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FERROMAGNETIC INSTABILITIES IN DISORDERED SYSTEMS IN THE LIMIT OF STRONG CORRELATIONS: APPLICATIONS TO TRANSITION METAL LIKE SYSTEMS AND ACTINIDES*

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ABSTRACT

One derives the criterion for ferromagnetic instabili - ties in hybridized disordered systems, e.g. transition metal like systems and actinides, within the Coherent Potential Approximation (CPA), the electron-electron correlations being described by Hu - bbard's approximation.

In the case of actinides, one treats approximately the motion of d electrons while the diagonal disorder within the f band is fully taken into account. In the case of a transition me- tal like system, except for Hubbard's approximation in dealing with d-d electron correlations, our procedure is exact within the

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spirit of CPA.

I. INTRODUCTION

In a previous work[1] the case of hybridized disordered systems described by two overlapping conduction bands was discussed, treating electron-electron correlations within the Hartree-Fock approach. This calculation[1] was intended to describe transition and actinide metals in the limit of large band widths and small correlations, i.e. $\Delta/U >> 1$.

In this paper, considering similar systems described by the same model Hamiltonian as before[1] and dealing with correlations within the Hubbard approximation[2] (in order to emphasize the strong correlation limit), we obtain the criterion for magnetic instabilities in these systems.

We recall that in our simple model[1] we have supposed that there exists diagonal disorder only within the α band (α = d in the case of transition metal like systems, and α = f in the actinides). Since the d band in the actinides "feels" the disorder only through the mixing, we have approximated the d occupation number $\langle n_{i-\sigma}^{(d)}\rangle$ by the self-consistent alloy occupation number $\langle n_{-\sigma}^{(d)}\rangle$ alloy. We emphasize that we have not taken into account the broad s band in these metals since it would only renormalize the d and f states through s-d and s-f mixing, respectively[3].

We have divided this work in the following way: in Section II we describe the model and obtain the relevant propagators and CPA equations. In the Section III we find the first order corrections due to the external magnetic fields, and in the last one we analyze the criterion of the ferromagnetic instability in special cases.

II. MODEL HAMILTONIAN AND CPA EQUATIONS

Consider a two band system of the type A_xB_{1-x} described by two hybridized α and β bands. We will suppose, as mentioned in the Introduction, that there is diagonal disorder only within the α band.

The Hamiltonian, in the Wannier representation, with usual notation, is:

$$\mathcal{H} = \sum_{i\sigma} \varepsilon_i^{(\alpha)} \alpha_{i\sigma}^{+}\alpha_{j\sigma} + \sum_{ij\sigma} T_{ij}^{(\alpha)} \alpha_{i\sigma}^{+} \alpha_{j\sigma} + \sum_i U_i^{(\alpha)} n_{i\uparrow}^{(\alpha)} n_{i\downarrow}^{(\alpha)} + \sum_{ij\sigma} T_{ij}^{(\beta)} \beta_{i\sigma}^{+}\beta_{j\sigma} +$$
$$+ U^{(\beta)} \sum_i n_{i\uparrow}^{(\beta)} n_{i\downarrow}^{(\beta)} + \sum_{ij\sigma} \{ V_{\alpha\beta}(R_i-R_j)\alpha_{i\sigma}^{+} \beta_{j\sigma} + V_{\beta\alpha}(R_i-R_j)\beta_{i\sigma}^{+}\alpha_{j\sigma} \} -$$
$$- h_0^{(\alpha)} \sum_{i\sigma} \sigma n_{i\sigma}^{(\alpha)} - h_0^{(\beta)} \sum_{i\sigma} \sigma n_{i\sigma}^{(\beta)} \qquad (1)$$

where $\beta_{i\sigma}^{+}(\beta_{i\sigma})$ and $\alpha_{i\sigma}^{+}(\alpha_{i\sigma})$ stand for the creation (annihilation) operators of β and α electrons respectively with spin σ at the ith lattice site. The energies $\varepsilon_i^{(\alpha)}$ and the Coulomb correlations $U_i^{(\alpha)}$ in the α band can take on values $\varepsilon_A^{(\alpha)}$, $\varepsilon_B^{(\alpha)}$ and $U_A^{(\alpha)}$, $U_B^{(\alpha)}$ respectively depending on the kind of related atoms, while the hopping integrals $T_{ij}^{(\beta)}$ and $T_{ij}^{(\alpha)}$ and mixing matrix elements $V_{\alpha\beta}(k)$ and $V_{\beta\alpha}(k)$ are assumed to have no randomness at all.

Following the equation of motion method[4,5,6] we obtain the following system of coupled equations for the propagator $G_{ij\sigma}^{\alpha\alpha}(\omega)$ and for $G_{ij\sigma}^{\beta\alpha}(\omega)$ (generated by hybridization):

$$\omega G_{ij\sigma}^{\alpha\alpha}(\omega) = \delta_{ij} + \varepsilon_i^{(\alpha)} G_{ij\sigma}^{\alpha\alpha}(\omega) + \sum_{\ell} T_{i\ell}^{(\alpha)} G_{\ell j\sigma}^{\alpha\alpha}(\omega) + U_i^{(\alpha)} \Gamma_{ij\sigma}^{\alpha\alpha}(\omega) +$$
$$+ \sum_{\ell} V_{\alpha\beta}(R_i-R_\ell) G_{\ell j\sigma}^{\beta\alpha}(\omega) - \sigma h_0^{(\alpha)} G_{ij\sigma}^{\alpha\alpha}(\omega) \qquad (2\text{-a})$$

and

$$\omega G^{\beta\alpha}_{ij\sigma}(\omega)=\sum_{\ell} T^{(\beta)}_{i\ell} G^{\beta\alpha}_{\ell j\sigma}(\omega)+U^{(\beta)}\Gamma^{\beta\alpha}_{ij\sigma}(\omega) + \sum_{\ell} V_{\beta\alpha}(R_i-R_\ell)G^{\alpha\alpha}_{\ell j\sigma}(\omega)- - \sigma h_o^{(\beta)}\, G^{\beta\alpha}_{ij\sigma}(\omega) \qquad (2\text{-}b)$$

where the Coulomb repulsion terms $U_i^{(\alpha)}$ and $U^{(\beta)}$ generate the new propagators

$$\Gamma^{\alpha\alpha}_{ij\sigma}(\omega)\equiv\langle\langle n^{(\alpha)}_{i-\sigma}\ \alpha_{i\sigma}\ ;\ \alpha^{+}_{j\sigma}\rangle\rangle_\omega \quad \text{and} \quad \Gamma^{\beta\alpha}_{ij\sigma}(\omega) = \langle\langle n^{(\beta)}_{i-\sigma}\ \beta_{i\sigma}\ ;\ \alpha^{+}_{j\sigma}\rangle\rangle_\omega .$$

