Magnetic excitation in the Hubbard-Hirsch model

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Based on the Hubbard-Hirsch model, we studied the dynamical susceptibility and spin excitation of an itinerant-electron system within the random-phase approximation by using a Green's-function technique. It is shown that the two-center matrix elements in the Hubbard-Hirsch model not only change the dynamic property of the susceptibility, but also widen the gap between two spin subbands, which suppresses the electron-hole single excitations. In contrast, the region of collective excitations of the spin becomes larger. [S0163-1829(96)02825-1]

I. INTRODUCTION

The origin of ferromagnetism in transition metals has been a controversial subject for quite a long time.[1,2] This controversy stems from the apparent dual character (itinerancy and localization properties) of the d electrons responsible for magnetism in transition metals. According to the molecular-field theory of ferromagnetism of Weiss,[3] the interaction giving rise to the spontaneous magnetic order can be represented by an internal molecular field. It was Heisenberg[4] who first realized that ferromagnetism is intrinsically a quantum many-body effect, and proposed the scenario that spin-independent Coulomb interaction and the Pauli exclusion principle result in the ''exchange interaction'' between electronic spins. From the Weiss-Heisenberg local model, the Curie-Weiss law is successfully explained. However, a nonintegral number of Bohr magnetons cannot be obtained for the atomic magnetic moment at $T=0$ K. Consequently, Stoner[5] and Slater[6] proposed an itinerant-electron model based on Bloch's work[7] in the free-electron gas. According to Stoner, the 3d electrons of transition metals, instead of being localized around particular nuclei, can move from one ion to another through the crystal lattice. This theory gives the nonintegral number of Bohr magnetons for the atomic magnetic moment at $T=0$ K, but fails at finite, nonzero temperature. In 1963 Hubbard[8] studied the electron correlation due to the strong Coulomb interaction, and proposed the famous Hubbard model. In this model, the hopping integral describes the itinerancy tendency of electrons, while the electron correlation describes the localization tendency. In terms of the Hubbard model, the metal-insulator transition is successfully explained,[8] and metal magnetic properties have been discussed. Within the mean-field approximation, the Stoner model can be deduced from the single-band Hubbard model. However, the single-band Hubbard model exhibits antiferromagnetism rather than ferromagnetism.[9–11]

Recently, Hirsch[12–14] proposed that certain two-center 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 to the Coulomb energy is negative. By adding this term to the Hubbard Hamiltonian, Hirsch obtained what we call the Hubbard-Hirsch Hamiltonian. He showed that partial spin polarization is naturally derived from the later model, which, we think, is an important improvement over the Stoner model.

However, in Hirsch's works, the metallic ferromagnetism is studied within the Hartree-Fock approximation (HFA), and the correlation of quasiparticles under thermal excitation is neglected. A more complete theory should go beyond the HFA and consider the electron-hole interaction. In fact, many people[15–17] have investigated the spin wave energy of a ferromagnet using the random-phase approximation (RPA) in the Stoner model. Based on the Hubbard-Hirsch Hamiltonian, in this paper we study the spin excitation in an itinerant-electron system with the RPA. The paper is organized as follows. In Sec. II we derive analytic expressions of the dynamical susceptibility. In Sec. III we give the spin excitation spectrum and some discussions. The conclusion is given in Sec. IV.

II. DYNAMICAL SUSCEPTIBILITY

The Hubbard-Hirsch Hamiltonian is expressed as

$$H=\sum_{i,j,\sigma} t_{ij}C^{+}_{i,\sigma}C_{j,\sigma}+\tfrac{1}{2}U\sum_{i,\sigma} n_{i,\sigma}n_{i,-\sigma}$$
$$+J\sum_{\langle i,j\rangle,\sigma,\sigma'} C^{+}_{i,\sigma}C^{+}_{j,\sigma'}C_{i,\sigma'}C_{j,\sigma}, \qquad (1)$$

where t_{ij} is the hopping integral, U is the usual Hubbard on-site repulsion, and 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. By Fourier transformation one can obtain the expression of the Hubbard-Hirsch Hamiltonian in the energy-momentum space

$$H=\sum_{k,\sigma}\varepsilon_k C^+_{k,\sigma}C_{k,\sigma}+\frac{U}{N}\sum_{k,k',q}C^+_{k+q,\uparrow}C^+_{k'-q,\downarrow}C_{k',\downarrow}C_{k,\uparrow}+\frac{JZ}{N}\sum_{k,k',q,\sigma,\sigma'}\gamma_q C^+_{k+q,\sigma}C^+_{k'-q,\sigma'}C_{k,\sigma'}C_{k',\sigma}, \quad (2)$$

where

$$\gamma_q=\frac{1}{Z}\sum_{\delta}e^{i\mathbf{q}\cdot\boldsymbol{\delta}} \quad (3)$$

with Z being the number of nearest neighbors, and δ the vectors that connect a site to its nearest neighbors.

