Local approach to the ferromagnetic ground state in the Hubbard-Hirsch model

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By using a Green's-function technique, the energy of the ferromagnetic ground state in the Hubbard-Hirsch model is calculated. The effect of electron correlation on the phase diagram and on the energy of the ground state is studied within the local approach. The results show that for a fixed Coulomb interaction U ($\neq 0$) between electrons with opposite spins at the same site, the region of the ferromagnetic ground state becomes smaller as compared with that of the Hartree-Fock approximation. For a fixed U ($\neq 0$) and electronic density n, the system goes successively from the paramagnetic, the weakly ferromagnetic, and the strongly ferromagnetic phase with increasing exchange interaction J between electrons of nearest-neighbor sites. The absolute value of the correlation energy is large in the paramagnetic region, small in the weakly ferromagnetic region, and zero in the strongly ferromagnetic region.

I. INTRODUCTION

The theory of the ferromagnetism in transition metals is still an interesting topic in condensed-matter physics. The ferromagnetic states of transition metals are rather complex due to both itinerant and localized properties of the d electrons. According to the molecular-field theory of ferromagnetism of Weiss,[1] the interaction responsible for the spontaneous order can be represented by an internal molecular field. Heisenberg[2] subsequently gave a physical origin about the molecular field using quantum theory. The Curie-Weiss law is successfully explained, although an integral number of Bohr magnetons is obtained for the magnetic moment at $T=0$ K from the Weiss-Heisenberg local model. Stoner[3] and Slater[4] have proposed an itinerant-electron model based on Bloch's work[5] on the free-electron gas. According to Stoner, the $3d$ electrons of transition metals, instead of being localized on particular nuclei, can move from one ion to another through the crystal lattice. This theory gives the nonintegral number of Bohr magnetons for the magnetic moment, but fails at finite, nonzero temperature. In 1963 Hubbard[6] studied the electron correlation due to the strong Coulomb interactions, and proposed the Hubbard model. In this model, the hopping integral describes the electron's itinerant property, while the electron correlation describes the electron's localized property. In terms of the Hubbard model, the metal-insulator transition is successfully explained[7] and metal magnetic properties has been discussed. Within the mean-field approximation, the Stoner model can be obtained from the single-band Hubbard model. However, the single-band Hubbard model exhibits antiferromagnetism rather than ferromagnetism.[8-10]

Recently, Hirsch[11] proposed that certain matrix elements that arise in the derivation of the Hubbard Hamiltonian from first-principles calculations play a fundamental role in metallic ferromagnetism. It is shown that when one electron is in the bonding state and the other in the antibonding state, the contribution of the exchange integral J is negative. He retains this term in the Hubbard Hamiltonian (which is called Hubbard-Hirsch model in this paper), and shows that partial spin polarization is naturally obtained even if one stays within the mean-field approximation and uses a constant density of states. It is an important improvement over the Stoner model. Hirsch also studied the properties of this model at finite, nonzero temperature,[12] and metallic ferromagnetism in a one-dimensional geometry, using an exact density of states.[13] Ivanov *et al.* studied the properties of this model for $U=\infty$.[14]

In Hirsch's works, the role of U in the tendency to ferromagnetism is overestimated because the ability of electrons of opposite spins to avoid each other has not been taken into account. A more complete theory should deal with the electron correlation in a narrow energy band. Many techniques have been used to investigate the electron correlation effect. The local approach, which has been developed from Gutzwiller variational method,[15] is more effective for smaller U in the narrow energy band. By using the local approach, we have studied the electron correlation effect in the Anderson lattice,[16,17] and the Hubbard model,[18,19] and the extended Hubbard model.[20,21] By using the local approach to the ferromagnetic phase of the Hubbard-Hirsch model, we study in this paper the effect of electron correlation on the phase diagram and on the energy of the ground state. The paper is organized as follows. In Sec. II we derive analytic expressions of the energy of the ground state and the condition which determines phase boundaries within the HF approximation and local approach. In Sec. III we give computation results and some discussions. Our conclusion is in Sec. IV.

