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A study of the Hubbard-Hirsch model within the Hartree-Fock Approximation (HFA)

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Abstract

Based on the Hubbard-Hirsch model, we studied the dynamical susceptibility and spin excitation of an itinerant electron system within the Hartree-Fock Approximation (HFA) by using a Green's function technique. We are able to arrive at the same results obtained by Zhang et al [1] who employed a Random-Phase Approximation (RPA).

1.0 Introduction

This paper shall be concerned with instability resulting from the repulsive Coulomb interactions. This is particularly likely to occur when the ionic potentials lead to the formation of narrow energy bands, and it can take various forms which, for a rigid lattice, are all magnetic in character. The effect of the instability is to produce a fundamental change in the symmetry of the ground state of the interacting system. The emphasis here shall be on the simplest form of the magnetic instability, namely ferromagnetism.

A more subtle form of instability occurs when the Coulomb interaction is localized at a point impurity inserted in the metal [1]. Here the instability is not a sharp one as in the uniform ferromagnetic case, but a gradual one which leads to new types of low-lying excitations in the system associated with the formation of a local magnetic moment.

As mentioned above, the band structure of a metal has an important influence on the stability of the electron gas in the metal. In order to discuss band structure effects, it is not enough to consider the simple Coulomb gas in a positive background, and one requires a theory of correlations, which takes into account the atomic structure of the solid [2]. In the presence of the ions the Coulomb problem becomes much more complicated owing to the multiband nature which is an essential feature in, say, the d-electrons of transition metals. An important physical simplification was introduced by J. Hubbard (1963) who pointed out that it is the short-ranged part of the Coulomb interaction which is dominant in leading to the instability [3].

He therefore proposed a model in which the electrons are considered to be in a narrow energy band with Bloch energies $\in_p$. Adopting the Wannier wave functions for an electron at site i

$$\psi_i(X) = N^{-1/2} \sum_{\vec{p}\in Zone} \exp(ip\cdot x_1)\, \psi_{\vec{p}}(X) \qquad (1.1)$$

where $\psi_p(X)$ are the Bloch states, and using the usual anticommutating properties of the Wannier destruction and creation operators, we can write the interaction Hamiltonian as

$$H_1 = UN + U\sum_i n_{i\uparrow}\, n_{i\downarrow} \qquad (1.2)$$

This automatically embodies the Pauli principle by asserting that only electrons of opposite spin will interact. It is this effect which leads to ferromagnetism, by aligning their spins the electrons can lower the strength of the repulsive potential.

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Recently, Hirsch [4-6] proposed that certain two-centre matrix elements that arise in the derivation of the Hubbard Hamiltonian from first-principles calculations play a fundamental role in metallic ferromagnetism. Hirsch was able to show that when one electron is in the bonding state and other in the antibonding state, the contribution of the exchange integral J to the Coulomb energy is negative. The final effect of including these extra matrix elements lead us to the so called Hubbard-Hirsch Hamiltonian. Zhang et al [1] have employed this Hamiltonian to study metallic ferromagnetism within the Random Phase Approximation. In this paper, we furnish an alternative derivation of the main result obtained by Zhang et. al. [1].

2.0 Dynamical Susceptibility

The Hubbard-Hirsch Hamiltonian is expressed as:

$$H = \sum_{ij\sigma} t_{ij}\, C^{+}_{i\sigma}\, C_{j\sigma} + \tfrac{1}{2}U \sum_{i\sigma} n_{i\sigma}\, n_{i-\sigma} + J \sum_{\langle ij\rangle\, \sigma\sigma'} C^{+}_{i\sigma} C^{+}_{j\sigma'}\, C_{i\sigma'}\, C_{j\sigma} \qquad (2.1)$$

where t_{ij} is the hopping integral, U is the Hubbard on-site repulsion, and J is an off diagonal matrix element of the Coulomb interaction between electrons on nearest-neighbour sites. Both U and J are taken to the positive. By Fourier transformation one can obtain the expression of the Hubbard-Hirsch Hamiltonian in the energy momentum space,

$$H = \sum_{k,\sigma} \in_{k}\, C^{+}_{k\sigma} C_{k\sigma} + \frac{U}{N} \sum_{K,K',q} C^{+}_{K+q,\uparrow}\, C_{K'-q\downarrow}\, C_{K'\downarrow}\, C_{K\uparrow} + \frac{JZ}{N} \sum_{KK'q\sigma\sigma'} Y_q\, C^{+}_{K+q\sigma}\, C_{K'-q\sigma'}\, C_{K\sigma'}\, C_{K'\sigma} \qquad (2.2)$$

where

$$Y_q = \frac{1}{Z} \sum_{\sigma} \exp(iq\delta) \qquad (2.3)$$

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

In order to calculate the dynamical susceptibility of the spin system, the spin densities where used:

$$\left.\begin{aligned} \tilde{S}^{+}_{(-q)} &= \sum_{k} C^{+}_{k-q,\uparrow}\, C_{k\downarrow} \\ \tilde{S}^{-}_{(q)} &= \sum_{k} C^{+}_{k+q\downarrow} C_{k\uparrow} \end{aligned}\right\} \qquad (2.4)$$

