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Theory of thermal expansion based on the localized paramagnon model

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We have investigated thermal volume expansion of nearly ferromagnetic metals by assuming localized spin fluctuations with wave vector independent damping constant. According to the Takahashi's theory of magneto-volume effect, thermal expansion is derived from the volume dependence of the free energy of spin fluctuations that consists of both the thermal and the zero-point components.

Keywords: spin fluctuation; localized paramagnon; thermal expansion; uranium; Gruneise's relation

1. Introduction

Many researchers have studied physical properties of U compounds theoretically [1, 2] and experimentally [3]. Moriya, Kawabata, and Takahashi developed the self-consistent renormalization theory of spin fluctuations (the SCR theory) that takes into account mode-mode couplings of spin fluctuations beyond the random phase approximation self-consistently [1]. 5f electrons of U ions in U compounds are more localized than 3d electrons of transition metal compounds and less localized than 4f electrons of Ce compounds. As the first starting point, we use the localized paramagnon model in the SCR theory where the damping constant of spin fluctuations is independent of wave numbers. Konno and Moriya examined specific heats of U compounds based on the localized paramagnon model [2]. This model is valid in UPt₃ and UAl₂. Their theory explained the specific heat experimental data qualitatively. Although it was experimentally reported that the short range antiferromagnetic correlation was important [3], the localized paramagnon model can consider both the nearly ferromagnetic and nearly antiferromagnetic metals because the damping constant is independent of wave numbers.

We feel that thermal expansion in U compounds has not been understood theoretically. We investigate thermal expansion based on the localized paramagnon model. By using Takahashi's method [1] thermal expansion is obtained. Whether the behavior of the specific heat is consistent with that of the thermal expansion coefficient is discussed.

This paper is organized. In the next section the formulation will be provided. In section 3 the numerical results will be shown. In the last section the conclusion will be provided.

2. Formulation

Spin fluctuations are composed of electron-hole pair excitations. These excitations are boson excitations. Because of the boson excitations, the free energy density of harmonic oscillators is used. The spin correlation function is related to the imaginary part of the dynamical susceptibility by the fluctuation-dissipation theorem that assumes the Lorentzian form. The free energy is

$$F_{sf} = \sum_q \int_0^{\omega_c} d\omega f(\omega) \frac{3}{\pi} \frac{\Gamma_q}{\Gamma_q^2 + \omega^2} \quad (1)$$

where $f(\omega)$ is given by

$$f(\omega) = \frac{\omega}{2} + T \ln(1 - e^{-\omega/T}) \quad (2)$$

and ω_c is the cut-off frequency. In the localized paramagnon model, the damping constant is independent of wave numbers q , $\Gamma_q = \Gamma$. According to Takahashi's theory [1], thermal expansion is given by

$$\omega_i = -K \frac{\partial F_{sf}}{\partial V}, \quad (3)$$

where K is the compressibility.

After integration with respect to frequency, thermal component of the volume expansion is given by

$$\omega_i = -K \frac{3N_0}{2\pi} \frac{\partial \Gamma}{\partial V} \left[\ln(1/\tau) - \frac{1}{2} \tau - \psi(1/\tau) \right] \quad (4),$$

$$\text{where } \tau = 2\pi T / \Gamma \quad (5)$$

is defined, and N_0 is the number of magnetic atoms.

The zero point component of thermal expansion is also given by

$$\omega_{zero} = -K \frac{3N_0}{4\pi} \frac{\partial \Gamma}{\partial V} \left[\ln \frac{\Gamma^2 + \omega_c^2}{\Gamma^2} + \frac{2\Gamma^2}{\Gamma^2 + \omega_c^2} - 2 \right]. \quad (6)$$

The thermal expansion coefficient is obtained as follows.

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$$\alpha = -K \frac{\partial \omega_i}{\partial T} \quad (7)$$

The zero point component does not contribute to the thermal expansion because it is independent of temperatures. The thermal expansion coefficient is, therefore, given by

$$\alpha = -3K \frac{N_0}{\Gamma} \frac{\partial \Gamma}{\partial V} \left[-\frac{1}{\tau} - \frac{1}{2} + \frac{1}{\tau^2} \psi'(1/\tau) \right] \quad (8),$$

where $\psi'(x)$ is the trigamma function. Numerically estimated these results are presented in the next section.