II. ANALYTIC DERIVATION

The Hubbard-Hirsch Hamiltonian is given by

$$H=\sum_{i,j,\sigma} t_{ij} C_{i\sigma}^{\dagger} C_{j\sigma} + \tfrac{1}{2} U \sum_{i,\sigma} n_{i\sigma} n_{i-\sigma} + \tfrac{1}{2} J \sum_{i,j,\sigma,\sigma'} C_{i\sigma}^{\dagger} C_{j\sigma'}^{\dagger} C_{i\sigma'} C_{j\sigma} , \quad (1)$$

where t_{ij} is the hopping integral, U is the usual Hubbard on-site repulsion, and the parameter J is an off-diagonal matrix element of the Coulomb interaction between electrons on nearest-neighbor sites. Both U and J are taken to be positive. In order to calculate the energy of ground state, we use the Green's-function technique developed by Zubarev.[22] The Green's function is defined as

$$G_{ij}^{\sigma\sigma'}=\langle\langle C_{i\sigma};C_{j\sigma'}^{\dagger}\rangle\rangle_{\omega} . \tag{2}$$

Within the HF approximation, it satisfies the equation of motion with

$$(\omega+\mu)G_{ij}^{\sigma\sigma'}=\delta_{ij}\delta_{\sigma\sigma'}+\sum_{l} t_{il}G_{ij}^{\sigma\sigma'}+(n_{-\sigma}U-n_{\sigma}ZJ)G_{ij}^{\sigma\sigma'} +JI_1\sum_{l} G_{lj}^{\sigma\sigma'} . \tag{3}$$

We have used the decoupling approximation

$$\langle\langle C_{i\sigma}n_{i-\sigma};C_{j\sigma'}^{\dagger}\rangle\rangle_{\omega}=n_{-\sigma}G_{ij}^{\sigma\sigma'} , \tag{4a}$$

$$\sum_{l,\sigma_1}\langle\langle C_{1\sigma_1}^{\dagger}C_{i\sigma_1}C_{1\sigma};C_{j\sigma'}^{\dagger}\rangle\rangle_{\omega}=I_1\sum_{l} G_{lj}^{\sigma\sigma'}-n_{\sigma}ZG_{ij}^{\sigma\sigma'} , \tag{4b}$$

where Z is the number of nearest neighbor and

$$n_{\sigma}=\langle n_{i\sigma}\rangle , \tag{5}$$

$$I_1=\sum_{\sigma}\langle C_{i\sigma}^{\dagger}C_{l\sigma}\rangle \quad (i,l \text{ are nearest neighbor}) . \tag{6}$$

With Fourier transformation one can obtain the expression of the Green's function in the energy-momentum space

$$G_{kk'}^{\sigma\sigma'}=\frac{\delta_{kk'}\delta_{\sigma\sigma'}}{\omega-E_{k\sigma}} , \tag{7}$$

where

$$E_{k\sigma}=(1-2jI_1)\varepsilon_k-n_{-\sigma}U+n_{\sigma}ZJ-\mu , \tag{8}$$

$$\varepsilon_k=-\frac{D}{2Z}\sum_{\delta} e^{i\mathbf{k}\cdot\delta} , \tag{9}$$

$$j=ZJ/D .$$

$E_{k\sigma}$ are the spectra of quasiparticle and D is the bandwidth.

We introduce the total occupation number and the ferromagnetic order parameter

$$n=n_{\uparrow}+n_{\downarrow} , \tag{10a}$$

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

The energy of the HF ground state and I_1 are easily obtained when we use the spectral theorem and a flat density of states. The energy of HF ground state per site is given by

$$E_{\mathrm{HF}}=\langle H\rangle/D=-\frac{I_1}{2}+ua_1+\frac{j}{2}(2a_1-n^2+I_1^2) , \tag{11}$$

where

$$I_1=n-n^2+2a_1 , \tag{12}$$

$$a_1=n_{\uparrow}n_{\downarrow}=(n^2-m^2)/4 , \tag{13}$$

$$u=U/D .$$

The ferromagnetic-order parameter can be calculated by using the minimization conduction of the ground-state energy $\partial E_{\mathrm{HF}}/\partial m$ or a self-consistency condition. The equation of m is given by

$$[1-u-(1+2I_1)]m=0 . \tag{14}$$

This equation is the same as the one derived from the condition where spin subband chemical potentials are equalized.[11]

Within the local approach the trial function for the correlation ground state $|\Psi_L\rangle$ is constructed by modulating the linear combination as

$$|\Psi_L\rangle=\prod_{i,j}\left[\prod_{m}(1-\eta_m O_{ij}^{(m)})\right]|\Phi_{\mathrm{HF}}\rangle , \tag{15}$$

where $\{\eta_m\}$ is a set of parameters, the indices i and j run over all sites, and $\{O_{ij}^{(m)}\}$ is a set of local operators. The ground-state energy per site is written as

$$E_G=\frac{1}{N}\frac{\langle\Psi_L|H|\Psi_L\rangle}{\langle\Psi_L|\Psi_L\rangle}=E_{\mathrm{HF}}+E_c . \tag{16}$$

