Spin-Wave Excitations in the weak Interacting Half-filled Narrow Band Systems

Hirotoshi WATANABE

渡 辺 丕 俊

〔内容抄録〕

遷移金属や遷移金属酸化物，及び有機伝導体等の磁性や輸送現象が最近色々な方面から研究されて来ている。ここでは狭い巾を持った単一バンドの場合を考え，良く知られているハバード・モデルを扱う。バンドが半分つまっていて相関の強い場合には，このモデルの基底状態ではスピンが局在し，反強磁性状態になっているということが一般的に知られている。しかしながら相関が弱い場合には，バンド・モデル的になっており磁性状態はあまり明確ではない。この論文において相関の弱い極限の場合にも，反強磁性のスピン波励起が存在し，この励起の考慮が物理量の計算に大切であることを示す。

The single-band Hubbard Hamiltonian is examined in the limit of intra-atomic Coulomb interaction much less than bandwidth. We make use of the well-known temperature Green's function method and the final estimation is performed only in the zero temperature limit. The purpose of this paper is to investigate the effect of electron correlation on the antiferromagnetic ground state of half-filled narrow band systems. We show that even in the weak correlation limit antiferromagnetic spin wave can be excited and it seems that the ground state is in the antiferromagnetic phase.

§ 1. Introduction

The properties of narrow band electron systems have been investigated in the last decade. It is because the magnetic and transport phenomena of the system are very different from the usual band theory.

To treat the narrow band electron systems, we consider the well-known Hubbard Hamiltonian[1)],

$$\bar{H} = \sum_{\substack{i,j \\ s}} t_{ij}\, c_{is}^{+}\, c_{js} + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow}, \tag{1.1}$$

which has received much attention in solid-state community for its importance to many phase transition phenomena. Until now many investigations were given to the Hamiltonian and we want the reader to consult the other papers[2)3)4)5)]. In the *Eq.* (1.1) n_{is} equals to $c_{is}^{+}c_{is}$ (c_{is} is the annihilation operator for a s-spin electron in a Wannier state on site i), t is the hopping term to nearest neighbors and U is the intra-atomic Coulomb interaction parameter. It is well-known that this system has an antiferromagnetic ground state in the half-filled band strong correlation limit $U \gg t$[6)7)]. In the $U \gg t$ limit electron localize at every lattice site and they interact each other by the effect of virtual transfer and single band breaks into two bands separated by a gap and the system show the antiferromagnetic and insulating metal. So it can be readily known that this system can be described by the Heisenberg Hamiltonian with antiferromagnetic coupling. The outhor investigated the strong correlation system in the previous paper[8)] and the many other people examined in this limit. On the other hand, however, the weak correlation system is not still so clear.

Recently Kubo *et al*[9)] investigated this weakly correlation system. They used the variational method and concluded that the ground state of half-filled band seems to be antiferromagnetic in the weak correlation limit. If the system is in the antiferromagnetic state, there must be spin-wave excitation. This indicate that it is necessary to consider all order of diagrams to examine the correlation effect even in the weakly correlated limit.

A brief outline of this paper follows. In Sec. 2, after definition of our notations, we derive the results of Hartree-Fock approximation. Then we consider the spin correlation function in the ladder approximation. In Sec. 3 we show that there are spin wave excitations even in the weak correlation limit. It seems that the ground state of half-filled band is antiferromagnetic in the limit, and the spin wave excitations are very important to consider many transport phenomena for real metals and transition metal oxides.

§ 2. Hubbard model Hamiltonian.

As we have mentioned in the previous section, we consider the Hubbard Hamiltonian (1.1) for the case of the weak correlation. To treat the Hamiltonian we describe our notations which we used in the previous paper[8)]. We consider a half-filled band system. As is usually done in the anti-ferromagnetic system, we assume two sublattices A and B which are doubly periodic in the crystal lattice. We transform the creation and annihilation operators of the A and B sublattices into momentum representation and the Hamiltonian can be written as follows

$$H=\bar{H}-\mu N=H_o+H_{int},$$

$$H_o=\sum_{qs}\varepsilon_q(b^+_{qs}a_{qs}+a^+_{qs}b_{qs})-\frac{U}{2}\sum_q\sigma\{(n^A_{q\uparrow}-n^A_{q\downarrow})-(n^B_{q\uparrow}-n^B_{q\downarrow})\},$$