To evaluate the Green's function

$$\chi^{-+}(k,q;t) = i\theta(t) \left\langle \left[C^{+}_{k+q\downarrow} C_{k\uparrow}, \tilde{S}^{+}(-q) \right] \right\rangle ,$$

we have adopted the equation of motion approach and solved it within a generalized Hartree-Fock Approximation (HFA). Clearly, the first derivative of the Green's Function is

$$i\frac{\partial}{\partial t}\chi^{-+}(k,q;t) = -\delta(t) \left\langle \left[C^{+}_{k+q\downarrow} C_{k\uparrow}, \tilde{S}^{+}(-q) \right] \right\rangle + i\theta(t) \left\langle \left[H, C^{+}_{k+q\downarrow} C_{k\uparrow} \right]; \tilde{S}^{+}(-q) \right\rangle \qquad (2.5)$$

From equation (2.2) above, the Hubbard-Hirsch Hamiltonian can be decoupled thus:

$$H = H_0 + H_1 + H_2$$

where $H_0 = \sum_{k\sigma} \varepsilon_k\, C^{+}_{k\sigma} C_{k\sigma}$

$$H_1 = \frac{U}{N} \sum_{kk'q} C^{+}_{k+q\uparrow}\, C_{k'-q\downarrow}\, C_{k'\downarrow}\, C_{k\uparrow} \text{ and } H_2 = \frac{JZ}{N} \sum_{kk'q\sigma\sigma'} Y_q\, C^{+}_{k+q\sigma}\, C^{+}_{k'-q\sigma'}\, C_{k\sigma'}\, C_{k'\sigma}$$

Now the first term of the RHS of equation (2.5), after some algebra, becomes

$$\delta(t) \left\langle \left[C^{+}_{k+q\downarrow} C_{k\uparrow}, \tilde{S}^{+}(-q) \right] \right\rangle = F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})} \qquad (2.6)$$

while the 2nd term becomes

$$i\theta(t) \left\langle \left[H, C^{+}_{k+q\downarrow} C_{k\uparrow} \right]; \tilde{S}^{+}(-q) \right\rangle = i\theta(t) \left\langle \left[H_0, C^{+}_{k+q\downarrow} C_{k\uparrow} \right] + \left[H_1, C^{+}_{k+q\downarrow} C_{k\uparrow} \right] + \left[H_2, C^{+}_{ki+q\downarrow} C_{k\uparrow} \right]; \tilde{S}^{+}(-q) \right\rangle$$

Invoking the generalized HFA which consists in replacing in the products of four operators, all pairs of type $C^{+}C$ by their expectation values and taking the sum over all averages, paying due regard to sign changes arising from changes in the order of anticommuting factors, and using the result

$$\left\langle C^{+}_{k\alpha} C_{k'\beta} \right\rangle = \delta_{kk'}\, \delta_{\alpha\beta}\, F_{(\in k\alpha)}$$

we get

$$\left\langle \left[H_0, C^{+}_{k+q\downarrow} C_{k\uparrow} \right]; \tilde{S}^{+}(-q) \right\rangle = \left\langle -\left(\in_{k} - \in_{k+q} \right) C^{+}_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^{+}(-q) \right\rangle$$

$$\left\langle \left[H_1, C^+_{k+q\downarrow} C_{k\uparrow}\right]; \tilde{S}^+(-q)\right\rangle = \left\langle \left[\frac{U}{N}\sum_{k'} \begin{Bmatrix} \left(F_{(\in_{k+q\downarrow})} - F_{\in_{k\uparrow}}\right) C^+_{k+k'+q\downarrow} C_{k+k'\uparrow} \\ +\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow})}\right) C^+_{k+q\downarrow} C_{k\uparrow} \end{Bmatrix}; \tilde{S}^+_{(-q)} \right] \right\rangle$$

and $$\left\langle \left[H_2, C^+_{k+q\downarrow} C_{k\uparrow}\right]; \tilde{S}^+(-q)\right\rangle = \left\langle \left[\frac{2JZ}{N} Y_q \sum_{k'} \begin{Bmatrix} \left(F_{(\in_{k\uparrow}')} - F_{(\in_{k'\downarrow})}\right) C^+_{k+q\downarrow} C_{k\uparrow} \\ +\left(F_{(\in_{k+q\downarrow})} - F_{(\in_{k\downarrow})}\right) C^+_{k+q\downarrow} C_{k\uparrow} \end{Bmatrix}; \bar{S}^+_{(-q)} \right] \right\rangle$$

