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MAGNETIC INSTABILITIES IN DISORDERED SYSTEMS IN HARTREE-FOCK:* APPLICATION TO TRANSITION METALS AND ACTINIDES

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ABSTRACT

The criterion for magnetic instabilities in disordered systems within the coherent potential approximation as derived by Hasegawa and Kanamori is extended in order to include hybridizations in two-band transition metals and actinides. In the last case the effect of intra-d-band correlations is treated approximately, while the disorder within the f band is fully taken into account. We recover the one band results and one shows that in the case of transition-like metals, s-d hybridization leaves the instability condition formally unaltered, just modifying the values of the functions involved. However, in the case of actinide metals, new terms appear directly connected to d-f hybridization and Coulomb repulsion in the d band which may considerably modify the condition for magnetic instability.

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I - INTRODUCTION

The problem of magnetic instabilities in disordered systems has been discussed by several authors[1,2,3] within various approximations to deal with Coulomb correlations. In these works, the metallic systems were always assumed to be described by a single non degenerate band. It is known from previous works that the existence of hybridized bands[4,5,6,7] modifies the conditions for magnetic instability respect to one-band systems. In particular, the case of actinide metals is a typical situation where d-f hybridization plays a central role in discussing the behaviour of the magnetism along the series of these metals[8].

In this paper we intend to discuss a simple model for dealing with the magnetic instabilities in disordered alloys which may be described by a hybridized two band system (transition or actinide metals). We adopt here the Hartree-Fock approximation to treat Coulomb correlations, consequently this calculation is to be compared to that of Hasegawa and Kanamori[1], which describes a one band system within the Hartree-Fock approach.

The model we consider includes the important assumption that no disorder exists in one of the bands. For transition metal systems this is precisely the model used by Brouers et al.[9,11] in the context of discussing transport properties of transition metal alloys. In the actinide metal case it is assumed that the f band, which is the narrowest, is the only one which exhibits randomness. It is hoped that this approximation (which considerably simplifies the calculation) will not destroy the main idea of disorder in such systems. In fact, one expects that the d band in actinides acts like a source of hybridization, shifts in the atomic levels of A and B atoms being expected to have a larger effect in the f states. In these metals we also neglect the existence of the broad s band, since its inclusion just renormalizes the d and f states through s-d and s-f mixing . As a last remark about actinide systems, in this calculation we approximately describe the d occupation numbers which appear in the d-d correlation introducing self-consistently the alloy occupation numbers, in order to restore the simple idea of one band randomness.

The plan of this work is as follows: in Sec. II we describe the model and obtain the relevant propagators and CPA (coherent potential approximation) conditions. Sec. III is devoted to calculate the first order corrections due to the external magnetic fields and finally, Sec. IV discusses applications of the results to transition and actinide systems.

II - MODEL HAMILTONIAN AND CPA EQUATIONS

Consider a binary alloy system of the type $A_x B_{1-x}$ described by two hybridized α and β bands which may correspond to situations encountered in transition or actinide metals. We assume, as discussed in the Introduction, that disorder exists only within the α band.

The one-electron Hamiltonian may be written in the Wannier representation as

$$\mathcal{H}_0 = \sum_{ij\sigma} T_{ij}^{(\beta)} \beta_{i\sigma}^{+} \beta_{j\sigma} + \sum_{i\sigma} \varepsilon_{i\sigma}^{(\alpha)} \alpha_{i\sigma}^{+} \alpha_{i\sigma} + \sum_{ij\sigma} T_{ij}^{(\alpha)} \alpha_{i\sigma}^{+} \alpha_{j\sigma} + $$

$$+ \sum_{i\sigma} \left\{ V_{\alpha\beta} \; \alpha_{i\sigma}^{+} \beta_{i\sigma} + V_{\beta\alpha} \; \beta_{i\sigma}^{+} \alpha_{i\sigma} \right\} , \qquad (1a)$$

$\beta_{i\sigma}^{+}(\beta_{i\sigma})$ and $\alpha_{i\sigma}^{+}$ $(\alpha_{i\sigma})$ being the creation (annihilation) operators of β and α electrons respectively with spin σ at the ith lattice site. $\varepsilon_i^{(\alpha)}$ is assumed to take on values $\varepsilon_A^{(\alpha)}$, $\varepsilon_B^{(\alpha)}$ depending on the kind of related atoms, while the hopping integrals $T_{ij}^{(\beta)}$ and $T_{ij}^{(\alpha)}$ and mixing matrix elements $V_{\alpha\beta}$ and $V_{\beta\alpha}$, which for simplicity are supposed to be k-independent, involve no randomness at all.