$$H_{int}=\frac{U}{N/2}\sum_q\sum_{p.p'}(a^+_{p\uparrow}a_{p-q\uparrow}a^+_{p'\downarrow}a_{p'+q\downarrow}+b^+_{p\uparrow}b_{p-q\uparrow}b^+_{p'\downarrow}b_{p'+q\downarrow})$$

$$-\frac{U}{2}\sum_{2s}\{(1-s\sigma)n^A_{qs}+(1+s\sigma)n^B_{qs}\}. \tag{2.1}$$

Here we divided the Hamiltonian into the Hartree-Fock part Ho and the remaining interaction part H_{int}. We considered that the chemical potential is equal to $U/2$ as we are dealing with the half-filled band. In this equation ε_q is the energy of the Bloch state q, n_q is the number operator, σ is the sublattice magnetization and s is the spin index which takes +1 or −1 depending on up or down electron spin. We apply the finite temperature Green's function method. As well-known the single-particle Green's function is denoted by

$$G_{\xi\eta,s}(k\,.\tau)=T\sum_n G_{\xi\eta,s}(k)e^{-i\omega_n\tau}$$

$$=-T_r(T\tau\ e^{-\beta H}\xi_{ks}(\tau)\,\eta^+_{ks}(o))/T_re^{-\beta H}, \tag{2.2}$$

where ξ and η are the annihilation operators in the Heisenberg representation and k denotes the four momentum $(k,i\omega_n)$, where

$$\omega_n=(2n+1)\pi T \qquad n:\text{ integer.}$$

The formula for the sublattice magnetization σ is

$$\sigma=\frac{1}{N/2}T\sum_k(G_{aa\uparrow}(k)-C_{aa.\downarrow}(k)). \tag{2.3}$$

The lowest order Green's function G^o can be easily calculated[8)]

$$G^o_{aa.s}(k)=\frac{i\omega_n-\frac{S\sigma U}{2}}{(i\omega_n)^2-E^2_k}$$

$$G^o_{bb.s}(k)=\frac{i\omega_n+\frac{S\sigma U}{2}}{(i\omega_n)^2-E^2_k}$$

$$G^o_{ab.s}(k)=G^o_{ba.s}(k)=\frac{\varepsilon_k}{(i\omega_n)^2-E^2_k} \tag{2.4}$$

where $E_k=\sqrt{\left(\frac{\sigma U}{2}\right)^2+\varepsilon_k^2}$

From *Eq.* (2.3) the self-consistent sublattice magnetization σ' in the Hartree-Fock approximation is

$$1=\frac{1}{N/2}\sum_q\frac{U}{2E_q}(\mathrm{f}(-E_q)-\mathrm{f}(E_q)), \qquad (2.5)$$

where $f(E_q)$ is the well-known Fermi distribution function. After a easy calculation the sublattice magnetization at zero temperature σ_0' is

$$\sigma_0'\approx\frac{2t\left(\frac{\pi}{2}\right)}{U/2}\mathrm{e}^{-\frac{2t}{U/2}\left(\frac{\pi}{2}\right)} \qquad \text{for 1 dimension,}$$

$$\sigma_0'\approx\frac{4t\left(\frac{\pi}{2}\right)^2}{U/2}\mathrm{e}^{-\left\{\frac{4t}{U/2}\left(\frac{\pi}{2}\right)^2\cdot 2\right\}^{1/2}} \qquad \text{for 2 dimention square lattice,}$$

$$\sigma_0'\approx\frac{8t\left(\frac{\pi}{2}\right)^3}{U/2}\mathrm{e}^{-\left\{\frac{8t}{U/2}\left(\frac{\pi}{2}\right)^3\cdot 3\right\}^{1/3}} \qquad \text{for 3 dimention b.c.c. lattice.} \qquad (2.6)$$

To discuss the correlation effect we must consider the higher order diagrams. For this purpose we examine the two-particle Green's function[8)]

$$\chi_{\underset{\uparrow\downarrow}{\xi\eta}}(\eta,\tau)=\sum_{p.p'}<T\tau(\xi^+_{p-q}\uparrow(\tau)\,\xi_p\downarrow(\tau)\,\eta^+_{p'}\downarrow(0)\,\eta_{p-q}\uparrow(0))>$$

and use the perturbation theory. Using the Bloch Dominicis theorem χ is written in the lowest order approximation as

$$\chi^0_{\xi\eta}(q)=-T\sum_p G^0_{\xi\eta,\uparrow}(p-q)\,G^0_{\eta\xi,\downarrow}(p). \qquad (2.7)$$

In the ladder approximation the graph of χ involves χ° as illustrated by Fig. 1.

