

Theory of the Maximum of the Magnetic Susceptibility in LuCo_2 Rikio Konno^{1*}, Kazuyoshi Yoshimura² and Chishiro Michioka³¹Kindai University Technical College, 7-1 Kasugaoka, Nabari-shi 518-0459, Japan.²Graduate School of Engineering, Division of Energy and Hydrocarbon Chemistry, Kyoto University, Kyoto daigaku-katsura, Nishikyo-ku, Kyoto 615-8530, Japan.³Department of Chemistry, Graduate School of Science, Kyoto University, Yoshida-honmachi, Sakyo-ku, Kyoto-shi, 606-8501, Kyoto, Japan.***Correspondence:**

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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 LuCo_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 LuCo_2 . We found that the temperature dependence of the magnetic susceptibility and that of $1/(T_1T)$ were consistent with the experimental data qualitatively.

KeywordsMagnetic Susceptibility, LuCo_2 , SCR theory, Metamagnetism.**Introduction**

The magnetic properties in nearly ferromagnetic metals have intrigued many researchers [1-15]. Yoshimura et al. investigated the temperature dependence of $1/(T_1T)$ where $1/T_1$ is the nuclear magnetic relaxation rate in LuCo_2 [16]. They show that LuCo_2 is the nearly ferromagnetic metal. They find that LuCo_2 has the anomaly of $1/(T_1T)$ corresponding to the maximum of the magnetic susceptibility.

Konno was successful in reproducing 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 [17]. We apply this theory to the magnetic properties in LuCo_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 [12,13,17,18]

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

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. 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.

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

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

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

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

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 $T = 0\text{K}$. 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 $S_L^2(T)$ [17,18] is

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

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

$$\begin{aligned} T_A &= Aq_B^2/2, \\ \Gamma &= A/C, \\ T_0 &= \Gamma q_B^3/(2\pi), \\ \gamma &= \alpha - \beta\chi_0\lambda^2, \\ y &= \frac{1}{2T_A\lambda\chi(0)}, \end{aligned} \quad [10]$$

$$t = T/T_0, u = x(x^2 + y/\gamma)/t. \quad [11]$$

where y is the inverse of the reduced magnetic susceptibility. q_B is the magnitude of the zone boundary wave vector. From Eqs. (1) and (9), the equations of the inverse of the reduced magnetic susceptibility are obtained.

$$\begin{aligned} y &= y_0 - y_1 A(y, t) + y_2 A^2(y, t), \\ A(y, t) &= \frac{1}{\gamma} \int_0^1 dx x^3 [\ln u - 1/(2u) - \psi(u)] \end{aligned} \quad [12]$$

Where

$$y_0 = \frac{1 - \alpha}{2T_A\lambda\chi_0}, \quad [13]$$

$$y_1 = \frac{15F_1 T_0}{2T_A^2}, \quad [13]$$

$$y_2 = \frac{315G_1 T_0^2}{2T_A^3}. \quad [14]$$

In Eq.(7), we rewrite λ by y and y_0 .

$$\lambda = \frac{1 - \sqrt{1 - 4\beta\chi_0(1 - \alpha)(1 - y/y_0)}}{2\beta\chi_0}. \quad [15]$$

$\chi_0(0)$ is the non-interacting magnetic susceptibility at the zero temperature.

We proceed to the nuclear magnetic relaxation rate. The nuclear magnetic relaxation rate $1/T_1$ [7,18] is

$$\frac{1}{T_1} = \gamma_N^2 T \frac{1}{N_0} \sum_q |A_q|^2 \frac{\text{Im}\chi(q, \omega_0)}{\omega_0} \quad [16]$$

where γ_N is the gyro-magnetic ratio, A_q is Fourier q component of the hyper-fine 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 $\omega_0 \rightarrow 0$, we obtain

$$\frac{1}{T_1} = \frac{3}{4\pi} \gamma_N^2 t / (\gamma T_A) A_{hf}^2 (\gamma/y - 1/(1 + (y/\gamma))). \quad [17]$$

The results will be provided in the next section.

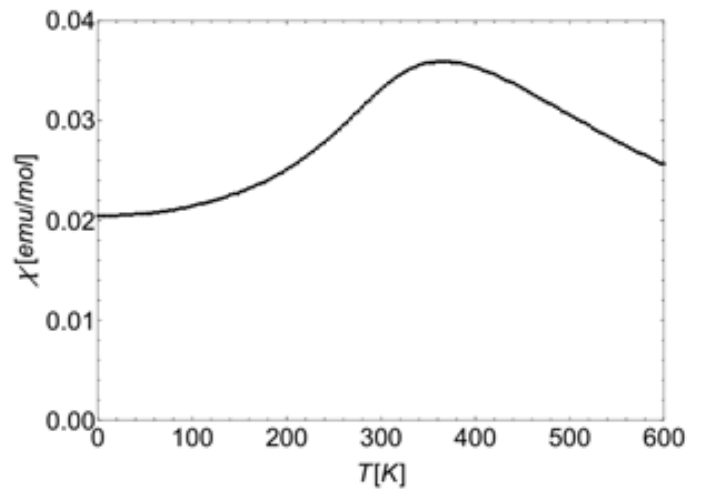


Figure 1: The temperature dependence of the magnetic susceptibility χ when $\alpha = 10/11$, $\beta = 1000$, $\chi(0) = 2.05 \times 10^{-2}$, $y_1 = 13.77$, $y_2 = 301.3$, $T_0 = 800\text{K}$, $T_A = 1000\text{K}$.

Results

In this section, the numerical results are provided by using the formulation in the previous section. According to Reference [17], we estimate the maximum of the magnetic susceptibility that is about 380K. Figure 1 shows the temperature dependence of the magnetic susceptibility with spin fluctuation parameters of

LuCo₂. From Figure 1, the maximum is around 380K. In elevated temperatures, the magnetic susceptibility obeys the Curie-Weiss law.

Figure 2 shows the temperature dependence of $1/(T_1T)$. The maximum is around 380K corresponding to the maximum of the magnetic susceptibility. These behaviors are good agreements with the experimental data qualitatively [16].

Conclusion

We have studied the maximum of the magnetic susceptibility and $1/(T_1T)$ where $1/T_1$ is the nuclear magnetic relaxation rate in LuCo₂ by using SCR theory that includes the electronic correlation beyond the random phase approximation. We have found that they are consistent with the experimental data qualitatively.

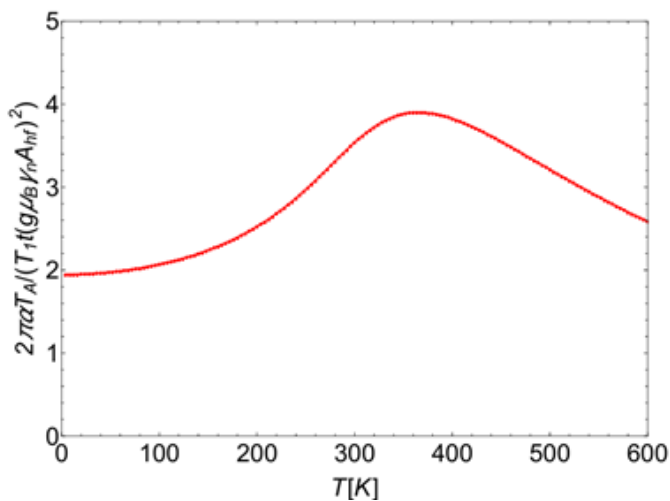


Figure 2: The temperature dependence of the $1/(T_1t)$ with the same parameter value as Figure 1.

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