Correlation effects of ferromagnetism

Hui-Quan Nie and Wei-Ying Zhou
Department of Physics, Box 326, Northeastern University, Shenyang, People's Republic of China
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Using the local approach, we have discussed the correlation effects of the ferromagnetic state in the Hamiltonian of a single band, and calculated the ground-state energy and the boundary condition of the phase diagram. The numerical results show that the exchange interaction j plays a decisive role for the existence of the ferromagnetic state; when Coulomb interaction u is increased, the correlation of electrons in both the paramagnetic and ferromagnetic states is increased; the larger the spin polarization m, the stronger the correlation of electrons; the Coulomb interaction w between nearest-neighbor sites depresses the correlation of electrons. [S0163-1829(97)01601-9]

I. INTRODUCTION

The ferromagnetism of transition metals are rather complex as the d electrons show both itinerant and localized properties. That complexity is due to strong Coulomb interactions. According to Hund's rule, they are local in nature and lead to the correlation of electrons and formation of local moments. This changes the criteria for the existence of a ferromagnetic state in a rather drastic way, as has been discussed in terms of second-order perturbation theory.[1] Since high-T_c superconductors have been discovered,[2] the correlation of electrons (or holes) in the narrow-band model has been extensively investigated[3,4] to explain the superconductivities. So far it is still of interest to study the electron correlation in the narrow-band model, the simplest of which is the Hubbard model.

The ground state of a half-filled Hubbard model is believed to be antiferromagnetic.[5] In the strong correlation limit, electrons localized and form a localized spin interacting by virtual hopping, they lead to an effective Heisenberg model with kinetic exchange interaction.[6] For the weak-coupling condition, the mechanism of the antiferromagnetism is not so clear. Kubo and Uchinami[7] with the perturbation expansion and the Gutzwiller approximation have shown that there is an antiferromagnetic ground state for any value U/D, on other hand, Oles and Spalek[8] have pointed out that in the case of $n=1$ the ground state is antiferromagnetic for any value of the ratio U/D and in the case of $n\neq 1$ the antiferromagnetism is destroyed and the ground state becomes paramagnetic for small ratio U/D. The extensive investigations on the Hubbard mode lead to the conclusion: the ferromagnetic state does not exist in the Hubbard model.

Hirsch[9] has proposed that certain matrix elements that arise in deriving from first-principles calculations play a fundamental role in the metallic ferromagnetism. These terms have been neglected in studies of ferromagnetism based on the Hubbard model. It is shown that if one electron is in bonding and the other is in the antibonding state, the contribution of the exchange integral J is negative. This will favor a situation where the Fermi surface for up and down electrons are in the regions at the Brillouin zone that correspond to states of opposite bonding character, and that favor spin polarization. As we well know, the correlation of electrons plays an important role in discussing the properties of the narrow-band system, however, Hirsch's work, in which the correlation effects of electrons are neglected, only gave a result in terms of mean-field theory for simplifying discussion.

In this paper, we use the local approach[10] which is developed from Gutzwiller variational method[11] to study the correlation effects of the ferromagnetic state in the single band Hamiltonian. The paper is organized as follows. In Sec. II we derive the formulas of the ground-state energy and the condition of the existence of the ferromagnetic state with the local approach. In Sec. III we show the numerical results and give some discussion. The conclusion is in Sec. IV.

II. FORMULATION

The Hamiltonian of single band model is given by

$$H=\sum_{ij\sigma} t_{ij}c_{i\sigma}^{+}C_{j\sigma}+\frac{U}{2}\sum_{i\sigma} n_{i\sigma}n_{i-\sigma}+\frac{W}{2}\sum_{ij\sigma\sigma'} n_{i\sigma}n_{j\sigma'} + \frac{J}{2}\sum_{ij\sigma\sigma'} c_{i\sigma}^{+}C_{j\sigma'}^{+}C_{i\sigma'}C_{j\sigma}, \tag{1}$$

where the first term denotes kinetic energy, the second term denotes Coulomb interaction of electrons onsite, the third term denotes Coulomb interaction of electrons between nearest-neighbor sites, and the fourth term denotes the exchange interaction.