In order to calculate the dynamical susceptibility of the spin system, we use the spin densities

$$\hat{S}^+(-q)=\sum_k C^+_{k-q,\uparrow}C_{k,\downarrow};\quad \hat{S}^-(q)=\sum_k C^+_{k+q,\downarrow}C_{k,\uparrow} \quad (4)$$

to define the Green's function

$$\langle\langle C^+_{k+q,\downarrow}C_{k,\uparrow};\hat{S}^+(q)\rangle\rangle_\omega .$$

In the RPA, the general equation of the Green's function,

$$\omega\langle\langle C^+_{k+q,\downarrow}C_{k,\uparrow};\hat{S}^+(-q)\rangle\rangle_\omega =\langle[C^+_{k+q,\downarrow}C_{k,\uparrow},\hat{S}^+(-q)]\rangle+\langle\langle[H,C^+_{k+q,\downarrow}C_{k,\uparrow}];\hat{S}^+(-q)\rangle\rangle_\omega , \quad (5)$$

is reduced to the following form:

$$\left\{\omega-\omega_{kq}-m(U+2ZJ)-\frac{2ZJ}{N}\sum_{q_1}\gamma_{q_1}(\langle n_{k+q+q_1}\rangle-\langle n_{k+q_1}\rangle)\right\}\langle\langle C^+_{k+q,\downarrow}C_{k,\uparrow};\hat{S}^+(-q)\rangle\rangle_\omega =(\langle n_{k+q,\downarrow}\rangle-\langle n_{k,\uparrow}\rangle)\left\{1+\left(\frac{U}{N}+\frac{2ZJ}{N}\gamma_q\right)\times\langle\langle\hat{S}^-(q);\hat{S}^+(-q)\rangle\rangle_\omega\right\}, \quad (6)$$

where

$$\omega_{kq}=\varepsilon_{k+q}-\varepsilon_k , \quad (7)$$

$$m=\langle n_\uparrow\rangle-\langle n_\downarrow\rangle, \quad (8)$$

$$\langle n_\sigma\rangle=\frac{1}{N}\sum_k\langle n_{k\sigma}\rangle. \quad (9)$$

Then we can obtain the Green's function

$$\langle\langle C^+_{k+q,\downarrow}C_{k,\uparrow};\hat{S}^+(-q)\rangle\rangle_\omega=\frac{f(E_{k+q,\downarrow})-f(E_{k,\uparrow})}{\omega-(E_{k+q,\downarrow}-E_{k,\uparrow})}\times\left\{1+\left(\frac{U}{N}+\frac{2ZJ}{N}\gamma_q\right)\times\langle\langle\hat{S}^-(q);\hat{S}^+(-q)\rangle\rangle_\omega\right\}. \quad (10)$$

where

$$\langle n_{k\sigma}\rangle=f(E_{k\sigma}), \quad (11)$$

$$E_{k\sigma}=\epsilon_k+(U+2ZJ)\langle n_\sigma\rangle+\frac{2ZJ}{N}\sum_{q_1}\gamma_{q_1}\langle n_{k+q_1}\rangle. \quad (12)$$

We find from the above results that in comparison with the Stoner model, the two-center matrix elements not only lead U to change into $(U+2ZJ)$, but also give rise to an additional term $(2ZJ/N)\Sigma_{q_1}\gamma_{q_1}\langle n_{k+q_1}\rangle$ in $E_{k\sigma}$.