The exact equations for these propagators are:

$$\omega\Gamma^{\alpha\alpha}_{ij\sigma}(\omega) =\langle n^{(\alpha)}_{i-\sigma}\rangle\ \delta_{ij} + \varepsilon_i^{(\alpha)}\ \Gamma^{\alpha\alpha}_{ij\sigma}(\omega) +\sum_{\ell} T^{(\alpha)}_{i\ell}\langle\langle n^{(\alpha)}_{i-\sigma}\alpha_{\ell\sigma};$$
$$\alpha^{+}_{j\sigma}\rangle\rangle_\omega + U_i^{(\alpha)}\ \Gamma^{\alpha\alpha}_{ij\sigma}(\omega) + \sum_{\ell} V_{\alpha\beta}(R_i-R_\ell)\langle\langle n^{(\alpha)}_{i-\sigma}\ \beta_{\ell\sigma}\ ;$$
$$\alpha^{+}_{j\sigma}\rangle\rangle_\omega - \sigma h_o^{(\alpha)}\ \Gamma^{\alpha\alpha}_{ij\sigma}(\omega) + \sum_{\ell} T^{(\alpha)}_{i\ell}\langle\langle(\alpha^{+}_{i-\sigma}\alpha_{\ell-\sigma}-\alpha^{+}_{\ell-\sigma}\alpha_{i-\sigma})\alpha_{i\sigma}\ ;$$
$$\alpha^{+}_{j\sigma}\rangle\rangle_\omega + \sum_{\ell}\{\ V_{\alpha\beta}(R_i-R_\ell)\langle\langle(\alpha^{+}_{i-\sigma}\beta_{\ell-\sigma})\alpha_{i\sigma}\ ;\ \alpha^{+}_{j\sigma}\rangle\rangle_\sigma - \qquad (3\text{-}a)$$
$$- V_{\beta\alpha}(R_i-R_\ell)\langle\langle(\beta^{+}_{\ell-\sigma}\alpha_{i-\sigma})\alpha_{i\sigma};\ \alpha^{+}_{j\sigma}\ \rangle\rangle_\omega\ \}$$

and

$$\omega\Gamma^{\beta\alpha}_{ij\sigma}(\omega)=\sum_{\ell} T^{(\beta)}_{i\ell}\langle\langle n^{(\beta)}_{i-\sigma}\beta_{\ell\sigma}\ ;\ \alpha^{+}_{j\sigma}\rangle\rangle_\omega + U^{(\beta)}\Gamma^{\beta\alpha}_{ij\sigma}(\omega) +$$
$$\sum_{\ell} V_{\beta\alpha}(R_i-R_\ell)\langle\langle n^{(\beta)}_{i-\sigma}\alpha_{\ell\sigma};\ \alpha^{+}_{j\sigma}\rangle\rangle_\omega - \sigma h_o^{(\beta)}\Gamma^{\beta\alpha}_{ij\sigma}(\omega) +$$
$$\sum_{\ell} T^{(\beta)}_{i\ell}\langle\langle(\beta^{+}_{i-\sigma}\ \beta_{\ell-\sigma}-\ \beta^{+}_{\ell-\sigma}\ \beta_{i-\sigma})\beta_{i\sigma};\alpha^{+}_{j\sigma}\rangle\rangle_\omega \qquad (3\text{-}b)$$

$$+ \sum_{\ell} \{V_{\beta\alpha}(R_i-R_\ell)\langle\langle(\beta^{+}_{i-\sigma}\alpha_{\ell-\sigma})\beta_{i\sigma};\alpha^{+}_{j\sigma}\rangle\rangle_\omega - V_{\alpha\beta}(R_i-R_\ell)\langle\langle(\alpha^{+}_{\ell-\sigma}\beta_{i-\sigma})\beta_{i\sigma}\,;\,\alpha^{+}_{j\sigma}\rangle\rangle_\omega$$

Neglecting "broadening corrections"[7] (the last two terms of 3-a and 3-b) and decoupling kinetic terms as:

$$\langle\langle n^{(\alpha)}_{i-\sigma}\,\alpha_{\ell\sigma};\alpha^{+}_{j\sigma}\rangle\rangle_\omega \simeq \langle n^{(\alpha)}_{i-\sigma}\rangle \quad G^{\alpha\alpha}_{\ell j\sigma}(\omega)$$

$$\langle\langle n^{(\alpha)}_{i-\sigma}\,\beta_{\ell\sigma};\,\alpha^{+}_{j\sigma}\rangle\rangle_\omega \simeq \langle n^{(\alpha)}_{i-\sigma}\rangle \quad G^{\beta\alpha}_{\ell j\sigma}(\omega)$$

Equations (3) can be rewritten, respectively, as:

$$(\omega-\varepsilon^{(\alpha)}_i - U^{(\alpha)}_i + \sigma h^{(\alpha)}_o)\Gamma^{\alpha\alpha}_{ij\sigma}(\omega) =$$

$$=\langle n^{(\alpha)}_{i-\sigma}\rangle\{\delta_{ij}+\sum_{\ell} T^{(\alpha)}_{i\ell}\; G^{\alpha\alpha}_{\ell j\sigma}(\omega) + \sum_{\ell} V_{\alpha\beta}(R_i-R_\ell)\; G^{\beta\alpha}_{\ell j\sigma}(\omega)\} \qquad (4\text{-a})$$

and

$$(\omega-U^{(\beta)}+\sigma h^{(\beta)}_o)\Gamma^{\beta\alpha}_{ij\sigma}(\omega) =$$

$$=\langle n^{(\beta)}_{i-\sigma}\rangle \;\{\sum_{\ell} T^{(\beta)}_{i\ell}\quad G^{\beta\alpha}_{\ell j\sigma}(\omega) + \sum_{\ell} V_{\beta\alpha}(R_i-R_\ell)\; G^{\alpha\alpha}_{\ell j\sigma}(\omega)\;\} \qquad (4\text{-b})$$

In the limit of strong correlations ($U^{(\beta)}\to\infty$, and $U^{(\alpha)}_i\to\infty$) one gets:

$$\lim_{U^{(\alpha)}_i\to\infty} U^{(\alpha)}_i\Gamma^{\alpha\alpha}_{ij\sigma}(\omega) \simeq -\langle n^{(\alpha)}_{i-\sigma}\rangle\{\delta_{ij}+\sum_{\ell} T^{(\alpha)}_{i\ell}\; G^{\alpha\alpha}_{\ell j\sigma}(\omega) +$$

$$+ \sum_{\ell} V_{\alpha\beta}(R_i-R_\ell)G^{\beta\alpha}_{\ell j\sigma}(\omega)\;\} \qquad (5\text{-a})$$

and

$$\lim_{U^{(\beta)}\to\infty} U^{(\beta)}\Gamma^{\beta\alpha}_{ij\sigma}(\omega) \simeq - \langle n^{(\beta)}_{i-\sigma}\rangle \{\sum_{\ell} T^{(\beta)}_{i\ell} G^{\beta\alpha}_{\ell j\sigma}(\omega) + $$

$$+\sum_{\ell} V_{\beta\alpha}(R_i - R_\ell) G^{\alpha\alpha}_{\ell j\sigma}(\omega) \} \qquad (5\text{-b})$$

Similarly, one obtains, using the same approximations, the follo wing system for the propagators $G^{\beta\beta}_{ij\sigma}(\omega)$ and $G^{\alpha\beta}_{ij\sigma}(\omega)$:

$$\omega G^{\beta\beta}_{ij\sigma}(\omega) = \delta_{ij} + \sum_{\ell} T^{(\beta)}_{i\ell} G^{\beta\beta}_{\ell j\sigma}(\omega) + U^{(\beta)}\Gamma^{\beta\beta}_{ij\sigma}(\omega) + \sum_{\ell} V_{\beta\alpha}(R_i - R_\ell) G^{\alpha\beta}_{\ell j\sigma}(\omega) -$$

$$- \sigma h^{(\beta)}_{o} G^{\beta\beta}_{ij\sigma}(\omega) \qquad (6\text{-a})$$

and

$$\omega G^{\alpha\beta}_{ij\sigma}(\omega) = \varepsilon^{(\alpha)}_{i} G^{\alpha\beta}_{ij\sigma}(\omega) + \sum_{\ell} T^{(\alpha)}_{i\ell} G^{\alpha\beta}_{\ell j\sigma}(\omega) + U^{(\alpha)}_{i}\Gamma^{\alpha\beta}_{ij\sigma}(\omega) +$$

$$+ \sum_{\ell} V_{\alpha\beta}(R_i - R_\ell) G^{\beta\beta}_{\ell j\sigma}(\omega) - \sigma h^{(\alpha)}_{o} G^{\alpha\beta}_{ij\sigma}(\omega) \quad , \qquad (6\text{-b})$$

the propagators generated by the Coulomb correlations satisfying the following approximate equations:

$$(\omega - U^{(\beta)} + \sigma h^{(\beta)}_{o})\Gamma^{\beta\beta}_{ij\sigma}(\omega) \simeq \langle n^{(\beta)}_{i-\sigma}\rangle \{\delta_{ij} + \sum_{\ell} T^{(\beta)}_{i\ell} G^{\beta\beta}_{\ell j\sigma}(\omega) + \sum_{\ell} V_{\beta\alpha}(R_i - R_\ell) G^{\alpha\beta}_{\ell j\sigma}(\omega)\}$$

$$(7\text{-a})$$

and

$$(\omega - U^{(\alpha)}_{i} + \sigma h^{(\alpha)}_{o})\Gamma^{\alpha\beta}_{ij\sigma}(\omega) \simeq \langle n^{(\alpha)}_{i-\sigma}\rangle \{\sum_{\ell} T^{(\alpha)}_{i\ell} G^{\alpha\beta}_{\ell j\sigma}(\omega) +$$

$$+ \sum_{\ell} V_{\alpha\beta}(R_i - R_\ell) G^{\beta\beta}_{\ell j\sigma}(\omega) \} \qquad (7\text{-b})$$

The last two equations become, in the limit of strong correlations:

$$\lim_{U^{(\beta)}\to\infty} U^{(\beta)}\Gamma^{\beta\beta}_{ij\sigma}(\omega) \simeq -\langle n^{(\beta)}_{i-\sigma}\rangle\{\delta_{ij}+\sum_{\ell} T^{(\beta)}_{i\ell}G^{\beta\beta}_{\ell j\sigma}(\omega) + \sum_{\ell} V_{\beta\alpha}(R_i-R_\ell)G^{\alpha\beta}_{\ell j\sigma}(\omega)\} \qquad (8\text{-a})$$

and

$$\lim_{U^{(\alpha)}_i\to\infty} U^{(\alpha)}_i\Gamma^{\alpha\beta}_{ij\sigma}(\omega) \simeq -\langle n^{(\alpha)}_{i-\sigma}\rangle\{\sum_{\ell} T^{(\alpha)}_{i\ell}G^{\alpha\beta}_{\ell j\sigma}(\omega)+\sum_{\ell} V_{\alpha\beta}(R_i-R_\ell)G^{\beta\beta}_{\ell j\sigma}(\omega)\} \qquad (8\text{-b})$$

At this point we make the approximation of replacing the occupation number $\langle n^{(\beta)}_{i-\sigma}\rangle$ by $\langle n^{(\beta)}_{-\sigma}\rangle_{alloy}$, which will be determined self-consistently through the configuration averaging of $G^{\beta\beta}_{ij\sigma}(\omega)$. This is a similar approximation to that used in a previous calculation[1] within the Hartree-Fock scheme. It corresponds physically to say that a β electron of spin σ interacts with the "effective occupation numbers of spin $-\sigma$". Such a procedure neglects the site dependence of the occupation numbers involved in the Coulomb terms. Since there is no disorder in the β band and disorder associated to the α electrons connects to the β band only through mixing, we expect that this will not be a very drastic approximation.

It should be noted that in the special case of transition metal alloys the α and β bands correspond to the d and s bands respectively. In this situation we can neglect the Coulomb correlation in the s band ($U^{(\beta)}=U^{(s)}=0$), thus making unnecessary the equations of motion (cf eqs. 3-b and 7-a) for the propagators $\Gamma^{\beta\alpha}_{ij\sigma}(\omega)$ and $\Gamma^{\beta\beta}_{ij\sigma}(\omega)$, respectively, generated by it. It should also be pointed out that, in this case, randomness has been completely removed from the s band, and there is no need any longer to do our previous approximation $<n^{(s)}_{i-\sigma}> = <n^{(s)}_{-\sigma}>$ alloy.

Substituting equations (5) into (2), we get the following system for the α-α propagator:

$$(\omega-\bar{\varepsilon}^{(\alpha)}_{i\sigma})G^{\alpha\alpha}_{ij\sigma}(\omega)=\bar{n}^{(\alpha)}_{i-\sigma}\{\delta_{ij}+\sum_{\ell}T^{(\alpha)}_{i\ell}\ G^{\alpha\alpha}_{\ell j\sigma}(\omega)+\sum_{\ell}V_{\alpha\beta}(R_i-R_\ell)G^{\beta\alpha}_{\ell j\sigma}(\omega)\} \qquad (9\text{-a})$$

and

$$(\omega+\sigma h^{(\beta)}_{o})G^{\beta\alpha}_{ij\sigma}(\omega)=\bar{n}^{(\beta)}_{-\sigma}\{\sum_{\ell}T^{(\beta)}_{i\ell}G^{\beta\alpha}_{\ell j\sigma}(\omega)+\sum_{\ell}V_{\beta\alpha}(R_i-R_\ell)G^{\alpha\alpha}_{\ell j\sigma}(\omega)\} \qquad (9\text{-b})$$

where we have defined:

$$\begin{aligned}\bar{\varepsilon}^{(\alpha)}_{i\sigma} &= \varepsilon^{(\alpha)}_{i}-\sigma h^{(\alpha)}_{o}\\ \bar{n}^{(\alpha)}_{i-\sigma} &= 1-<n^{(\alpha)}_{i-\sigma}>\\ \bar{n}^{(\beta)}_{-\sigma} &= 1-<n^{(\beta)}_{i-\sigma}> \simeq 1-<n_{-\sigma}> \text{ alloy.}\end{aligned} \qquad (9\text{-c})$$

Fourier transforming (9-b) we have:

$$G^{\beta\alpha}_{kk'\sigma}(\omega) = \frac{V_{\beta\alpha}(k)\bar{n}^{(\beta)}_{-\sigma}}{\omega - \bar{\varepsilon}^{(\beta)}_{k\sigma}}\ G^{\alpha\alpha}_{kk'\sigma}(\omega) \qquad (10)$$

$\bar{\varepsilon}^{(\beta)}_{k\sigma}$ being:

$$\bar{\varepsilon}^{(\beta)}_{k\sigma} = \bar{n}^{(\beta)}_{-\sigma}\varepsilon^{(\beta)}_{k} - \sigma h^{(\beta)}_{o} \qquad (11)$$

or transforming back equation (10) to site representation:

$$G^{\beta\alpha}_{ij\sigma}(\omega)=\bar{n}^{(\beta)}_{-\sigma}\sum_{\ell}\left\{\sum_{k}\frac{V_{\beta\alpha}(k)}{\omega-\bar{\varepsilon}^{(\beta)}_{k\sigma}}\ e^{-ik(R_i-R_\ell)}\right\}G^{\alpha\alpha}_{\ell j\sigma}(\omega)\ \equiv$$

$$\equiv \bar{n}_{-\sigma}^{(\beta)} \sum_{\ell} T_{i\ell\sigma}^{mix}(\omega)\ G_{\ell j\sigma}^{\alpha\alpha}(\omega) \quad ,$$

where we note that, within this approximation, $T_{i\ell\sigma}^{mix}(\omega)$ contains no disorder at all. Defining:

$$\tilde{T}_{i\ell\sigma}^{(\alpha)}(\omega) = T_i^{(\alpha)} + \bar{n}_{-\sigma}^{(\beta)} \sum_{m} V_{\alpha\beta}(R_i - R_m)\ T_{m\ell\sigma}^{mix}(\omega) \tag{12}$$

and the "locator" $F_i^{\sigma}(\omega)$ as:

$$F_i^{\sigma}(\omega) = \frac{\omega - \bar{\varepsilon}_{i\sigma}^{(\alpha)}}{1 - \langle n_{i-\sigma}^{(\alpha)} \rangle} = \omega - \frac{\bar{\varepsilon}_{i\sigma}^{(\alpha)} - \omega \langle n_{i-\sigma}^{(\alpha)} \rangle}{\bar{n}_{i-\sigma}^{(\alpha)}} \equiv \omega - \tilde{\varepsilon}_{i\sigma}^{(\alpha)}(\omega) \tag{13}$$

one gets for the α-α propagator:

$$G_{ij\sigma}^{\alpha\alpha}(\omega) = \frac{1}{F_i^{\sigma}(\omega)} \left[\delta_{ij} + \sum_{\ell} \tilde{T}_{i\ell\sigma}^{(\alpha)}(\omega)\ G_{\ell j\sigma}^{\alpha\alpha}(\omega) \right] \tag{14}$$

