THE EXCHANGE INTERACTION EFFECT ON MAGNETISM FOR ITINERANT ELECTRON SYSTEM

Wen Yu, K.Y. Zhang
Department of Physics, Northeast University of Technology, Shenyang Liaoning, China

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The magnetism of itinerant electron systems, i.e., the extended Hubbard model, is
investigated by the perturbation theory. In this paper, we have considered three
dimensions. The results are in good agreement with the approximate solution of
the problem.

1. Introduction

The magnetism of itinerant electron systems has been investigated by many
authors. Some authors have neglected the problem with the usual a-band Hubbard
model. All of these methods are based on the assumption of a half-filled band.
Whether the ferromagnetic state exists or not and what conditions are necessary
for the ferromagnetism are the questions of interest. For the many-body problem in
arbitrary electron density, the problem is complex. Hence, we have considered the
three-dimensional system and assumed that there is only a small change from
antiferromagnetic to paramagnetic phases with the electron density increasing
and decreasing. This is the second-order perturbation. The results are consistent
with the approximate solution of many-body problems in this density range.

2. Perturbation Expansion

We follow the method adopted by Kohn et al.

Equations to consider are:

$$\sum_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \rho_{\mathbf{k}, \sigma} - \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', \sigma} J_{\mathbf{k}, \mathbf{k}', \sigma} n_{\mathbf{k}, \sigma} n_{\mathbf{k}', \sigma}$$

The exchange interaction is divided into two parts: the transfer integral term
and the exchange term. The exchange term is divided into two parts: the
exchange interaction and the transfer term. The former can be neglected, especially
in the case of half-filled band.
and \( z \) is the coordination number. We should be aware that the atomic spins here are denoted by \( s \). The local spins are defined by the Heisenberg Hamiltonian, which persists for a period long enough to be compared with the relaxation times in their magnitude and direction.

The magnetic moment \( \mathbf{m} \) can be derived from the local spins in this way, as we shall treat the interactions between the spins in the perturbations.

The grand thermodynamic potential \( \Omega \) of the system per lattice site is expressed in terms of \( \mathbf{m} \) as:

\[
\Omega = -\beta J \sum_{\langle i,j \rangle} \mathbf{m}_i \cdot \mathbf{m}_j + \sum_{i} \left( -\mu_B \mathbf{H} \cdot \mathbf{m}_i + \frac{1}{2} \mathbf{m}_i \cdot \mathbf{m}_i \right)
\]

where \( \beta = \frac{1}{k_B T} \) is the reduced temperature, \( J \) is the exchange integral, and \( \mathbf{H} \) is the external magnetic field.

A reciprocal lattice \( \mathbf{G} \) is all of the usual connected reciprocal lattice points. The diagrams corresponding to terms up to second order are shown in Fig. 1.

**Fig. 1** Diagrams contributing to the perturbational series of the grand thermodynamic potential up to second order in \( \mathbf{G} \). The corresponding \( \mathbf{G} \) terms are shown in each diagram.

The grand thermodynamic potential per lattice site is expressed in terms of contributions corresponding to the diagrams in Fig. 1:

\[
\Omega = -\beta J \sum_{\langle i,j \rangle} \mathbf{m}_i \cdot \mathbf{m}_j + \sum_{i} \left( -\mu_B \mathbf{H} \cdot \mathbf{m}_i + \frac{1}{2} \mathbf{m}_i \cdot \mathbf{m}_i \right)
\]

where:

\[
\mathbf{Q}_a = \left( \mathbf{G}_a \cdot \mathbf{m}_i \right) \left( \mathbf{G}_a \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_b = \left( \mathbf{G}_b \cdot \mathbf{m}_i \right) \left( \mathbf{G}_b \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_c = \left( \mathbf{G}_c \cdot \mathbf{m}_i \right) \left( \mathbf{G}_c \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_d = \left( \mathbf{G}_d \cdot \mathbf{m}_i \right) \left( \mathbf{G}_d \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_e = \left( \mathbf{G}_e \cdot \mathbf{m}_i \right) \left( \mathbf{G}_e \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_f = \left( \mathbf{G}_f \cdot \mathbf{m}_i \right) \left( \mathbf{G}_f \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_g = \left( \mathbf{G}_g \cdot \mathbf{m}_i \right) \left( \mathbf{G}_g \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_h = \left( \mathbf{G}_h \cdot \mathbf{m}_i \right) \left( \mathbf{G}_h \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_i = \left( \mathbf{G}_i \cdot \mathbf{m}_i \right) \left( \mathbf{G}_i \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_j = \left( \mathbf{G}_j \cdot \mathbf{m}_i \right) \left( \mathbf{G}_j \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_k = \left( \mathbf{G}_k \cdot \mathbf{m}_i \right) \left( \mathbf{G}_k \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_l = \left( \mathbf{G}_l \cdot \mathbf{m}_i \right) \left( \mathbf{G}_l \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_m = \left( \mathbf{G}_m \cdot \mathbf{m}_i \right) \left( \mathbf{G}_m \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_n = \left( \mathbf{G}_n \cdot \mathbf{m}_i \right) \left( \mathbf{G}_n \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_o = \left( \mathbf{G}_o \cdot \mathbf{m}_i \right) \left( \mathbf{G}_o \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_p = \left( \mathbf{G}_p \cdot \mathbf{m}_i \right) \left( \mathbf{G}_p \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_q = \left( \mathbf{G}_q \cdot \mathbf{m}_i \right) \left( \mathbf{G}_q \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_r = \left( \mathbf{G}_r \cdot \mathbf{m}_i \right) \left( \mathbf{G}_r \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_s = \left( \mathbf{G}_s \cdot \mathbf{m}_i \right) \left( \mathbf{G}_s \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_t = \left( \mathbf{G}_t \cdot \mathbf{m}_i \right) \left( \mathbf{G}_t \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_u = \left( \mathbf{G}_u \cdot \mathbf{m}_i \right) \left( \mathbf{G}_u \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_v = \left( \mathbf{G}_v \cdot \mathbf{m}_i \right) \left( \mathbf{G}_v \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_w = \left( \mathbf{G}_w \cdot \mathbf{m}_i \right) \left( \mathbf{G}_w \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_x = \left( \mathbf{G}_x \cdot \mathbf{m}_i \right) \left( \mathbf{G}_x \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_y = \left( \mathbf{G}_y \cdot \mathbf{m}_i \right) \left( \mathbf{G}_y \cdot \mathbf{m}_j \right)
\]

