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On the zero-point spin-fluctuations in itinerant-electron metamagnetism

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Abstract

The effect on the magnetic equation-of-state of the zero-point spin fluctuations, together with the thermal ones, in an itinerant-electron system is discussed on the Landau-Ginzburg theory. It is shown that the zero-point spin fluctuations do not affect the results obtained previously by the spin fluctuation model for the itinerant-electron metamagnetism, when the Landau coefficients renormalized by the zero-point spin fluctuations are made use of. It is also shown that the contributions from the zero-point spin fluctuations at high temperatures are included in the results obtained on the static Gaussian statistics.

Recently, high magnetic fields of about 100 T are used in the fundamental research on magnetism in an itinerant-electron system. For instance, the field-induced metamagnetic transition (MT) from the paramagnetic to ferromagnetic state has been observed in Co compounds, YCo_2, $LuCo_2$, CoS_2 and others, [1-4] at low temperature under strong magnetic fields of about 100 T. These compounds also show susceptibility maximum phenomena. That is, a broad maximum in a temperature dependence of paramagnetic susceptibility is observed in these compounds at a room temperature.

These anomalous magnetic properties were previously discussed on the phenomenological Landau theory by Wohlfarth and Rhodes[5] and Shimizu[6]. However, in these theories the effect of spin fluctuations, which plays an important role in the temperature dependence of magnetic properties, was not taken into account. On the Landau-Ginzburg theory expanded up to the sixth order term with respect to the magnetization density, Moriya[7] has discussed the magnetic phase diagram at finite temperatures, by taking into account the effect of spin fluctuations. He found that the metamagnetic phase is stabilized when the coefficient of the fourth order term of the magnetization density in the free energy density is negative.

The present author[8] has discussed the relation between the susceptibility maximum phenomenon and the MT at finite temperatures, by taking into account the thermal spin fluctuations. Goto et al.[3] and Saitoh et al.[4] have recently applied this model to the analyses of their observed results for $Co(S, Se)_2$ and $Lu(Co, Ga)_2$ and a good agreement is obtained. More recently, Mushnikov et al.[9] have also applied the model to the analyses of their observed results for UCoAl under high pressures. This model for the MT based on the Landau-Ginzburg theory has recently been extended to the case of the MT for MnSi under high pressures.[10] However, the effect of the zero-point spin fluctuations is perfectly neglected in the theory, as criticized by Takahashi and Sakai[11]. In this short paper, it is shown that the zero-point spin fluctuations do not affect the results obtained by the spin fluctuation model for the MT[8], when the Landau coefficients renormalized by the zero-point spin fluctuations are made use of.

The magnetic free energy is given by

$$\Delta F=\frac{1}{V}\int d^3r\,\Delta f(\mathbf{r}), \tag{1}$$

where the free energy density $\Delta f(\mathbf{r})$ is written as

$$\Delta f(\mathbf{r})=\frac{1}{2}a|\mathbf{m}(\mathbf{r})|^2+\frac{1}{4}b|\mathbf{m}(\mathbf{r})|^4+\frac{1}{6}c|\mathbf{m}(\mathbf{r})|^6+\frac{1}{2}D|\nabla\cdot\mathbf{m}(\mathbf{r})|^2. \tag{2}$$

Here, $\mathbf{m}(\mathbf{r})$ and V are the magnetization density and the volume of crystal. The coefficients a, b, c, and D in (2) are Landau-Ginzburg coefficients.

The equation-of-state for the magnetic field H and the bulk magnetization M is given by

$$H=\left\langle\frac{\partial\Delta F}{\partial M}\right\rangle=A(T)M+B(T)M^3+C(T)M^5, \tag{3}$$

where $\langle\cdots\rangle$ denotes a thermal average and

$$\begin{aligned} A(T)&=a+\frac{5}{3}b\xi(T)^2+\frac{35}{9}c\xi(T)^4,\\ B(T)&=b+\frac{14}{3}c\xi(T)^2,\\ C(T)&=c, \end{aligned} \tag{4}$$

Here, $\xi(T)^2$ in (4) is the mean square amplitude of spin fluctuations defined as

$$\xi(T)^2=\xi_{\parallel}(T)^2+2\xi_{\perp}(T)^2, \tag{5}$$

where

$$\begin{aligned} \xi_{\parallel}(T)^2&=\frac{1}{V}\sum_{q(\neq0)}\langle|m_{\parallel}(\mathbf{q})|^2\rangle,\\ \xi_{\perp}(T)^2&=\frac{1}{V}\sum_{q(\neq0)}\langle|m_{\perp}(\mathbf{q})|^2\rangle, \end{aligned} \tag{6}$$

and $m_{\parallel}(\mathbf{q})$ and $m_{\perp}(\mathbf{q})$ are Fourier components of magnetization densities, $m_{\parallel}(\mathbf{r})$ and $m_{\perp}(\mathbf{r})$, parallel and perpendicular to the direction of H, respectively.