Summing over all wave numbers, from Eq. (10) we obtain the dynamical spin susceptibility in the RPA,

$$\chi^{-+}(q,\omega)=\langle\langle\hat{S}^-(q)|\hat{S}^+(-q)\rangle\rangle_\omega =\frac{\Gamma^{-+}(q,\omega)}{1-\left(\frac{U}{N}+\frac{2ZJ}{N}\gamma_q\right)\Gamma^{-+}(q,\omega)}, \quad (13)$$

where

$$\Gamma^{-+}(q,\omega)=\sum_k\frac{f(E_{k+q,\downarrow})-f(E_{k,\uparrow})}{\omega-(E_{k+q,\downarrow}-E_{k,\uparrow})+i0^+}, \quad (14)$$

$$E_{k+q,\downarrow}-E_{k,\uparrow}=\omega_{kq}+m(U+2ZJ)+L(k,q), \quad (15)$$

$$L(k,q)=\frac{2ZJ}{N}\sum_{q_1}\gamma_{q_1}(\langle n_{k+q_1}\rangle-\langle n_{k+q+q_1}\rangle). \quad (16)$$

For the paramagnetic phase,

$$\langle n_\uparrow\rangle=\langle n_\downarrow\rangle;\quad E_{k+q,\downarrow}-E_{k,\uparrow}=E_{k+q}-E_k , \quad (17)$$

where

$$E_k=\varepsilon_k+\frac{2ZJ}{N}\sum_{q_1}\gamma_{q_1}\langle n_{k+q_1}\rangle. \quad (18)$$

Then

$$Re\Gamma^{-+}(q=0,\omega=0)=\sum_k\left[-\frac{\partial f}{\partial E_k}\right]=2\chi_p(T). \quad (19)$$

$\chi_p(T)$ in Eq. (19) is the Pauli paramagnetic susceptibility of the free-electron gas.

III. MAGNETIC EXCITATION

The magnetic excitation spectrum is determined by the poles of the dynamical susceptibility, i.e., from

$$\chi^{-+}(q,\omega)^{-1}=0, \quad (20)$$

namely,

$$F(\omega)=\left(\frac{U}{N}+\frac{2ZJ}{N}\gamma_q\right)\sum_k \frac{f(E_{k+q,\downarrow})-f(E_{k,\uparrow})}{\omega-\omega_{kq}-m(U+2ZJ)-L(k,q)}=1. \tag{21}$$

This equation has solutions corresponding to the single or the Stoner excitations as well as the spin-wave modes. First, we discuss the Stoner excitation. The poles of $F(\omega)$ are

$$\omega=\epsilon_{k+q}-\epsilon_k+(U+2ZJ)(\langle n_\uparrow\rangle-\langle n_\downarrow\rangle)+\frac{2ZJ}{N}\sum_{q_1}\gamma_{q_1}(\langle n_{k+q_1}\rangle-\langle n_{k+q+q_1}\rangle). \tag{22}$$

Thus the thermal excitations resulting from the electronic spin-flip excitations across the Fermi surface, which create single-particle electron-hole pairs with opposite spins, must exist in an itinerant magnet. Such excitations are called single or Stoner excitations. Taking into account the effect of two-center matrix elements, the gaps which the spin flips must overcome are widened, so that the single excitations will be suppressed. In the Stoner continuum the imaginary part of $\Gamma^{-+}(q,\omega)$ is not zero, however, it vanishes outside of the Stoner continuum. This means that in the Stoner excitations in Hubbard-Hirsch's model the damping still exists.

In order to study the collective excitations outside of the Stoner continuum, we expand $(E_{k+q}-E_k)$ and $(\langle n_{k+q+q_1}\rangle-\langle n_{k+q}\rangle)$ in the long-wavelength limit as follows:

$$E_{k\pm q}-E_k\approx\pm(\mathbf{q}\cdot\boldsymbol{\nabla})E_k+\tfrac{1}{2}(\mathbf{q}\cdot\nabla)^2E_k, \tag{23}$$

$$\langle n_{k\pm q+q_1}\rangle-\langle n_{k+q_1}\rangle\approx\pm(\mathbf{q}\cdot\boldsymbol{\nabla})\langle n_{k+q_1}\rangle+\tfrac{1}{2}(\mathbf{q}\cdot\boldsymbol{\nabla})^2\langle n_{k+q_1}\rangle. \tag{24}$$