In the perturbation theory, the energy of a given system can be divided into two parts

$$E_g=E_{\mathrm{HF}}+E_{\mathrm{corr}}, \tag{2}$$

where E_{HF} is the energy for Hartree-Fock (HF) approximation, and E_{corr} is the correlation energy. Fourier transformation of Eq. (1) yields

$$H=\sum_{k\sigma}\varepsilon_k C^+_{k\sigma}C_{k\sigma}+\frac{U}{2N}\sum_{kk'q\sigma}C^+_{k+q\sigma}C^+_{k'-q-\sigma}C_{k'-\sigma}C_{k\sigma}+\frac{W}{2N}\sum_{kk'q\delta\sigma\sigma'}e^{iq\delta}C^+_{k+q\sigma}C^+_{k'-q\sigma'}C_{k'\sigma'}C_{k\sigma}+\frac{J}{2N}\sum_{kk'q\delta\sigma\sigma'}e^{i(k-k'+q)\delta}C^+_{k+q\sigma}C^+_{k'-q\sigma'}C_{k'\sigma'}C_{k\sigma}, \tag{3}$$

where

$$\varepsilon_k=-\frac{D}{2Z}\sum_{\delta}e^{ik\delta} \tag{4}$$

is the kinetic energy in the tight-binding approximation and $D=2Zt$ is the bandwidth, δ are the vectors that connect a site to its nearest neighbors, z is a number of nearest-neighbor sites. To calculate the HF energy at zero temperature, we consider a ''reduced Hamiltonian'' for ferromagnetism as in the BCS theory of superconductivity. For antiparallel spins we take the terms of the exchange interaction in Eq. (3) with $q=0$ only, for the parallel spin we keep $q=0$ and $q=k'-k$,[9] then the Hamiltonian (3) becomes

$$H=\sum_{k\sigma}E_{k\sigma}C^+_{k\sigma}C_{k\sigma} \tag{5}$$

and

$$E_{k\sigma}=\varepsilon_k-\frac{2J}{ND}\sum_{\delta}e^{ik\delta}\sum_{k'\sigma'}\varepsilon_{k'}n_{k'\sigma'}+\frac{1}{N}\sum_{k'}\left(Un_{k'-\sigma}-ZJn_{k'\sigma}+ZW\sum_{\sigma'}n_{k'\sigma'}\right). \tag{6}$$

To obtain the analytic results, we introduce the rectangular density of states

$$\rho(\varepsilon)=\frac{1}{D}\quad\text{for}\quad|\varepsilon|\leqslant\frac{D}{2} \tag{7}$$

and the occupation number of electrons

$$n=n_\uparrow+n_\downarrow, \tag{8}$$

then, the HF energy of the ground state is easily calculated, and Eqs. (5), (6), and (7) lead to the boundary condition of the phase diagram by minimization of the HF ground-state energy with respect to m. It yields

$$1+j[m^2+(n-1)^2-2]-u=0, \tag{9}$$

where m is defined as magnetization

$$m=n_\uparrow-n_\downarrow \tag{10}$$

and $u=U/D$, $j=ZJ/D$, and $w=ZW/D$.

We note that Eq. (9) does not include the terms of the Coulomb interaction w between nearest-neighbor sites. This equation is same as the result given by Hirsch.[9] This means that in mean-field theory the Coulomb interaction w between nearest-neighbor sites does not influence the existence of the ferromagnetic state, but if we consider the correlation of electrons, it will show that the Coulomb interaction w between nearest-neighbor sites depresses the correlation of electrons which mainly depends on the Coulomb interaction u.

To calculate the correlation energy $E_{\rm corr}$ with the local approach, one first decomposes the HF ground state $|\psi_{\rm HF}\rangle$ into a linear combination of configurations. The trial function for the ground state $|\psi_L\rangle$ is constructed by modulating the linear combination as

$$|\psi_L\rangle=\prod_{ij}\left(\prod_m(1-\eta_m O^{(m)}_{ij})\right)|\psi_{\rm HF}\rangle, \tag{11}$$

where (η_m) is a set of variational parameters, i and j run over all sites, and $(O^{(m)}_{ij})$ is a set of local operators. For simplicity, we only consider the single site correlation, then $O^{(m)}_{ij}$ reduces to $O=n_{i\uparrow}n_{i\downarrow}$ and η_m to η.

For a given local operator, the ground-state energy per site can be written as

$$E_g=\frac{1}{N}\frac{\langle\psi_L|H|\psi_L\rangle}{\langle\psi_L|\psi_L\rangle}=E_{\rm HF}+E_{\rm corr}. \tag{12}$$

The first term in Eq. (12) is the HF ground-state energy, the second term is the correlation energy.

