

# Theory of the Minimum of the Temperature Dependence of the Inverse of the Magnetic Susceptibility in Nearly Ferromagnetic Metals

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## ABSTRACT

*We investigated the minimum of the temperature dependence of the inverse of the magnetic susceptibility by using self-consistent renormalisation theory of spin fluctuations in nearly ferromagnetic metals that includes the electronic correlation beyond the random phase approximation. We used the Landau expansion of the magnetic free energy up to the 6th order term of the magnetisation. We found that the inverse of the magnetic susceptibility had the minimum at low temperatures at maximum of the square of the local spin amplitude. We succeeded in reproducing the Curie-Weiss law at elevated temperatures.*

## Introduction

Many experimental and theoretical researchers have been interested in the magnetic properties of nearly ferromagnetic metals [1-15]. Kawakami and Okiji examined the minimum of the temperature dependence of the magnetic susceptibility based on the degenerate impurity Anderson model by the exact solution. They found that the orbital degeneracy leads to the minimum [16].

Ishigaki and Moriya studied the effect of zero point spin fluctuations [17]. Moriya [18] and Yamada [19] investigated the relationship between metamagnetism and the minimum of the temperature dependence of the inverse of the magnetic susceptibility. They used the Landau expansion of the magnetic free energy up to 6th-order term of the magnetisation. However, the minimum of the temperature dependence of the inverse of the magnetic susceptibility in nearly ferromagnetic metals has yet been unanswered theoretically where it appears in YCo<sub>2</sub>, Pd, UPt<sub>3</sub>, UTe<sub>2</sub>, and LuCo<sub>2</sub> [6]. We use the self-consistent renormalisation theory of spin fluctuations in nearly ferromagnetic metals including the electronic correlations beyond the random phase approximation. In order to explain the minimum of the temperature dependence of the inverse of the magnetic susceptibility, we consider the Landau expansion of the magnetic free energy up to the 6th-order term of the magnetisation like Moriya [17] and Yamada [18]. The inverse of the magnetic susceptibility is investigated. Throughout this

paper, we use units of energy, such that  $\hbar = 1$ ,  $k_B = 1$ , and  $g\mu_B = 1$  where  $g$  is the  $g$ -factor of the conduction electron, unless explicitly stated. We assume that the  $c$ -axis is the axis of easy magnetisation.

This paper is organized as follows: the formulation will be provided in section 2.

The results will be supplied in section 3. The conclusions will be given in section 4.

## Formulation

Let's begin with the following equation of the inverse of the magnetic susceptibility [18,19]

$$\frac{1}{\chi(T)} = \frac{1-\alpha}{\chi_0} - \frac{5}{3}F_1S_L^2(T) + \frac{35}{9}G_1S_L^4(T) \quad (1)$$

where  $F_1$  and  $G_1$  are the coefficients of the Landau expansion of the magnetic free energy.  $(1-\alpha)^{-1}$  is the Stoner's enhancement factor.  $\chi_0$  is the non-interacting magnetic susceptibility.  $S_L^2(T)$  is the square of the local spin amplitude.

In order to consider  $S_L^4(T)$  self-consistently, the following dynamical susceptibility is introduced.

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - I\chi_0(q, \omega) - \lambda + \beta\lambda^2\chi_0(q, \omega)} \quad (2)$$

where  $I$  is the on-site Coulomb coupling. From Eq.(1),  $\lambda$  is determined by the limit  $q \rightarrow 0$  and  $\omega \rightarrow 0$

$$\lambda = \frac{5}{3}F_1S_L^2(T) \quad (3)$$

$$\beta\lambda^2 = \frac{35}{9}G_1S_L^4(T) \quad (4)$$

From Eqs. (3) and (4),

$$\beta = \frac{7G_1}{5\chi_0^2F_1^2} \quad (5)$$

$\lambda$  is determined by the following equation.

$$\beta\chi_0\lambda^2 - \lambda + 1 - \alpha = 0 \quad (6)$$

$$\lambda = \frac{1 - \sqrt{1 - 4\beta\chi_0(1 - \alpha - \chi_0/\chi)}}{2\beta\chi_0} \quad (7)$$

