NOTAS DE FÍSICA
VOLUME XX
Nº 9

REMARKS ON THE CONDITIONS FOR MAGNETIC INSTABILITIES IN ACTINIDES; STRONG CORRELATIONS

by
M.A. Continentino and A.A. Gomes
Centro Brasileiro de Pesquisas Físicas

CENTRO BRASILEIRO DE PESQUISAS FÍSICAS
Av. Wenceslau Braz, 71 - Botafogo - ZC-82
Rio de Janeiro, Brazil
1973

q-dependent magnetic field. In this sense the present work extends the previous calculation of Hubbard and Jain |3| for the strongly correlated transition metal-like system, to the case of a two band (d and f) with intra and interband Coulomb interactions. An essentially different aspect here is that one has d-f hybridization, which has been shown to be of great importance in explaining the magnetic properties of actinide metals |4|. The one electron propagators for this situation have been discussed by the authors |5|, and here we use these results in computing the response to the magnetic field. The plan of this paper is as follows: firstly we discuss briefly the equation of motion for the one-electron propagators in presence of the magnetic field, and this part is a rather trivial generalization of |5|. Secondly the first order correction due to the external field is calculated, and the self-consistency problem approximately solved, giving then the expression for the static, wave-number dependent susceptibility. Finally we search for the poles of the susceptibility in order to obtain the conditions for magnetic instability. It turns out from this procedure a two-band generalization of the criterion of Hubbard and Jain, the effect of the d-f hybridization being then qualitatively discussed.

II - FORMULATION OF THE PROBLEM

We start defining the Hamiltonian we adopt for the actinide metal:

$$\mathcal{H}_0 = \sum_{i,j,\sigma} T^{(d)}_{ij} \overset{+}{d}_{i\sigma} d_{j\sigma} + \sum_{i,j,\sigma} T^{(f)}_{ij} \overset{+}{f}_{i\sigma} f_{j\sigma} + U_d \sum_i n^{(d)}_{i\uparrow} n^{(d)}_{i\downarrow} + U_f \sum_i n^{(f)}_{i\uparrow} n^{(f)}_{i\downarrow} + I_{df} \sum_i \{ n^{(d)}_{i\uparrow} n^{(f)}_{i\downarrow} + n^{(d)}_{i\downarrow} n^{(f)}_{i\uparrow} \} + \sum_{i,\sigma} \{ V_{df} \overset{+}{d}_{i\sigma} f_{i\sigma} + V_{fd} \overset{+}{f}_{i\sigma} d_{i\sigma} \} \qquad (1)$$

where the notation is the usual one |1| and here for simplicity we have assumed k-independent mixing matrix elements. The external, static, wave number dependent magnetic field contributes with the term:

$$\mathcal{H}_1 = h_o \sum_{i,\sigma} \sigma(n_{i\sigma}^{(d)} + n_{i\sigma}^{(f)})\ell^{-iq.R_i} \quad (2)$$

the magnetic field being applied parallel to the Z-axis. Now we firstly obtain the general equations of motion for the one-electron propagators $<<d_{i\sigma};d_{j\sigma}^+>>$ and $<<f_{i\sigma};f_{j\sigma}^+>>_\omega$ in presence of the magnetic field. Then the first order correction due to the external field is obtained, the zero-order solution being discussed in |1|. Firstly we obtain two <u>exact</u> equations for the propagators $<<d_{i\sigma};d_{j\sigma}^+>>$ and $<<f_{i\sigma};d_{j\sigma}^+>>_\omega$; using (1) and (2) one has:

$$\omega << d_{i\sigma}; d_{j\sigma}^+>>_\omega = \frac{1}{2\pi}\delta_{ij} + \sum_\ell T_{i\ell}^{(d)} <<d_{\ell\sigma}; d_{j\sigma}^+>>_\omega + V_{df} <<f_{i\sigma}; d_{j\sigma}^+>>_\omega + h_o\sigma\,\ell^{-iq.R_i} <<d_{i\sigma}; d_{j\sigma}^+>>_\omega + U_d<<n_{i-\sigma}^{(d)} d_{i\sigma}; d_{j\sigma}^+>>_\omega + I_{df}<<n_{i-\sigma}^{(f)} d_{i\sigma};d_{j\sigma}^+>>_\omega \quad (3)$$

$$\omega <<f_{i\sigma}; d_{j\sigma}^+>>_\omega = \sum_\ell T_{i\ell}^{(f)} <<f_{\ell\sigma};d_{j\sigma}^+>>_\omega + V_{fd}<<d_{i\sigma}; d_{j\sigma}^+>>_\omega + h_o\sigma\,\ell^{-iq.R_i}<<f_{i\sigma}; d_{j\sigma}^+>>_\omega + U_f<<n_{i-\sigma}^{(f)}f_{i\sigma}; d_{j\sigma}^+>>_\omega + I_{df}<<n_{i-\sigma}^{(d)}f_{i\sigma}; d_{j\sigma}^+>>_\omega \quad (4)$$

From (3) and (4) one sees that four new propagators are generated by the electron-electron interaction, so now we intend to completely determine each of these propagators.

a) <u>Determination of the propagator</u> $<<n^{(d)}_{i-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}>>_{\omega}$

The equation of motion for this propagator is:

$$\begin{aligned}
\omega << n^{(d)}_{i-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}>>_{\omega} &= \frac{1}{2\pi} <n^{(d)}_{i-\sigma}>\delta_{ij} + U_d << n^{(d)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} + \\
&+ I_{df} << n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} + h_o \sigma\, \ell^{-iq.R_i} << n^{(d)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} + \\
&+ \sum_{\ell} T^{(d)}_{i\ell} << n^{(d)}_{i-\sigma} d_{\ell\sigma}; d^{+}_{j\sigma}>>_{\omega} + \sum_{\ell} T^{(d)}_{i\ell} << \left[d^{+}_{i-\sigma} d_{\ell-\sigma} - d^{+}_{\ell-\sigma} d_{i-\sigma}\right] d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} \\
&\quad V_{df} << n^{(d)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} + V_{df} << d^{+}_{i-\sigma} f_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} - V_{fd} << f^{+}_{i-\sigma} d_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega}
\end{aligned} \tag{5}$$

In the equation (5) there are several new terms; the kinetic terms are Hubbard |2| decoupled, namely:

$$\sum_{\ell} T^{(d)}_{i\ell} << n^{(d)}_{i-\sigma} d_{\ell\sigma}; d^{+}_{j\sigma}>>_{\omega} = <n^{(d)}_{i-\sigma}> \sum_{\ell} T^{(d)}_{i\ell} << d_{\ell\sigma}; d^{+}_{j\sigma}>>_{\omega} \tag{6-a}$$

$$\begin{aligned}
\sum_{\ell} T^{(d)}_{i\ell} << \left[d^{+}_{i-\sigma} d_{\ell-\sigma} - d^{+}_{\ell-\sigma} d_{i-\sigma}\right] d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} &\cong \sum_{\ell} T^{(d)}_{i\ell} \{<d^{+}_{i-\sigma} d_{\ell-\sigma}> - \\
&- < d^{+}_{\ell-\sigma} d_{i-\sigma}>\} << d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega} = <S^{(d)}_{i-\sigma}> << d_{i\sigma}; d^{+}_{j\sigma}>>_{\omega}
\end{aligned} \tag{6-b}$$