\[
\mathbf{Q}_z = \left( \mathbf{G}_z \cdot \mathbf{m}_i \right) \left( \mathbf{G}_z \cdot \mathbf{m}_j \right)
\]
Host we turn our attention to the Extended Hubbard Model system. Let's first review the perturbational Hamiltonian $H$. It has two parts: an isotropic interaction $V$ and a term $J$ that describes the exchange interaction. The first term is the nearest neighbor lattice interaction potential $H_V$, while the second term is the non-isotropic exchange field. The exchange interaction term $J$ is present only if the system is in a magnetic phase. The Hamiltonian for the system is given by:

$$H = -V\sum_{\langle i,j \rangle} \langle \sigma_i \sigma_j \rangle - J\sum_{\langle i,j \rangle} \langle \sigma_i \sigma_j \rangle$$

where $\sigma_i$ is the spin at site $i$, $V$ is the nearest neighbor repulsion, and $J$ is the exchange interaction.

To study the magnetic properties of this system, we can calculate the magnetic susceptibility:

$$\chi = \frac{\langle \sigma_i \sigma_j \rangle}{2J}$$

where $\langle \sigma_i \sigma_j \rangle$ is the average magnetization.

The magnetic susceptibility is given by the susceptibility of the density of states at the Fermi level. It is related to the density of states at the Fermi level, which is proportional to the number of states occupied by the electrons.

The magnetic susceptibility is given by:

$$\chi = \frac{N(E_F)}{2J}$$

where $N(E_F)$ is the density of states at the Fermi level.

We can then study the magnetic properties of the system by calculating the magnetic susceptibility as a function of the exchange interaction strength $J$. The magnetic susceptibility is given by:

$$\chi = \frac{N(E_F)}{2J}$$

where $N(E_F)$ is the density of states at the Fermi level.

The magnetic susceptibility is given by:

$$\chi = \frac{N(E_F)}{2J}$$

where $N(E_F)$ is the density of states at the Fermi level.
number on the diagrams are the same as on Fig. 2. From these figures, we can find that besides the common features with Figs. 1 : 4 , where the current decreases as the T/J increases and the decreasing rate is proportional related to 1/J, in other cases, the more ferromagnetic phase is

Furthermore, the increasing T/J makes the antiferromagnetic phase move to higher range of the density, like the case of Hubbard model. This situation also depends on the ratio of T/J, and is demonstrated in Fig. 6.

Fig. 5 The phase diagram is projected in T'/m plane for BCC lattice.

In this Fig. 5, we project the phase diagram on T'/m plane, which there have been three areas curved (A, 1/J, b) and (A, b, 1/J), where the first A is antiferro-ferromagnetic transition, the second A is antiferromagnetic and ferromagnetic transition. The second and third areas are phase transitions corresponding to 1/J = 0.0, 0.05 respectively. A, A, are the antiferro-ferromagnetic transition, B, C, are the ferro-ferromagnetic phase transitions. It is important to point out that for 1/J = 0.0 there is no transition. Because at the lower density, the antiferromagnetic phase does not have the correct density for the antiferromagnetic phase. The former occupied the order in lower n, the paramagnetic phase is hindered in small range of high density and antiferromagnetic phase. But when we consider the exchange interaction, the ferromagnetic coupling occurs at the same time as the antiferromagnetic does. The former occupied the correct density in lower n, the paramagnetic phase is hindered in small range of high density and weaker coupling. This has turned out that the J/0 makes the system become antiferromagnetic ordering at lower n and ferromagnetic ordering at lower n.

The distance between A, A, is too far at strong correlation, but too close when the correlation weaken at the same time all will attach on A, which means the J/0 in a small range to the competition of ferro- and antiferromagnetic coupling. It should also be noted that we have the same results at this case for 2.2.

The ferromagnetic phase beyond 1/J < n < 1, and the phase transition from ferro-ferromagnetic state at low density limit Infinite system difference from the Hubbard model system.

Finally, we can conclude that the exchange interaction J affects the antiferromagnetic coupling between high density and low density, but the configuration cannot be identified. It shows the ferromagnetic phase transition under the perturbation of antiferromagnetic phase transition, which occurs to the competition of ferro- and antiferromagnetic coupling. This competition depends not only on 1/J, m, but also on T/J. In short, it is not so complicated.

We would like to emphasize that there are not qualitative differences between high density and low density. It can be suggested that the conclusion of this paper also holds for the two dimensional system, and the different magnetic states in these systems could be observed at high density limit. This work will be done in future.

Though the K term doesn't have an influence on antiferromagnetic, but the exchange term WJ does obviously. Next we are asking to research on this case.

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