The Coulomb correlation terms are

$$\mathcal{H}_{Coul} = \sum_i U_i^{(\alpha)} n_{i\uparrow}^{(\alpha)} \; n_{i\downarrow}^{(\alpha)} + U^{(\beta)} \sum_i \; n_{i\uparrow}^{(\beta)} n_{i\downarrow}^{(\beta)} \quad , \quad n_{i\sigma}^{(\lambda)} = \lambda_{i\sigma}^{+} \lambda_{i\sigma} ,$$

$$(\lambda = \alpha \text{ or } \beta), \qquad (1b)$$

where the Coulomb interaction parameter $U_i^{(\alpha)}$ may assume values $U_A^{(\alpha)}$ or $U_B^{(\alpha)}$.

Finally, the interaction with the external magnetic fields is described through

$$\mathcal{H}_{mag} = - h_o^{(\alpha)} \sum_{i\sigma} \sigma\, n_{i\sigma}^{(\alpha)} - h_o^{(\beta)} \sum_{i\sigma} \sigma\, n_{i\sigma}^{(\beta)} \quad . \qquad (1c)$$

The complete Hamiltonian is then

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_{Coul} + \mathcal{H}_{mag} \quad . \qquad (2)$$

We follow now the equation of motion method[2,3] to obtain the coupled set of equations for the relevant propagators $G_{ij\sigma}^{\alpha\alpha}(\omega)$ and $G_{ij\sigma}^{\beta\beta}(\omega)$. Within the Hartree-Fock scheme one gets for the α -α propagator

$$\omega\, G_{ij\sigma}^{\alpha\alpha}(\omega) = \delta_{ij} + \sum_\ell T_{i\ell}^{(\alpha)} G_{\ell j\sigma}^{\alpha\alpha}(\omega) + \varepsilon_i^{(\alpha)} G_{ij\sigma}^{\alpha\alpha}(\omega) + U_i^{(\alpha)} \langle n_{i-\sigma}^{(\alpha)} \rangle G_{ij\sigma}^{\alpha\alpha}(\omega) +$$

$$+ V_{\alpha\beta}\, G_{ij\sigma}^{\beta\alpha}(\omega) - h_o^{(\alpha)}\sigma\, G_{ij\sigma}^{\alpha\alpha}(\omega) \qquad (3a)$$

and

$$\omega\, G_{ij\sigma}^{\beta\alpha}(\omega) = \sum_\ell T_{i\ell}^{(\beta)} G_{\ell j\sigma}^{\beta\alpha}(\omega) + U^{(\beta)} \langle n_{i-\sigma}^{(\beta)} \rangle G_{ij\sigma}^{\beta\alpha}(\omega) + V_{\beta\alpha}\, G_{ij\sigma}^{\alpha\alpha}(\omega) -$$

$$- h_o^{(\beta)}\sigma\, G_{ij\sigma}^{\beta\alpha}(\omega) \qquad (3b)$$

while the β - β propagator satisfies

$$\omega\, G^{\beta\beta}_{ij\sigma}(\omega) = \delta_{ij} + \sum_{\ell} T^{(\beta)}_{i\ell}\, G^{\beta\beta}_{\ell j\sigma}(\omega) + U^{(\beta)} \langle n^{(\beta)}_{i-\sigma}\rangle G^{\alpha\beta}_{ij}(\omega) +$$

$$+ V_{\beta\alpha}\, G^{\alpha\beta}_{ij\sigma}(\omega) - h^{(\beta)}_{o}\sigma\; G^{\beta\beta}_{ij\sigma}(\omega) \tag{4a}$$

and

$$\omega\, G^{\alpha\beta}_{ij\sigma}(\omega) = \sum_{\ell} T^{(\alpha)}_{i\ell}\, G^{\alpha\beta}_{\ell j\sigma}(\omega) + \varepsilon^{(\alpha)}_{i}\, G^{\alpha\beta}_{ij\sigma}(\omega) + U^{(\alpha)}_{i} \langle n^{(\alpha)}_{i-\sigma}\rangle\, G^{\alpha\beta}_{ij\sigma}(\omega) +$$

$$+ V_{\alpha\beta}\, G^{\beta\beta}_{ij\sigma}(\omega) - h^{(\alpha)}_{o}\sigma\; G^{\alpha\beta}_{ij\sigma}(\omega) \tag{4b}$$