The first term is the HF ground-state energy and the second term is the correlation energy. Substituting (15) into (16), then expanding (16) in powers of η_m up to second order, one can obtain the expression for the correlation energy as

$$E_c=-\frac{2}{N}\sum_{i,j,m}\eta_m\langle O_{ij}^{(m)}H\rangle +\frac{1}{N}\sum_{\substack{i,j,m,\\ i',j',m'}}\eta_m\eta_{m'}\langle O_{ij}^{(m)}HO_{i'j'}^{(m')}\rangle +\frac{1}{N}\sum_{\substack{i,j,m,\\ i',j',m'}}\eta_m\eta_{m'}\langle O_{ij}^{(m)}O_{i'j'}^{(m')}H\rangle . \tag{17}$$

The third term summation of the right-hand side in Eq. (17) is forbidden if $\{i,j,m\}=\{i',j'm'\}$. In order to give the main characteristic feature of the electron correlation effect, we only consider the single-site correlations, then, $O_{ij}^{(m)}$ reduces to $O=n_{i\uparrow}n_{i\downarrow}$, and η_m to η which is determined by minimizing the ground-state energy. Within the $R=0$ approximation,[23] by using Wick's theorem, η and the correlation energy are given, respectively, as

$$\eta=\frac{u}{1+ua_3} , \tag{18}$$

$$E_c/D=-\frac{u^2a_1a_2}{1+ua_3} , \tag{19}$$

where

$$a_2=1-n+a_1 , \tag{20}$$

$$a_3=1-2n+4a_1 . \tag{21}$$

Considering the electron correlation one can obtain a new equation of m from minimization of E_G with respect to m as the following:

$$j=\frac{1-u}{1+2I_1}+\frac{u^2}{1+2I_1}\left[\frac{a_1+a_2}{1+ua_3}-\frac{4ua_1a_2}{(1+ua_3)^2}\right]. \tag{22}$$

Equation (22) is important for determining the ground-state phase boundaries. The first term of the right-hand side in Eq. (22) is from the HF approximation; the second term is the correction due to the electron correlation. It is important to notice that the condition $0\le\eta<1$ when Eqs. (16) and (22) are solved self-consistently.

III. COMPUTATION RESULTS AND DISCUSSION

The computation results are shown in Figs. 1–3. In these figures three groups of curves a, b, and c correspond to $u=0$, 0.3, and 0.6, respectively. The solid lines correspond to the results of the local approach, and the dashed lines to the ones of HF approximation. From these figures we see that the results are identical in both different approximations when $u=0$. This is easily explained since there is not the electron correlation when $u=0$.

In Figs. 1(a) and 1(b) the exchange interaction j vs n is plotted for $m=0$ and n, respectively. Due to the electron-hole symmetry in the Hamiltonian (1), we only take $0\le n\le 1$. From Fig. 1 we can see that the curves which are given by the local approach are over ones given by the HF approximation for $u\neq 0$. It is shown that considering the electron correlation effect, the values of j required to obtain the ferromagnetic phase are larger than ones of the HF approximation when $u\neq 0$. For fixed n, the larger the value of u, the larger is the difference of values of j given by both approximations. In other words the role of u in the tendency to ferromagnetic becomes smaller when the effect of electron correlations is taken into account. In addition we also see that for fixed $u\neq 0$, considering electron correlation the correction over the HF approximation decreases with increasing n. In the case of the half-filled band ($n=1$) and the full spin polarization ($m=1$) the correction is zero. This effect is similar to the one found for the antiferromagnetism within the local approach.[24] It is due to relatively strong correlation of electrons in the paramagnetic state. Figure 1(a) indicates that the most likely case to occur after the ferromagnetic-paramagnetic transition is the half-filled band in both approximations. From Fig. 1(b) one can find that the electron density n_c, where it is most likely to achieve full spin polarization, increases with increasing u in the local approach, while $n_c=0.5$ in the HF approximation, which is independent of u.