Collecting together the various components, we get $w\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle = F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})} - \left(\in_k - \in_{k+q}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w$

$$+\left(F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}\right)\frac{U}{N}\sum_{k'}\left\langle C^+_{k+k'+q\downarrow} C_{k+k'\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

$$+\frac{U}{N}\sum_{k'}\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow})}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w + \frac{2JZ}{N} Y_q \sum_{k'}\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow})}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

$$+\frac{2JZ}{N} Y_q \sum_{k'}\left(F_{(\in_{k+q\downarrow})} - F_{(\in_{k'\uparrow})}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

which can be further simplified to

$$w\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w + \left(\in_k - \in_{k+q}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w - \frac{U}{N}\sum_{k'}\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow})}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

$$+\frac{2JZ}{N} Y_q \sum_{k'}\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow})}\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w = F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})} + \left(F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}\right)\frac{U}{N}\sum_{k'}\left\langle C^+_{k+k'+q\downarrow} C_{k+k'\downarrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

$$F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}\frac{2JZ}{N} Y_q \sum_{k}\left\langle C^+_{k+q\downarrow} C_{k\downarrow}; \tilde{S}^+_{(-q)}\right\rangle_w$$

Factorizing, and introducing the spin densities we have;

$$\left\{W - \left(\in_{k+q} - \in_k\right) - \left(\frac{U}{N} + \frac{2JZ}{N} Y_q\right)\sum_{k'}\left(F_{(\in_{k'\uparrow})} - F_{(\in_{k'\downarrow}}\right)\right\}\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w =$$

$$F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}\left\{1 + \left(\frac{U}{N} + \frac{2JZ}{N} Y_q\right)\left\langle \tilde{S}^-_{(q)}; \tilde{S}^+_{(-q)}\right\rangle\right\}_w \qquad (2.7)$$

Now define the modified one-particle energy (modified by the exchange self energy), where

$$\in_{k\uparrow} = \in_k - \left(\frac{U}{N} + \frac{2JZ}{N} Y_q\right)\sum_{k'} F_{(\in_{k'\uparrow})} \quad \text{and} \quad \in_{k+q\downarrow} = \in_{k+q} - \left(\frac{U}{N} - \frac{2JZ}{N} Y_q\right)\sum_{k'} F_{(\in_{k'\downarrow})}$$

Equation (2.7) reduces to

$$\left(W - \left(\in_{k+q\downarrow} - \in_{k\uparrow}\right)\right)\left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w = \left(F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}\right)\left\{1 + \left(\frac{U}{N} + \frac{2JZ}{N} Y_q\right)\left\langle \tilde{S}^-_{(q)}; \tilde{S}^+_{(-q)}\right\rangle_w\right.$$

$$\therefore \quad \left\langle C^+_{k+q\downarrow} C_{k\uparrow}; \tilde{S}^+_{(-q)}\right\rangle_w = \frac{F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}}{W - \left(\in_{k+q\downarrow} - \in_{k\uparrow}\right)}\left\{1 + \left(\frac{U}{N} + \frac{2JZ}{N} Y_q \left\langle \tilde{S}^-_{(q)}; \tilde{S}^+_{(-q)}\right\rangle\right)\right\} W - \left(\in_{k+q\downarrow} - \in_{k\uparrow}\right)$$

Summing over all wave numbers in the equation above, we have:

$$\left\langle \tilde{S}^-_{(q)} \middle| \tilde{S}^+_{(-q)}\right\rangle_w = \Gamma^{-+}_{(q,w)}\left[1 + \left(\frac{U}{N} + \frac{2JZ}{N} Y_q\right)\left\langle \tilde{S}^-_{(q)} \middle| \tilde{S}^+_{(-q)}\right\rangle_w\right] \qquad (2.8)$$

where $\Gamma^{-+}_{(q,w)} = \sum_k \frac{F_{(\in_{k+q\downarrow})} - F_{(\in_{k\uparrow})}}{W - \left(\in_{k+q\downarrow} - \in_{k\uparrow}\right) + io^+}$

From equation (2.8), collecting like terms, we have:

$$\left\langle \tilde{S}^{-}_{(q)} \,|\tilde{S}^{+}_{(-q)} \right\rangle_{w} \left[1 - \left(\frac{U}{N} + \frac{2JZ}{N} Y_q \right) \Gamma^{-+}_{(q,w)} \right] = \Gamma^{-+}_{(q,w)}$$

but $$\left\langle \tilde{S}^{-}_{(q)} \middle| \tilde{S}^{+}_{(-q)} \right\rangle_{w} = \chi^{-+}_{(q,w)}$$

hence $$\chi^{-+}_{(q,w)} = \frac{\Gamma^{-+}_{(q,w)}}{1 - \left(\frac{U}{N} + \frac{2JZ}{N} \right) \Gamma^{-+}_{(q,w)}} \qquad (2.9)$$

Equation (2.9) is the analytic expression for the dynamical susceptibility of the interacting electron gas under the Hubbard-Hirsch model.

3.0 Conclusion

Based on the magnetic excitation in the Hubbard-Hirsch model, we have studied the spin excitation in an itinerant electron system within the Hartree-Fock approximation . Interestingly the result obtained for the dynamical spin susceptibility agrees exactly with the RPA result of Zhang et al [1].

References

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