At this point we introduce the approximation of supposing that as far Coulomb terms are concerned, the occupation numbers $\langle n^{(\beta)}_{i-\sigma}\rangle$ will be replaced by $\langle n^{(\beta)}_{-\sigma}\rangle_{\text{alloy}}$. This quantity will be self consistently determined from the solution of the configuration average of $G^{\beta\beta}_{ij\sigma}(\omega)$ and corresponds physically to say that an 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 no disorder is present 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 absence of $U^{(\beta)}$ Coulomb interaction our procedure is exact. Introducing the Hartree-Fock renormalized energies

$$\bar{\varepsilon}^{(\alpha)}_{i\sigma} = \varepsilon^{(\alpha)}_{i} + U^{(\alpha)}_{i} \langle n^{(\alpha)}_{i-\sigma}\rangle - \sigma\, h^{(\alpha)}_{o} \tag{5a}$$

and effective hopping energy

$$T_{ij\sigma}^{(\beta)} = T_{ij}^{(\beta)} + \left\{ U^{(\beta)} \langle n_{-\sigma}^{(\beta)} \rangle_{alloy} - \sigma h_o^{(\beta)} \right\} \delta_{ij} \tag{5b}$$

the equations of motion determining the $\alpha - \alpha$ propagator become

$$(\omega - \bar{\varepsilon}_{i\sigma}^{(\alpha)}) G_{ij\sigma}^{\alpha\alpha}(\omega) = \delta_{ij} + \sum_{\ell} T_{i\ell}^{(\alpha)} G_{\ell j\sigma}^{\alpha\alpha}(\omega) + V_{\alpha\beta} G_{ij\sigma}^{\beta\alpha}(\omega) \tag{6a}$$

and

$$(\omega - \bar{\varepsilon}_{k\sigma}^{(\beta)}) G_{kk'\sigma}^{\beta\alpha}(\omega) = V_{\beta\alpha} G_{kk'\sigma}^{\alpha\alpha}(\omega) \quad , \tag{6b}$$

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

$$\bar{\varepsilon}_{k\sigma}^{(\beta)} = \sum_{\ell} T_{i\ell\sigma}^{(\beta)} \; e^{ik.(R_i - R_\ell)} \quad .$$

Transforming back equation (6b) to site representation and defining $T_{i\ell\sigma}^{mix}$ through

$$T_{i\ell\sigma}^{mix} = \sum_k \frac{e^{-ik.(R_i - R_\ell)}}{\omega - \bar{\varepsilon}_{k\sigma}^{(\beta)}} \quad ,$$

one finally gets for the $\alpha - \alpha$ propagator

$$(\omega - \bar{\varepsilon}_{i\sigma}^{(\alpha)})\ G_{ij\sigma}^{\alpha\alpha}(\omega) = \delta_{ij} + \sum_{\ell} \tilde{T}_{i\ell\sigma}^{(\alpha)}\ G_{\ell j\sigma}^{\alpha\alpha}(\omega) \tag{7a}$$

where

$$\tilde{T}_{i\ell\sigma}^{(\alpha)} = T_{i\ell}^{(\alpha)} + |V_{\alpha\beta}|^2\ T_{i\ell\sigma}^{mix} \tag{7b}$$

or introducing the locator $F_i^{\sigma}(\omega)$,

$$F_i^{\sigma}(\omega) = \omega - \bar{\varepsilon}_{i\sigma}^{(\alpha)} \tag{7c}$$

one arrives to the standard form of Ref.[3]

$$G_{ij\sigma}^{\alpha\alpha}(\omega) = \frac{1}{F_i^{\sigma}(\omega)} \left[\delta_{ij} + \sum_{\ell} \tilde{T}_{i\ell\sigma}^{(\alpha)} \langle G_{\ell j\sigma}^{\alpha\alpha}(\omega)\rangle\right] , \tag{7d}$$

where we emphasize that no disorder is present in the "effective hopping" Configuration averaging equation (7d) one has

$$F^{\sigma}(\omega)\ \langle G_{ij\sigma}^{\alpha\alpha}(\omega)\rangle = \delta_{ij} + \sum_{\ell} \tilde{T}_{i\ell\sigma}^{(\alpha)} \langle G_{\ell j\sigma}^{\alpha\alpha}(\omega)\rangle \tag{8a}$$

and Fourier transforming (8a):

$$\langle G_{ij\sigma}^{\alpha\alpha}(\omega)\rangle_k = \frac{1}{F^{\sigma}(\omega) - \tilde{\varepsilon}_{k\sigma}^{(\alpha)}} , \tag{8b}$$

where $\tilde{\varepsilon}_{k\sigma}^{(\alpha)}$ is the β - α renormalized α energy

$$\tilde{\varepsilon}_{k\sigma}^{(\alpha)} = \varepsilon_k^{(\alpha)} + \frac{|V_{\alpha\beta}|^2}{\omega - \varepsilon_k^{(\beta)} - U^{(\beta)}\langle n_{-\sigma}^{(\beta)}\rangle_{alloy} + \sigma\, h_o^{(\beta)}} . \qquad (8c)$$