$\lambda$  represents the electronic correlation beyond the random phase approximation. We take the minus sign because  $S_L^2(0) = 0$  and  $\lambda = 0$  when  $T = 0K$ . By using Moriya's expression [15] based on the single band Hubbard model, the non-interacting dynamical susceptibility  $\chi_0(q, \omega)$  is obtained as follows:

$$\chi_0(q, \omega) = \chi_0(0, 0)(1 - Aq^2 + iC\frac{\omega}{q}), \quad (8)$$

$q$  and  $\omega$  are the magnitude of the wave vector and the frequency, respectively. The square of the local spin amplitude  $S_L^2(T)$  is

$$S_L^2(T) = \frac{3}{2\pi} \sum_q \int_0^\infty d\omega \frac{1}{e^{\omega/T} - 1} \text{Im}\chi(q, \omega). \quad (9)$$

From Eq.(8),  $\text{Im}\chi(q, \omega)$  is

$$\text{Im}\chi(q, \omega) = \frac{T_0}{2\alpha T_A} \frac{\omega}{u_1^2 + \omega^2} \quad (10)$$

with

$$u_1 = 2\pi T_0(1/(2\gamma T_A \chi(0)) + (q/q_B)^2), \quad (11)$$

$$T_A = Aq_B^2/2,$$

$$\Gamma = A/C,$$

$$T_0 = \Gamma q_B^3/(2\pi)$$

$$\gamma = \beta\chi_0\lambda^2$$

$q_B$  is the magnitude of the zone boundary wave vector. From Eq.(9),  $S_L^2(T)$  is

$$S_L^2(T) = \frac{3T_0}{\alpha T_A} \int_0^1 dx x^3 (\ln u - \frac{1}{2u} - \psi(u)) \quad (12)$$

where  $\psi(u)$  is the digamma function.

$$y = \frac{1}{2\alpha T_A \chi(0)}, \quad (13)$$

$$t = T/T_0, u = x(x^2 + y/\gamma)/t. \quad (14)$$

where  $y$  is the inverse of the reduced magnetic susceptibility. From Eqs.(1) and (12), the equations of the inverse of the reduced magnetic susceptibility are obtained.

$$y = y_0 - y_1 A(y, t) + y_2 A^2(y, t) \quad (15)$$

$$A(y, t) = \int_0^1 dx x^3 [\ln u - 1/(2u) - \psi(u)]$$

where

$$y_0 = \frac{1 - \alpha}{2\alpha T_A \chi_0}, \quad (16)$$

$$y_1 = \frac{15F_1T_0}{2\gamma T_A^2}, \quad (17)$$

$$y_2 = \frac{315G_1T_0}{2\gamma T_A^2}, \quad (18)$$

In Eq. (7), we rewrite  $\lambda$  by  $y$  and  $y_0$ .

$$\lambda = \frac{1 - \sqrt{1 - 4\beta\chi_0(1 - \alpha)(1 - y/y_0)}}{2\beta\chi_0} \quad (19)$$

$\chi_0(0)$  is the non-interacting magnetic susceptibility at the zero temperature. The results will be provided in the next section.

## Results

In this section, the numerical results are provided by using the formulation in the previous section. In order to roughly estimate the minimum of the temperature dependence of the inverse of the magnetic susceptibility at low temperatures  $t \ll 1$ , we use the following asymptotic expansion of the digamma function in the integrand of Eq. (15).

$$\ln u - 1/(2u) - \psi(u) \simeq \frac{1}{12u^2} + \dots \quad (20)$$

$$A(y, t) \simeq \gamma t^2/(24y_0), \gamma \simeq \alpha(t \ll 1) \quad (21)$$

$$y \simeq y_0 - \frac{y_1\alpha}{24y_0} t^2 + \frac{y_2\alpha^2}{24^2y_0^2} t^4 \quad (22)$$

If the inverse of the reduced magnetic susceptibility has the minimum at  $t = t_M$ ,  $\frac{\partial y}{\partial t} = 0$  at  $t = t_M$ .

$$t_M = 2\sqrt{\frac{3y_0y_1}{\alpha y_2}}. \quad (23)$$

The  $y > 0$  at  $t = t_M$ .