Substituting Eq. (11) into Eq. (12) and expanding Eq. (12) in powers of η up to second order η^2, one can obtain the expression for the ground-state energy per site as

$$E_g=E_{\rm HF}-2\eta\langle OH\rangle+\eta^2(\langle OHO\rangle+\langle OOH\rangle), \tag{13}$$

where η is determined by minimization of the ground-state energy E_g in Eq. (13) with respect to η, then we obtain the correlation energy as

$$E_{\rm corr}=-\frac{\langle OH\rangle^2}{\langle OHO\rangle+\langle OOH\rangle}. \tag{14}$$

As we have mentioned[12] the term $\langle OOH\rangle$ represents the off-diagonal elements of the density matrix. When the term $\langle OOH\rangle$ is included for calculating the correlation energy in second-order perturbation theory, one can obtain more accurate results in the so-called $R=0,\alpha$ approximation than the results where the term $\langle OOH\rangle$ is neglected. With Wick''s theorem and the linked diagram rule, one can obtain the analytic expressions of the ground-state energy by complicated calculation, and then the boundary condition of phase diagram is obtained by minimization of the ground-state energy E_g with respect to m, i.e., $\partial E_g/\partial m=0$. These expressions are too complicated to present here, we will show the numerical results as follows.

III. NUMERICAL RESULTS

The numerical results are shown in Figs. 1, 2, and 3, respectively, where the solid lines correspond to the local approach and the dashed lines correspond to the mean-field theory. From pattern A of Fig. 1, we found that for the case of $u=0$ the solid lines are very close to the dashed lines for $m=0.0$, 0.5, and 1.0, respectively. It means that when the Coulomb interaction $u=0$, the correlation of electrons is very weak, in other words, the contribution of the exchange interaction j to the correlation effects is small in both paramag-

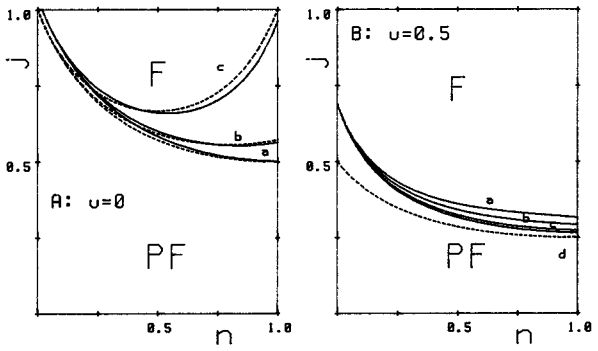

FIG. 1. Exchange interaction j vs electron number n for fixed u, where solid lines correspond to the local approach, dashed lines to mean-field theory; pattern A: curves a, b, and c correspond to $m=0.0$, 0.5, and 1.0; pattern B: Curves a, b, c, and d to $w=0.0$, 0.2, 0.4, and 0.5, respectively.

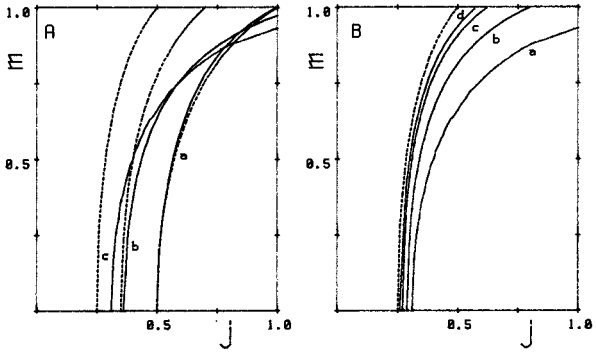

FIG. 3. Spin polarization m vs exchange interaction j for fixed $n=1$, where dashed lines correspond to mean-field theory, solid lines to the local approach. Pattern A: Curves a, b, and c correspond to $u=0.0$, 0.3, and 0.5; pattern B: Curves a, b, c, and d correspond to $w=0.0$, 0.2, 0.4, and 0.5 for $u=0.5$.

