NOTAS DE FÍSICA
VOLUME XX
Nº 5

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by

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RIO DE JANEIRO, BRAZIL
1973

Notas de Física - Volume XX - Nº 5

ONE-ELECTRON PROPAGATORS FOR ACTINIDE METALS: STRONG CORRELATION LIMIT

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(Received 8th July, 1973)

INTRODUCTION

The electronic structure of actinide metals has been the subject of several studies in recent years. [1,2] Actinide metals are characterized by the existence of two overlapping bands of d and f type and a strong hybridization among them [2]. The magnetic properties arise fundamentally from the competition among kinetic and Coulomb terms, but in actinides, these properties are also strongly connected to the amount of d-f mixing. In a previous calculation [3] the magnetic instability conditions are discussed within the Hartree-Fock picture which is expected to hold for large bands and relatively weak Coulomb repulsions. In this work we discuss in detail the calculation of the one-electron propagators for f and d electrons in the opposite case of [3], namely a strongly correlated limit. The strongly correlated limit was already discussed [2] within Roth's variational method for intra-band correlations or inter-band correlations. Here we adopt a simpler procedure namely a Hubbard-like approximation. This method has been previously used to discuss correlation effects in degenerate transition metals [4], and here we improve it to take account of the hybridization effect, which seems to be one of the most important parameters in discussing actinide metals. The calculation of the one electron propagators is the first step of the calculation of the magnetic instabilities within a Hubbard like approximation. The application of this method to the instability problem is the subject of a forthcoming paper [5]. The plan of this paper is as follows: firstly we derive the equations of motion for these propagators within the Hubbard-like approximation. In the second part these equations are solved using Fourier transformation and finally the self-consistency problem is briefly discussed.

II. FORMULATION OF THE PROBLEM

We start from the hamiltonian for the pure metal [2]:

$$= \sum_{i,j,\sigma} T_{ij}^{(d)} d_{i\sigma}^{+} d_{j\sigma} + \sum_{i,j,\sigma} T_{ij}^{(f)} f_{i\sigma}^{+} f_{j\sigma} + U_d \sum_i n_{i\uparrow}^{(d)} n_{i\downarrow}^{(d)} + U_f \sum_i n_{i\uparrow}^{(f)} n_{i\downarrow}^{(f)}$$

$$+ I_{df} \sum_i \left\{ n_{i\uparrow}^{(d)} n_{i\downarrow}^{(f)} + n_{i\downarrow}^{(d)} n_{i\uparrow}^{(f)} \right\} + \sum_i \left\{ V_{df} d_{i\sigma}^{+} f_{i\sigma} + V_{fd} f_{i\sigma}^{+} d_{i\sigma} \right\} \qquad (1)$$

where the notation is the usual one (in the Wannier representation), and for simplicity we took the mixing matrix elements as k independent.. The last approximation may be easily removed as in [3]. We intend to obtain the equations of motion for the one-electron propagator $\langle\langle d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_{\omega}$ and $\langle\langle f_{i\sigma}; f_{j\sigma}^{+}\rangle\rangle_{\omega}$. We consider here in detail only the first propagator since the f propagator can be obtained just by replacing d by f in the equations of motion.

From (1) one can derive the following exact equations of motion:

$$\omega \langle\langle d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = \frac{1}{2\pi}\delta_{ij} + \sum_\ell T_{i\ell}^{(d)} \langle\langle d_{\ell\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega + V_{df} \langle\langle f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega$$

$$+ U_d \langle\langle n_{i-\sigma}^{(d)} \; d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega + I_{df} \langle\langle n_{i-\sigma}^{(f)} \; d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \qquad (2)$$

and

$$\omega \langle\langle f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = \sum_\ell T_{i\ell}^{(f)} \langle\langle f_{\ell\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega + V_{fd} \langle\langle d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega$$

$$+ U_f \langle\langle n_{i-\sigma}^{(f)} \; f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega + I_{df} \langle\langle n_{i-\sigma}^{(d)} \; f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \qquad (3)$$

Equations (2) and (3) involve four unknown propagators, which we label as:

$$\begin{aligned} G_{ij}^{dd,d}(\omega) &= \langle\langle n_{i-\sigma}^{(d)} \; d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \\ G_{ij}^{fd,d}(\omega) &= \langle\langle n_{i-\sigma}^{(f)} \; d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \\ G_{ij}^{ff,d}(\omega) &= \langle\langle n_{i-\sigma}^{(f)} \; f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \\ G_{ij}^{df,d}(\omega) &= \langle\langle n_{i-\sigma}^{(d)} \; f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \end{aligned} \qquad (4)$$

Now contrary to the Hartree-Fock approximation [3] we do not decouple propagators (4) but instead we write down new equations of motion for them. Hamiltonian (1) has translational invariance, the propagators are diagonal in Bloch representation so:

$$(\omega - \varepsilon_k^{(d)})\, G_k^{dd}(\omega) = \frac{1}{2\pi} + V_{df}\, G_k^{fd}(\omega) + U_d\, G_k^{dd,d}(\omega) + I_{df}\, G_k^{fd,d}(\omega) \qquad (5\text{-a})$$

$$(\omega - \varepsilon_k^{(f)})\, G_k^{fd}(\omega) = V_{fd}\, G_k^{dd}(\omega) + U_f\, G_k^{ff,d}(\omega) + I_{df}\, G_k^{df,d}(\omega) \qquad (5\text{-b})$$

a) *DETERMINATION OF THE PROPAGATOR* $G_{ij}^{dd,d}(\omega)$

The exact equation of motion is:

$$(\omega-U_d)G_{ij}^{dd,d}(\omega)=\frac{1}{2\pi}<n_{-\sigma}^{(d)}>\delta_{ij}+I_{df}<<n_{i-\sigma}^{(d)}\,n_{i-\sigma}^{(f)}\,d_{i\sigma};\,d_{j\sigma}^{+}>>_{\omega}+\sum_{\ell}T_{i\ell}^{(d)}<<n_{i-\sigma}^{(d)}d_{\ell\sigma};d_{j\sigma}^{+}>>_{\omega}$$

$$+\sum_{\ell}T_{i\ell}^{(d)}<<\left[d_{i-\sigma}^{+}\,d_{\ell-\sigma}-d_{\ell-\sigma}^{+}\,d_{i-\sigma}\right]d_{i\sigma};d_{j\sigma}^{+}>>_{\omega}+V_{df}\,G_{ij}^{df,d}(\omega)$$

$$+V_{df}<<d_{i-\sigma}^{+}\,f_{i-\sigma}\,d_{i\sigma};\,d_{j\sigma}^{+}>>_{\omega}-V_{fd}<<f_{i-\sigma}^{+}\,d_{i-\sigma}\,d_{i\sigma};\,d_{j\sigma}^{+}>>_{\omega}\tag{6-a}$$