We observe that associated to the existence of strong Coulomb correlations a factor $\bar{n}_{i-\sigma}^{(\alpha)}$ has been introduced multiplying the right-hand side of equation (9-a). This factor has an important consequence in the definition of the locator, and subsequently in the form of the self-energy. From equation (13) one sees that if the locator is to be rewritten as $(\omega - \tilde{\varepsilon}_{i\sigma})$, this effective level energy is frequency dependent. In the absence of Coulomb interaction $\tilde{\varepsilon}_{i\sigma}^{(\alpha)}(\omega)$ would reduce to $(\varepsilon_i^{(\alpha)} - \sigma h_0^{(\alpha)})$, and in the Hartree-Fock approximation[1] the effective level energy would be simply $\varepsilon_i^{(\alpha)} + U_i^{(\alpha)} \langle n_{i-\sigma}^{(\alpha)} \rangle - \sigma h_0^{(\alpha)}$. Then the frequency dependence is a clear feature of the Hubbard strong correlation limit (e.g., $\frac{U}{\Delta} \gg 1$).

Taking the configuration average and Fourier transforming equation (14), we have in the Bloch representation:

$$<G^{\alpha\alpha}_{ij\sigma}(\omega)>_k = \frac{1}{F^{\sigma}(\omega) - \tilde{\varepsilon}^{(\alpha)}_{k\sigma}(\omega)}$$

with

$$\tilde{\varepsilon}^{(\alpha)}_{k\sigma}(\omega) = \varepsilon^{(\alpha)}_{k} + \frac{\bar{n}^{(\beta)}_{-\sigma}|V_{\alpha\beta}(k)|^2}{\omega - \bar{n}^{(\beta)}_{-\sigma}\varepsilon^{(\beta)}_{k} + \sigma h_o^{(\beta)}} \tag{15}$$

$F^{\sigma}(\omega)$ being the "configuration averaged locator".

Or, coming back to the Wannier representation:

$$<G^{\alpha\alpha}_{ij\sigma}(\omega)> = \sum_k \frac{e^{ik(R_i-R_j)}}{F^{\sigma}(\omega) - \tilde{\varepsilon}^{(\alpha)}_{k\sigma}(\omega)} \tag{16}$$

Setting i=j we obtain:

$$<G^{\alpha\alpha}_{jj\sigma}(\omega)> = \sum_k \frac{1}{F^{\sigma}(\omega) - \tilde{\varepsilon}^{(\alpha)}_{k\sigma}(\omega)} \equiv H^{\sigma}_{(\alpha)}(\omega) \tag{17}$$

According to Ref.[5] the self-consistency condition reads:

$$C_A<G^{\alpha\alpha}_{\ell j\sigma}(\omega)>_A + C_B<G^{\alpha\alpha}_{\ell j\sigma}(\omega)>_B = <G^{\alpha\alpha}_{\ell j\sigma}(\omega)> \text{ , with } C_A \equiv x \text{ and } C_B \equiv 1-x$$

(18-a)

where

$$<G^{\alpha\alpha}_{\ell j\sigma}(\omega)>_i = <G^{\alpha\alpha}_{\ell j\sigma}(\omega)> + <G^{\alpha\alpha}_{\ell i\sigma}(\omega)> \cdot \frac{F^{\sigma}(\omega) - F^{\sigma}_i(\omega)}{1 - [F^{\sigma}(\omega) - F^{\sigma}_i(\omega)] <G^{\alpha\alpha}_{ii\sigma}(\omega)>} <G^{\alpha\alpha}_{ij\sigma}(\omega)>$$

(18-b)

From equations (18) we can rewrite the self-consistency equation as:

$$\Sigma^{\sigma}_{(\alpha)}(\omega) = C_A\tilde{\varepsilon}^{(\alpha)}_{A\sigma}(\omega) + C_B\tilde{\varepsilon}^{(\alpha)}_{B\sigma}(\omega) - (\tilde{\varepsilon}^{(\alpha)}_{A\sigma}(\omega) - \Sigma^{\sigma}_{(\alpha)}) H^{\sigma}_{(\alpha)}(\omega) (\tilde{\varepsilon}^{(\alpha)}_{B\sigma}(\omega) - \Sigma^{\sigma}_{(\alpha)})$$

(19)

where we have introduced the self-energy $\Sigma^{\sigma}_{(\alpha)}(\omega)$ through the "configuration averaged locator":

$$F^{\sigma}(\omega) = \omega - \Sigma^{\sigma}_{(\alpha)}(\omega) \tag{20}$$

In order to find the β-β propagator we, firstly, substitute equations (8) into (6), getting:

$$(\omega+\sigma h_0^{(\beta)})G^{\beta\beta}_{ij\sigma}(\omega)=\bar{n}^{(\beta)}_{-\sigma}\left[\delta_{ij}+\sum_{\ell}T_i^{(\beta)}G^{\beta\beta}_{\ell j\sigma}(\omega)+\sum_{\ell}V_{\beta\alpha}(R_i-R_\ell)G^{\alpha\beta}_{\ell j\sigma}(\omega)\right] \tag{21-a}$$

and

$$(\omega-\bar{\varepsilon}^{(\alpha)}_{i\sigma})G^{\alpha\beta}_{ij\sigma}(\omega) = \bar{n}^{(\alpha)}_{i-\sigma}\left[\sum_{\ell} T^{(\alpha)}_{i\ell}G^{\alpha\beta}_{\ell j\sigma}(\omega)+\sum_{\ell}V_{\alpha\beta}(R_i-R_\ell)G^{\beta\beta}_{\ell j\sigma}(\omega)\right] \tag{21-b}$$

Configuration averaging and Fourier transforming equations (21) one obtains:

$$(\omega-\bar{n}^{(\beta)}_{-\sigma}\varepsilon_k^{(\beta)}+\sigma h_0^{(\beta)})\langle G^{\beta\beta}_{ij\sigma}(\omega)\rangle_k=\bar{n}^{(\beta)}_{-\sigma}\left[1+V_{\beta\alpha}(k)\langle G^{\alpha\beta}_{ij\sigma}(\omega)\rangle_k\right] \tag{22-a}$$

and

$$V_{\beta\alpha}(k)\langle G^{\alpha\beta}_{ij\sigma}(\omega)\rangle_k = \frac{|V_{\alpha\beta}(k)|^2}{\omega-\varepsilon_k^{(\alpha)}-\Sigma^{\sigma}_{(\alpha)}}\langle G^{\beta\beta}_{ij\sigma}(\omega)\rangle_k \tag{22-b}$$

Substituting the last equation into (22-a) one finally gets:

$$\langle G^{\beta\beta}_{ij\sigma}(\omega)\rangle_k=\frac{\bar{n}^{(\beta)}_{-\sigma}(\omega-\varepsilon_k^{(\alpha)}-\Sigma^{\sigma}_{(\alpha)})}{(\omega-\bar{n}^{(\beta)}_{-\sigma}\varepsilon_k^{(\beta)}+\sigma h_0^{(\beta)})(\omega-\varepsilon_k^{(\alpha)}-\Sigma^{\sigma}_{(\alpha)})-\bar{n}^{(\beta)}_{-\sigma}|V_{\alpha\beta}(k)|^2} \tag{23}$$

