The self-consistent renormalization theory of spin fluctuations for itinerant antiferromagnetism in quasi-one dimensional metals

Rikio Konno [a,1]

[a] *Cross Tec, 2-4-1 Shinoharakita, Kohhoku-ku, Yokohama 222-0021, Japan, and Kinki University Technical College, 2800 Arima-cho, Kumano-shi, Mie Prefecture 519-4395, Japan*

Abstract

We introduce a three dimensional character to the transfer of one dimensional conduction electrons within the self-consistent renormalization theory of spin fluctuations for itinerant antiferromagnetism. We study how the three dimensional character influences the Néel temperature and the temperature dependence of the inverse staggered susceptibility at low temperatures. From these investigations, we find that the Néel temperature and the temperature dependence of the inverse staggered susceptibility are controlled by the three dimensional character.

Key words: the Néel temperature ; the staggered susceptibility ; quasi-one dimensional metals ;

The magnetic properties in itinerant electron systems have been investigated on the Hubbard model theoretically[1-5]. It is understood that the effects of spin fluctuations on the magnetic properties in three dimensional(3-D) nearly ferromagnetic metals, nearly antiferromagnetic metals, weak ferromagnetic metals, and weak antiferromagnetic metals are important. On the other hand, these effects in one dimensional(1-D) itinerant electron systems have been discussed in relation to 1-D organic conductors[6]. However, we have the unanswered questions how the magnetic properties are influenced by the introduction of the 3-D character to the 1-D conduction electrons within the self-consistent renormalization theory of spin fluctuations(the SCR theory) for itinerant antiferromagnetism. The SCR theory enables us to treat the dynamical effects of spin fluctuations beyond the random phase approximation. We investigate how the three dimensional character influences the temperature dependence of the inverse staggered susceptibility at low temperatures above the Néel temperature $T_{\rm N}$ and $T_{\rm N}$.

We introduce the 3-D character to the transfer of the 1-D conduction electrons. So we enter an additional parameter A_1 in the expression for the dynamical susceptibility of non-interacting electrons in 1-D metals. A_1 represents 3-D character of the conduction electrons. For $T \geq T_{\rm N}$, the dynamical susceptibility can be expressed as

$$\chi(Q+q,\omega) = \frac{\chi(Q+q)}{1-{\rm i}\omega/\Gamma_{\rm Q+q}} \qquad (1)$$

with

$$\Gamma_{\rm Q+q} = \Gamma_0(\kappa_{\rm s}^2 + q_{\rm z}^2 + \frac{A_1}{A}q^2), \Gamma_0 = \frac{A}{C} \qquad (2)$$

$$\kappa_{\rm s}^2 = \frac{\chi_0(Q)}{\alpha_{\rm s}A\chi(Q)}, \alpha_{\rm s} = 2I\chi_0(Q) > 1 \qquad (3)$$

where $q = \sqrt{q_{\rm x}^2 + q_{\rm y}^2}$. $\Gamma_{\rm Q+q}$ is the wave vector dependent damping constant for the antiferromagnetic spin fluctuation mode. The other notations is standard[7]. For convenience we now introduce, in place of Γ_0, A and A_1, the parameters T_0, $T_{\rm A}$, and $T_{\rm A_1}$ which are defined as follows:

[1] Corresponding author. Present address: Division of General Education, Kinki University Technical College, 2800 Arima-cho, Kumano-shi, Mie Prefecture 519-4395, Japan E-mail:r-konno@ktc.ac.jp

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$$\bar{A}_1 = \frac{A_1}{2\chi_0(Q)}, \bar{A} = \frac{A}{2\chi_0(Q)}, \tag{4}$$

$$T_0 = \frac{\Gamma_0}{2\pi} q_{\rm C}^2, T_{\rm A} = \bar{A} q_{\rm C}^2, T_{\rm A_1} = \bar{A}_1 q_{\rm B}^2 \tag{5}$$

where $q_{\rm B}$ and $q_{\rm C}$ are the cutoff wave number of q and q_z, respectively.We take $v_0 = \frac{8\pi^2}{q_{\rm B}^2 q_{\rm C}}$ where v_0 is the volume per magnetic atoms. Next, we advance to the inverse reduced staggered susceptibility. According to the prescriptions of the SCR theory[1,4-7] with Eqs.(1-5), The inverse staggered susceptibility is reduced to the following form:

$$y = -y_0 + \frac{1}{2}(1+\delta_s) y_1 t \int_0^1 {\rm d}z \; [\phi(\frac{B(z,y)}{t}) - \phi(\frac{B(z,y) + \frac{T_{\rm A_1}}{T_{\rm A}}}{t})] \tag{6}$$