The new terms that appear in equation (6-a) must now be treated in a certain approximation; the kinetic like terms are Hubbard [6] decoupled:

$$\sum_{\ell}T_{i\ell}^{(d)}<<n_{i-\sigma}^{(d)}\,d_{\ell\sigma};\,d_{j\sigma}^{+}>>_{\omega}\cong<n_{-\sigma}^{(d)}>\sum_{\ell}T_{i\ell}^{(d)}\,G_{\ell j}^{dd}(\omega)\tag{6-b}$$

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

$$\cong\sum_{\ell}T_{i\ell}^{(d)}\left\{<d_{i-\sigma}^{+}\,d_{\ell-\sigma}>-<d_{\ell-\sigma}^{+}\,d_{i-\sigma}>\right\}G_{ij}^{dd}(\omega)=0\tag{6-c}$$

where (6-c) follows from the existence of translational symmetry. Now, the terms arising from the hybridization are of two types: the first one $V_{df}\,G_{ij}^{df,d}(\omega)$ is not decoupled since it appears in equation (3) as generated by the electron correlation, and consequently is separately determined. The second type of terms are the last two of (6-a); these are decoupled as:

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

$$\cong\left\{V_{df}<d_{i-\sigma}^{+}\,f_{i-\sigma}>-V_{fd}<f_{i-\sigma}^{+}\,d_{i-\sigma}>\right\}G_{ij}^{dd}(\omega)=0\tag{6-d}$$

where (6-d) follows also from the translation symmetry (cf. below).

Then one obtain for (6-a):

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

$$+<n_{-\sigma}^{(d)}>\sum_{\ell}T_{i\ell}^{(d)}\;G_{\ell j}^{dd}(\omega) \qquad (7\text{-a})$$

or Fourier transformed:

$$(\omega-U_d)\;G_{k}^{dd,d}(\omega)=\frac{1}{2\pi}<n_{-\sigma}^{(d)}>+I_{df}<<(n_{i-\sigma}^{(d)}\;n_{i-\sigma}^{(f)}\;d_{i\sigma})_k;d_{k\sigma}^{+}>>_{\omega}+<n_{-\sigma}^{(d)}>\varepsilon_k^{(d)}G_k^{dd}(\omega)$$

$$+V_{df}\,G_k^{df,d}(\omega) \qquad (7\text{-b})$$

Equations (7) still involve the propagator $<<n_{i-\sigma}^{(d)}\;n_{i-\sigma}^{(f)}\;d_{i\sigma};d_{j\sigma}^{+}>>_{\omega}$; we now determine it completely. It satisfies the following equation of motion:

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

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

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

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

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

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

$$(8\text{-a})$$

The terms involving kinetic effects are easily decoupled; due to translational symmetry only the first term survives (cf. 6-c) and one gets:

$$\sum_\ell T_{i\ell}^{(d)} \langle\langle n_{i-\sigma}^{(d)} \; n_{i-\sigma}^{(f)} \, d_{\ell\sigma}; \, d_{j\sigma}^{+}\rangle\rangle_\omega \cong \langle n_{-\sigma}^{(d)} \; n_{-\sigma}^{(f)}\rangle \sum_\ell T_{i\ell}^{(d)} \, G_{\ell j}^{dd}(\omega) \quad (8\text{-b})$$

The last four terms, which involve d-f hybridization can be handled exactly just using the properties of d and f operators. One may write:

$$V_{df}\langle\langle d_{i-\sigma}^{+} \, f_{i-\sigma} n_{i-\sigma}^{(f)} \, d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = V_{df}\langle\langle d_{i-\sigma}^{+} f_{i-\sigma} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \quad (8\text{-c})$$

$$V_{df}\langle\langle n_{i-\sigma}^{(d)} \; d_{i-\sigma}^{+} \; f_{i-\sigma} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = V_{df} \; \langle\langle d_{i-\sigma}^{+} \; f_{i-\sigma} \; d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \quad (8\text{-d})$$

where we used $f_{i-\sigma} \, n_{i-\sigma}^{(f)} = f_{i-\sigma}$ and $n_{i-\sigma}^{(d)} \; d_{i-\sigma}^{+} = d_{i-\sigma}^{+}$. One has also:

$$V_{fd}\langle\langle f_{i-\sigma}^{+} d_{i-\sigma} n_{i-\sigma}^{(f)} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = V_{fd}\langle\langle f_{i-\sigma}^{+} n_{i-\sigma}^{(f)} d_{i-\sigma} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \equiv 0 \quad (8\text{-e})$$

$$V_{fd}\langle\langle n_{i-\sigma}^{(d)} f_{i-\sigma}^{+} d_{i-\sigma} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = - \, V_{fd}\langle\langle n_{i-\sigma}^{(d)} \; d_{i-\sigma} f_{i-\sigma}^{+} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \equiv 0 \quad (8\text{-f})$$