We should observe that in the case of transition metal alloys, where $U^{(\beta)}=0$, the equations of motion for the propagators $G^{\beta\alpha}_{ij\sigma}(\omega)$ and $G^{\beta\beta}_{ij\sigma}(\omega)$ (see equation 2-b and 6-a) reduce, respectively, to:

$$(\omega+\sigma h_o^{(\beta)})G_{ij\sigma}^{\beta\alpha}(\omega) = \sum_\ell T_{i\ell}^{(\beta)}G_{\ell j\sigma}^{\beta\alpha}(\omega) + \sum_\ell V_{\beta\alpha}(R_i-R_\ell)G_{\ell j\sigma}^{\alpha\alpha}(\omega)$$

and

$$(\omega+\sigma h_o^{(\beta)})G_{ij\sigma}^{\beta\beta}(\omega) = \delta_{ij}+\sum_\ell T_{i\ell}^{(\beta)}G_{\ell j\sigma}^{\beta\beta}(\omega) + \sum_\ell V_{\beta\alpha}(R_i-R_\ell)G_{\ell j\sigma}^{\alpha\beta}(\omega)$$

One can easily verify that our previous equations and definitions still remain valid for this special case if we simply make $\bar{n}_{-\sigma}^{(\beta)} = 1$.

Having determined the propagators $G_{ij\sigma}^{\alpha\alpha}(\omega)$ and $G_{ij\sigma}^{\beta\beta}(\omega)$, we can evaluate the first order corrections due to the magnetic fields in the occupation numbers $n_A^{(\alpha)}$ and $n_B^{(\alpha)}$.

III. FIRST ORDER CORRECIONS IN THE MAGNETIC FIELDS

Next, we proceed as Ref. [8] , and collect first order terms in $h_o^{(\alpha)}$and $h_o^{(\beta)}$. So, we introduce the following definitions:

$$\Sigma_{(\alpha)}^{\sigma} = \Sigma_{(\alpha)}^{p} - \sigma\delta\Sigma_{(\alpha)}$$

$$\langle n_{i-\sigma}^{(\alpha)}\rangle = \langle n_i^{(\alpha)}\rangle_p - \sigma\delta n_i^{(\alpha)} \quad \text{or} \quad \langle \bar{n}_{i-\sigma}^{(\alpha)}\rangle = \langle \bar{n}_i\rangle_p^{(\alpha)} + \sigma\delta n_i^{(\alpha)} \tag{24}$$

$$\langle n_{-\sigma}^{(\beta)}\rangle_{alloy} = \langle n^{(\beta)}\rangle_p - \sigma\delta n^{(\beta)} \quad \text{or} \quad \langle \bar{n}_{-\sigma}^{(\beta)} = \langle \bar{n}^{(\beta)}\rangle_p + \sigma\delta n^{(\beta)}\rangle$$

where the sub-script (or super-script) p stands for paramagnetic phase.

Substituting definition (15) into equation (17) one has:

$$H_{(\alpha)}^{o}(\omega) = \sum_k \frac{\omega-\bar{n}_{-\sigma}^{(\beta)}\epsilon_k^{(\beta)}+\sigma h_o^{(\beta)}}{(\omega-\epsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^{\sigma})(\omega-\bar{n}_{-\sigma}^{(\beta)}\epsilon_k^{(\beta)}+\sigma h_o^{(\beta)})-\bar{n}_{-\sigma}^{(\beta)}|V_{\alpha\beta}(k)|^2} \tag{25}$$

Using definitions (24) we can expand $H^{\sigma}_{(\alpha)}(\omega)$ to first order in the magnetic fields as:

$$H^{\sigma}_{(\alpha)}(\omega)=H_p(\omega)-\sigma\left[<\bar{n}^{(\beta)}>_p\ h_o^{(\beta)}-\omega\delta n^{(\beta)}\right]\ H_1^{(1)}(\omega)-\sigma\delta\Sigma_{(\alpha)}\ H_1^{(2)}(\omega) \quad (26)$$

where we have defined:

$$H_p(\omega) = \sum_k \frac{(\omega-<\bar{n}^{(\beta)}>_p\varepsilon_k^{(\beta)})}{(\omega-\Sigma^p_{(\alpha)}-\varepsilon_k^{(\alpha)})(\omega-<\bar{n}^{(\beta)}>_p\varepsilon_k^{(\beta)})-<\bar{n}^{(\beta)}>_p|V_{\alpha\beta}(k)|^2} \quad (27\text{-a})$$

$$H_1^{(1)}(\omega) = \sum_k \frac{|V_{\alpha\beta}(k)|^2}{\left[(\omega-\Sigma^p_{(\alpha)}-\varepsilon_k^{(\alpha)})(\omega-<\bar{n}^{(\beta)}>_p\varepsilon_k^{(\beta)})-<\bar{n}^{(\beta)}>_p|V_{\alpha\beta}(k)|^2\right]^2} \quad (27\text{-b})$$

$$H_1^{(2)}(\omega) = \sum_k \frac{(\omega-<\bar{n}^{(\beta)}>_p\varepsilon_k^{(\beta)})^2}{\left[(\omega-\Sigma^p_{(\alpha)}-\varepsilon_k^{(\alpha)})(\omega-<\bar{n}^{(\beta)}>_p\varepsilon_k^{(\beta)})-<\bar{n}^{(\beta)}>_p|V_{\alpha\beta}(k)|^2\right]^2} \quad (27\text{-c})$$

One should note (see below) that the full k-dependence of the hybridization is included only in the above well defined functions. If one approximates the mixing to a constant, then we can use the Kishore and Joshi approximation of homothetic bands and rewrite these functions in terms of the density of states[9].

Again, using (24) and (9c) we get for $\tilde{\varepsilon}^{(\alpha)}_{i\sigma}(\omega)$:

$$\tilde{\varepsilon}^{(\alpha)}_{i\sigma}(\omega) = \frac{\varepsilon_i^{(\alpha)}-\omega<n_i^{(\alpha)}>_p-\sigma h_o^{(\alpha)}+\sigma\omega\delta n_i^{(\alpha)}}{<\bar{n}_i^{(\alpha)}>_p+\sigma\delta n_i^{(\alpha)}} \quad ;\ i = A \text{ or } B$$

And keeping terms of first order only, we have:

$$\tilde{\varepsilon}^{(\alpha)}_{i\sigma}(\omega) = \varepsilon^{(\alpha)}_{ip}(\omega) - \frac{1}{<\bar{n}_i^{(\alpha)}>_p}\ \sigma h_o^{(\alpha)} + \frac{\omega-\varepsilon_i^{(\alpha)}}{(<\bar{n}_i^{(\alpha)}>_p)^2}\sigma\delta n_i^{(\alpha)} \quad (28)$$

$\varepsilon^{(\alpha)}_{ip}(\omega)$ being defined as:

$$\varepsilon_{ip}^{(\alpha)}(\omega) = \frac{\varepsilon_i^{(\alpha)} - \omega \langle n_i^{(\alpha)} \rangle_p}{\langle \bar{n}_i^{(\alpha)} \rangle_p} \tag{29}$$