The terms associated to the hybridization are of two types; the first one $<<n^{(d)}_{i-\sigma} f_{i\sigma};d^{+}_{j\sigma}>>_{\omega}$ is <u>not</u> decoupled since it appears in equation (4) as generated by the electron correlation, and will be determined separately. The second type of terms are the last two terms of (5), they are decoupled as:

$$V_{df} <<d^{+}_{i-\sigma} f_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} - V_{fd} <<f^{+}_{i-\sigma} d_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} \cong$$

$$\cong \{ V_{df} <d^{+}_{i-\sigma} f_{i-\sigma}> - V_{fd} < f^{+}_{i-\sigma} d_{i-\sigma}>\} <<d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} = \qquad (6\text{-}c)$$

$$= <T_{i-\sigma}> <<d_{i\sigma};d^{+}_{j\sigma}>>_{\omega}$$

Equation (6-c) is just a Hubbard like approximation as in (6-b) and we only perform this type of approximation for V_{df} terms when the corresponding propagators are not generated previously by the electron correlation. One gets then:

$$(\omega-U_d) <<n^{(d)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>> \cong \frac{1}{2\pi} <n^{(d)}_{i-\sigma}>\delta_{ij} + I_{df}<<n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} +$$

$$+ h_o \sigma \, \ell^{-iq.R_i} <<n^{(d)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} + <n^{(d)}_{i-\sigma}> \sum_{\ell} T_{i\ell} <<d_{\ell\sigma};d^{+}_{j\sigma}>>_{\omega} \qquad (7)$$

$$\{ < S^{(d)}_{i-\sigma}> + <T_{i-\sigma}>\} <<d_{i\sigma};d^{+}_{j\sigma}>>_{\omega} + V_{df}<<n^{(d)}_{i-\sigma} f_{i\sigma};d^{+}_{j\sigma}>>_{\omega}$$

In equation (7) one still has two unknown propagators namely

$<< n^{(d)}_{i-\sigma} f^{+}_{i\sigma};d_{j\sigma}>>$ and $<<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega$; the former propagator appears already in equation (4) and will be discussed later on. Now we discuss the equation of motion for $<< n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_\omega$. One has:

$$(\omega-U_d-I_{df}) <<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega = \frac{1}{2\pi} <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}> \delta_{ij} +$$

$$+ \sum_\ell T^{(d)}_{i\ell} <<n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{\ell\sigma};d^{+}_{j\sigma}>>_\omega + \sum_\ell T^{(d)}_{i\ell} <<\left[d^{+}_{i-\sigma}d_{\ell-\sigma} - d^{+}_{\ell-\sigma} d_{i-\sigma}\right]n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_\omega$$

$$+ \sum_\ell T^{(f)}_{i\ell} << \left[f^{+}_{i-\sigma} f_{\ell-\sigma} - f^{+}_{\ell-\sigma} f_{i-\sigma}\right] n^{(d)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_\omega +$$

$$+ V_{df} <<n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma};d^{+}_{j\sigma}>>_\omega + h_o\sigma\, \ell^{-iq.R_i} <<n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma} >>_\omega$$

$$+ V_{df} <<d^{+}_{i-\sigma}f_{i-\sigma}n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_\omega - V_{fd}<<f^{+}_{i-\sigma}d_{i-\sigma}n^{(f)}_{i-\sigma} d_{i\sigma};d^{+}_{j\sigma}>>_\omega$$

$$+ V_{fd} <<n^{(d)}_{i-\sigma}f^{+}_{i-\sigma} d_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega - V_{df}<<n^{(d)}_{i-\sigma}d^{+}_{i-\sigma}f_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega \qquad (8)$$

Now the terms involving kinetic energy are easily decoupled as follows:

$$\sum_\ell T^{(d)}_{i\ell} <<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{\ell\sigma};d^{+}_{j\sigma}>>_\omega \cong <n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma}> \sum_\ell <<T^{(d)}_{i\ell} <<d_{\ell\sigma};d^{+}_{j\sigma}>>_\omega \qquad (9\text{-a})$$

$$\sum_{\ell} T^{(d)}_{i\ell} \ll \left[d^{+}_{i-\sigma}d_{\ell-\sigma}-d^{+}_{\ell-\sigma}d_{i-\sigma}\right] n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \cong \langle S^{(d)}_{i-\sigma}\rangle \ll n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \quad (9\text{-b})$$

$$\sum_{\ell} T^{(f)}_{i\ell} \ll \left[f^{+}_{i-\sigma}f_{\ell-\sigma}-f^{+}_{\ell-\sigma}f_{i-\sigma} \right] n^{(d)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \cong \langle S^{(f)}_{i-\sigma}\rangle \ll n^{(d)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \quad (9\text{-c})$$

The last four terms involving V_{df} matrix elements can be handled <u>exactly</u> just using the properties of the d and f operators. One has:

$$\ll f^{+}_{i-\sigma}d_{i-\sigma}n^{(f)}_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} = - \ll d_{i-\sigma}f^{+}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \equiv 0 \qquad (9\text{-d})$$

since $f^{+}_{i-\sigma}\, n^{(f)}_{i-\sigma} = 0$; similarly

$$\ll n^{(d)}_{i-\sigma}\, f^{+}_{i-\sigma}\, d_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} \equiv 0 \qquad (9\text{-e})$$

Since $n^{(d)}_{i-\sigma}\, d_{i-\sigma} = 0$

Finally:

$$\ll d^{+}_{i-\sigma}\, f_{i-\sigma}\, n^{(f)}_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} = \ll d^{+}_{i-\sigma}\, f_{i-\sigma}\, d_{i\sigma}\, ;d^{+}_{j\sigma}\gg_{\omega}$$

$$(9\text{-f})$$

$$\ll n^{(d)}_{i-\sigma}\, d^{+}_{i-\sigma}\, f_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega} = \ll d^{+}_{i-\sigma}\, f_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}\gg_{\omega}$$

Then all of these terms cancel out, and equation (8) can be rewritten as:

$$(\omega-U_d-I_{df}) <<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}>>_\omega \cong \frac{1}{2\pi} <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}> +$$

$$+ <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}> \sum_\ell T^{(d)}_{i\ell} <<d_{\ell\sigma};d^{+}_{j\sigma}>>_\omega + <S^{(f)}_{i-\sigma}> <<n^{(d)}_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}>>_\omega +$$

$$+ <S^{(d)}_{i-\sigma}> <<n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega + V_{df} <<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma};d^{+}_{j\sigma}>>_\omega +$$

$$+ h_o\sigma\, \ell^{-iq.R_i} <<n^{(d)}_{i-\sigma}\, n^{(f)}_{i-\sigma}\, d_{i\sigma};d^{+}_{j\sigma}>>_\omega \qquad (10)$$

Now everything in equation (10) is known or will have an equation of motion, including the propagator $<<n^{(d)}_{i-\sigma}\, n^{(f)}_{i-\sigma}\, f_{i\sigma};\, d^{+}_{j\sigma}>>_\omega$ which will appear naturally as resulting from the Coulomb repulsion in subsequent equations. Then (10) and (7) complete the determination of the propagator $<< n^{(d)}_{i-\sigma}\, d_{i\sigma};\, d^{+}_{j\sigma}>>_\omega$

b) <u>Determination of the propagator</u> $<<n^{(f)}_{i-\sigma}\, d_{i\sigma};\, d^{+}_{j\sigma}>>_\omega$