Then all the four last terms *cancel out exactly* and there is no need in making approximations. The final equation of motion is then:

$$(\omega - U_d - I_{df})\langle\langle n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)} d_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega = \frac{1}{2\pi} \langle n_{-\sigma}^{(d)} \; n_{-\sigma}^{(f)}\rangle \; \delta_{ij} + \langle n_{-\sigma}^{(d)} n_{-\sigma}^{(f)}\rangle \sum_\ell T_{i\ell}^{(d)} G_{\ell j}^{dd}(\omega)$$

$$+ \; V_{df} \; \langle\langle n_{i-\sigma}^{(d)} \; n_{i-\sigma}^{(f)} \; f_{i\sigma}; d_{j\sigma}^{+}\rangle\rangle_\omega \quad (9\text{-a})$$

or in Fourier transformed version:

$$(\omega - U_d - I_{df})\langle\langle (n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)} d_{i\sigma})_k; d_{k\sigma}^{+}\rangle\rangle_\omega = \frac{1}{2\pi} \langle n_{-\sigma}^{(d)} \; n_{-\sigma}^{(f)}\rangle + \langle n_{-\sigma}^{(d)} n_{-\sigma}^{(f)}\rangle \varepsilon_k^{(d)} \; G_k^{dd}(\omega)$$

$$+ \; V_{df} \; \langle\langle (n_{i-\sigma}^{(d)} \; n_{i-\sigma}^{(f)} \; f_{i\sigma})_k; \; d_{k\sigma}^{+}\rangle\rangle_\omega \quad (9\text{-b})$$

To complete the determination of the $G_k^{dd,d}(\omega)$ one just needs to find out the equation of motion for the last propagator in (9-b). One has:

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

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

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

$$+ V_{fd}<<n^{(d)}_{i-\sigma}\ n^{(f)}_{i-\sigma}\ d_{i\sigma};d^+_{j\sigma}>>_\omega \qquad (10\text{-a})$$

In equation (10-a) we have dropped the terms in V_{df} which cancel out exactly as in equations (8-c) to (8-f). The kinetic terms are Hubbard decoupled and one gets:

$$(\omega-U_f-I_{df})<<n^{(d)}_{i-\sigma}n^{(f)}_{i-\sigma}f_{i\sigma};d^+_{j\sigma}>>_\omega = <n^{(d)}_{-\sigma}\ n^{(f)}_{-\sigma}> \sum_\ell T^{(f)}_{i\ell}\ G^{fd}_{\ell j}(\omega)$$

$$+ V_{fd}<<n^{(d)}_{i-\sigma}\ n^{(f)}_{i-\sigma}\ d_{i\sigma};\ d^+_{j\sigma}>>_\omega \qquad (10\text{-b})$$

Fourier transforming:

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

$$+ V_{fd}\ <<(n^{(d)}_{i-\sigma}\ n^{(f)}_{i-\sigma}d_{i\sigma})_k;\ d^+_{k\sigma}>>_\omega \qquad (11)$$

One sees that equations (7-b), (9-b) and (10-b) completely determine the propagator $G^{dd,d}_k(\omega)$ in terms of $G^{dd}_k(\omega)$ and $G^{fd}_k(\omega)$.

b) *DETERMINATION OF THE PROPAGATOR* $G^{fd,d}_{ij}(\omega)$

This propagator satisfies:

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

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

$$+ V_{fd}<<f^+_{i-\sigma}d_{i-\sigma}d_{i\sigma};d^+_{j\sigma}>>_\omega-V_{df}<<d^+_{i-\sigma}f_{i-\sigma}d_{i\sigma};d^+_{j\sigma}>>_\omega \qquad (12\text{-a})$$

The kinetic terms and the last two terms are decoupled exactly as in equations (6-a, b, c); one gets:

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

$$+<n_{-\sigma}^{(f)}>\sum_{\ell}T_{i\ell}^{(d)}\,G_{\ell j}^{dd}(\omega)+V_{df}\,G_{ij}^{ff,d}(\omega) \qquad (12\text{-b})$$

Fourier transforming:

$$(\omega-I_{df})G_{k}^{fd,d}(\omega)=\frac{1}{2\pi}<n_{-\sigma}^{(f)}>+<n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}\,G_k^{dd}(\omega)+V_{df}\,G_k^{ff,d}(\omega)$$

$$+U_d<<(n_{i-\sigma}^{(d)}\,n_{i-\sigma}^{(f)}\,d_{i\sigma})_k;\,d_{k\sigma}^{+}>>_{\omega} \qquad (13)$$

c) *DETERMINATION OF THE PROPAGATOR* $G_{ij}^{df,d}(\omega)$

One has:

$$(\omega-I_{df})G_{ij}^{df,d}(\omega)=U_f<<n_{i-\sigma}^{(d)}\,n_{i-\sigma}^{(f)}\,f_{i\sigma};\,d_{j\sigma}^{+}>>_{\omega}+\sum_{\ell}T_{i\ell}^{(f)}<<n_{i-\sigma}^{(d)}\,f_{\ell\sigma};d_{j\sigma}^{+}>>_{\omega}$$

$$+\sum_{\ell}T_{i\ell}^{(d)}<<\left[d_{i-\sigma}^{+}\,d_{\ell-\sigma}-d_{\ell-\sigma}^{+}\,d_{i-\sigma}\right]f_{i\sigma};d_{j\sigma}^{+}>>_{\omega}+V_{fd}\,G_{ij}^{dd,d}(\omega)$$

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

(14-a)

Quite similarly to (12) one obtains:

$$(\omega-I_{df})G_{ij}^{df,d}(\omega)=U_f<<n_{i-\sigma}^{(d)}\,n_{i-\sigma}^{(f)}\,f_{i\sigma};d_{j\sigma}^{+}>>_{\omega}+<n_{-\sigma}^{(d)}>\sum_{\ell}T_{i\ell}^{(f)}\,G_{\ell j}^{fd}(\omega)$$

$$+V_{fd}\,G_{ij}^{dd,d}(\omega) \qquad (14\text{-b})$$

Or Fourier transforming:

$$(\omega-I_{df})G_{k}^{df,d}(\omega)=<n_{-\sigma}^{(d)}>\varepsilon_k^{(f)}\,G_k^{fd}(\omega)+V_{fd}\,G_k^{dd,d}(\omega)+U_f<<(n_{i-\sigma}^{(d)}\,n_{i-\sigma}^{(f)}\,f_{i\sigma})_k;d_{k\sigma}^{+}>>_{\omega}$$

