Research Article

ISSN 2639-9466

Nanotechnology & Applications

Theory of the Maximum of the Magnetic Susceptibility in YCo_2

Rikio Konno[1], Kazuyoshi Yoshimura[2] and Chishiro Michioka[3]

[1]*Kindai University Technical College, 7-1 Kasugaoka, Nabari-shi 518-0459, Japan.*

[2]*Graduate School of Engineering, Department of Energy and Hydrocarbon Chemistry, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan.*

[3]*Department of Chemistry, Graduate School of Science, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto-shi, 606-8501, Kyoto, Japan.*

***Correspondence:**
Rikio Konno, Kindai University Technical College, 7-1 Kasugaoka, Nabari-shi 518-0459, Japan.

Received: 04 Jul 2025; **Accepted:** 10 Jul 2025; **Published:** 16 Jul 2025

Citation: Konno R, Yoshimura K, Michioka C. Theory of the Maximum of the Magnetic Susceptibility in YCo_2. Nano Tech Appl. 2025; 8(2): 1-3.

ABSTRACT

We investigated the temperature dependence of the magnetic susceptibility and that of $1/(T_1T)$ where $1/T_1$ was the nuclear magnetic relaxation rate in YCo_2 theoretically. The self-consistent renormalization theory of spin fluctuations (SCR theory) was used. The SCR theory includes the electronic correlations beyond the random phase approximation. The Landau expansion of the magnetic free energy was used up to 6th order of the magnetization because of the metamagnetism in YCo_2. We found that the temperature dependence of the magnetic susceptibility and that of $1/(T_1T)$ were consistent with the experimental data qualitatively.

Keywords
SCR theory, Magnetic susceptibility.

Introduction

Many researchers have been interested in nearly ferromagnetic metals [1-13] Yoshimura et al. investigated the temperature dependence of $1/(T_1T)$ where $1/T_1$ is the nuclear magnetic relaxation rate in YCo_2 [14,15]. They show that YCo_2 is the nearly ferromagnetic metal. They find that YCo_2 has the anomaly of $1/(T_1T)$ corresponding to the maximum of the magnetic susceptibility.

Konno explains the minimum of the inverse of the magnetic susceptibility in nearly ferromagnetic metals by using the self-consistent renormalization theory of spin fluctuations (the SCR theory) that includes the electronic correlations beyond the random phase approximation [16]. We apply this theory to the magnetic properties in YCo_2

Throughout this paper, we use units of the 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 easy axis of the magnetization.

This paper is organized as follows: the formulation will be supplied in section 2. The results will be provided 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 [12,13,16]

$$\frac{1}{\chi(T)} = \frac{1-\alpha}{\chi_0} - \frac{5}{3}F_1 S_L^2(T) + \frac{35}{9}G_1 S_L^4(T) \tag{1}$$

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. χ_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.

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

where I is the on-site Coulomb coupling. From Eq.(1), λ is determined by the limit

$q \to 0$ and $\omega \to 0$

$$\lambda = \frac{5}{3}\chi_0 F_1 S_L^2(T) \quad (3)$$

$$\beta\lambda^2 = \frac{35}{9}G_1 S_L^4(T) \quad (4)$$

From Eqs.(3) and (4),

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

λ is determined by the following equation.

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

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

λ represents the electronic correlation beyond the random phase approximation. We take the minus sign because $S_L^2(0) = 0$ and $\lambda = 0$ when $T = 0$K. By using Moriya's expression [11] 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 ω are the magnitude of the wave vector and the frequency, respectively. The square of the local spin amplitude $S_L^2(T)$ is

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

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

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

With

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

$$TA = \frac{Aq\_B^2}{2}$$

$$\Gamma = A/C,$$

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

$$\gamma = \alpha - \beta\chi_O\lambda^2$$

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

$$S_L^2(T) = \frac{9T_0}{\gamma T_A}\int_0^1 dx x^3(\ln u - \frac{1}{2u} - \psi(u)) \quad (12)$$

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.

$$y = y_0 - y_1 A(y,t) + y_2 A^2(y,t)$$
$$A(y,t) = \frac{1}{\gamma}\int^1 dx x^3[\ln u - 1/(2u) - \psi(u)] \quad (15)$$

where

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

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

$$y_2 = \frac{315G_1T_0^2}{2\alpha T_A^3}, \quad (18)$$

In Eq.(7), we rewrite λ 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.

We proceed to the nuclear magnetic relaxation rate. The nuclear magnetic relaxation rate $1/T_1$ [7,8] is

$$\frac{1}{T_1} = \gamma_N T\frac{1}{N_0}\sum_q |A_q|^2\frac{\mathrm{Im}\chi^{-+}(\mathrm{q},\omega_0)}{\omega_0} \quad (20)$$

where γ_N is the gyro-magnetic ratio, A_q is the Fourier q component of the hyperfine coupling, ω_0 is the nuclear magnetic resonance frequency, and N_0 is the number of magnetic ions. When q dependence of A_q is neglected and $\omega_0 \to 0$, we obtain

$$\frac{1}{T_1} = \frac{3}{4\pi}\gamma_N t/(\gamma T_A)A_{hf}^2(\gamma/y - 1/(1+(y/\gamma))) \quad (21)$$

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. According to Ref. [16], we estimate the maximum of the magnetic susceptibility that is about 250K. Figure 1 shows the temperature dependence of the magnetic susceptibility with spin fluctuation parameters of $Y(Co_{1-x}Al_x)_2$ at $x = 0.13$ [4]. From Figure1, the maximum is around 250K. In elevated temperatures, the magnetic susceptibility obeys the Curie-Weiss law. Figure 2 shows the temperature dependence of the spin fluctuations λ. λ is the maximum corresponding to the maximaum of the magnetic susceptibility.