In the site representation it follows that

$$\langle G_{ij\sigma}^{\alpha\alpha}(\omega)\rangle = \sum_k \frac{e^{ik\cdot(R_i-R_j)}}{F^{\sigma}(\omega) - \tilde{\varepsilon}_{k\sigma}^{(\alpha)}} \qquad (8d)$$

or in particular

$$\langle G_{ii\sigma}^{\alpha\alpha}(\omega)\rangle = \sum_k \frac{1}{F^{\sigma}(\omega) - \tilde{\varepsilon}_{k\sigma}^{(\alpha)}} = H_{(\alpha)}^{\sigma}(\omega) . \qquad (8e)$$

The self-consistency condition is derived in the way obtained in Refs.[3] namely

$$c_A \langle G_{\ell j\sigma}(\omega)\rangle_A + c_B \langle G_{\ell j\sigma}(\omega)\rangle_B = \langle G_{\ell j\sigma}(\omega)\rangle , \quad c_A \equiv x, \quad c_B \equiv 1 - x \qquad (9a)$$

where

$$\langle G_{\ell j\sigma}^{\alpha\alpha}(\omega)\rangle_A = \langle G_{\ell j\sigma}^{\alpha\alpha}(\omega)\rangle + \langle G_{\ell i\sigma}^{\alpha\alpha}(\omega)\rangle \frac{F^{\sigma}(\omega) - F_A^{\sigma}(\omega)}{1-\left[F^{\sigma}(\omega) - F_A^{\sigma}(\omega)\right] \langle G_{ii\sigma}^{\alpha\alpha}(\omega)\rangle} \langle G_{ij\sigma}^{\alpha\alpha}(\omega)\rangle, \qquad (9b)$$

and

$$<G^{\alpha\alpha}_{\ell j\sigma}(\omega)>_B = <G^{\alpha\alpha}_{\ell j\sigma}(\omega)> + <G^{\alpha\alpha}_{\ell i\sigma}(\omega)> \frac{F^{\sigma}(\omega) - F^{\sigma}_B(\omega)}{1- \left[F^{\sigma}(\omega) - F^{\sigma}_B(\omega)\right]<G^{\alpha\alpha}_{ii\sigma}(\omega)>} < G^{\alpha\alpha}_{ij\sigma}(\omega)>. \qquad (9c)$$

From equations (9) the self-consistency equation is easily derived. One obtains

$$\Sigma^{\sigma}_{(\alpha)} = \bar{\varepsilon}^{(\alpha)}_{\sigma} - (\bar{\varepsilon}^{(\alpha)}_{A\sigma} - \Sigma^{\sigma}_{(\alpha)})\, H^{\sigma}_{(\alpha)}(\omega)\, (\bar{\varepsilon}^{(\alpha)}_{B\sigma} - \Sigma^{\sigma}_{(\alpha)}) , \qquad (10a)$$

where we defined

$$\bar{\varepsilon}^{(\alpha)}_{\sigma} = c_A\, \bar{\varepsilon}^{(\alpha)}_{A\sigma} + c_B\, \bar{\varepsilon}^{(\alpha)}_{B\sigma} \qquad (10b)$$

and introduced the self energy $\Sigma^{\sigma}_{(\alpha)}$ through

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

Now we solve the equations which determine the β - β propagator. From equations (4) and using (5a) one gets

$$(\omega-U^{(\beta)}<n_{-\sigma}>_{alloy} + h^{(\beta)}_{o}\sigma)\, G^{\beta\beta}_{ij\sigma}(\omega) = \delta_{ij} + \sum_{\ell} T^{(\beta)}_{i\ell}\, G^{\beta\beta}_{\ell j\sigma}(\omega) + V_{\beta\alpha}\, G^{\alpha\beta}_{ij\sigma}(\omega) , \qquad (11a)$$

$$G^{\alpha\beta}_{ij\sigma}(\omega) = \frac{1}{F^{\sigma}_{i}(\omega)} \left\{ \sum_{\ell} T^{(\alpha)}_{i\ell} \; G^{\alpha\beta}_{\ell j\sigma}(\omega) + V_{\alpha\beta} \; G^{\beta\beta}_{ij\sigma}(\omega) \right\} . \qquad (11b)$$