Substituting expansions (26) and (28) in the self-consistency condition (19) one has:

$$\delta \textstyle\sum_{(\alpha)} = - \frac{(\omega - \varepsilon_A^{(\alpha)})}{\langle \bar{n}_A^{(\alpha)} \rangle_p} T_A(\omega) \delta n_A^{(\alpha)} - \frac{(\omega - \varepsilon_B^{(\alpha)})}{\langle \bar{n}_B^{(\alpha)} \rangle_p} T_B(\omega)\, \delta n_B^{(\alpha)} +$$

$$+ \left[T_A(\omega) + T_B(\omega) \right] h_o^{(\alpha)} - k(\omega) \langle \bar{n}^{(\beta)} \rangle_p h_o^{(\beta)} + \omega k(\omega) \delta n^{(\beta)} \tag{30}$$

where we have used the following definitions:

$$T_i(\omega) = \frac{C_i - H_p(\omega)\left[\varepsilon_{jp}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p\right]}{\langle \bar{n}_i^{(\alpha)} \rangle_p \{1 + (\varepsilon_{Ap}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p) H_1^{(2)}(\omega)(\varepsilon_{Bp}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p) - H_p(\omega)(\varepsilon_{Ap}^{(\alpha)}(\omega) + \varepsilon_{Bp}^{(\alpha)}(\omega) - 2\sum_{(\alpha)}^p} \tag{31-a}$$

$i,j = A, B \quad ; \quad j \neq i$

and

$$k(\omega) = \frac{(\varepsilon_{Ap}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p) H_1^{(1)}(\omega)(\varepsilon_{Bp}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p)}{1 + (\varepsilon_{Ap}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p) H_1^{(2)}(\omega)(\varepsilon_{Bp}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p) - H_p(\omega)(\varepsilon_{Ap}^{(\alpha)}(\omega) + \varepsilon_{Bp}^{(\alpha)}(\omega) - 2\sum_{(\alpha)}^p)} \tag{31-b}$$

And the self-energy in the paramagnetic phase $\sum_{(\alpha)}^p$ satisfies:

$$\textstyle\sum_{(\alpha)}^p(\omega) = C_A \varepsilon_{Ap}^{(\alpha)}(\omega) + C_B \varepsilon_{Bp}^{(\alpha)}(\omega) - \left[\varepsilon_{Ap}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p\right] H_p(\omega) \left[\varepsilon_{Bp}^{(\alpha)}(\omega) - \sum_{(\alpha)}^p\right] \tag{32}$$

Now, we proceed to determine the change in the β-occupation number $\delta n^{(\beta)}$ through the expression:

$$\delta n^{(\beta)} = \mathcal{F}_{\omega} \{\sum_{k} <\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k\} \tag{33}$$

where

$$<G^{\beta\beta}_{ij\sigma}(\omega)>_k = <G^{\beta\beta}_{ij}(\omega)>^p_k + \sigma < \delta G^{\beta\beta}_{ij\sigma}(\omega)>_k \tag{34}$$

and $\mathcal{F}_{\omega}$ denotes[10]:

$$\mathcal{F}_{\omega}\left[<\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k\right] =$$

$$\frac{i}{2\pi} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} d\omega f(\omega) \left[<\delta G^{\beta\beta}_{ij\sigma}(\omega+i\varepsilon)>_k - <\delta G^{\beta\beta}_{ij\sigma}(\omega-i\varepsilon)>_k\right] \tag{35}$$

$f(\omega)$ being the Fermi distribution function.

Remembering equation (23) and definitions (24) we get, in the first order in the magnetic fields, the following expression for $<\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k$:

$$<\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k =$$

$$- \frac{(\omega - \varepsilon^{(\alpha)}_k - \Sigma^p_{(\alpha)})^2}{\left[(\omega - <\bar{n}^{(\beta)}>_p \varepsilon^{(\beta)}_k)(\omega - \varepsilon^{(\alpha)}_k - \Sigma^p_{(\alpha)}) - <\bar{n}^{(\beta)}>_p |V_{\alpha\beta}(k)|^2\right]^2} (<\bar{n}^{(\beta)}>_p h^{(\beta)}_o - \omega \delta n^{(\beta)})$$

$$- \frac{(<\bar{n}^{(\beta)}>_p)^2 |V_{\alpha\beta}(k)|^2}{\left[(\omega - <\bar{n}^{(\beta)}>_p \varepsilon^{(\beta)}_k)(\omega - \varepsilon^{(\alpha)}_k - \Sigma^p_{(\alpha)}) - <\bar{n}^{(\beta)}>_p |V_{\alpha\beta}(k)|^2\right]^2} \delta\Sigma_{(\alpha)} \tag{36}$$

Using equations (30), (33) and the definitions in the Appendix, one has:

$$\delta n^{(\beta)} = - \frac{\Lambda_4^A}{1 + \Lambda_3} \delta n_A^{(\alpha)} - \frac{\Lambda_4^B}{1 + \Lambda_3} \delta n_B^{(\alpha)}$$

$$+ \frac{(\Lambda_2^A + \Lambda_2^B)}{1+\Lambda_3} h_o^{(\alpha)} + \frac{\Lambda_1}{1+\Lambda_3} h_o^{(\beta)} \qquad (37)$$

In order to obtain explicit expressions for $\delta n_A^{(\alpha)}$ and $\delta n_B^{(\alpha)}$ in terms of the magnetic fields and $\delta n^{(\beta)}$ we have to expand $\langle G_{ij\sigma}^{\alpha\alpha}(\omega)\rangle_i$ (i=A or B). To do this we take l=j and i=j in equation (18-b) and rearrange the terms getting:

$$\langle G_{jj\sigma}^{\alpha\alpha}(\omega)\rangle_i = \frac{H_{(\alpha)}^{\sigma}(\omega)}{1-(\tilde{\varepsilon}_{i\sigma}^{(\alpha)}(\omega) - \Sigma_{(\alpha)}^{\sigma})\, H_{(\alpha)}^{\sigma}(\omega)} \qquad i=A \text{ or } B \qquad (38)$$

From the expressions

$$\langle G_{jj\sigma}^{\alpha\alpha}(\omega)\rangle_i = \langle G_{jj}^{\alpha\alpha}(\omega)\rangle_i^p + \sigma\langle \delta G_{jj\sigma}^{\alpha\alpha}(\omega)\rangle_i \qquad i=A \text{ or } B$$

and

$$\delta n_i^{(\alpha)} = \mathcal{G}_\omega\left[\langle \delta G_{jj\sigma}^{\alpha\alpha}(\omega)\rangle_i\right]$$

and using expansions (26), (28), (30) we obtain:

$$\delta n_i^{(\alpha)} = - \lambda_i^A \delta n_A^{(\alpha)} - \lambda_i^B \delta n_B^{(\alpha)} - \alpha_i \delta n_i^{(\alpha)} + \Gamma_i \delta_n^{(\beta)}$$

$$+ (\xi_i + \zeta_i^A + \zeta_i^B)\, h_o^{(\alpha)} \qquad (39)$$

where the quantities λ_i^j, ζ_i^j, Γ_i, ξ_i, α_i and η_i are defined in the Appendix.

Substituting equation (37) in (39) one finally has:

$$\delta n_i^{(\alpha)} = - \left\{\lambda_i^A + \frac{\Gamma_i \Lambda_4^A}{1+\Lambda_3}\right\} \delta n_A^{(\alpha)} - \left\{\lambda_i^B + \frac{\Gamma_i \Lambda_4^B}{1+\Lambda_3}\right\} \delta n_B^{(\alpha)} - \alpha_i \delta n_i^{(\alpha)}$$

$$+\left\{\xi_i+\zeta_i^A+\zeta_i^B+\frac{\Gamma_i(\Lambda_2^A+\Lambda_2^B)}{1+\Lambda_3}\right\} h_o^{(\alpha)}+\left\{\eta_i+\frac{\Gamma_i\Lambda_1}{1+\Lambda_3}\right\} h_o^{(\beta)} \qquad (40)$$

Taking i=A and B in (40) one gets the following system:

$$(1+M_A)\delta n_A^{(\alpha)}+N_B\delta n_B^{(\alpha)}=\tau_A h_o^{(\beta)}+Q_A h_o^{(\alpha)} \qquad (41\text{-a})$$

$$N_A\delta n_A^{(\alpha)}+(1+M_B)\delta n_B^{(\alpha)}=\tau_B h_o^{(\beta)}+Q_B h_o^{(\alpha)} \qquad (41\text{-b})$$

where the functions M_i, N_i, τ_i and Q_i are defined in the Appendix.