(15)

d) *DETERMINATION OF THE PROPAGATOR* $G_{ij}^{ff,d}(\omega)$

The calculation is quite similar to the previous cases so we only quote the result:

$$(\omega-U_f)G_{ij}^{ff,d}(\omega)=<n_{-\sigma}^{(f)}> \sum_\ell T_{i\ell}^{(f)} G_{\ell j}^{fd}(\omega)+V_{fd}G_{ij}^{fd,d}(\omega)+I_{df}<<n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}f_{i\sigma};d_{j\sigma}^{+}>>_\omega \quad (16\text{-a})$$

or in Fourier transformed form:

$$(\omega-U_f)G_{k}^{ff,d}(\omega)=<n_{-\sigma}^{(f)}> \varepsilon_k^{(f)}\ G_k^{fd}(\omega)+V_{fd}\ G_k^{fd,d}(\omega)+I_{df}<<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ f_{i\sigma})_k;d_{k\sigma}^{+}>>_\omega \quad (16\text{-b})$$

III. SOLUTION OF THE COUPLED EQUATIONS

Since the propagators $<<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ d_{i\sigma})_k,\ d_{k\sigma}^{+}>>_\omega$ and $<<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ f_{i\sigma})_k,\ d_{k\sigma}^{+}>>_\omega$ are present in almost all equations of motion we firstly determine them in terms of $G_k^{dd}(\omega)$ and $G_k^{fd}(\omega)$.

Combining equations (9-a) and (11) one gets:

$$\left\{1-\frac{|V_{df}|^2}{(\omega-U_d-I_{df})(\omega-U_f-I_{df})}\right\}<<(n_{i-\sigma}^{(d)}\cdot n_{i-\sigma}^{(f)}\ d_{i\sigma})_k;\ d_{k\sigma}^{+}>>_\omega = \frac{1}{2\pi}\ \frac{<n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}>}{\omega-U_d-I_{df}}$$

$$+\frac{<n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}>}{\omega-U_d-I_{df}}\ \varepsilon_k^{(d)}\ G_k^{dd}(\omega)+\frac{<n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}>\ \varepsilon_k^{(f)}}{(\omega-U_d-I_{df})(\omega-U_f-I_{df})}\ V_{df}\ G_k^{fd}(\omega) \quad (17\text{-a})$$

and

$$\left\{1-\frac{|V_{df}|^2}{(\omega-U_d-I_{df})(\omega-U_f-I_{df})}\right\}<<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ f_{i\sigma})_k;\ d_{k\sigma}^{+}>>_\omega = \frac{<n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}>}{\omega-U_f-I_{df}}\ \varepsilon_k^{(f)}G_k^{fd}(\omega)$$

$$+\frac{1}{2\pi}V_{fd}\ \frac{<n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}>}{(\omega-U_d-I_{df})(\omega-U_f-I_{df})}+\frac{<n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}}{(\omega-U_f-I_{df})(\omega-U_d-I_{df})}\ V_{fd}\ G_k^{dd}(\omega) \quad (17\text{-b})$$

The solutions (17-a) and (17-b) can now be substituted in the pertinent equations of motion. Now we completely determine the last two terms of equations (5-a).

a) *DETERMINATION OF* $U_d\, G_k^{dd,d}(\omega)$

Combining equations (7-b) and (15) one has:

$$\left\{1-\frac{|V_{df}|^2}{(\omega-U_d)(\omega-I_{df})}\right\} U_d\, G_k^{dd,d}(\omega) = \frac{1}{2\pi}\frac{U_d}{\omega-U_d}\langle n_{-\sigma}^{(d)}\rangle + \frac{U_d}{\omega-U_d}\langle n_{-\sigma}^{(d)}\rangle\varepsilon_k^{(d)}\, G_k^{dd}(\omega)$$

$$+\frac{U_d}{\omega-U_d}\,\frac{\langle n_{-\sigma}^{(d)}\rangle\varepsilon_k^{(f)}}{\omega-I_{df}}\, V_{df}\, G_k^{fd}(\omega)$$

$$+\frac{U_d}{\omega-U_d}\, I_{df}\langle\langle (n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, d_{i\sigma})_k ;\, d_{k\sigma}^{+}\rangle\rangle_\omega$$

$$+\frac{U_d}{\omega-U_d}\,\frac{U_f}{\omega-I_{df}}\, V_{df}\langle\langle (n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, f_{i\sigma})_k ;\, d_{k\sigma}^{+}\rangle\rangle_\omega \tag{18}$$

Equation (18) together with equations (17) provide the complete determination of $U_d\, G^{dd,d}(\omega)$ in terms of G_k^{dd} and G_k^{fd}. Now one determines the contribution $I_{df}\, G^{fd,d}(\omega)$ to equation (5-a)

b) *DETERMINATION OF* $I_{df}\, G_k^{fd,d}(\omega)$

One starts combining equations (13) and (16-b) to get:

$$\left\{1-\frac{|V_{df}|^2}{(\omega-U_f)(\omega-I_{df})}\right\} I_{df}\, G_k^{fd,d}(\omega) = \frac{1}{2\pi}\frac{I_{df}}{\omega-I_{df}}<n_{-\sigma}^{(f)}> + \frac{I_{df}}{\omega-I_{df}}<n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}\, G_k^{dd}(\omega)$$

$$+\frac{I_{df}}{\omega-I_{df}}\frac{<n_{-\sigma}^{(f)}>\varepsilon_k^{(f)}}{\omega-U_f} V_{df}\, G_k^{fd}(\omega)$$

$$+\frac{I_{df}}{\omega-I_{df}} U_d <<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, d_{i\sigma})_k ;\, d_{k\sigma}^{+}>>_\omega$$

$$+\frac{I_{df}}{\omega-I_{df}}\frac{I_{df}}{\omega-U_f} V_{df} <<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)} f_{i\sigma})_k ; d_{k\sigma}^{+}>>_\omega \qquad (19)$$

Equations (19) and (17) completely determine $I_{df}\, G_k^{fd,d}(\omega)$ in terms of G_k^{dd} and G_k^{fd}, and also complete the determination of the propagators appearing in (5-a). Now we start calculating the propagators involved in (5-b).