Configuration averaging equations (11) and Fourier transforming one gets

$$(\omega - U^{(\beta)} <n^{(\beta)}_{-\sigma}>_{alloy} + h^{(\beta)}_{o}\sigma - \varepsilon^{(\beta)}_{k}) <G^{\beta\beta}_{ij\sigma}(\omega)>_{k} = 1 + V_{\beta\alpha}<G^{\alpha\beta}_{ij\sigma}(\omega)>_{k} \qquad (11c)$$

and

$$(\omega - \Sigma^{\sigma}_{(\alpha)} - \varepsilon^{(\alpha)}_{k}) <G^{\alpha\beta}_{ij\sigma}(\omega)>_{k} = V_{\alpha\beta} <G^{\beta\beta}_{ij\sigma}(\omega)>_{k} , \qquad (11d)$$

where $\Sigma^{\sigma}_{(\alpha)}$ was determined already through equation (10a). Recalling the previous definition of $\overline{\varepsilon}^{(\beta)}_{k\sigma}$ one finally obtains

$$<G^{\beta\beta}_{ij\sigma}(\omega)>_{k} = \frac{\omega - \varepsilon^{(\alpha)}_{k} - \Sigma^{\sigma}_{(\alpha)}}{(\omega - \overline{\varepsilon}^{(\beta)}_{k\sigma}) \; (\omega - \varepsilon^{(\alpha)}_{k} - \Sigma^{\sigma}_{(\alpha)}) - |V_{\alpha\beta}|^{2}} . \qquad (12)$$

These results complete the determination of the propagators $G^{\alpha\alpha}_{ij\sigma}(\omega)$ and $G^{\beta\beta}_{ij\sigma}(\omega)$.

III - FIRST ORDER CORRECTIONS IN THE MAGNETIC FIELDS.

Next, we follow strictly Ref.[1] and collect first order terms in the magnetic fields. To do that we define

$$\Sigma^{\sigma}_{(\alpha)} = \Sigma^{p}_{(\alpha)} - \sigma\delta\, \Sigma_{(\alpha)} \quad ,$$

$$\langle n^{(\alpha)}_{i-\sigma}\rangle = \langle n^{(\alpha)}_{i}\rangle_{p} - \sigma\delta\, n^{(\alpha)}_{i} \quad ,$$

$$\langle n^{(\beta)}_{-\sigma}\rangle_{alloy} = \langle n^{(\beta)}\rangle_{p} - \sigma\delta\, n^{(\beta)} \quad ,$$

$$\bar{\varepsilon}^{(\alpha)}_{i\sigma} = \varepsilon^{(\alpha)}_{i} + U^{(\alpha)}_{i}\langle n^{(\alpha)}_{i}\rangle_{p} - \sigma\, U^{(\alpha)}_{i}\, \delta n^{(\alpha)}_{i} - \sigma h^{(\alpha)}_{o} = \varepsilon^{(\alpha)}_{ip} - \sigma\, U^{(\alpha)}_{i}\, \delta n^{(\alpha)}_{i} - \sigma\, h^{(\alpha)}_{o} \quad ,$$

$$\bar{\varepsilon}^{(\beta)}_{k\sigma} = \varepsilon^{(\beta)}_{k} + U^{(\beta)}\langle n^{(\beta)}\rangle_{p} - \sigma\, U^{(\beta)}\, \delta n^{(\beta)} - \sigma h^{(\beta)}_{o} \quad . \qquad (13)$$

From equation (8e) and using definition of the self-energy one has

$$H^{\sigma}_{(\alpha)}(\omega) = \sum_{k} \frac{\omega - \varepsilon^{(\beta)}_{k} - U^{(\beta)}\langle n^{(\beta)}_{-\sigma}\rangle_{alloy} + \sigma\, h^{(\beta)}_{o}}{(\omega - \Sigma^{\sigma}_{(\alpha)} - \varepsilon^{(\alpha)}_{k})(\omega - \varepsilon^{(\beta)}_{k} - U^{(\beta)}\langle n^{(\beta)}_{-\sigma}\rangle_{alloy} + \sigma h^{(\beta)}_{o}) - |V_{\alpha\beta}|^{2}} \quad . \qquad (14)$$

At this point it is useful to introduce the model of homothetic bands proposed by Kishore and Joshi[4], namely

$$\varepsilon^{(\beta)}_{k} = \varepsilon_{k}$$

$$\varepsilon^{(\alpha)}_{k} = A\varepsilon_{k} + B$$

since this simplifies te calculation of (14). If $\rho_o(\varepsilon)$ is the density of states associated to the dispersion relation $\varepsilon_{\mathbf{k}}$, equation (14) can be rewritten as

$$H^{\sigma}_{(\alpha)}(\omega) = \int d\,\varepsilon\, \rho_o(\varepsilon) \frac{\omega - \varepsilon - U^{(\beta)} \langle n^{(\beta)}_{-\sigma}\rangle_{alloy} + \sigma h_o^{(\beta)}}{(\omega - \Sigma^{\sigma}_{(\alpha)} - A\varepsilon - B)(\omega - \varepsilon - U^{(\beta)} \langle n^{(\beta)}_{-\sigma}\rangle_{alloy} + \sigma h_o^{(\beta)}) - |V_{\alpha\beta}|^2} \tag{15}$$

