaluate higher derivatives of y

Instead of directly evaluating higher derivatives $y^{(n)}(\sigma, 1)$ for $3 \leqslant n$, we numerically evaluate them from the values of $y^{(2)}(\sigma, t)$ evaluated at several values of t. For a given function $f(t)$, let us define following functions:

$$F(h) = \frac{4f(1+h/2) - f(1+h) - 3f(1)}{h}$$

$$G(h) = \frac{2f(1+h/2) - f(1+h) - f(1)}{h^2/4}$$

$$H(h) = \frac{8f(1+h/4) - 6f(1+h/2) + f(1+h) - 3f(1)}{h^3/16}.$$

Then the derivatives of $f(t)$ at $t = 1$ can be estimated by

$$f'(1) = \frac{4F(h/2) - F(h)}{3} - \frac{h^3}{192} f^{(4)}(1) + \cdots$$

$$f''(1) = \frac{6G(h/2) - G(h) - 8G(h/4)}{3} - \frac{h^3}{256} f^{(5)}(1) + \cdots$$

$$f^{(3)}(1) = 2H(h/2) - H(h) + \frac{7h^2}{512} f^{(4)}(1) + \cdots .$$

In this paper we have estimated $y^{(3)}$, $y^{(4)}$ and $y^{(5)}$ from this formula by assuming $f(t) = y''(\sigma, t)$ and $h = \frac{1}{4}$ for $y^{(3)}$ and $y^{(4)}$, and $h = \frac{1}{2}$ for $y^{(5)}$. We suppose that relative accuracy will be maintained. We have checked the validity of the results by evaluating summation (3.1) up to the fifth order and comparing it with the value of $y(\sigma, 2)$ directly obtained by solving equation (2.9).

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