netic ($m=0$) and ferromagnetic phases ($m=0.5$, 1.0). Pattern B of Fig. 1 shows the exchange interaction j versus band filling for various values of w. For the case of large u, the solid lines are always above the dashed line. It implies that the electron correlation in the paramagnetic phase ($m=0$) mainly depends on the Coulomb interaction u, and it enhances the boundary of the phase diagram. When the Coulomb interaction w between nearest-neighbor sites is increased, the boundary of the phase diagram is decreased, that is, the Coulomb interaction w depresses the correlation effects of electrons. The numerical results for exchange interaction j versus electron number n in the ferromagnetic phase are shown in Fig. 2, from which we can see that in ferromagnetic states ($m=0.5$, 1.0) all solid lines are always above the dashed lines. It means that when we consider the correlation effects of electrons, a large value j is needed to keep a certain spin polarization. For the case of $w=0.0$, the Hamiltonian is reduced to the one given by Hirsch,[9] where the dashed line corresponds to the numerical results of Hirsch and the solid line (a) corresponds to the results of the local approach. From patterns A and B, it is seen that when the Coulomb interaction w between nearest-neighbor sites is increased, the solid lines are decreased, i.e., the boundary of phase diagram is decreased. It means that the Coulomb interaction w depresses the correlation of electrons in the ferromagnetic phase. Comparing Fig. 2 with Fig. 1, we found that the correlation of electrons in the ferromagnetic phase is stronger than in paramagnetic phase for fixed u and n; the larger the spin polarization m, the stronger the correlation of electrons. The numerical results for spin polarization m vs exchange interaction j are shown in Fig. 3 where solid lines correspond to the local approach, dashed lines to mean-field theory, and curves a, b and c to $u=0.0$, 0.3, and 0.5, respectively. In pattern A, it is shown that when u is increased, the correlation effect is increased; in pattern B, we show that for $u=0.5$, the correlation effect is decreased with increasing w.

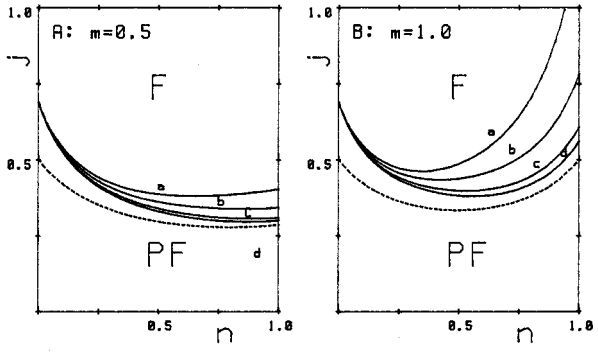

FIG. 2. Exchange interaction j vs electron number n for fixed $u=0.5$, where dashed lines correspond to mean-field theory, solid lines to the local approach, curves a, b, c, and d to $w=0.0$, 0.2, 0.4, and 0.5, respectively.

In general discussions, one uses the Hubbard model to describe the electron correlation; it is believed that the ground state of the Hubbard mode is antiferromagnetic for $n=1$, and the ground state is paramagnetic for the case of $n\neq 1$ and small u;[8] when we consider the exchange interaction j between nearest-neighbor sites, the Hamiltonian becomes Hirsch's type; then one can obtain the condition of the existence of the ferromagnetic phase. It means that exchange interaction j plays a decisive role for the existence of the ferromagnetic phase and the correlation of electrons mainly depends on the Coulomb interaction u. When u is large, the correlation of electrons is strong. The correlation of electrons is unfavorable to the existence of ferromagnetic phase, while it favors the existence of the antiferromagnetic phase. When we consider Coulomb interaction w between nearest-neighbor sites, we found that Coulomb interaction w depresses the correlation of electrons which mainly depends on the Coulomb interaction u.

Finally, the ground state of a given system is a para-, ferro- or antiferromagnetic phase which depends on the competition of the contribution of exchange interaction j, and Coulomb interactions u and w.

IV. CONCLUSION

With the local approach, we have discussed the correlation of electrons in the Hamiltonian of a single band model. We found that the exchange interaction j plays a decisive role for the existence of ferromagnetism; the correlation ef-

fects of electrons mainly depend on the Coulomb interaction u and the contribution of the exchange interaction j to the correlation is very small; when Coulomb interaction u is increased, the correlation of electrons in both the paramagnetic and ferromagnetic phases is increased; the larger the spin polarization m, the stronger the correlation effects; the Coulomb interaction w between nearest-neighbor sites depresses the correlation of electrons.

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