3. Results and discussions

To begin with, the behavior of the thermal expansion coefficient is shown at low temperatures from Eq. (8). In order to show the behavior of thermal expansion coefficient at low temperatures, the trigamma function is expanded by

$$\psi'(u) \approx 1/u + 1/2u^2 + 1/6u^3 - 1/30u^4$$

with $u = 1/\tau$.

At low temperatures, the thermal expansion coefficient is obtained by

$$\alpha \approx -K \frac{N_0}{2\Gamma} \frac{\partial \Gamma}{\partial V} \tau \left(1 - \frac{1}{5} \tau^2 \right) \quad (9)$$

We find that the thermal expansion coefficient has T -linear dependence at low temperature. **Figure 1** shows its temperature dependence for $\Gamma = 58\text{K}$ and $\frac{\partial \Gamma}{\partial V} = 0.1$ from the T -linear coefficient of the specific heat [2] and the sign of the thermal expansion coefficient, respectively. The red line and the dotted line represent numerical results in Eq. (8) and the expansion at low temperatures in Eq.(9).

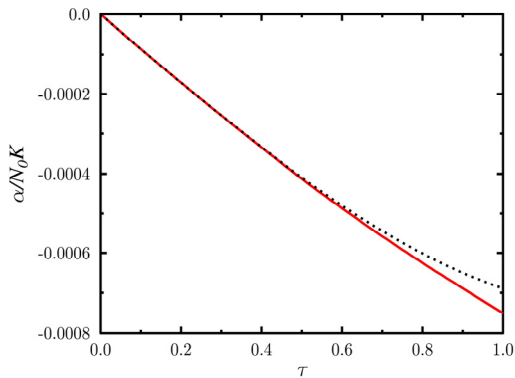


Figure 1. The temperature dependence of the thermal expansion coefficient where Γ is 58K and $\frac{\partial \Gamma}{\partial V}$ is 0.1. The red line and the dotted line represent numerical results in Eq. (8) and the expansion at low temperatures in Eq.(9), respectively.

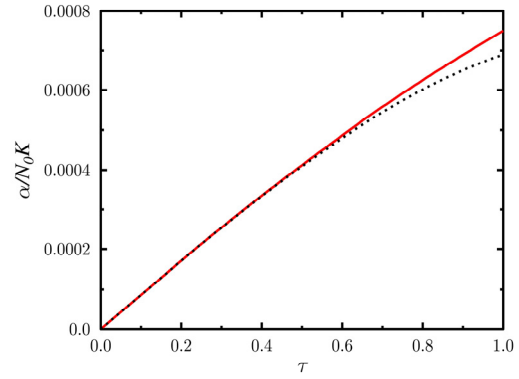


Figure 2. The temperature dependence of the thermal expansion coefficient where Γ is 58K and $\frac{\partial \Gamma}{\partial V}$ is -0.1. The red line and the dotted line represent numerical results in Eq. (8) and the expansion at low temperatures in Eq.(9), respectively.

Figure 2 shows the temperature dependence of the thermal expansion coefficient for $\Gamma = 58\text{K}$ and $\frac{\partial \Gamma}{\partial V} = -0.1$.

From Figure 1 and Figure 2, the sign of the thermal expansion coefficient depends on the sign of $\frac{\partial \Gamma}{\partial V}$. This result is qualitatively consistent with the experimental data of UPT_3 [4].

On the other hand, the temperature dependence of the specific heat is given as follows,

$$C_m = 3N_0 \left[-\frac{1}{\tau} - \frac{1}{2} + \frac{1}{\tau^2} \psi'(1/\tau) \right] \quad (10)$$

This is the same temperature dependence as that of the thermal expansion coefficient in Eq. (8). The reason is thermo-dynamic Gruneisen's relation is satisfied for them because the specific heat and the thermal expansion coefficient are derived from the same free energy.

4. Conclusion

We have investigated the thermal expansion based on the localized paramagnon model. We find that the thermal expansion coefficient has T -linear dependence at low temperatures. The thermo-dynamic Gruneisen's relation is automatically satisfied.

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