Solving the system (41), we can get the "partial static susceptibilities" defined by:

$$\chi_i^{\alpha\beta}=\frac{\delta n_i^{(\alpha)}}{h_o^{(\beta)}} \quad ; \quad \chi_i^{\alpha\alpha}=\frac{\delta n_i^{(\alpha)}}{h_o^{(\alpha)}} \qquad i=A,B$$

They are:

$$\chi_i^{\alpha\beta}=\frac{\tau_i(1+M_j)-\tau_j N_j}{(1+M_A)(1+M_B)-N_A N_B} \qquad (42\text{-a})$$

$i,j=A,B$; $i\neq j$

and

$$\chi_i^{\alpha\alpha}=\frac{Q_i+Q_iM_j-Q_jN_j}{(1+M_A)(1+M_B)-N_A N_B} \qquad (42\text{-b})$$

$i,j=A,B$; $i\neq j$

From the equations above, the condition for ferromagnetic instability reads:

$$(1+M_A)(1+M_B)-N_A N_B=0$$

or

$$-(M_A+M_B)+(N_AN_B-M_AM_B)=1 \qquad (43)$$

IV. APPLICATION TO SPECIFIC CASES

i) Reduction to one band model

If we switch-off the mixing $|V_{\alpha\beta}(k)|^2$ and the external magnetic field $h_0^{(\beta)}$ (which acts only on the β states) we obtain the case of a single α band with diagonal randomness submitted to an external magnetic field $h_0^{(\alpha)}$.

In this case, the propagator α-α (see equation 14) remains the same except for the term $\tilde{T}_{i l \sigma}^{(\alpha)}(\omega)$ which becomes simply $T_{il}^{(\alpha)}$, the locator $F_i^{\sigma}(\omega)$ being unaltered. Since we are considering only the α band the equation of motion (23) for the propagator β-β turns out to be useless.

In this limit, the self-consistency condition remains the same except for the function $H_{(\alpha)}^{\sigma}(\omega)$ which reduces to:

$$H_{(\alpha)}^{\sigma}(\omega) = \sum_k \frac{1}{F^{\sigma}(\omega)-\varepsilon_k^{(\alpha)}} \simeq H_p(\omega) - \sigma\delta\Sigma_{(\alpha)} H_1^{(2)}(\omega)$$

The functions $H_p(\omega)$ and $H_1^{(2)}(\omega)$ become formally identical to the Hartree-Fock ones[1], namely:

$$H_p(\omega) = \sum_k \frac{1}{\omega-\Sigma_{(\alpha)}^{p}-\varepsilon_k^{(\alpha)}}$$

and

$$H_1^{(2)}(\omega) = \sum_k \frac{1}{(\omega-\Sigma_{(\alpha)}^{p}-\varepsilon_k^{(\alpha)})^2}$$

In this case, we can write the first order change in the self-energy as:

$$\delta\Sigma_{(\alpha)} = -\frac{(\omega-\varepsilon_A^{(\alpha)})}{\langle\bar{n}_A^{(\alpha)}\rangle_p} T_A(\omega)\delta n_A^{(\alpha)} - \frac{(\omega-\varepsilon_B^{(\alpha)})}{\langle\bar{n}_B^{(\alpha)}\rangle_p} T_B(\omega)\delta n_B^{(\alpha)} + \left[T_A(\omega)+T_B(\omega)\right] h_0^{(\alpha)}$$

where the functions $T_i(\omega)$ are the same as in equation (31-a) with the redefined $H_p(\omega)$ and $H_i^{(2)}(\omega)$. Similarly eq. (37), as the above mentioned eq. (23), becomes unnecessary.

Finally, the change in the occupation numbers $\delta n_i^{(\alpha)}$ (cf. eq. 40) turn out to be:

$$\delta n_i^{(\alpha)} = -\sum_{j=A,B} \lambda_i^j \delta n_j^{(\alpha)} - \alpha_i \delta n_i^{(\alpha)} + (\xi_i+\zeta_i^A+\zeta_i^B)\, h_0^{(\alpha)} \qquad (44)$$

And the condition for magnetic instability is again:

$$-(M_A+M_B)+(N_A N_B-M_A M_B) = 1 \qquad (45)$$

with

$$M_i = \alpha_i + \lambda_i^i \qquad (46\text{-a})$$

and

$$N_i = \lambda_j^i \qquad (i \neq j) \qquad (46\text{-b})$$

We note that this condition is formally identical to the result obtained by Hasegawa and Kanamori[8], although the functions involved are different due to the assumption of strong correlations.

ii) Transition Metal Like Systems

In the transition metal alloys we neglect the Coulomb correlations ($U^{(\beta)}=U^{(s)}=0$), but maintain the mixing ($|V_{\alpha\beta}|=|V_{sd}|\neq 0$). In this situation, as discussed in Section II, the previous equations of motion remain valid provided one replaces $\bar{n}_{-\sigma}^{(\beta)}$ by 1. Consequently the function $H_{(\alpha)}^{\sigma}(\omega)$ reads:

$$H_{(\alpha)}^{\sigma}(\omega) = \sum_k \frac{\omega-\epsilon_k^{(\beta)}+\sigma h_0^{(\beta)}}{(\omega-\epsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^{\sigma})(\omega-\epsilon_k^{(\beta)}+\sigma h_0^{(\beta)})-|V_{\alpha\beta}(k)|^2}$$

...

where we emphasize that the β energies $\varepsilon_k^{(\beta)}$ have no "Hubbard band narrowing". The lack of Hubbard band narrowing makes the term in $\delta n^{(\beta)}$ to disappear in the expansions of $H^{\sigma}_{(\alpha)}(\omega)$ and $\delta\sum_{(\alpha)}$. Hence, if we make $<\bar{n}^{(\beta)}>_p=1$ and switch-off the terms $\omega\delta n^{(\beta)}$ in the equations (26) and (30), we obtain the expressions for $H^{\sigma}_{(\alpha)}(\omega)$ and $\delta\sum_{(\alpha)}$ adequate for transition metal like systems.

Since these expansions are used in equation (38) to calculate the first order corrections $<\delta G^{\alpha\alpha}_{jj\sigma}(\omega)>_i$, the term involving $\delta n^{(\beta)}$ will also be absent, which implies its absence also in the change in occupation numbers $\delta n_i^{(\alpha)}$. Consequently, one gets an equation similar to (44) but with the extra contribution arising from the $h_o^{(\beta)}$ term, namely: $\eta_i\ h_o^{(\beta)}$.

Then, due to hybridization, the partial susceptibilities χ_i^{ds} do exist, but the condition for ferromagnetic instability is still given by (45) with the definitions (46). However it should be emphasized that the functions α_i and λ_j^i (i,j=A,B) differ from those in the one band case by corrections associated to the mixing $|V^{sd}|^2$.

iii) Actinide Alloys

In the actinide alloys the α and β bands are the f and d bands respectively. We have assumed that randomness exists only in the f band, the d band acting as a source of hybridization. In this case, the presence of the Coulomb correlation in the d band ($U^d \neq 0$) influences explicitly the criterion for ferromagnetic instabilities. Recalling the definitions of the functions which appear in this criterion, one can rewrite M_i and N_i as:

$$M_i = (\alpha_i+\lambda_i^i) + \frac{\Gamma_i\Lambda_4^i}{1+\Lambda_3} \equiv (\alpha_i+\lambda_i^i)+\delta M_i \equiv M_i^{(t)}+\delta M_i \qquad (47\text{-a})$$

and

$$N_i = \lambda_j^i + \frac{\Gamma_j\Lambda_4^i}{1+\Lambda_3} \equiv \lambda_j^i + \delta N_i \equiv N_i^{(t)}+\delta N_i \qquad (47\text{-b})$$

$i,j = A,B \; ; \; i \neq j$

We should note that the functions δM_i and δN_i are proportional to the fourth order in mixing since Γ_i and Λ_4^i contain explicitly the term $|V_{df}|^2$. We also want to emphasize that the quantities δM_i and δN_i involve the function $\Gamma_i=f(H_1^{(1)}(\omega))$, which is completely absent in the transition metal alloys, being a characteristic of strong correlations in the d band. On the contrary, the functions $M_i^{(t)}$ and $N_i^{(t)}$ do exist in the cases i) and ii).