From (21), (23), and (24), we can obtain the following equation, from which the dispersion of spin waves are determined:

$$\begin{aligned}1=F(\omega)=&-\frac{\widetilde{U}_q}{m\widetilde{U}}\left(1+\frac{\omega}{m\widetilde{U}}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})-\frac{\widetilde{U}_q}{m^2\widetilde{U}^2}\sum_k(f_{k\uparrow}-f_{k\downarrow})(\mathbf{q}\cdot\boldsymbol{\nabla})E_k-\frac{\widetilde{U}_q}{2m^2\widetilde{U}^2}\sum_k(f_{k\uparrow}-f_{k\downarrow})(\mathbf{q}\cdot\boldsymbol{\nabla})^2E_k\\&+\frac{\widetilde{U}_q}{m^3\widetilde{U}^3}\sum_k(f_{k\uparrow}-f_{k\downarrow})(\mathbf{q}\cdot\boldsymbol{\nabla}E_k)^2-\frac{\widetilde{U}_q}{m^2\widetilde{U}^2}\left(\frac{2ZJ}{N}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})\sum_{q_1}\gamma_{q_1}(\mathbf{q}\cdot\boldsymbol{\nabla})\langle n_{k+q_1}\rangle\\&-\frac{\widetilde{U}_q}{2m^2\widetilde{U}^2}\left(\frac{2ZJ}{N}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})\sum_{q_1}\gamma_{q_1}(\mathbf{q}\cdot\nabla)^2\langle n_{k+q_1}\rangle+\frac{\widetilde{U}_q}{m^3\widetilde{U}^3}\left(\frac{2ZJ}{N}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})\sum_{q_1}\gamma_{q_1}^2(\mathbf{q}\cdot\boldsymbol{\nabla}\langle n_{k+q_1}\rangle)^2,\end{aligned} \tag{25}$$

where

$$\widetilde{U}_q=\frac{U}{N}+\frac{2ZJ}{N}\gamma_q, \tag{26}$$

$$\widetilde{U}=U+2ZJ. \tag{27}$$

For a cubic crystal in the long-wavelength limit, we have

$$\gamma_q=1-\frac{1}{Z}a^2q^2; \tag{28}$$

then

$$\widetilde{U}_q=\frac{1}{N}[(U+2ZJ)-2Ja^2q^2]. \tag{29}$$

Let E_k be at the spherical Fermi surface. From (29) and (25), we can obtain the collective excitation spectrum of the spin system,

$$\begin{aligned}\omega=&\,2mJa^2q^2+\frac{q^2}{6mN}\sum_k(f_{k\uparrow}-f_{k\downarrow})\boldsymbol{\nabla}^2E_k-\frac{q^2}{3m^2N(U+2ZJ)}\sum_k(f_{k\uparrow}-f_{k\downarrow})(\boldsymbol{\nabla}E_k)^2\\&+\frac{q^2}{6mN}\left(\frac{2ZJ}{N}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})\sum_{q_1}\gamma_{q_1}\boldsymbol{\nabla}^2\langle n_{k+q_1}\rangle-\frac{q^2}{3Nm^2(U+2ZJ)}\left(\frac{2ZJ}{N}\right)\sum_k(f_{k\uparrow}-f_{k\downarrow})\sum_{q_1}\gamma_{q_1}(\boldsymbol{\nabla}\langle n_{k+q_1}\rangle)^2\\&+\frac{4mJ^2a^4q^4}{U+2ZJ}+\cdots.\end{aligned} \tag{30}$$

Comparing our result with the collective excitation in Stoner theory, we find that the effect of two-center matrix elements not only change the dispersion of spin waves by $[U/N \rightarrow (U/N)+(2ZJ/N)\gamma_q]$, but also broaden the region of collective excitations. That is to say, the collective excitations become stronger when the effect of two-center matrix elements are accounted for.

IV. CONCLUSION

Based on the spin-polarization ferromagnetism theory of Hirsch, we have studied the dynamical susceptibility and magnetic excitations of an itinerant-electron system with the random-phase approximation. It has been found that the dynamical susceptibility $\chi^{-+}(q,\omega)$ is modified greatly, the gap of spin flip is increased by $2ZJ(\langle n_\uparrow\rangle - \langle n_\downarrow\rangle)$, and in $E_{k\sigma}$ an additional term $(2ZJ/N)\Sigma_{q_1}\gamma_{q_1}\langle n_{k+q_1}\rangle$ appears, when the effect of two-center matrix elements are taken into account. Thus the single excitations of the electron-hole pairs are suppressed, while the region of collective excitations becomes larger.

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