c) *DETERMINATION OF* $U_f\, G_k^{ff,d}(\omega)$

One combines equations (16-b) and (13) to get:

$$\left\{1-\frac{|V_{df}|^2}{(\omega-U_f)(\omega-I_{df})}\right\} U_f\, G_k^{ff,d}(\omega) = \frac{U_f}{\omega-U_f}<n_{-\sigma}^{(f)}>\varepsilon_k^{(f)}\, G_k^{fd}(\omega) + \frac{1}{2\pi}\frac{U_f <n_{-\sigma}^{(f)}> V_{fd}}{(\omega-U_f)(\omega-I_{df})}$$

$$+\frac{U_f}{\omega-U_f}\frac{<n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}}{\omega - I_{df}} V_{fd}\, G_k^{dd}(\omega) + \frac{U_f}{\omega-U_f} I_{df} <<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)} f_{i\sigma})_k ; d_{k\sigma}^{+}>>_\omega$$

$$+\frac{U_f}{\omega-U_f}\frac{U_d}{\omega-I_{df}} V_{fd} <<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, d_{i\sigma})_k ;\, d_{k\sigma}^{+}>>_\omega \qquad (20)$$

Quite similarly, from equation (15) one has:

$$I_{df}\, G_k^{df,d}(\omega) = \frac{I_{df}}{\omega - I_{df}} \langle n_{-\sigma}^{(d)}\rangle\, \varepsilon_k^{(f)}\; G_k^{fd}(\omega) + \frac{I_{df}}{\omega - I_{df}} V_{fd}\, G_k^{dd,d}(\omega)$$

$$+ \frac{I_{df}}{\omega - I_{df}} U_f \langle\langle (n_{i-\sigma}^{(d)}\; n_{i-\sigma}^{(f)}\, f_{i\sigma})_k ; d_{k\sigma}^{+} \rangle\rangle_\omega \qquad (21)$$

Since the propagator $G_k^{dd,d}(\omega)$ is completely defined in (18) equation (21) defines $G_k^{df,d}(\omega)$. Equations (20) and (21) complete the solution of equation (5-b).

d) *LIMIT OF STRONG CORRELATIONS*

In this paper we are interested in the limit of Coulomb repulsions much larger than the band widths. We consider then the limit of the above equations when U_d, U_f and I_{df} are equal and tend to infinity.

From equations (17) one sees that:

$$\lim_{U\to\infty} \langle\langle (n_{i-\sigma}^{(d)}\; n_{i-\sigma}^{(f)}\; d_{i\sigma})_k ; d_{k\sigma}^{+}\rangle\rangle_\omega = \lim_{U\to\infty} \langle\langle (n_{i-\sigma}^{(d)}\; n_{i-\sigma}^{(f)}\; f_{i\sigma})_k ; d_{k\sigma}^{+}\rangle\rangle_\omega = 0 \qquad (22\text{-a})$$

Showing that simultaneous occupancy with opposite spins is inhibited. Quite similarly one derives from (18) and (19) that:

$$\lim_{U\to\infty} G_k^{dd,d}(\omega) = \lim_{U\to\infty} G_k^{fd,d}(\omega) = 0 \qquad (22\text{-b})$$

and also that:

$$\lim_{U\to\infty} U_d\, G_k^{dd,d}(\omega) = -\frac{1}{2\pi} \langle n_{-\sigma}^{(d)}\rangle - \langle n_{-\sigma}^{(d)}\rangle \varepsilon_k^{(d)}\; G_k^{dd}(\omega) - \lim_{U\to\infty} I_{df} \langle\langle (n_{i-\sigma}^{(d)}\; n_{i-\sigma}^{(f)}\; d_{i\sigma})_k ; d_{k\sigma}^{+}\rangle\rangle_\omega$$

$$= -\frac{1}{2\pi} \langle n_{-\sigma}^{(d)}\rangle + \frac{1}{2\pi}\, \frac{\langle n_{-\sigma}^{(d)}\; n_{-\sigma}^{(f)}\rangle}{2} - \langle n_{-\sigma}^{(d)}\rangle \varepsilon_k^{(d)}\; G_k^{dd}(\omega) + \frac{\langle n_{-\sigma}^{(d)}\; n_{-\sigma}^{(f)}\rangle}{2}\, \varepsilon_k^{(d)}\; G_k^{dd}(\omega) \qquad (22\text{-c})$$

$$\lim_{U\to\infty} I_{df}\, G_k^{fd,d}(\omega) = -\frac{1}{2\pi} <n_{-\sigma}^{(f)}> - <n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}\, G_k^{dd}(\omega) - \lim_{U\to\infty} U_d <<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, d_{i\sigma})_k ; d_{k\sigma}^{+}>>_\omega$$

$$= -\frac{1}{2\pi} <n_{-\sigma}^{(f)}> + \frac{1}{2\pi}\, \frac{<n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}>}{2} - <n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}\, G_k^{dd}(\omega) + \frac{<n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}>}{2}\, \varepsilon_k^{(d)}\, G_k^{dd}(\omega) \tag{22-d}$$

Using (22-d) and (22-c) and defining:

$$\alpha^{-\sigma} = <n_{-\sigma}^{(d)}> + <n_{-\sigma}^{(f)}> - <n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}>$$

one obtains for the last two terms of (5-a) in this limit:

$$\lim_{U\to\infty} \left\{ U_d\, G_k^{dd,d}(\omega) + I_{df}\, G_k^{fd,d}(\omega) \right\} = -\frac{1}{2\pi}\alpha^{-\sigma} - \alpha^{-\sigma}\varepsilon_k^{(d)}\, G_k^{dd}(\omega) \tag{22-e}$$

Equation (5-a) can be rewritten using these results as:

$$\left\{ \omega - \varepsilon_k^{(d)}(1-\alpha^{-\sigma}) \right\} G_k^{dd}(\omega) = \frac{1}{2\pi}(1-\alpha^{-\sigma}) + V_{df}\, G_k^{fd}(\omega) \tag{23}$$

Now from equations (20) and (21) one derives that:

$$\lim_{U\to\infty} G_k^{ff,d}(\omega) = \lim_{U\to\infty} G_k^{df,d}(\omega) = 0 \tag{24-a}$$

and that

$$\lim_{U\to\infty} \left\{ U_f\, G_k^{ff,d}(\omega) + I_{df}\, G_k^{df,d}(\omega) \right\} = -\alpha^{-\sigma}\, \varepsilon_k^{(f)}\, G_k^{fd}(\omega) \tag{24-b}$$