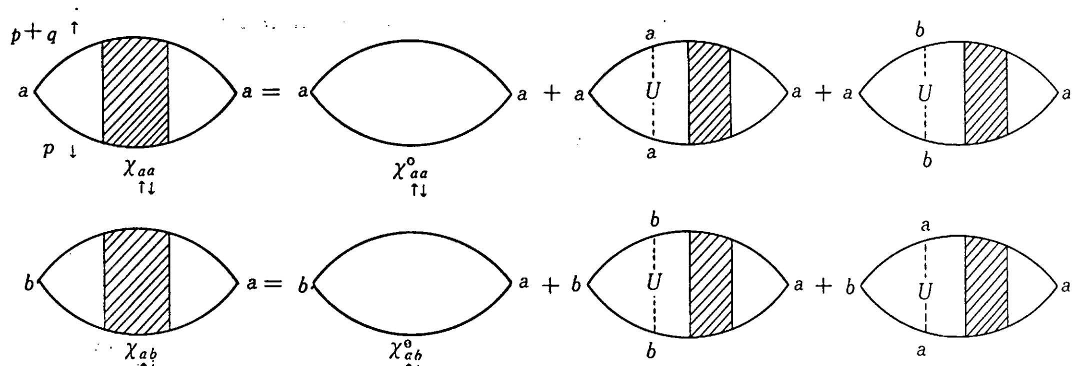

Fig. 1 The ladder diagrams leading to spin correlation function χ .

$$\chi_{\substack{aa\\ \uparrow\downarrow}}(q)=\frac{1}{D}\left[\chi^{\circ}_{\substack{aa\\ \uparrow\downarrow}}(q)\left(1-\frac{U}{N/2}\chi^{\circ}_{\substack{bb\\ \uparrow\downarrow}}(q)\right)+\frac{U}{N/2}\chi^{\circ}_{\substack{ab\\ \uparrow\downarrow}}(q)\chi^{\circ}_{\substack{ba\\ \downarrow\uparrow}}(q)\right]$$

$$\chi_{\substack{bb\\ \uparrow\downarrow}}(q)=\frac{1}{D}\left[\chi^{\circ}_{\substack{bb\\ \uparrow\downarrow}}(q)\left(1-\frac{U}{N/2}\chi^{\circ}_{\substack{aa\\ \uparrow\downarrow}}(q)\right)+\frac{U}{N/2}\chi^{\circ}_{\substack{ba\\ \uparrow\downarrow}}(q)\chi^{\circ}_{\substack{ab\\ \uparrow\downarrow}}(q)\right]$$

$$\chi_{\substack{ab\\ \uparrow\downarrow}}(q)=\chi_{\substack{ba\\ \uparrow\downarrow}}(q)=\frac{1}{D}\chi^{\circ}_{\substack{ab\\ \uparrow\downarrow}}(q) \qquad (2.8)$$

where $D=\left(1-\frac{U}{N/2}\chi^{\circ}_{\substack{aa\\ \uparrow\downarrow}}(q)\right)\left(1-\frac{U}{N/2}\chi^{\circ}_{\substack{bb\\ \uparrow\downarrow}}(q)\right)-\left(\frac{U}{N/2}\right)^2\chi^{\circ}_{\substack{ab\\ \uparrow\downarrow}}(q)\chi^{\circ}_{\substack{ba\\ \uparrow\downarrow}}(q).$ (2.9)

The dispersion relation can be found if we estimate the denominator D.

§3 Antiferromagnetic spin-wave excitation.

In this section we want to calculate the spin-wave correlation function at zero temperature. From Eqs. (2.5), (2.7) and (2.9), the denominator D is

$$D(q,\omega)=\frac{1}{N/2}\sum_p\left[\frac{U}{2E_p}-U\frac{E_p+E_{p-q}}{2E_pE_{p-q}}\,\frac{-\frac{\omega\sigma_0' U}{2}-\left(\frac{\sigma_0' U}{2}\right)^2-E_pE_{p-q}}{\omega^2-(E_p+E_{p-q})^2}\right]$$

$$\cdot\frac{1}{N/2}\sum_p\left[\frac{U}{2E_p}-U\frac{E_p+E_{p-q}}{2E_pE_{p-q}}\,\frac{\frac{\omega\sigma_0' U}{2}-\left(\frac{\sigma_0' U}{2}\right)^2-E_pE_{p-q}}{\omega^2-(E_p+E_{p-q})^2}\right].$$

$$-\left[\frac{U}{N/2}\sum_p\frac{E_p+E_{p-q}}{2E_pE_{p-q}}\,\frac{\varepsilon_p\,\varepsilon_{p-q}}{\omega^2-(E_p+E_{p-q})^2}\right]^2 \qquad (3.1)$$