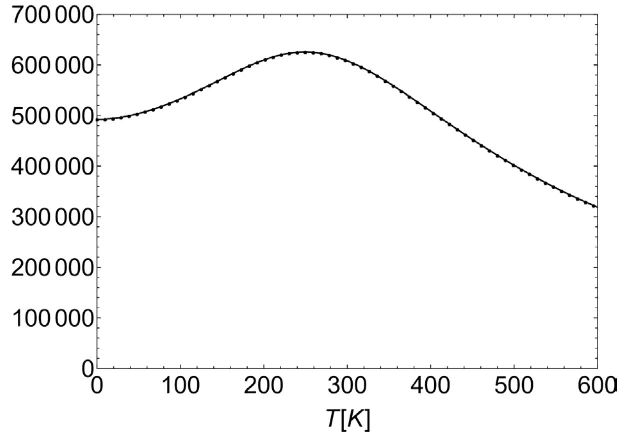

Figure 1: The temperature dependence of the reduced magnetic susceptibility χ when α = 0.75, β = 120.17, χ_0 = 0.0003266[1/K], y_0=0.03747, y_1=1.4952, y_2=70, T_0= 1920K, T_A= 12300K.

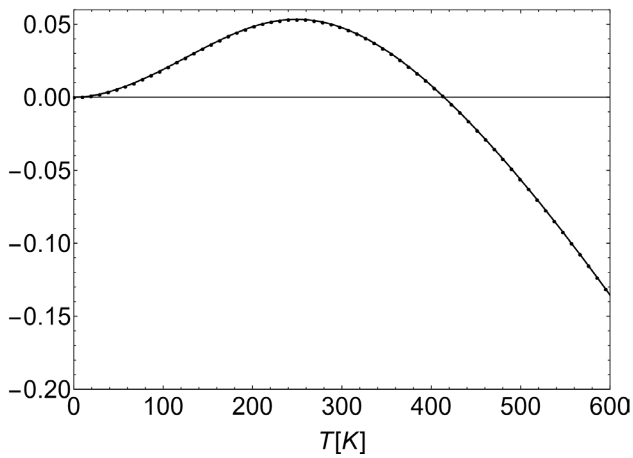

Figure 2: The temperature dependence of the λ with the same parameter value as Figure 1.

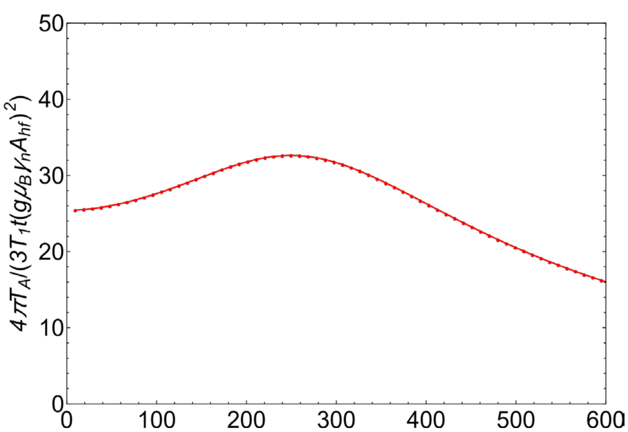

Figure 3: The temperature dependence of the $1/(T_1T)$ with the same parameter value as Figure 1.

Figure 3 shows the temperature dependence of $1/(T_1T)$. The maximum is around 250K corresponding to the maximum of the magnetic susceptibility. These behaviors are good agreements with the experimental data qualitatively.

Conclusions

We have studied the maximum of the magnetic susceptibility and $1/(T_1T)$ where $1/T_1$ is the nuclear magnetic relaxation rate in YCo_2 by using SCR theory that includes the electronic correlation beyond the random phase approximation. We have found that they are good agreements with the experimental data qualitatively.

Acknowledgments

This work is supported by Kindai University Technical College grants. The authors dedicate this work to Michael Bonitz on his 65th birthday and the late T. Moriya. One of the authors (R.K.) would like to thank Y. Takahashi, F. Honda, and S. Demura for fruitful discussions. He would like to also thank Y. Tokunaga, Y. Haga, H. von Lohneysen, M. Brando, F. Steglich, C. Geibel, J. Flouquet, A. de Visser, S. Murayama, K. Ishida, E. Bauer, M. Grosche, K. Gofryk, P. Canfield, V. Sechovsky, D. Legut, and S. Khmelevskyi for stimulating conversations.

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