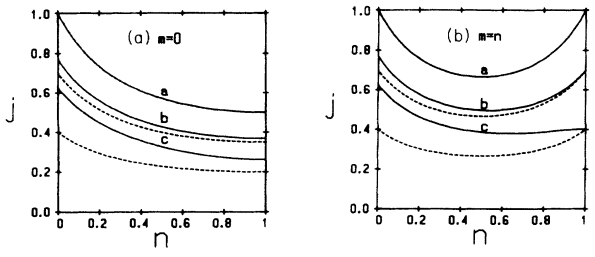

FIG. 1. Ground-state phase boundaries, where three groups of curves a, b, and c correspond to $u=0$, 0.3, and 0.6, respectively. The solid lines correspond to the local approach and the dashed lines correspond to the HF approximation. (a) Without spin polarization $m=0$; (b) full spin polarization $m=n$.

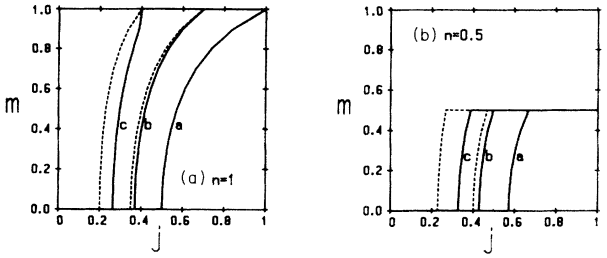

FIG. 2. The ferromagnetic-order parameter m vs j; same as plotted in Fig. 1, but (a) half-filled band $n=1$; (b) quarter-filled band $n=0.5$.

In Figs. 2(a) and 2(b) the ferromagnetic order parameter m is plotted vs the exchange interaction j for $n=1$ and 0.5, respectively. The bent part of curves corresponds to the range of j required for existence of partial spin polarization when both u and n are fixed. Figure 2 indicates that for the correlation of electrons the value of j_c required for the onset of spin polarization is larger than that in the HF approximation. The larger the u, the larger is the difference of j_c given by both different approximations. j_c decreases with increasing u, as is the case for the HF approximation.

Figures 3(a) and 3(b) show the ground-state energy versus the exchange interaction j for $n=1$ and 0.5, respectively. With increasing j, the curves are first straight segments, and the system is the paramagnetic phase where the separated degree between a solid line and a corresponding dashed line is larger. Then the curves become bent, and the system is in the weakly ferromagnetic phase where the separated degree of lines is smaller. Finally, the curves again become straight, but with a steeper ratio of the slopes, and the system is a strongly ferromagnetic phase where the correlation ground-state energy is the same as the HF ground-state energy. From the physics viewpoint, it is easy to understand that there

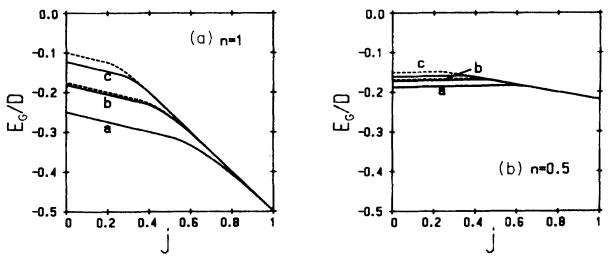

FIG. 3. The ground-state energy E_G/D vs j, same as plotted in Fig. 2.

is no correlation between electrons because the system only has single-spin electrons (for $n > 1$, single-spin hole) for full spin polarization. Thus the correlation effect of electrons is stronger in the paramagnetic region but weaker in the weakly ferromagnetic region. From Figs. 3(a) and 3(b) one can see that the range for partial spin polarization becomes smaller with increasing u or decreasing n.

IV. CONCLUSION

By using the local approach to the ferromagnetic phase in the Hubbard-Hirsch model, we have studied the effect of electron correlations on the phase diagram and on the ground-state energy. We considered the single-site electron correlations and performed a second-order expansion within $R=0$ approximation. Comparing with those of the HF approximation, when the Coulomb interaction U ($\neq 0$) between electrons with opposite spin at the same site is fixed, the values of the exchange interaction J of nearest-neighbor sites required to obtain the ferromagnetic phase are larger, the ferromagnetic region becomes smaller, and the paramagnetic region becomes larger. The effect of electron correlations greatly reduces the role of U in the tendency to ferromagnetism and stabilizes paramagnetism.

For fixed U ($\neq 0$) and electron density n, the absolute value of the correlation energy is large in the paramagnetic region, small in the weakly ferromagnetic region, and zero in the strongly ferromagnetic region. It is shown that the electron correlation effect is stronger in the paramagnetic region and is weaker in the weakly ferromagnetic region.

Although we have considered only single-site electron correlations in this paper, we do not expect the main characteristic features of the electron correlation effect to change greatly when electron correlation and spin correlation between nearest-neighbor sites are taken into account.

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