The equation of motion is:

$$(\omega-I_{df}) <<n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega = \frac{1}{2\pi} <n^{(f)}_{i-\sigma}> \delta_{ij} + U_d<<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma};d^{+}_{j\sigma}>>_\omega +$$

$$\sum_\ell T^{(d)}_{i\ell} <<n^{(f)}_{i-\sigma}d_{\ell\sigma};d^{+}_{j\sigma}>>_\omega + \sum_\ell T^{(f)}_{i\ell} <<\left[f^{+}_{i-\sigma}f_{\ell-\sigma}-f^{+}_{\ell-\sigma}f_{i-\sigma}\right]d_{i\sigma};d^{+}_{j\sigma}>>_\omega +$$

$$+ h_o \sigma \ell^{-iq.R_i} \langle\langle n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + V_{df} \langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ V_{fd} \langle\langle f^+_{i-\sigma} d_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega - V_{df} \langle\langle d^+_{i-\sigma} f_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega \qquad (11)$$

Now the kinetic terms are decoupled as in (6-a) and the last two terms involving mixing are decoupled as in (6-c).

We retain without decoupling the propagator $\langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega$ since it appears naturally in equation (4) generated by the Coulomb repulsion, and the propagator $\langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega$ was determined in equation (10). Then equation (11)becomes:

$$(\omega - I_{df}) \langle\langle n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega = \frac{1}{2\pi} \langle n^{(f)}_{i-\sigma} \rangle \delta_{ij} + U_d \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ \langle n^{(f)}_{i-\sigma} \rangle \sum_\ell T^{(d)}_{i\ell} \langle\langle d_{\ell\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + h_o \sigma \ell^{-iq.R_i} \langle\langle n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ V_{df} \langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + \{ \langle S^{(f)}_{i-\sigma} \rangle - \langle T_{i-\sigma} \rangle \} \langle\langle d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega . \qquad (12)$$

c) <u>Determination of the propagators</u> $\langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega$

The equation of motion is:

$$(\omega - I_{df}) \langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega = U_f \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + \sum_\ell T^{(f)}_{i\ell} \langle\langle n^{(d)}_{i-\sigma} f_{\ell\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ h_0 \sigma\, e^{-iq.R_i} \langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega + \sum_\ell T^{(d)}_{i\ell} \langle\langle \left[d^{+}_{i-\sigma} d_{\ell-\sigma} - d^{+}_{\ell-\sigma} d_{i-\sigma} \right] f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega +$$

$$+ V_{fd} \langle\langle n^{(d)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega + V_{df} \langle\langle d^{+}_{i-\sigma} f_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega - V_{fd} \langle\langle f^{+}_{i-\sigma} d_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega \tag{13}$$

Here we conserve the propagator $\langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega$ without decoupling, the kinetic and the last two hybridization terms being decoupled as usually. The final results is:

$$(\omega - I_{df}) \langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega = U_f \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega + \langle n^{(d)}_{i-\sigma} \rangle \sum_\ell T^{(f)}_{i\ell} \langle\langle f_{\ell\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega +$$

$$+ \{ \langle S^{(d)}_{i-\sigma} \rangle + \langle T_{i-\sigma} \rangle \} \langle\langle f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega + V_{fd} \langle\langle n^{(d)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega +$$

$$+ h_0 \sigma\, e^{-iq.R_i} \langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega \tag{14}$$

Now it remains to determine the propagator $\langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega$; one has:

$$(\omega - U_f - I_{df}) \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega = \sum_\ell T^{(f)}_{i\ell} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{\ell\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega +$$

$$+ \sum_\ell T^{(d)}_{i\ell} \langle\langle \left[d^{+}_{i-\sigma} d_{\ell-\sigma} - d^{+}_{\ell-\sigma} d_{i-\sigma} \right] n^{(f)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega +$$

$$+ \sum_\ell T^{(f)}_{i\ell} \langle\langle \left[f^{+}_{i-\sigma} f_{\ell-\sigma} - f^{+}_{\ell-\sigma} f_{i-\sigma} \right] n^{(d)}_{i-\sigma} f_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega + V_{fd} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma}; d^{+}_{j\sigma} \rangle\rangle_\omega$$

$$+ h_o \sigma e^{-iq.R_i} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega \quad (15)$$

Where we have dropped the terms in V_{df} which cancel out exactly as in equation (9). The other terms are Hubbard decoupled to get finally:

$$(\omega - U_f - I_{df}) \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega = \langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} \rangle \sum_\ell T^{(f)}_{i\ell} \langle\langle f_{\ell\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ \langle S^{(d)}_{i-\sigma} \rangle \langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + \langle S^{(f)}_{i-\sigma} \rangle \langle\langle n^{(d)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + V_{fd} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ h_o \sigma e^{-iq.R_i} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega \quad (16)$$

d) <u>Determination of the propagator</u> $\langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega$

The calculation is quite similar to the previous ones so we just quote the results:

$$(\omega - U_f) \langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega = I_{df} \langle\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + \langle n^{(f)}_{i-\sigma} \rangle \sum_\ell T^{(f)}_{i\ell} \langle\langle f_{\ell\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ \{ \langle S^{(f)}_{i-\sigma} \rangle - \langle T_{i-\sigma} \rangle \} \langle\langle f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega + V_{fd} \langle\langle n^{(f)}_{i-\sigma} d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega +$$

$$+ h_o \sigma e^{-iq.R_i} \langle\langle n^{(f)}_{i-\sigma} f_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega \quad (17)$$

As a conclusion of this paragraph one sees that the system of coupled equations (3), (4), (7), (10), (12), (14), (16) and (17) solve completely the problem of determining the one electron propagator $\langle\langle d_{i\sigma}; d^+_{j\sigma} \rangle\rangle_\omega$ in presence of correlations and the external magnetic field. Next step is to obtain the first order correction due to the magnetic field.

III) FIRST ORDER CORRECTION DUE TO h_o : SOLUTION BY FOURIER TRANSFORM

In this paragraph we present the main results of the solution of coupled equations above by Fourier transformation. Equations (3) and (4) to first order in the magnetic field are:

$$(\omega-\varepsilon_k^{(d)})G_{kk'}^{dd(1)}(\omega) = V_{df}\, G_{kk'}^{fd(1)}(\omega) + U_d\, G_{kk'}^{dd,d(1)}(\omega) + I_{df}\, G_{kk'}^{fd,d(1)}(\omega) +$$

$$+ h_o\sigma\, \delta_{k-q,k'}\, g_{k'}^{dd(o)}(\omega) \tag{18-a}$$

and

$$(\omega-\varepsilon_k^{(f)})G_{kk'}^{fd(1)}(\omega) = V_{fd}\, G_{kk'}^{dd(1)}(\omega) + U_f\, G_{kk'}^{ff,d(1)}(\omega) + I_{df}\, G_{kk'}^{df,d(1)}(\omega) +$$

$$+ h_o\sigma\delta_{k-q,k'}\, g_{k'}^{fd(o)}(\omega) \tag{18-b}$$

Now the propagator $G_{kk'}^{dd,d(1)}$ satisfies to first order the following equation:

$$(\omega-U_d)G_{kk'}^{dd,d(1)}(\omega) = \frac{1}{2\Pi}\,\Delta\, n_{kk'}^{-\sigma(d)} + I_{df}\, \langle\langle (n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)} d_{i\sigma})_k ; d_{k'\sigma}^{+}\rangle\rangle_{\omega}^{(1)} +$$

$$+ \langle n_{-\sigma}^{(d)}\rangle\, \varepsilon_k^{(d)}\, G_{kk'}^{dd(1)}(\omega) + V_{df}\, G_{kk'}^{df,d(1)}(\omega) + \{\, \Delta n_{kk'}^{-\sigma(d)}\, \varepsilon_{k'}^{(d)} + \Delta S_{kk'}^{-\sigma(d)} +$$

$$+ \Delta T_{kk'}^{-\sigma}\,\}\, g_{k'}^{dd(o)}(\omega) + h_o\sigma\, \delta_{k-q,k'}\, g_{k'}^{dd,d(o)}(\omega) \tag{19-a}$$

and this equation should be simultaneously solved together with:

$$(\omega-U_d-I_{df})<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(1)} = \frac{1}{2\Pi}<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}>^{(1)}_{kk'} +$$

$$+ <n^{(d)}_{-\sigma}n^{(f)}_{-\sigma}>\varepsilon^{(d)}_k G^{dd(1)}_{kk'}(\omega) + V_{df}<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(1)}_{\omega}$$

$$+ <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}>^{(1)}_{kk'}\varepsilon^{(d)}_{k'}g^{dd(o)}_{k'}(\omega) + \Delta S^{-\sigma(f)}_{kk'}g^{dd,d(o)}_{k'}(\omega) + \Delta S^{-\sigma(d)}_{kk'}g^{fd,d(o)}_{k'}(\omega) +$$

$$+ h_o\sigma\,\delta_{k-q,k'}<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(o)}_{\omega} \qquad (19\text{-b})$$

which in turn should be simultaneously solved together with:

$$(\omega-U_f-I_{df})<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(1)}_{\omega} = <n^{(d)}_{-\sigma}n^{(f)}_{-\sigma}>\varepsilon^{(f)}_k G^{fd(1)}_{kk'}(\omega) +$$

$$+ V_{fd}<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(1)} + <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}>^{(1)}_{kk'}\varepsilon^{(f)}_{k'}g^{fd(o)}_{k'}(\omega) +$$

$$+ \Delta S^{-\sigma(d)}_{kk'}g^{ff,d(o)}_{k'}(\omega) + \Delta S^{-\sigma(f)}_{kk'}g^{df,d(o)}_{k'}(\omega) + h_o\sigma\,\delta_{k-q,k'}<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma})_k;$$

$$;d^{+}_{k'\sigma}>>^{(o)}_{\omega} \qquad (19\text{-c})$$

Since the propagators to zero order in the magnetic field are known (cf.[5]) equations (19-c) and (19-b) completely determine the propagators $<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d_{i\sigma})k,d^{+}_{k'\sigma}>>^{(1)}_{\omega}$ and $<<(n^{(d)}_{i-\sigma}\,n^{(f)}_{i-\sigma}\,f_{i\sigma})_k;d^{+}_{k'\sigma}>>^{(1)}_{\omega}$ in terms of

$G^{dd(1)}_{kk'}(\omega)$ and $G^{fd(1)}_{kk'}(\omega)$. Substituing this result in (19-a) one gets $G^{dd,d(1)}_{kk'}(\omega)$ in terms of these propagators, $G^{df,d(1)}_{kk'}(\omega)$ and known quantities. Now the propagator $G^{df,d(1)}_{kk'}(\omega)$ satisfies:

$$(\omega-I_{df})G^{df,d(1)}_{kk'}(\omega) = U_f\langle\langle(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f^{+}_{i\sigma})_k;d^{(1)}_{k'\sigma}\rangle\rangle_\omega + \langle n^{(d)}_{-\sigma}\rangle\varepsilon^{(f)}_k G^{fd(1)}_{kk'}(\omega) +$$

$$+ V_{fd}G^{dd,d(1)}_{kk'}(\omega)+\left[\Delta n^{-\sigma(d)}_{kk'}\varepsilon^{(f)}_{k'} + \Delta S^{-\sigma(d)}_{kk'} + \Delta T^{-\sigma}_{kk'}\right]g^{fd(o)}_{k'}(\omega) +$$

$$h_o\sigma\,\delta_{k-q,k'}\,g^{df,d(o)}_{k'}(\omega) \qquad (19\text{-d})$$

Then one sees that equation (19-d) substituted in (19-a) together with the solutions for (19-b) and (19-c) completely specify $G^{dd,d(1)}_{kk'}(\omega)$ in terms of known quantities, $G^{dd(1)}_{kk'}$ and $G^{fd(1)}_{kk}(\omega)$. Next step is to determine $G^{fd,d(1)}_{kk'}(\omega)$ which appears in equation (18-a); this propagator satisfies:

$$(\omega-I_{df})G^{fd,d(1)}_{kk'}(\omega) = \frac{1}{2\Pi}\Delta n^{-\sigma(f)}_{kk'} + U_d\langle\langle(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}d^{+}_{i\sigma})_k;d^{(1)}_{k'\sigma}\rangle\rangle_\omega +$$

$$+ \langle n^{(f)}_{-\sigma}\rangle\varepsilon^{(d)}_k G^{dd(1)}_{kk'}(\omega) + V_{df}G^{ff,d(1)}_{kk'}(\omega) + \{\Delta n^{-\sigma(f)}_{kk'}\varepsilon^{(d)}_{k'} + \Delta S^{-\sigma(f)}_{kk'} -$$

$$-\Delta T^{-\sigma}_{kk'}\}\,g^{dd(o)}_{k'}(\omega) + h_o\sigma\,\delta_{k-q,k'}\,g^{fd,d(o)}_{k'}(\omega) \qquad (20\text{-a})$$

Equation (20-a) involves also the propagator $G^{ff,d(1)}_{kk'}(\omega)$ which in turn satisfies the following equation of motion:

$$(\omega-U_f)G^{ff,d(1)}_{kk'}(\omega) = I_{df}<<(n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma})^{(1)}_k;d_{k'\sigma}>>_\omega + <n^{f}_{-\sigma}>\varepsilon^{(f)}_k G^{fd(1)}_{kk'}(\omega) +$$

$$+ V_{fd}G^{fd,d(1)}_{kk'}(\omega)+\{\Delta n^{-\sigma(f)}_{kk'}\varepsilon^{(f)}_{k'} + \Delta S^{-\sigma(f)}_{kk'} - \Delta T^{-\sigma}_{kk'}\} g^{fd\,(o)}_{k'}(\omega) +$$

$$+ h_o\sigma\,\delta_{k-q,k'}\,g^{ff,d(o)}_{k'}(\omega) \tag{20-b}$$

Equation (20-b) substituted in (20-a) solves for $G^{fd,d}_{kk'}(\omega)$ in terms of $G^{dd(1)}_{kk'}$ and $G^{fd(1)}_{kk'}$ provided one makes use of the solution of (19-b) and (19-c). Substituing all these results in equation (18-a) one obtains the propagator $G^{dd(1)}_{kk'}(\omega)$ in terms of $G^{fd(1)}_{kk'}(\omega)$ and known quantities of zero order. The result is however very complicated and at this point we introduce the strong correlation limit namely: $U_f, U_d \to \infty$ and $I_{df} \to \infty$. By this limit we mean physically that the Coulomb repulsions are very large as compared to the band width. Introducing the definitions:

$$\alpha^{-\sigma} = <n^{(d)}_{-\sigma}> + <n^{(f)}_{-\sigma}> - <n^{(d)}_{-\sigma}n^{(f)}_{-\sigma}> \tag{21-a}$$

and

$$\Delta\,\alpha^{-\sigma}_{kk'} = \Delta n^{-\sigma(d)}_{kk'} + \Delta n^{-\sigma(f)}_{kk'} - <n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}>^{(1)}_{kk'} \tag{21-b}$$

one gets for the $G^{dd(1)}_{kk'}(\omega)$ propagator in the infinite repulsion limit the result:

$$\{\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})\}\, G_{kk'}^{dd(1)}(\omega) = h_o\sigma\, \delta_{k-q,k'}\, g_{k'}^{dd(o)}(\omega) - \frac{1}{2\Pi}\Delta\alpha_{kk'}^{-\sigma} -$$

$$\{\Delta\,\alpha_{kk'}^{-\sigma}\,\varepsilon_{k'}^{(d)} + \Delta\,S_{kk'}^{-\sigma(d)} + \Delta\,S_{kk'}^{-\sigma(f)}\}\; g_{k'}^{dd(o)}(\omega) + V_{df}\, G_{kk'}^{fd(1)}(\omega) \qquad (22)$$

Equation (22) shows a great similarity with previously obtained results |1| |3| , |6| and it is the first step of the complete determination of the first order correction. Now we return back to equation (18-b) in order to calculate $G_{kk'}^{fd(1)}(\omega)$ in terms of $G_{kk'}^{dd(1)}(\omega)$. In order to perform this calculations one just needs to use equations (20-b), (20-a), equation (19-d) and the coupled equations (19-b) and (19-c). Performing the algebra and taking the limits one obtains:

$$\{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\}\, G_{kk'}^{fd(1)}(\omega) = V_{fd}\, G_{kk'}^{dd(1)}(\omega) + h_o\sigma\, \delta_{k-q,k'}\, g_{k'}^{fd(o)}(\omega) -$$

$$-\{\Delta\,\alpha_{kk'}^{-\sigma}\,\varepsilon_{k'}^{(f)} + \Delta\,S_{kk'}^{-\sigma(d)} + \Delta\,S_{kk'}^{-\sigma(f)}\}\; g_{k'}^{fd(o)}(\omega) \qquad (23)$$

Equations (22) and (23) solve then the problem of determining the first order correction in the propagator $G_{kk'}^{dd(1)}(\omega)$ due to the magnetic field. The explicit form for this correction is obtained substituing (23) in (22); if one defines:

$$\bar{g}_k^{dd}(\omega) = \frac{1}{\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma}) - \dfrac{|V_{df}|^2}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})}} = \frac{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})}{\left[\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right]-|V_{df}|^2} \qquad (24\text{-a})$$

and

$$g_k^{dd(o)}(\omega) = \frac{1}{2\Pi}(1-\alpha^{-\sigma})\bar{g}_k^{dd}(\omega) \tag{24-b}$$

and using the results of |5| , namely:

$$g_k^{fd(o)}(\omega) = \frac{V_{fd}}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})} g_k^{dd(o)}(\omega) \tag{24-c}$$

one gets for the propagator:

$$G_{kk'}^{dd(1)}(\omega) = -\frac{1}{2\Pi}\bar{g}_k^{dd}(\omega)\,\Delta\alpha_{kk'}^{-\sigma} - \frac{1}{2\Pi}\bar{g}_k^{dd}(\omega)(1-\alpha^{-\sigma})\,\{-h_o\sigma\delta_{k-q,k'} +$$

$$+\Delta\alpha_{kk'}^{-\sigma}\varepsilon_{k'}^{(d)} + \Delta S_{kk'}^{-\sigma(d)} + \Delta S_{kk'}^{-\sigma(f)}\}\,\bar{g}_k^{dd}(\omega) +$$

$$+\frac{1}{2\Pi}|V_{df}|^2\,\bar{g}_k^{dd}(\omega)\frac{(1-\alpha^{-\sigma})}{[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})]\,[\omega-\varepsilon_{k'}^{(f)}(1-\alpha^{-\sigma})]}\{h_o\sigma\,\delta_{k-q,k'}-\Delta\alpha_{kk'}^{-\sigma}\,\varepsilon_{k'}^{(f)} -$$

$$-\Delta S_{kk'}^{-\sigma(d)} - \Delta S_{kk'}^{-\sigma(f)}\}\,\bar{g}_{k'}^{dd}(\omega) \tag{25}$$

A quite similar expression can be obtained for the $G_{kk'}^{ff(1)}(\omega)$ propagator, just by making $d \rightarrow f$ and $f \rightarrow d$ in expression (25). It should be noted that the terms $\Delta T_{kk'}^{-\sigma}$ cancel out in the calculation, as it can be verified in equations (19-a) and (20-a) where they appear with opposite signs.

IV) SELF-CONSISTENCY PROBLEM: CALCULATION OF THE STATIC SUSCEPTIBILITY

We now take $k' = k$ and $k = k + q$ in equation (25) and remember that $\Delta n_{kk'}^{-\sigma(\alpha)} = \Delta n_q^{-\sigma(\alpha)}$ and $\Delta S_{kk'}^{-\sigma(\alpha)} = \Delta S_q^{-\sigma(\alpha)}$ $\alpha = d,f$. Using the explicit form of $\Delta\alpha_q^{-\sigma}$ as defined in (21-b) one gets:

$$G_{k+q,k}^{dd(1)}(\omega) = -\frac{1}{2\Pi}\left\{\Delta n_q^{-\sigma(d)} + \Delta n_q^{-\sigma(f)} - \langle n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)}\rangle_q^{(1)}\right\}\bar{g}_{k+q}^{dd}(\omega) -$$

$$-\frac{1}{2\Pi}\bar{g}_{k+q}^{dd}(\omega)(1-\alpha^{-\sigma})\left\{-h_o\sigma + (\Delta n_q^{-\sigma(d)} + \Delta n_q^{-\sigma(f)} - \langle n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)}\rangle_q^{(1)})\varepsilon_k^{(d)} +\right.$$

$$\left. + \Delta S_q^{-\sigma(d)} + \Delta S_q^{-\sigma(f)}\right\}\bar{g}_k^{dd}(\omega) + \frac{1}{2\Pi}|V_{df}|^2\,\bar{g}_{k+q}^{dd}(\omega) \quad X$$

$$X\,\frac{1-\alpha^{-\sigma}}{\left[\omega-\varepsilon_{k+q}^{(f)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right]}\left\{h_o\sigma - (\Delta n_q^{-\sigma(d)} + \Delta n_q^{-\sigma(f)} - \langle n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)}\rangle_q^{(1)})\varepsilon_k^{(f)}\right.$$

$$\left. - \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)}\right\}\bar{g}_k^{dd}(\omega) \qquad (26)$$