Equation (24-b) enables us to write instead of (5-b):

$$\left\{ \omega - \varepsilon_k^{(f)}(1-\alpha^{-\sigma}) \right\} G_k^{fd}(\omega) = V_{fd}\, G_k^{dd}(\omega) \tag{25}$$

The final solution for the $G_k^{dd}(\omega)$ propagator is obtained combining equations (23) and (25) to get:

$$G_k^{dd}(\omega) = \frac{1}{2\pi}\, \frac{1 - \alpha^{-\sigma}}{\omega - \varepsilon_k^{(d)}(1-\alpha^{-\sigma}) - \dfrac{|V_{df}|^2}{\omega - \varepsilon_k^{(f)}(1-\alpha^{-\sigma})}} = \frac{1}{2\pi}(1-\alpha^{-\sigma})\left\{ \omega - \varepsilon_k^{(f)}(1-\alpha^{-\sigma}) \right\} \bar{g}_k(\omega) \tag{26}$$

The propagator (26) is a clear generalization of Hubbard propagator [6] for two bands, mixing and all Coulomb correlations. An expression for the $G_k^{ff}(\omega)$ can be obtained from (26) just replacing d by f and f by d. Incidentally one notes that

$$G_k^{fd}(\omega) = \frac{1}{2\pi} \frac{V_{fd}(1-\alpha^{-\sigma})}{\left[\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right]-|V_{df}|^2} = V_{fd}(1-\alpha^{-\sigma})\bar{g}_k(\omega) \quad (27\text{-a})$$

and

$$G_k^{df}(\omega) = \frac{1}{2\pi} \frac{V_{df}(1-\alpha^{-\sigma})}{\left[\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right]-|V_{df}|^2} = V_{df}(1-\alpha^{-\sigma})\bar{g}_k(\omega) \quad (27\text{-b})$$

From equations (27) one concludes that:

$$V_{df}\langle d_\sigma^+ f_\sigma\rangle = |V_{df}|^2(1-\alpha^{-\sigma})F_\omega\left[\bar{g}_k(\omega)\right] = V_{fd}\langle f_\sigma^+ d_\sigma\rangle \quad (27\text{-c})$$

justifying then the result of equation (6-d).

IV. SELF-CONSISTENCY CONDITIONS

The propagators $G_k^{dd}(\omega)$ and $G_k^{ff}(\omega)$ contain the occupation numbers $\langle n_{-\sigma}^{(d)}\rangle$, and $\langle n_{-\sigma}^{(f)}\rangle$ and the correlation function $\langle n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}\rangle$. The first two quantities can be self-consistently determined using:

$$\langle n_\sigma^{(d)}\rangle = \sum_k F_\omega\left\{G_{k\sigma}^{dd}(\omega)\right\}$$

$$\langle n_\sigma^{(f)}\rangle = \sum_k F_\omega\left\{G_{k\sigma}^{ff}(\omega)\right\} \quad (28)$$

It remains however to determine the correlation function $\langle n_{-\sigma}^{(d)}\ n_{-\sigma}^{(f)}\rangle$. Since this quantity cannot be determined from the propagators discussed in paragraph II, we use here a method due to Roth [7] to explicitly calculate $<n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}>$. One notes that defining $\beta_{j\sigma} = n_{j\sigma}^{(f)}\, d_{j\sigma}^{+}$, and considering the propagator $<<d_{i\sigma};\, \beta_{j\sigma}>>_{\omega}$ one gets:

$$<d_{j\sigma}^{+}\, d_{i\sigma}\, n_{j\sigma}^{(f)}> = F_{\omega}\, <<d_{i\sigma};\beta_{j\sigma}>>_{\omega} \qquad (29)$$

from which taking i = j the correlation function can be determined. Since the only modification is the choice of the operator on the right, the equations of motion discussed in paragraph II are unchanged, except for the anticommutators $\frac{1}{2\pi} < \left[A_i,\, \beta_j\right]_+ >$. In appendix I we quote the equations of motion necessary to determine the propagator $<<d_{i\sigma};\, \beta_{j\sigma}>>_{\omega}$. The solution of these coupled equations follow exactly the same steps as in paragraph II. One obtains in the limit of infinite Coulomb interactions the following result:

$$\left\{\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})-\frac{|V_{df}|^2}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})}\right\}G_k^{d\beta}(\omega) = \frac{1}{2\pi}\left\{<n_{\sigma}^{(f)}>-<n_{-\sigma}^{(d)}n_{\sigma}^{(f)}> + \right.$$

$$\left. + <n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}n_{\sigma}^{(f)}>-<n_{-\sigma}^{(f)}n_{\sigma}^{(f)}>\right\} + \frac{1}{2\pi}\,\frac{V_{df}}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})}\left\{<f_{\sigma}d_{\sigma}^{+}> - \right.$$

$$\left. - <n_{-\sigma}^{(f)}\, f_{\sigma}\, d_{\sigma}^{+}> - <n_{-\sigma}^{(d)}\, f_{\sigma}\, d_{\sigma}^{+}> + <n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}\, f_{\sigma}\, d_{\sigma}^{+}>\right\} \qquad (30)$$

The propagator (30) still involves correlation functions which now we connect to propagators determined in paragraph III. One has:

$$<n_{-\sigma}^{(f)}\, n_{\sigma}^{(f)}> = <n_{-\sigma}^{(f)}\, f_{\sigma}^{+}\, f_{\sigma}> = \sum_k F_{\omega}\left\{G_k^{ff,f}(\omega)\right\} = 0 \qquad (31\text{-a})$$

since $\lim_{U\to\infty} G_k^{ff,f}(\omega) = 0$ (cf. 22-b). Quite similarly

$$<n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}\, n_{\sigma}^{(f)}> \;=\; <n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}\, f_{\sigma}^{+}\, f_{\sigma}> \;=\; \sum_k F_{\omega}\{<<(n_{i-\sigma}^{(d)} n_{i-\sigma}^{(f)} f_{i\sigma})_k ;\, f_{k\sigma}^{+}>>_{\omega}\} = 0 \tag{31-b}$$

$$<n_{-\sigma}^{(f)}\, f_{\sigma}\, d_{\sigma}^{+}> = \sum_k F_{\omega}\,\{G_k^{ff,d}(\omega)\} = 0 \tag{31-c}$$

$$<n_{-\sigma}^{d}\, f_{\sigma}\, d_{\sigma}^{+}> = \sum_k F_{\omega}\,\{G_k^{df,d}(\omega)\} = 0$$

$$<n_{-\sigma}^{d}\, n_{\sigma}^{(f)}> = \sum_k F_{\omega}\,\{G_k^{df,f}(\omega)\} = 0 \tag{31-d}$$

and finally:

$$<n_{-\sigma}^{(d)}\, n_{-\sigma}^{(f)}\, f_{\sigma}\, d_{\sigma}^{+}> = \sum_k F_{\omega}\,\{<<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, f_{i\sigma})_k ;\, d_{k\sigma}^{+}>>_{\omega}\} = 0$$