Now, using definitions (13), we collect first order terms in the magnetic field and expand equation (15). One gets

$$H^{\sigma}_{(\alpha)}(\omega) = F_p(\omega) - \sigma \left\{ h_o^{(\beta)} |V_{\alpha\beta}|^2 + U^{(\beta)}\, \delta n^{(\beta)}\, |V_{\alpha\beta}|^2 \right\} H_1(\omega) -$$

$$- \sigma\, \delta\, \Sigma_{(\alpha)}\, H_p(\omega) \quad , \tag{16}$$

where we defined

$$F_p(\omega) = \int d\,\varepsilon\,\, \rho_o(\varepsilon) \frac{\omega - \varepsilon - U^{(\beta)} \langle n^{(\beta)}\rangle_p}{(\omega - \Sigma^{(\alpha)}_p - A\varepsilon - B)(\omega - \varepsilon - U^{(\beta)} \langle n^{(\beta)}\rangle_p) - |V_{\alpha\beta}|^2} \, , \tag{17a}$$

$$H_1(\omega) = \int d\,\varepsilon\, \rho_o(\varepsilon) \frac{1}{\left[(\omega - \Sigma^{(\alpha)}_p - A\varepsilon - B)(\omega - \varepsilon - U^{(\beta)} \langle n^{(\beta)}\rangle_p) - |V_{\alpha\beta}|^2\right]^2} \tag{17b}$$

$$H_p(\omega) = \int d\varepsilon\, \rho_o(\varepsilon) \frac{(\omega-\varepsilon-U^{(\beta)}\langle n^{(\beta)}\rangle_p)^2}{\left[(\omega-\Sigma_p^{(\alpha)}-A\varepsilon-B)(\omega-\varepsilon-U^{(\beta)}\langle n^{(\beta)}\rangle_p)-|V_{\alpha\beta}|^2\right]^2} \quad (17c)$$

Using the result (16) and definitions (13) the first order contributions to the self-consistency equation reads

$$\delta\Sigma_{(\alpha)} = K_A(\omega)\, U_A^{(\alpha)}\, \delta n_A^{(\alpha)} + K_B(\omega)\, U_B^{(\alpha)}\, \delta n_B^{(\alpha)} + \left[K_A(\omega) + K_B(\omega)\right] h_o^{(\alpha)} -$$

$$- |V_{\alpha\beta}|^2 K(\omega)\, (h_o^{(\beta)} + U^{(\beta)}\, \delta n^{(\beta)}) \quad (18a)$$

where we defined

$$K_i(\omega) = \frac{\left[C_i - F_p(\omega)\, (\varepsilon_{jp}^{(\alpha)} - \Sigma_{(\alpha)}^p)\right]}{1 + (\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, H_p(\omega)\, (\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^p) - F_p(\omega)\, (\varepsilon_{Ap}^{(\alpha)} + \varepsilon_{Bp}^{(\alpha)} - 2\Sigma_{(\alpha)}^p)} \quad (18b)$$

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

and

$$K(\omega) = \frac{(\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, H_1(\omega)(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^p)}{1 + (\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, H_p(\omega)(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^p) - F_p(\omega)(\varepsilon_{Ap}^{(\alpha)} + \varepsilon_{Bp}^{(\alpha)} - 2\Sigma_{(\alpha)}^p)} \quad (18c)$$

the self-energy in the paramagnetic phase, $\Sigma_{(\alpha)}^p$, satisfying

$$\Sigma^{p}_{(\alpha)} = \bar{\varepsilon}^{(\alpha)}_{p} - (\varepsilon^{(\alpha)}_{Ap} - \Sigma^{p}_{(\alpha)})\, F_p(\omega)\, (\varepsilon^{(\alpha)}_{Bp} - \Sigma^{p}_{(\alpha)}) \tag{18d}$$

and

$$\bar{\varepsilon}^{(\alpha)}_{p} = c_A\ \varepsilon^{(\alpha)}_{Ap} + c_B\, \varepsilon^{(\alpha)}_{Bp} \tag{18e}$$