At this point we introduce an approximation, which although not necessary (cf. |5|), simplifies considerally the mathematics of the problem. This approximation involves the correlation function $\langle n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)}\rangle_q^{(1)}$. Since parallel spin Coulomb correlations are not present we take:

$$\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} \rangle \cong \langle n^{(d)}_{i-\sigma} \rangle \langle n^{(f)}_{i-\sigma} \rangle \tag{27-a}$$

which implies that the first order correction is given by:

$$\langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} \rangle^{(1)} \cong \left(\langle n^{(d)}_{i-\sigma} \rangle \langle n^{(f)}_{i-\sigma} \rangle\right)^{(1)} = \langle n^{(d)}_{-\sigma} \rangle \, \Delta n^{(f)}_{i-\sigma} + \langle n^{(f)}_{-\sigma} \rangle \Delta n^{(d)}_{i-\sigma} \tag{27-b}$$

Using the result (27-b) one gets:

$$\Delta n_q^{-\sigma(d)} + \Delta n_q^{-\sigma(f)} - \langle n^{(d)}_{i-\sigma} n^{(f)}_{i-\sigma} \rangle_q^{(1)} \cong (1-\langle n^{(f)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(f)} \tag{27-c}$$

These results substituted in equation (26) give:

$$G^{dd(1)}_{k+q,k}(\omega) = \frac{1}{2\Pi} \{(1-\langle n^{(f)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(f)} \} \, \bar{g}^{dd}_{k+q}(\omega) -$$

$$- \frac{1}{2\Pi} \bar{g}^{dd}_{k+q}(\omega) \, (1-\alpha^{-\sigma}) \, \{-h_o\sigma + \Big[(1-\langle n^{(f)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(d)} +$$

$$+ (1-\langle n^{(d)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(f)} \Big] \varepsilon_k^{(d)} + \Delta S_q^{-\sigma(d)} + \Delta S_q^{-\sigma(f)} \} \, \bar{g}^{dd}_{k}(\omega) +$$

$$+ \frac{1}{2\Pi} |V_{df}|^2 \, \bar{g}^{dd}_{k+q}(\omega) \frac{1-\alpha^{-\sigma}}{\left[\omega-\varepsilon^{(f)}_{k+q}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon^{(f)}_{k}(1-\alpha^{-\sigma})\right]} \{ h_o\sigma -$$

$$\left[(1-\langle n^{(f)}_{-\sigma} \rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma} \rangle) \, \Delta n_q^{-\sigma(f)} \right] \varepsilon_k^{(f)} -$$

$$- \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)} \} \, \bar{g}^{dd}_k(\omega) \tag{28}$$

A quite similar equation can be obtained for $G^{ff(1)}_{k+q,k}(\omega)$ just by replacing in (28) d by f and f by d. Now we recall the relations:

$$\Delta n_q^{-\sigma(d)} = \sum_k F_\omega \left[G^{dd(1)}_{k+q,k}(\omega) \right]$$

$$\Delta S_q^{-\sigma(d)} = \sum_k \left(\varepsilon^{(d)}_{k+q} - \varepsilon^{(d)}_k\right) F_\omega \left[G^{dd(1)}_{k+q,k}(\omega) \right] \tag{29}$$

Before explicitly calculating (29) let us rewrite equation (28) in a more convenient form; the first two terms can be rewriten as:

$$- \frac{1}{2\Pi} \bar{g}^{dd}_{k+q}(\omega) \left\{ (1- \langle n^{(f)}_{-\sigma}\rangle \Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma}\rangle) \Delta n_q^{-\sigma(f)} \right\} \{ 1+(1-\alpha^{-\sigma})\varepsilon^{(d)}_k \bar{g}^{dd}_k(\omega)\} =$$

$$= - \frac{1}{2\Pi} \bar{g}^{dd}_{k+q}(\omega) \left\{ (1-\langle n^{(f)}_{-\sigma}\rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma}\rangle)\Delta n_q^{-\sigma(f)} \right\} \left\{ \omega - \frac{|V_{df}|^2}{\omega-\varepsilon^{(f)}_k(1-\alpha^{-\sigma})} \right\} \bar{g}^{dd}_k(\omega)$$

Then (28) becomes:

$$G^{dd(1)}_{k+q,k}(\omega) = - \frac{1}{2\Pi} \bar{g}^{dd}_{k+q}(\omega) \left\{ (1-\langle n^{(f)}_{-\sigma}\rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n^{(d)}_{-\sigma}\rangle)\Delta n_q^{-\sigma(f)} \right\} \left\{ \omega - \frac{|V_{df}|^2}{\omega-\varepsilon^{(f)}_k(1-\alpha^{-\sigma})} \right\} \bar{g}^{dd}_k(\omega) - \frac{1}{2\Pi} \bar{g}^{dd}_{k+q}(\omega)(1-\alpha^{-\sigma}) \{-h_o\sigma + \Delta S_q^{-\sigma(d)} + \tag{30-a}$$

$$+ \Delta S_q^{-\sigma(f)} \} \bar{g}_k^{dd}(\omega) + \frac{1}{2\Pi} |V_{df}|^2 \bar{g}_{k+q}^{dd}(\omega) \frac{1-\alpha^{-\sigma}}{\left[\omega-\varepsilon_{k+q}^{(f)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right]} \times \qquad (30\text{-b})$$

$$\times \{h_o\sigma - \left[(1-<n_{-\sigma}^{(f)}>)\Delta n_q^{-\sigma(d)} + (1-<n_{-\sigma}^{(d)}>)\Delta n_q^{-\sigma(f)}\right]\varepsilon_k^{(f)} - \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)}\} \bar{g}_k^{dd}(\omega)$$

Now we introduce the following definitions:

$$\chi_d(k,q) = F_\omega\left[\frac{1}{2\Pi}\,\omega\,\bar{g}_{k+q}^{dd}(\omega)\bar{g}_k^{dd}(\omega)\right] \quad ; \quad \chi_d(q) = \sum_k \chi_d(k,q) \qquad (31\text{-a})$$

$$\tilde{\chi}_d(k,q) = F_\omega\left[\frac{1}{2\Pi}\bar{g}_{k+q}^{dd}(\omega)\frac{1}{\omega-\tilde{\varepsilon}_k^{(f)}}\bar{g}_k^{dd}(\omega)\right] \quad ; \quad \tilde{\chi}_d(q) = \sum_k \tilde{\chi}_d(k,q) \qquad (31\text{-b})$$

where $\tilde{\varepsilon}_k^{(f)} = \varepsilon_k^{(f)}(1-\alpha^{-\sigma})$

$$\tilde{\tilde{\chi}}_d(k,q) = F_\omega\left[\frac{1}{2\Pi}\bar{g}_{k+q}^{dd}(\omega)\,\bar{g}_k^{dd}(\omega)\right] \quad ; \quad \tilde{\tilde{\chi}}_d(q) = \sum_k \tilde{\tilde{\chi}}_d(k,q) \qquad (31\text{-c})$$

$$\chi(k,q) = F_\omega\left[\frac{1}{2\Pi}\bar{g}_{k+q}^{dd}(\omega)\frac{1}{(\omega-\tilde{\varepsilon}_{k+q}^{(f)})(\omega-\tilde{\varepsilon}_k^{(f)})}\bar{g}_k^{dd}(\omega)\right] \quad ; \quad \chi(q) = \sum_k \chi(k,q) \qquad (31\text{-d})$$