We assume throughout our calculation that the d band does not sustain magnetism independently of the f band, which means that $1+\Lambda_3 \neq 0$. But if the d band is near the condition of magnetic instability, the denominator of δM_i and δN_i assume small values, thus making the corrections proportional to $|V_{df}|^4$ to become relevant.

Substituting (47-a) and (47-b) in the general condition for ferromagnetic instability (43), one obtains:

$$-(M_A^{(t)}+M_B^{(t)}) + (N_A^{(t)}N_B^{(t)}-M_A^{(t)}M_B^{(t)}) - (\delta M_A+\delta M_B) +$$
$$+\{(\delta N_A N_B^{(t)} + \delta N_B N_A^{(t)})-(\delta M_A M_B^{(t)} + \delta M_B M_A^{(t)}) + \theta(|V_{df}(k)|^8) = 1 \qquad (48)$$

Hence, we can see from (48) that the two first terms including only hybridization effects behave like a transition metal in presence of mixing. The last two terms contain the intrinsic feature of the actinide alloys, namely: the existence of correlated d bands which hybridize with the f band. A similar expression was obtained in the limit of the Hartree-Fock approach[1].

APPENDIX

i) Definition of the Functions λ_i^j , ζ_i^j, Γ_i, ξ_i, α_i and η_i (i,j=A,B)

These functions are defined as follows:

$$\lambda_i^j = \mathcal{F}_\omega \left\{ \frac{-(\omega-\varepsilon_j^{(\alpha)})\ T_j(\omega)\ \left[H_1^{(2)}(\omega) - (H_p(\omega))^2\right]}{\langle \bar{n}_j^{(\alpha)}\rangle_p \left[1-(\varepsilon_{ip}^{(\alpha)}(\omega)-\Sigma_{(\alpha)}^p)\ H_p(\omega)\right]^2} \right\} \tag{A-1}$$

$$\zeta_i^j = \mathcal{F}_\omega \left\{ \frac{-T_j(\omega)\left[H_1^{(2)}(\omega) - (H_p(\omega))^2\right]}{\left[1-\left(\varepsilon_{ip}^{(\alpha)}(\omega) - \Sigma_{(\alpha)}^p\ H_p(\omega)\right)\right]^2} \right\} \tag{A-2}$$

$$\Gamma_i = \mathcal{F}_\omega \left\{ \frac{-\omega\left[k(\omega)\ \left[H_1^{(2)}(\omega) - (H_p(\omega))^2\right] - H_1^{(1)}(\omega)\right]}{\left[1-(\varepsilon_{ip}^{(\alpha)}(\omega)-\Sigma_{(\alpha)}^p)\ H_p(\omega)\right]^2} \right\} \tag{A-3}$$

$$\xi_i = \mathcal{F}_\omega \left\{ \frac{-\ (H_p(\omega))^2}{\langle \bar{n}_i^{(\alpha)}\rangle_p \left[1-(\varepsilon_{ip}^{(\alpha)}(\omega) - \Sigma_{(\alpha)}^p) H_p(\omega)\right]^2} \right\} \tag{A-4}$$

$$\alpha_i = \mathcal{F}_\omega \left\{ \frac{-\ (\omega-\varepsilon_i^{(\alpha)})(H_p(\omega))^2}{(\langle \bar{n}_i^{(\alpha)}\rangle_p)^2\ \left[1-(\varepsilon_{ip}^{(\alpha)}(\omega) - \Sigma_{(\alpha)}^p) H_p(\omega)\right]^2} \right\} \tag{A-5}$$

$$\eta_i = \mathcal{F}_\omega \left\{ \frac{-\langle \bar{n}^{(\beta)}\rangle_p \left[H_1^{(1)}(\omega) - k(\omega)\ \left[H_1^{(2)}(\omega)-(H_p(\omega))^2\right]\right]}{\left[1-(\varepsilon_{ip}^{(\alpha)}(\omega) - \Sigma_{(\alpha)}^p) H_p(\omega)\right]^2} \right\} . \tag{A-6}$$

ii) Definition of the Functions Λ_{ℓ}^{i} (l=1 a 4; i=A,B)

$$\Lambda_1 = -\langle\bar{n}^{(\beta)}\rangle_p \mathcal{F}_\omega \left\{ \sum_k \frac{(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)^2-(\langle\bar{n}^{(\beta)}\rangle_p)^2|V_{\alpha\beta}(k)|^2 k(\omega)}{\left[(\omega-\langle\bar{n}^{(\beta)}\rangle_p\varepsilon_k^{(\beta)})(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)-\langle\bar{n}^{(\beta)}\rangle_p|V_{\alpha\beta}(k)|^2\right]^2} \right\} \tag{A-7}$$

$$\Lambda_2^i = -(\langle\bar{n}^{(\beta)}\rangle_p)^2 \mathcal{F}_\omega \left\{ \sum_k \frac{|V_{\alpha\beta}(k)|^2\ T_i(\omega)}{\left[(\omega-\langle\bar{n}^{(\beta)}\rangle_p\varepsilon_k^{(\beta)})(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)-\langle\bar{n}^{(\beta)}\rangle_p|V_{\alpha\beta}(k)|^2\right]^2} \right\} \tag{A-8}$$

$$\Lambda_3 = -\mathcal{F}_\omega \left\{ \sum_k \frac{\omega\left[(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)^2-(\langle\bar{n}^{(\beta)}\rangle_p)^2|V_{\alpha\beta}(k)|^2 k(\omega)\right]}{\left[(\omega-\langle\bar{n}^{(\beta)}\rangle_p\varepsilon_k^{(\beta)})(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)-\langle\bar{n}^{(\beta)}\rangle_p|V_{\alpha\beta}(k)|^2\right]^2} \right\} \tag{A-9}$$

and

$$\Lambda_4^i = -\frac{(\langle\bar{n}^{(\beta)}\rangle_p)^2}{\langle\bar{n}_i^{(\alpha)}\rangle_p} \mathcal{F}_\omega \left\{ \sum_k \frac{|V_{\alpha\beta}(k)|^2(\omega-\varepsilon_i^{(\alpha)})T_i(\omega)}{\left[(\omega-\langle\bar{n}^{(\beta)}\rangle_p\varepsilon_k^{(\beta)})(\omega-\varepsilon_k^{(\alpha)}-\Sigma_{(\alpha)}^p)-\langle\bar{n}^{(\beta)}\rangle_p|V_{\alpha\beta}(k)|^2\right]^2} \right\} \tag{A-10}$$

iii) Definition of the functions M_i, N_i, τ_i and Q_i; (i,j=A,B; i ≠ j)

$$M_i = \alpha_i + \lambda_i^i + \frac{\Gamma_i \Lambda_4^i}{1+\Lambda_3} \tag{A-11}$$

$$N_i = \lambda_j^i + \frac{\Gamma_j \Lambda_4^i}{1+\Lambda_3} \tag{A-12}$$

$$\tau_i = \eta_i + \frac{\Gamma_i \Lambda_1}{1+\Lambda_3} \qquad \text{(A-13)}$$

and

$$Q_i = \xi_i + \zeta_i^A + \xi_i^B + \frac{\Gamma_i(\Lambda_2^A + \Lambda_2^B)}{1 + \Lambda_3} \qquad \text{(A-14)}$$

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