Whence the result (18a) is obtained, one needs to obtain explicit expressions for $\delta n^{(\alpha)}_{A}$ and $\delta n^{(\alpha)}_{B}$ in terms of the magnetic fields, $\delta n^{(\beta)}$ and the change $\delta\Sigma_{(\alpha)}$ in the self-energy. One starts from the result (obtained from (9b) and (9c) taking l=j=i):

$$\langle G^{\alpha\alpha}_{ii\sigma}(\omega)\rangle_i = \frac{H^{\sigma}_{(\alpha)}(\omega)}{1 - (\bar{\varepsilon}^{(\alpha)}_{i\sigma} - \Sigma^{\sigma}_{(\alpha)})\, H^{\sigma}_{(\alpha)}(\omega)} \tag{19a}$$

Collecting first order terms, which we denote by $\langle\delta G^{\alpha\alpha}_{ii\sigma}(\omega)\rangle$, one gets

$$\delta n^{(\alpha)}_{i} = \mathcal{F}_{\omega}\left[\langle\delta G^{\alpha\alpha}_{ii\sigma}(\omega)\rangle_i\right] \quad , \quad i = A,B \tag{19b}$$

where

$$\langle G^{\alpha\alpha}_{ii\sigma}(\omega)\rangle_i = \langle G_{ii\sigma}(\omega)\rangle^{p}_{i} + \sigma\langle\delta G^{\alpha\alpha}_{ii\sigma}(\omega)\rangle_i$$

and $\mathcal{F}_{\omega}$ denotes

$$\mathcal{F}_{\omega}\left[G^{\alpha\alpha}_{ij\sigma}(\omega)\right] = \frac{i}{2\pi}\int_{-\infty}^{+\infty} d\omega\ f(\omega)\ \left[G^{\alpha\alpha}_{ij\sigma}(\omega+i\varepsilon) - G^{\alpha\alpha}_{ij\sigma}(\omega - i\varepsilon)\right],\ \varepsilon \to 0$$

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

The result of the explicit calculation of (19b) using (19a) is

$$\delta n_i^{(\alpha)} = U_A^{(\alpha)}(\zeta_i^A - \lambda_i^A)\ \delta n_A^{(\alpha)} + U_B^{(\alpha)}(\zeta_i^B - \lambda_i^B)\ \delta n_B^{(\alpha)} + U_i^{(\alpha)}\ \xi_i\ \delta n_i^{(\alpha)} +$$
$$+ (\zeta_i^A + \zeta_i^B - \lambda_i^A - \lambda_i^B + \xi_i)\ h_o^{(\alpha)} + |V_{\alpha\beta}|^2\ (\eta_i - \pi_i + \Gamma_i)(h_o^{(\beta)} +$$
$$+ U^{(\beta)}\ \delta n^{(\beta)})\ , \qquad (20)$$

where the quantities ζ_i^j, λ_i^j, π_i, ξ_i, Γ_i and η_i are defined explicitly in the Appendix. Equation (20) is quite similar to that obtained by Hasegawa and Kanamori[1] with the difference that now, due to mixing effects, the contribution of the change in β occupation number appears explicitly. As shown in equation (12) the β occupation number involves, through the change in self-energy, the quantities $\delta n_A^{(\alpha)}$ and $\delta n_B^{(\alpha)}$. So in order to obtain the coupled linear equations determining $\delta n_i^{(\alpha)}$, one must firstly obtain explicit results for the quantity $\delta n^{(\beta)}$. From equation (12) one has

$$<\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k = - \frac{(\omega-\varepsilon_k^{(\alpha)} - \Sigma^p_{(\alpha)})^2}{\left[(\omega-\varepsilon_{kp}^{(\beta)})(\omega-\varepsilon_k^{(\alpha)} - \Sigma^p_{(\alpha)})|V_{\alpha\beta}|^2\right]^2} \left\{ U^{(\beta)}\ \delta n^{(\beta)} + h_o^{(\beta)} \right\} +$$

$$- \frac{|V_{\alpha\beta}|^2}{\left[(\omega-\varepsilon_{kp}^{(\beta)})(\omega-\varepsilon_k^{(\alpha)} - \Sigma^p_{(\alpha)}) - |V_{\alpha\beta}|^2\right]^2}\ \delta\ \Sigma_{(\alpha)} \quad , \qquad (21a)$$

where we used

$$<G^{\beta\beta}_{ij\sigma}(\omega)>_k = <G^{\beta\beta}_{ij\sigma}(\omega)>^p_k + \sigma<\delta G^{\beta\beta}_{ij\sigma}(\omega)> \qquad (21b)$$