The explicit form of these "susceptibilities" will be discussed latter on; from (30-b) and using definitions (31) one obtains:

$$F_\omega\left[G_{k+q,k}^{dd(1)}(\omega)\right] = -\{(1-<n_{-\sigma}^{(f)}>)\Delta n_q^{-\sigma(d)} + (1-<n_{-\sigma}^{(d)}>)\Delta n_q^{-\sigma(f)}\}\{\chi_d(k,q) -$$

$$- |V_{df}|^2 \quad \tilde{\chi}_d(k,q)\} \; - (1-\alpha^{-\sigma})\{ - h_o\sigma + \Delta S_q^{-\sigma(d)} + \Delta S_q^{-\sigma(f)} \} \; \tilde{\tilde{\chi}}_d(k,q) \; +$$

$$+|V_{df}|^2 \; (1-\alpha^{-\sigma}) \; \{h_o\sigma - \left[(1-\langle n_{-\sigma}^{(f)}\rangle \, \Delta n_q^{-\sigma(d)} + (1-\langle n_{-\sigma}^{(d)}\rangle)\Delta n_q^{-\sigma(f)}\right] \varepsilon_k^{(f)} \; -$$

$$- \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)} \} \, \chi \, (k,q) \qquad (32)$$

Equation (32) together with equations (29) enable us to self-consistently, determine Δn_q^{σ} and ΔS_q^{σ}. Using the definitions (31) one gets from (32)

$$\Delta n_q^{\sigma(d)} = - \left[(1-\langle n_{-\sigma}^{(f)}\rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n_{-\sigma}^{(d)}\rangle)\Delta n_q^{-\sigma(f)} \right]\{ \chi_d(q) - |V_{df}|^2 \, \tilde{\chi}_d(q) \; +$$

$$+|V_{df}|^2 \, \chi_d^{(1)}(q)\} \; + (1-\alpha^{-\sigma})\{h_o\sigma - \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)} \} \, \{\tilde{\tilde{\chi}}_d(q) + |V_{df}|^2 \, \chi(q)\} \qquad (33\text{-a})$$

where $\chi_d^{(1)}(q)$ is defined as:

$$\chi_d^{(1)}(q) = \sum_k \tilde{\varepsilon}_k^{(f)} \; \chi(k,q) \qquad (33\text{-b})$$

A quite similar expression holds for the f electrons; interchanging d with f one has:

$$\Delta n_q^{\sigma(f)} = - \left[(1-\langle n_{-\sigma}^{(d)}\rangle)\Delta n_q^{-\sigma(f)} + (1-\langle n_{-\sigma}^{(f)}\rangle)\Delta n_q^{-\sigma(d)} \right] \{ \chi_f(q) - |V_{df}|^2 \, \tilde{\chi}_f(q) \; +$$

$$+ |V_{df}|^2 \; \chi_f^{(1)}(q)\} +(1-\alpha^{-\sigma}) \; \{h_o\sigma - \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)} \} \; \{\tilde{\tilde{\chi}}_f(q) +|V_{df}|^2 \, \chi(q)\} \qquad (33\text{-c})$$

where the f susceptibilities are defined in (31) just by interchanging d with f. Now it remains to determine the quantities $\Delta S_q^{-\sigma(d)}$. To do that we define:

$$S_d(q) = \sum_k (\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)})\, \chi_d(k,q) \tag{34-a}$$

$$\tilde{S}_d(q) = \sum_k (\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)})\, \tilde{\chi}_d(k,q) \tag{34-b}$$

$$\tilde{\tilde{S}}_d(q) = \sum_k (\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)})\, \tilde{\tilde{\chi}}_d(k,q) \tag{34-c}$$

$$\bar{S}_d(q) = \sum_k (\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)})\, \chi(k,q) \tag{34-d}$$

$$\bar{S}_d^{(1)}(q) = \sum_k (\varepsilon_{k+q}^{(d)} - \varepsilon_k^{(d)})\, \tilde{\varepsilon}_k^{(f)}\, \chi(k,q) \tag{34-e}$$

Using these definitions one has :

$$\Delta S_q^{\sigma(d)} = - \left[(1-\langle n_{-\sigma}^{(f)}\rangle)\Delta n_q^{-\sigma(d)} + (1-\langle n_{-\sigma}^{(d)}\rangle)\Delta n_q^{-\sigma(f)}\right] \{ S_d(q) - |V_{df}|^2\, \tilde{S}_d(q) +$$

$$|V_{df}|^2\, \bar{S}_d^{(1)}(q)\} + \{h_o\sigma - \Delta S_q^{-\sigma(d)} - \Delta S_q^{-\sigma(f)}\}\, (1-\alpha^{-\sigma})\, \{\tilde{\tilde{S}}_d(q) +$$

$$+ |V_{df}|^2\, \bar{S}_d(q)\} \tag{35}$$

and a similar equation for $\Delta S_q^{\sigma(f)}$. Equations (35) and (33) together with the fact that for external magnetic fields |3|

$$\Delta n_q^{-\sigma(i)} = - \Delta n_q^{\sigma(i)} \qquad i = d,\ f$$

$$\Delta S_q^{-\sigma(i)} = - \Delta S_q^{\sigma(i)}$$

can be written in the paramagnetic phase as:

$$\left[1 + (1-<n^{(f)}>) \chi_d^c \right] \Delta n_q^{\sigma(d)} = -(1-<n^{(d)}>) \chi_d^c(q) \Delta n_q^{\sigma(f)} + \tilde{\chi}_d^c(q) \Delta S_q^{\sigma(d)}$$

$$+ \tilde{\chi}_d^c(q) \Delta S_q^{\sigma(f)} + h_o \sigma \tilde{\chi}_d^c(q) \qquad (36\text{-a})$$

$$\left[1 + (1-<n^{(d)}>) \chi_f^c \right] \Delta n_q^{\sigma(f)} = -(1-<n^{(f)}>) \chi_f^c(q) \Delta n_q^{\sigma(d)} + \tilde{\chi}_f^c(q) \Delta S_q^{\sigma(f)} +$$

$$+ \tilde{\chi}_f^c(q) \Delta S_q^{\sigma(d)} + h_{o\sigma} \tilde{\chi}_f^c(q) \qquad (36\text{-b})$$

$$\left[1 - \tilde{S}_d^c(q) \right] \Delta S_q^{\sigma(d)} = -(1-<n^{(f)}>) S_d^c(q) \Delta n_q^{\sigma(d)} - (1-<n^{(d)}>) S_d^c(q) \Delta n_q^{\sigma(f)}$$

$$+ \tilde{S}_d^c(q) \Delta S_q^{\sigma(f)} + h_o \sigma \tilde{S}_d^c(q) \qquad (36\text{-c})$$

$$\left[1 - \tilde{S}_f^c(q) \right] \Delta S_q^{\sigma(f)} = -(1-<n^{(d)}>) S_f^c(q) \Delta n_q^{\sigma(f)} - (1-<n^{(f)}>) S_f^c(q) \Delta n_q^{\sigma(d)}$$

$$+ \tilde{S}_f^c(q) \Delta S_q^{\sigma(d)} + h_o \sigma \tilde{S}_f^c(q) \qquad (36\text{-d})$$

where we have defined:

$$\chi_d^c(q) = -\chi_d(q) + |V_{df}|^2 \left\{ \tilde{\chi}_d(q) - \chi_d^{(1)}(q) \right\} \qquad (36\text{-e})$$

$$\tilde{\chi}_d^{c}(q) = (1-\alpha^{-\sigma}) \{\tilde{\tilde{\chi}}_d(q) + |V_{df}|^2 \chi(q)\}$$

$$S_d^c(q) = - S_d(q) + |V_{df}|^2 \{\tilde{S}_d(q) - \bar{S}_d^{(1)}(q)\} \tag{36-e}$$

$$\tilde{S}_d^c(q) = (1-\alpha^{-\sigma}) \{\tilde{\tilde{S}}_d(q) + |V_{df}|^2 \bar{S}_d(q)\}$$