Using these results (30) can be written as:

$$\left\{\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma}) - \frac{|V_{df}|^2}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})}\right\} G_k^{d\beta}(\omega) = \frac{1}{2\pi} <n_{\sigma}^{(f)}> - \frac{1}{2\pi}\, \frac{V_{df} <d_{\sigma}^{+}\, f_{\sigma}>}{\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})} \tag{32}$$

Now we recall from (27-a) that:

$$V_{df}<d_{\sigma}^{+}\, f_{\sigma}> = \frac{1}{2\pi}\, |V_{df}|^2 (1-\alpha^{-\sigma}) \sum_k F_{\omega}\{\overline{g}_k(\omega)\} = |V_{df}|^2 (1-\alpha^{-\sigma})\, N(\alpha^{-\sigma}) \tag{33-a}$$

$$N(\alpha^{-\sigma}) = \frac{1}{2\pi} \sum_k F_{\omega}\{\overline{g}_k(\omega)\} \tag{33-b}$$

$$\overline{g}_k(\omega) = \frac{1}{\left[\omega-\varepsilon_k^{(d)}(1-\alpha^{-\sigma})\right]\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right] - |V_{df}|^2} \tag{33-c}$$

Using equations (33) one gets from (32):

$$G_k^{d\beta}(\omega) = \frac{1}{2\pi}\,\{<n_{\sigma}^{(f)}>\left[\omega-\varepsilon_k^{(f)}(1-\alpha^{-\sigma})\right] - |V_{df}|^2 (1-\alpha^{-\sigma})\, N(\alpha^{-\sigma})\}\, \overline{g}_k(\omega) \tag{34}$$

Equation (34) enables us to determine the correlation function $<n_{\sigma}^{(d)}\, n_{\sigma}^{(f)}>$;

one gets:

$$\langle n_\sigma^{(d)} n_\sigma^{(f)} \rangle = \langle n_\sigma^{(f)} \rangle N_2(\alpha^{\sigma}) - |V_{df}|^2 (1-\alpha^{-\sigma}) \{N(\alpha^{-\sigma})\}^2 \quad (35\text{-a})$$

where

$$N_2(\alpha^{-\sigma}) = \frac{1}{2\pi} \sum_k F_\omega \{ \left[\omega - \varepsilon_k^{(f)} (1-\alpha^{-\sigma})\right] \bar{g}_k(\omega) \} \quad (35\text{-b})$$

Now from equations (28) one gets:

$$\langle n_\sigma^{(f)} \rangle = (1-\alpha^{-\sigma}) N_1(\alpha^{-\sigma}) \quad (36\text{-a})$$

where

$$N_1(\alpha^{-\sigma}) = \frac{1}{2\pi} \sum_k F_\omega \left\{ \left[\omega - \varepsilon_k^{(d)} (1-\alpha^{-\sigma})\right] \bar{g}_k(\omega) \right\} \quad (36\text{-b})$$

and also:

$$\langle n_\sigma^{(d)} \rangle = (1-\alpha^{-\sigma}) N_2(\alpha^{-\sigma}) \quad (36\text{-c})$$

The coupled equations (35-a), (36-a) and (36-c) solve the self-consistency problem. Now if one is interested in the paramagnetic region (as in the case of the conditions for magnetic instability [5]) the coupled system can be simplified to give:

$$\langle n^{(d)} n^{(f)} \rangle = \langle n^{(f)} \rangle N_2(\alpha) - |V_{df}|^2 (1-\alpha) \left[N(\alpha)\right]^2 \quad (37\text{-a})$$

$$\langle n^{(d)} \rangle = (1-\alpha) N_2(\alpha)$$

$$\langle n^{(f)} \rangle = (1-\alpha) N_1(\alpha) \quad (37\text{-b})$$

This system can be solved to give the self-consistency condition:

$$\frac{\alpha}{1-\alpha} = N_1(\alpha) + N_2(\alpha) - N_1(\alpha) N_2(\alpha) + |V_{df}|^2 \left[N(\alpha)\right]^2 \quad (38)$$

Given the band structure ($\varepsilon_k^{(d)}$ and $\varepsilon_k^{(f)}$), the mixing $|V_{df}|^2$, equation (38) must now be numerically solved in order to get the parameter α. It sould be emphasized that the results are to be expressed in terms of the number of electrons (d and f) as discussed in ref. 3.