We estimate this in the limit $q\approx0,\omega\approx0$ and $\frac{U}{t}\approx0$. The detailed calculation is found in Appendix 1. We obtain the result,

$$D_1=\frac{U}{4\pi t}\,\frac{1}{(\sigma_0' U)^2}\left[-\omega^2+c_1^2(1-\cos^2 q)\right]$$

where

$$c_1^2=\frac{\pi t(\sigma_0' U)^2}{2U}\left(1-\frac{U}{\pi t}\right)^2$$

in the case of 1 dimension.

$$D_2=\frac{U}{\pi^2 t(\sigma_0' U)^2}\log\frac{2\pi^2 t}{\sigma_0' U}\left[-\omega^2+c_2^2(1-\cos^2 q_x\cdot\cos^2 q_y)\right]$$

where

$$c_2^2=\frac{\pi^2 t(\sigma_0 U)^2}{2U}\ \log^{-1}\frac{2\pi^2 t}{\sigma_0' U}\left(1-\frac{U}{\pi^2 t}\ \log\ \frac{2\pi^2 t}{\sigma_0' U}\right)^2$$

in the case of 2 dimension square lattice,

$$D_3=\frac{U}{2\pi^3 t(\sigma_0' U)^2}\log^2\frac{2\pi^3 t}{\sigma_0' U}\left[-\omega^2+c_3^2(1-\cos^2 q_x\cdot\cos^2 q_y\cdot\cos^2 q_z)\right]$$

where

$$c_3^2=\frac{\pi^3 t(\sigma_0' U)^2}{U}\ \log^{-2}\frac{2\pi^3 t}{\sigma_0' U}\left(1-\frac{U}{2\pi^3 t}\ \log^2\frac{2\pi^3 t}{\sigma_0' U}\right)^2$$

in the case of 3 dimension b.c.c. lattice.

(3.2)

These equations show that there is spin-wave excitation at zero temperature for very small interaction term of U.

It is not difficult to calculate the sublattice spin correlation functions from the *Eqs.* (2.8) and (3.1) when q and ω are very small.

$$\chi_{\underset{\uparrow\downarrow}{aa}}=\frac{N/2}{D}\left[\frac{1}{2U}-\frac{1}{4}\left(\frac{\sigma_0' U}{2}\right)^2\frac{1}{N/2}\sum_p\frac{1}{E_p^3}\right]$$

$$=\chi_{\underset{\uparrow\downarrow}{bb}}=-\chi_{\underset{\uparrow\downarrow}{ab}} \qquad (3.3)$$

These equations lead to

$$\chi_{\underset{\uparrow\downarrow}{aa}}=\frac{N/2}{D_1}\left[\frac{1}{2U}-\frac{1}{2\pi t}\right]$$

for 1 dimensional case,

$$\chi_{\underset{\uparrow\downarrow}{aa}}=\frac{N/2}{D_2}\left[\frac{1}{2U}-\frac{1}{2\pi^2 t}\ \log\ \frac{2\pi^2 t}{\sigma_0' U}\right]$$

for 2 dimensional square lattice case.

$$\chi_{\underset{\uparrow\downarrow}{aa}}=\frac{N/2}{D_3}\left[\frac{1}{2U}-\frac{1}{4\pi^3 t}\ \log^2\ \frac{2\pi^3 t}{\sigma_0' U}\right]$$

for 3 dimensional b.c.c. lattice case.

(3.4)

Also we can calculate the expectation value of the interacting Hamiltonian by the formula[8)]

$$\langle Hint\rangle_{U'}=-\frac{U'}{N/2}T\sum_{q=0}(\chi_{\underset{\uparrow\downarrow}{aa}}(q)+\chi_{\underset{\uparrow\downarrow}{bb}}(q)) \qquad (3.5)$$

$$=U' \sum_{q \neq 0} \frac{\partial \ln D(q, \omega_n)}{\partial U'} \quad .$$

When we use the energy theorem for the free-energy

$$F=\int_0^U \frac{dU'}{U'} \langle Hint \rangle_{U'} \quad , \tag{3.6}$$

we can derive the free energy, although it needs a little tedious calculations to estimate the value of free-energy. It is not so difficult to show the spin wave excitation is very important for these calculations. We represent only the result of the calculation of $\langle H_{int} \rangle$ in the Appendix 2.