The fluctuation-dissipation theorem gives

$$\xi(T)^2=\frac{4\hbar}{V}\sum_q\int_0^\infty\frac{d\omega}{2\pi}\left\{n(\omega)+\frac{1}{2}\right\}\mathrm{Im}\chi_i(\mathbf{q},\omega) \tag{7}$$

where $n(\omega)$ is the Bose-Einstein distribution function and $\chi_i(\mathbf{q},\omega)$ is the i-component of the dynamical spin susceptibility approximately given by[12,13)]

$$\begin{aligned}&\chi_i(\mathbf{q},\omega)=\chi_i(\mathbf{q})/[1-i\hbar\omega/\Gamma_i(\mathbf{q})],\\&\chi_i(\mathbf{q})^{-1}=\chi_i(0)^{-1}+Dq^2,\\&\Gamma_i(\mathbf{q})^{-1}=\gamma\chi_i(\mathbf{q})/q.\end{aligned} \tag{8}$$

The summation over $\mathbf{q}$ in (6) should be limited within a cut-off wavevector, which is introduced by the use of the approximate form (8) for $\chi_i(\mathbf{q},\omega)$. In deriving (4) we assumed that $\xi_{\parallel}(T)^2=\xi_{\perp}(T)^2$. That is, the spin fluctuations are assumed to be isotropic. Furthermore, the dependence of $\xi_i(T)^2$ on M is neglected here.

From (7), $\xi(T)^2$ is found to be a sum of the contributions of the zero-point spin fluctuations $\xi_o{}^2$ and thermal spin fluctuations $\delta\xi(T)^2$ as

$$\xi(T)^2=\xi_0{}^2+\delta\xi(T)^2, \tag{9}$$

where the first and second terms in the right-hand side come from the terms of 1/2 and $n(\omega)$ in the curly bracket in (7), respectively. $\delta\xi(T)^2$ is known as a monotonically increasing function of T, being proportional to T^2 at low temperature and to T at high temperature.[12,13)] On the other hand, the mean square amplitude of the zero-point spin fluctuations $\xi_0{}^2$ is finite even at $T=0$. And $\xi_0{}^2$ shows a temperature dependence as $\chi_i(\mathbf{q},\omega)$ depends on T. However, the temperature dependence of $\xi_0{}^2$ is much weaker than that of $\delta\xi(T)^2$. This is because the Bose distribution function $n(\omega)$ is included in $\delta\xi(T)^2$, as shown in (7). The temperature dependent term in $\xi_0{}^2$ can be anyhow included into $\delta\xi(T)^2$. That is, the temperature dependent part of the mean square amplitude of spin fluctuations is denoted by $\delta\xi(T)^2$. $\xi_0{}^2$ in (9) denotes the temperature independent part.

Inserting (9) into (4), one gets the Landau coefficients renormalized by the zero-point and thermal spin fluctuations as

$$\begin{aligned}&A(T)=\tilde{a}+\delta A(T),\\&B(T)=\tilde{b}+\delta B(T),\\&C(T)=\tilde{c},\end{aligned} \tag{10}$$

where

$$\begin{aligned}&\tilde{a}=a+\frac{5}{3}b\xi_0{}^2+\frac{35}{9}c\xi_0{}^4,\\&\tilde{b}=b+\frac{14}{3}c\xi_0{}^2,\end{aligned} \tag{11}$$

$$\tilde{c}=c,$$

and

$$\delta A(T)=\frac{5}{3}\tilde{b}\ \delta\xi(T)^2+\frac{35}{9}\tilde{c}\ \delta\xi(T)^4, \tag{12}$$

$$\delta B(T)=\frac{14}{3}\tilde{c}\delta\xi(T)^2. \tag{13}$$

The Landau coefficients $A(T)$, $B(T)$, and $C(T)$ in the equation-of-state (3) are then written in the same forms as (4), by replacing a, b, and c by the renormalized $\tilde{a}$, $\tilde{b}$, and $\tilde{c}$, respectively. In this way it is concluded that the results obtained for the metamagnetic properties[8] are available even if the effect of the zero-point spin fluctuations is taken into account, when the coefficients a, b, and c are replaced by the renormalized ones by $\xi_0{}^2$.

It should be noted that, at high temperatures, the renormalized coefficients $\tilde{a}$, $\tilde{b}$, and $\tilde{c}$ in (11) tend to a, b, and c without the renormalization of zero-point spin fluctuations. At high temperatures, the Bose distribution function in (7) can be expanded as

$$n(\omega)=\frac{k_{\mathrm{B}}T}{\hbar\omega}-\frac{1}{2}+O\left(\frac{1}{T}\right). \tag{14}$$

It is found that the second term in the right hand side is cancelled out by the zero-point term in (7). Then we get

$$\xi_i(T)^2=\frac{k_{\mathrm{B}}T}{V}\sum_q\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\pi}\ \frac{\mathrm{Im}\chi_i(\mathbf{q},\ \omega)}{\omega}. \tag{15}$$

Here, we made use of the relation ;

$$\mathrm{Im}\chi_i(\mathbf{q},\ -\omega)=-\mathrm{Im}\chi_i(\mathbf{q},\ \omega). \tag{16}$$

By making use of the Kramers-Kronig relation, (15) is rewritten as

$$\xi_i(T)^2=\frac{k_{\mathrm{B}}T}{V}\sum_q\mathrm{Re}\chi_i(\mathbf{q},\ 0). \tag{17}$$

This is just the result obtained by using the Gaussian statistics. In this way, the contribution to $\xi(T)^2$ of the zero-point spin fluctuations is shown to be included in (17) at high temperatures. Then, the Landau coefficients $A(T)$, $B(T)$, and $C(T)$ in the magnetic equation-of-state (3) are given by (4) with (17) at high temperatures, as obtained previously[8] in the Gaussian statistics.

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