DISCUSSION AND CONCLUSIONS

In the above paragraphs the one-electron propagators G_k^{dd} and G_k^{ff} have been calculated within the Hubbard model. This is a natural extension for a two band problem, of the usual Hubbard approach for narrow bands. It should be emphasized that the same type of inconvenients of a Hubbard like picture are still present here, and some of these difficulties, if one intends to discuss ferro-magnetic cases have been removed previously using Roth's method [2]. We want to stress that this calculation is intended to be applied to non-magnetic cases (as the calculation of the susceptibility in the paramagnetic phase) where many of the above problems disappear. The formal expression for the propagator is the expected one; one has a narrow band, through the factor $1-\alpha^{-\sigma}$ and the hybridization correction where, say, a d-electron is d-f admixed into the f-band, propagates within it and is admixed back into the d band. The narrowing factor involves $<n_d>$, $<n_f>$ and a correction for simultaneous occupancy of a site by d and f states. This correction arises from the existence of simultaneous interactions. Physically one can say that the d-band is narrowed by $<n_{-\sigma}^d>$ due to U_d interaction, or by $<n_{-\sigma}^f>$ if there were only I_{df} interaction. In presence of both interactions, the band is narrowed by $<n_{-\sigma}^d> + <n_{-\sigma}^f> - <n_{-\sigma}^d\, n_{-\sigma}^f>$, the last term accounting for double occupancy of site i. Finally it should be stressed that higher order propagators generated by d-f mixing were not decoupled when they corresponded to propagators generated by the Coulomb rep ulsions, ensuring then correct behaviour in the limit of strong interaction. In the last paragraph the self-consistency problem was discussed, including the complete determination of the correction $<n^d_{-\sigma}\, n^f_{-\sigma}>$ to the band narrowing. The final self-consistent relation determining $\alpha^{-\sigma}$ was calculated only in the paramagnetic case, since it is the only one of interest in the determination of the magnetic instabilities through the susceptibility. The magnetism conditions as obtained from the poles of the susceptibility is the subject of the next paper.

APPENDIX I

EQUATIONS OF MOTION FOR THE PROPAGATOR $<<d_{i\sigma};\, \beta_{j\sigma}>>_\omega$

One has:

$$(\omega-\varepsilon_k^{(d)})G_k^{d\beta}(\omega) = \frac{1}{2\pi} <n_\sigma^{(f)}> + V_{df}\, G_k^{f\beta}(\omega) + U_d\, G_k^{dd,\beta}(\omega) + I_{df}\, G_k^{fd,\beta}(\omega) \quad \text{(A-1)}$$

$$(\omega-\varepsilon_k^{(f)})G_k^{f\beta}(\omega) = \frac{1}{2\pi} <f_\sigma d_\sigma^+> + V_{fd}\, G_k^{d\beta}(\omega) + U_f\, G_k^{ff,\beta}(\omega) + I_{df}\, G_k^{df,\beta}(\omega) \quad \text{(A-2)}$$

i) Determination of the $G_k^{dd,\beta}$ *Propagator*

$$(\omega-U_d)G_k^{dd,\beta}(\omega) = \frac{1}{2\pi} <n_{-\sigma}^{(d)}n_\sigma^{(f)}> + I_{df}<<(n_{i-\sigma}^{(d)}n_{i-\sigma}^{(f)}d_{i\sigma})_k;\beta_{k\sigma}>>_\omega + <n_{-\sigma}^{(d)}>\varepsilon_k^{(d)}G_k^{d\beta}(\omega) +$$

$$+ V_{df}\, G_k^{df,\beta}(\omega) \quad \text{(A-3)}$$

$$(\omega-U_d-I_{df})<<(n_{i-\sigma}^{(d)}n_{i-\sigma}^{(f)}d_{i\sigma})_k;\beta_{k\sigma}^+>>_\omega = \frac{1}{2\pi} <n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}n_\sigma^{(f)}> + <n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}>\varepsilon_k^{(d)}G_k^{d\beta}(\omega)$$

$$+ V_{df}<<(n_{i-\sigma}^{(d)}\, n_{i-\sigma}^{(f)}\, f_{i\sigma})_k;\, \beta_{k\sigma}>>_\omega \quad \text{(A-4)}$$

$$(\omega-U_f-I_{df})<<(n_{i-\sigma}^{(d)}n_{i-\sigma}^{(f)}f_{i\sigma})_k\ \beta_{k\sigma}^{+}>>_\omega=\frac{1}{2\pi}<n_{i-\sigma}^{(d)}n_{i-\sigma}^{(f)}f_{i\sigma}d_{i\sigma}^{+}>+<n_{-\sigma}^{(d)}n_{-\sigma}^{(f)}>\varepsilon_k^{(f)}G_k^{f\beta}(\omega)$$

$$+\ V_{fd}\ <<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ d_{i\sigma})_k;\ \beta_{k\sigma}>>_\omega \qquad \text{(A-5)}$$

ii) Determination of the $G_k^{fd,\beta}(\omega)$

$$(\omega-I_{df})G_k^{fd,\beta}(\omega)=\frac{1}{2\pi}<n_{i-\sigma}^{(f)}\ n_{i\sigma}^{(f)}>+<n_{-\sigma}^{(f)}>\ \varepsilon_k^{(d)}\ G_k^{d\beta}(\omega)+V_{df}\ G_k^{ff,\beta}(\omega)$$

$$+\ U_d<<(n_{i-\sigma}^{(d)}\ n_{i-\sigma}^{(f)}\ f_{i\sigma})_k;\ \beta_{k\sigma}>>_\omega \qquad \text{(A-6)}$$

iii) Determination of the Propagator $G_k^{df,\beta}(\omega)$

$$(\omega-I_{df})G_k^{df,\beta}(\omega)=\frac{1}{2\pi}<n_{i-\sigma}^{(d)}\ f_{i\sigma}d_{j\sigma}^{+}>+<n_{-\sigma}^{(d)}>\varepsilon_k^{(f)}G_k^{f\beta}(\omega)+V_{fd}\ G_k^{dd,\beta}(\omega)$$

$$+\ U_f\ <<(n_{i-\sigma}^{(d)}n_{i-\sigma}^{(f)}f_{i\sigma})_k;\ \beta_{k\sigma}>>_\omega \qquad \text{(A-7)}$$

iv) Determination of $G_k^{ff,\beta}(\omega)$

$$(\omega-U_f)G_k^{ff,\beta}(\omega)=\frac{1}{2\pi}<n_{i-\sigma}^{(f)}\ f_{i\sigma}d_{j\sigma}^{+}>+<n_{-\sigma}^{(f)}>\ \varepsilon_k^{(f)}\ G_k^{f\beta}(\omega)+V_{fd}\ G_k^{fd,\beta}(\omega)$$

$$+\ I_{df}<<(n_{i-\sigma}^{(d)}\ \ n_{i-\sigma}^{(f)}\ \ f_{i\sigma})_k;\ \beta_{k\sigma}>>_\omega \qquad \text{(A-8)}$$

Equations (A-1) to (A-8) determine completely the propagator $<<d_{i\sigma};\ \beta_{k\sigma}>>_\omega$.

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