Appendix 1: Calculation of *Eq.* (3.2).

In this section we present the details of the calculation leading to *Eq.* (3.2). From *Eq.* (3.1) it is clear that D (q = 0, ω = 0) = 0.

If we expand D for small ω when q=0,

$$D(q=o,\omega\approx o)=\frac{U}{N/2}\ \omega^2\ \frac{-1}{8}A. \tag{A.1}$$

Here

$$A=\sum_p \frac{1}{E_p^3} \tag{A.2}$$

In the same way for small q at ω=0,

$$D(q\approx o,\ \omega=o)=\left(\frac{U}{N/2}\right)^2\frac{1}{8}\left(2\frac{N/2}{U}-\left(\frac{\sigma_0' U}{2}\right)^2 A\right)^2(1-Q^2), \tag{A.3}$$

where

$Q=$ coq q for 1 dimension,

$Q=$ cog $q_x \cdot$ cos q_y for 2 dimension square lattice,

$Q=$ cos $q_x \cdot$ cos $q_y \cdot$ cos q_x. for 3 dimension b.c.c. lattice.

Thus for small q and ω,

$$D=\frac{U}{N/2}\ \omega^2\ \frac{-1}{8}A+\left(\frac{U}{N/2}\right)^2\frac{1}{8}\left(2\frac{N/2}{U}-\left(\frac{\sigma_0 U}{2}\right)^2 A\right)^2(1-Q^2). \tag{A.4}$$

If we calculate A of Eq. (A.2) using the approximation sin $q\approx q$, we get the result of Eq. (3.2).

Appendix 2: The result of calculation of $\langle H_{int} \rangle$.

If we take into account only the effect of spin wave excitations, it is straightforward to calculate the value of $\langle H_{int} \rangle$ of *Eq.* (3.5).

$$\langle Hint\rangle = -\frac{N}{2}\sqrt{\frac{2\pi t}{U}}\,\frac{\sigma_0' U}{2}\,\frac{1}{\pi/2}\int_0^{\pi/2}\frac{dq}{(1-\cos^2 q)^{1/2}}\left[\frac{\sinh[\beta c_1(1-\cos^2 q)^{1/2}]}{-1+\cosh[\beta c_1(1-\cos^2 q)^{1/2}]}\right] \quad \text{1 dim.}$$

$$\langle Hint\rangle = -\frac{N}{2}\sqrt{\frac{2\pi^2 t}{U\log\left(\frac{2\pi^2 t}{\sigma_0' U}\right)}}\,\frac{\sigma_0' U}{2}\,\frac{1}{(\pi/2)^2}\int_0^{\pi/2}\frac{dq_x dq_y}{(1-\cos^2 q_x\cdot\cos^2 q_y)^{1/2}}\left[\frac{\sinh[\beta c_2(1-\cos^2 q_x\cdot\cos^2 q_y)^{1/2}]}{-1+\cosh[\beta c_2(1-\cos^2 q_x\cdot\cos^2 q_y)^{1/2}]}\right] \quad \text{2 dim.}$$

$$\langle Hint\rangle = -\frac{N}{2}\sqrt{\frac{4\pi^3 t}{U\log^2\left(\frac{2\pi^3 t}{\sigma_0' U}\right)}}\,\frac{\sigma_0' U}{2}\,\frac{1}{(\pi/2)^3}\int_0^{\pi/2}\frac{dq_x dq_y dq_z}{(1-\cos^2 q_x\cdot\cos^2 q_y\cdot\cos^2 q_z)^{1/2}}\left[\frac{\sinh[\beta c_3(1-\cos^2 q_x\cdot\cos^2 q_y\cdot\cos^2 q_z)^{1/2}]}{-1+\cosh[\beta c_3(1-\cos^2 q_x\cdot\cos^2 q_y\cdot\cos^2 q_z)^{1/2}]}\right] \quad \text{3 dim.}$$

We only notice that the same integrations appear when we calculate the anti-ferromagnetic Heisenberg model.

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