$$y_M = y_0 - \frac{y_1^2}{4y_2} > 0. \quad (24)$$

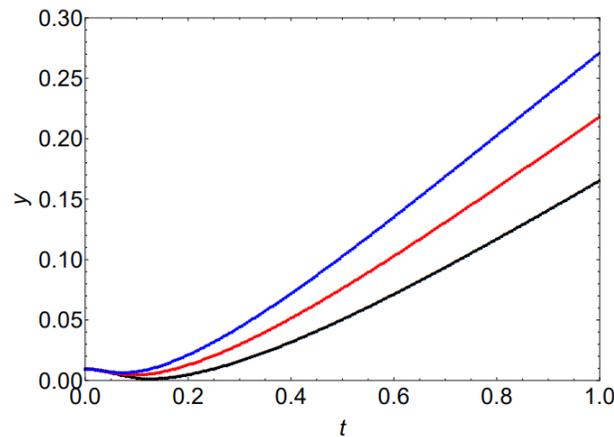
Then  $y_2 > y_1^2/(4y_0)$ . Figure 1 shows the temperature dependence of  $y$  when  $\beta = 10^{-4}$ ,  $\chi_0 = 1000[1/K]$ ,  $y_0 = 0.01$ ,  $y_1 = 1$ ,  $y_2 = 30$  (the black line), 50 (the red line), 80 (the blue line), respectively. These parameters are typical of nearly ferromagnetic metals [6]. From Figure 1, the inverse of the reduced magnetic susceptibility has the minimum as function  $t$  at low temperatures. In elevated temperatures it has  $T$ -linear dependence. Figure 2 shows the temperature dependence of  $\lambda$  with the same parameters as Figure 1. From Figure 2, the maximum of the temperature dependence of  $\lambda$  corresponds to the minimum of the temperature dependence of the reduced magnetic susceptibility. In other words, the minimum of the temperature dependence of the reduced magnetic susceptibility appears in the maximum of the square of the local spin amplitude. In elevated temperatures,  $\lambda$  has  $T$ -linear dependence.

## Conclusion

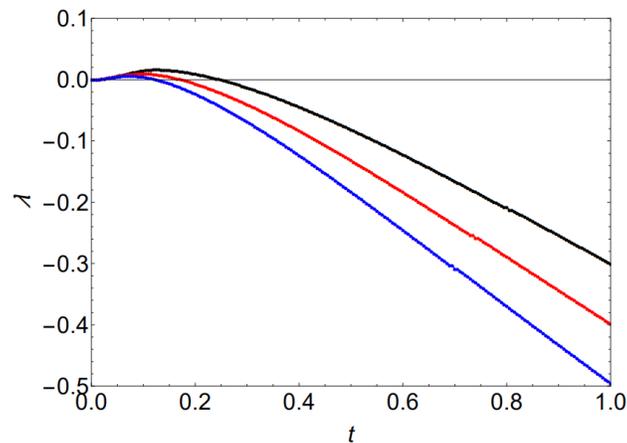
We have studied the minimum of the temperature dependence of the inverse of the magnetic susceptibility. We have succeeded in producing the minimum of the temperature dependence of the inverse of the magnetic susceptibility at low temperatures. At higher temperatures, the inverse of the magnetic susceptibility obeys the Curie-Weiss law. This theory explains the behaviors of the inverse of the magnetic susceptibility in Pd, YCo<sub>2</sub>, UPt<sub>3</sub>, UTe<sub>2</sub>, and LuCo<sub>2</sub>.

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**Figure 1:** The temperature dependence of the inverse of the reduced magnetic susceptibility  $y$  when  $\alpha = 0.98$ ,  $\beta = 10^{-4}$ ,  $\chi_0 = 1000[1/K]$ ,  $y_0 = 0.01$ ,  $y_1 = 1$ ,  $y_2 = 30$  (the black line), 50 (the red line), 80 (the blue line), respectively.



**Figure 2:** The temperature dependence of the  $\lambda$  when  $\alpha = 0.98$ ,  $\beta = 10^{-4}$ ,  $\chi_0 = 1000[1/K]$ ,  $y_0 = 0.01$ ,  $y_1 = 1$ ,  $y_2 = 30$  (the black line), 50 (the red line), 80 (the blue line), respectively.

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