with

$$y = \frac{1}{2\alpha_{\rm s} T_{\rm A} \chi(Q)}, y_0 = \frac{\alpha_{\rm s} - 1}{2\alpha_{\rm s} T_{\rm A} \chi_0(Q)}, y_1 = \frac{5T_0}{\alpha_s^2 T_{\rm A} T_{\rm A1}} F_{\rm s},$$
$$B(z,y) = z^2 + y, t = \frac{T}{T_0}, \delta_s = \frac{\chi_0(Q)}{\alpha_{\rm s}\chi(Q)},$$
$$\phi(x) = -(x - \frac{1}{2}) \ln x + x + \ln \Gamma(x) - \ln \sqrt{2\pi}. \tag{7}$$

$F_{\rm s}$ is the mode-mode coupling constant for the Fourier components of spin density around the antiferromagnetic wave vecter Q. The first term in Eq.(6) is related to the staggered magnetization $M_s^2(0)$ at $T = 0$. y_0 is positive because of $\alpha_{\rm s} > 1$. The second term in Eq.(6)is equal to the effect of antiferromagnetic spin fluctuations $(5/3)F_{\rm s} S_{\rm L}^2(T)$ where $S_{\rm L}^2$ is a mean square local amplitude of thermal spin fluctuations. The inverse reduced staggered susceptibility in the 1-D isotropic model can be derived from Eqs.(6) and (7) for $\frac{T_{\rm A_1}}{T_{\rm A}} \to 0$ when we note that $T_{\rm A_1}$ is included in y_1.

We study the inverse reduced staggered susceptibility in $\frac{T_{\rm N}}{T_0} < t << 1$. When $\frac{T_{\rm N}}{T_0} < t << 1$, the inverse reduced staggered susceptibility is given by

$$y \simeq -y_0 + \frac{1}{24} y_1 t^2 [\frac{1}{\sqrt{y}} \arctan \frac{1}{\sqrt{y}} - \frac{1}{\sqrt{y + \frac{T_{\rm A_1}}{T_{\rm A}}}} \arctan \frac{1}{\sqrt{y + \frac{T_{\rm A_1}}{T_{\rm A}}}}] \tag{8}$$

with

$$\ln \Gamma(x) \simeq (x - \frac{1}{2}) \ln x - x + \frac{1}{12x} (x >> 1) \tag{9}$$

From Eq.(8), we find that the inverse staggered susceptibility is proportional to T^2 and that the inverse staggered susceptibility is reduced by introducing $T_{\rm A_1}$ i.e. the 3-D character when $\frac{T_{\rm N}}{T_0} < t << 1$.

We proceed to investigate how the Néel temperature behaves by introducing $T_{\rm A_1}$ that expresses the 3-D character in the quasi-one dimensional systems. In order to study the behavior, we derive $S_{\rm L}^2(T_{\rm N})$. From Eq.(6), Eqs.(2.1) and (2.3) in Ref.[7], $S_{\rm L}^2(T_{\rm N})$ is given by

$$S_{\rm L}^2(T_{\rm N}) = \frac{3T_{\rm N}}{2\pi\alpha_{\rm s} T_{\rm A_1}} \sqrt{\frac{T_{\rm N}}{2\pi T_0}} \int_0^\infty {\rm d}t \int_0^{\sqrt{\frac{2\pi T_0}{T_{\rm N}}}} {\rm d}z \int_0^{\frac{2\pi T_0 T_{\rm A_1}}{T_{\rm N} T_{\rm A}}} {\rm d}x \; \frac{1}{e^t - 1} \frac{t}{(z^2 + x)^2 + t^2} \tag{10}$$

because of $y = 0$ at $T_{\rm N}$. From Eqs.(10) and (2.1) in Ref.[7], we find that

$$T_{\rm N} \propto (\frac{T_{\rm A_1}}{T_{\rm A}})^{\frac{2}{3}} \tag{11}$$

for $(T_{\rm A_1}/T_{\rm A}) \to 0$. This behavior is different from that of the introduction of the 3-D character into two dimensional isotropic model[7]. This shows that $T_{\rm N}$ increase more steeply by introducing the 3-D character into the 1-D isotropic model than that into the two dimensional isotropic model.

In conclusion, we find that the inverse staggered susceptibility is reduced by the introduction of three dimensional character into the one dimensional systems when $\frac{T_{\rm N}}{T_0} < t << 1$. We also find that the Néel temperature is proportional to $(T_{\rm A_1}/T_{\rm A})^{\frac{2}{3}}$ for $(T_{\rm A_1}/T_{\rm A}) \to 0$ where $T_{\rm A_1}$ represents the three dimensional character in the quasi-one dimensional systems.

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