The coupled system (36) is solved after a straighforward algebraic manipulation giving:

$$\Delta n_q^{\sigma(d)} = h_o\sigma \frac{\left[\tilde{\chi}_d^c(q)+(1-\langle n_d\rangle)(\chi_f^c(q)\tilde{\chi}_d^c(q)-\chi_d^c(q)\tilde{\chi}_f^c(q))\right](1+\bar{p}(q))}{1 + (1-\langle n_d\rangle)(\chi_f^c(q)+p(q)\tilde{\chi}_f^c(f))+(1-\langle n_f\rangle)(\chi_d^c(q)+p(q)\tilde{\chi}_d^c(q))} \tag{37}$$

where we have defined:

$$p(q) = \frac{S_d^c(q)+S_f^c(q)}{1-\tilde{S}_d^c(q)-\tilde{S}_f^c(q)} \tag{38-a}$$

and

$$\bar{p}(q) = \frac{\tilde{S}_d^c(q)+\tilde{S}_f^c(q)}{1-\tilde{S}_d^c(q)-\tilde{S}_f^c(q)} \tag{38-b}$$

Quite similarly one obtains one expression for $\Delta n_q^{\sigma(f)}$ which has identical denominator (it should be noted that $p(q)$ and $\bar{p}(q)$ are independent of the fact that (37) was derived for d electrons).

III) CRITERION FOR MAGNETIC INSTABILITY

The condition for occurence of a magnetic instability characterized by wave vector q is provided by:

$$1 + (1-\langle n_d\rangle)(\chi^c_f(q)+p(q)\,\tilde{\chi}^c_f(q)) + (1-\langle n_f\rangle)(\chi^c_d(q)+p(q)\,\tilde{\chi}^c_d(q)) = 0 \qquad (39)$$

Expression (39) can be written in a more illustrative way; define:

$$\chi^{(i)}(q) = \chi^c_{(i)}(q) + p(q)\,\tilde{\chi}^c_{(i)}(q) \qquad i=d,f \qquad (40\text{-a})$$

$$\chi^{(f)}_{eff} = \chi^{(f)}(q)\,\{1 + \frac{1-\langle n_f\rangle}{1-\langle n_d\rangle}\,\frac{\chi^{(d)}(q)}{\chi^{(f)}(q)}\} \qquad (40\text{-b})$$

so the instability criterion is (if one wants to emphasize f-states):

$$1 + (1-\langle n_d\rangle)\,\chi^{(f)}_{eff}(q) = 0 \qquad (41)$$

where it should be emphasized that $\chi^{(f)}_{eff}(q)$ is not a true susceptibility but a quantity with the dimension of a number (cf.Hubbard and Jain |3|). Now we discuss in more detail the quantities involved in the criterion (41). To do that we consider the particular case of a ferromagnetic instability (q=0). This is a particularly simple case since one notes from equations (34) that all the functions S(q) are zero in this case. Consequently, according to equations (36-e) and the definition (38-a), p(q) = 0. Then the ferromagnetic instability condition reads:

$$1 + (1-\langle n_d\rangle)\,\chi^{(f)}_{eff}(0) = 0 \qquad (42\text{-a})$$

$$\chi^{(f)}_{eff}(0) = \chi^c_{(f)}(0)\ \{1 + \frac{1-\langle n_f\rangle}{1-\langle n_d\rangle}\,\frac{\chi^c_{(d)}(0)}{\chi^c_{(f)}(0)}\} \qquad (42\text{-b})$$

and

$$\chi_d^c(0) = -\chi_d(0) + |V_{df}|^2\{\tilde{\chi}_d(0) - \chi_d^{(1)}(0)\}$$

$$\chi_f^c(0) = -\chi_f(0) + |V_{df}|^2\{\tilde{\chi}_f(0) - \chi_f^{(1)}(0)\} \qquad (42\text{-c})$$

Now the "susceptibilities" $\chi_d(0)$, $\tilde{\chi}_d(0)$ and $\tilde{\chi}_f(0)$ are defined in equations (31-a) and (31-b) respectively, the quantities $\chi_d^{(1)}(0)$ and $\chi_f^{(1)}(0)$ being defined in (33-b). The procedure to explicitly calculate these"susceptibilities" is strictly similar to that used in the Hartree-Fock case |1| and we do not repeat here. Finally it should be emphasized that the complete definition of the criterion of magnetism as a function of the number of electrons still involves the self-consistent determination of the chemical potential and the correlation function $<n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}>^{(0)}$. The method to be used has been discussed in detail in |1| and, the one-electron propagators together with the discussion of the correlation function $<n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}>^{(0)}$is the subject of the previous calculation |5|.

CONCLUSIONS AND DISCUSSION

In paragraph III the instability criterion was derived from the poles of the static susceptibility of wave vector q. This result is a natural extension, for a coupled two band problem, of the results derived by Hubbard and Jain |3| within the strong correlation limit.

It should be emphasized that due to the existence of inter-band Coulomb repulsion I_{df}, some propagators generated by the hybridization effect are also generated by correlations, and no decoupling is performed. As discussed in |5| this procedure ensures the correct behaviour in the strong repulsion limit. In the case of the ferromagnetic instability one can verify that in the absence of V_{df} the "susceptibilities" $\chi_d^c(0)$ and $\chi_f^c(0)$ reduce to values formally identical to those obtained by Hubbard and Jain |3|. This shows that the effect of the I_{df} interaction is two fold: firstly it introduces the narrowing coefficient $(1-<n_d>)$ that appears in equation (42-a); secondly the effective susceptibility (42-b) involves the ratio of the χ_d^c and χ_f^c. The origin of the narrowing factor is associated to the approximate treatment of the correction $<n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)}>^{(1)}$ associated to the simultaneous occupation of a site by d and f electrons, and the coupling I_{df}. This is one of the more interesting features of the coupling of the bands. Finally the explicit effect of the mixing is quite similar to that obtained previously |1|.

ACKNOWLEDGEMENTS

One of the authors (M.A.C.) would like to thank the CNPq for a research fellowship.

REFERENCES

1. M.A. Continentino and A.A. Gomes, Notas de Física, Vol.XX, nº 4 (1973).

2. J. Hubbard Proc.Roy.Soc. (London) A276 238,(1963).

3. J. Hubbard and K.P. Jain, J.Phys. C., 1, 1950, (1968).

4. R. Jullien, E. Galleani d'Agliano and B. Coqblin, Phys. Rev. B 6,-2139(1972)

5. M.A. Continentino and A.A. Gomes, Notas de Física, Vol.XX nº 5 (1973).

6. X.A. da Silva and A.A. Gomes, Notas de Física, Vol. 18, nº (1972) and to be published.

* * *