From $\delta n^{(\beta)} = \mathcal{F}_\omega\left[\sum_k <\delta G^{\beta\beta}_{ij\sigma}(\omega)>_k\right]$, using the result (18a) and the definitions in the Appendix, one gets

$$\delta n^{(\beta)} = |V_{\alpha\beta}|^2 \frac{U_A^{(\alpha)}\ \phi_2^A}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\ \phi_3)}\ \delta n_A^{(\alpha)} +$$

$$+ |V_{\alpha\beta}|^2 \frac{U_B^{(\alpha)}\ \phi_2^B}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\ \phi_3)}\ \delta n_B^{(\alpha)} +$$

$$+ |V_{\alpha\beta}|^2 \frac{\phi_2^A + \phi_2^B}{1-U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\ \phi_3)}\ h_o^{(\alpha)} + \frac{\phi_1 - |V_{\alpha\beta}|^2\ \phi_3}{1-U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\ \phi_3)}\ h_o^{(\beta)}$$

(22)

It is clear from (22) that the last term of it corresponds to the response of β electrons to the magnetic field $h_o^{(\beta)}$ (as renormalized through $V_{\alpha\beta}$ mixing to α electrons which move in presence of the paramagnetic self--energy $\Sigma^p_{(\alpha)}$. It will be assumed that the β band *do not develop* a magnetic instability in the Stoner criterion, namely $1 \neq U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4 \phi_3)$. Now we are in position to get the coupled equations determining the quantities $\delta n_A^{(\alpha)}$ and $\delta n_B^{(\alpha)}$. Combining equations (22) and (20) one obtains

$$\delta n_i^{(\alpha)} = \sum_{j=A,B} U_j^{(\alpha)} \left[\zeta_i^j - \lambda_i^j + |V_{\alpha\beta}|^4 \frac{U^{(\beta)} \phi_2^j (\eta_i - \pi_i + \Gamma_i)}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4 \phi_3)} \right] \delta n_j^{(\alpha)} +$$

$$+ U_i^{(\alpha)} \xi_i \, \delta n_i^{(\alpha)} + \left[\zeta_i^A + \zeta_i^B - \lambda_i^A - \lambda_i^B + \xi_i + \right.$$

$$\left. + |V_{\alpha\beta}|^4 \frac{U^{(\beta)} (\eta_i - \Pi_i + \Gamma_i)(\phi_2^A + \phi_2^B)}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4 \phi_3)} \right] h_o^{(\alpha)} +$$

$$+ |V_{\alpha\beta}|^2 \left[(\eta_i - \pi_i + \Gamma_i) \frac{1}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4 \phi_3)} \right] h_o^{(\beta)} . \qquad (23)$$

Taking i=A and B in (23) and collecting terms proportional to $\delta n_A^{(\alpha)}$, $\delta n_B^{(\alpha)}$ and to the magnetic fields one has the coupled equations

$$(1 - U_A^{(\alpha)} M_A)\, \delta n_A^{(\alpha)} - U_B^{(\alpha)} N_A \;\delta n_B^{(\alpha)} = Q_A\, h_o^{(\beta)} + (N_A + M_A)\, h_o^{(\alpha)} \quad ,$$

$$- U_A^{(\alpha)} N_B\, \delta n_A^{(\alpha)} + (1 - U_B^{(\alpha)} M_B)\, \delta n_B^{(\alpha)} = Q_B\, h_o^{(\beta)} + (N_B + M_B)\, h_o^{(\alpha)} \quad , \qquad (24)$$

where we defined

$$M_i = \zeta_i^i - \lambda_i^i + \xi_i + |V_{\alpha\beta}|^4 \; \frac{U^{(\beta)}\, \phi_2^{(i)} (n_i - \pi_i + \Gamma_i)}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\, \phi_3)} \,, \qquad i=A,B \qquad (25a)$$

$$N_i = \zeta_i^j - \lambda_i^j + |V_{\alpha\beta}|^4 \; \frac{U^{(\beta)}\, \phi_2^{(j)} (n_i - \pi_i + \Gamma_i)}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\, \phi_3)} \,, \qquad i,j = A,B; \;\; j \neq i$$

$$(25b)$$

$$Q_i = |V_{\alpha\beta}|^2 \; \frac{n_i - \pi_i + \Gamma_i}{1 - U^{(\beta)}(\phi_1 - |V_{\alpha\beta}|^4\, \phi_3)} \,. \qquad , \; i = A, B \qquad (25c)$$

From (24), solving the linear system and recalling the definition of the "partial static susceptibilities"

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

it follows that

$$\chi_i^{\alpha\beta} = \frac{Q_i(1 - U_j^{(\alpha)} M_j) + Q_j U_j^{(\alpha)} N_i}{1 - \left[U_A^{(\alpha)} M_A + U_B^{(\alpha)} M_B + U_A^{(\alpha)} U_B^{(\alpha)}(N_A N_B - M_A M_B)\right]}, \quad i,j = A \text{ or } B, \quad i \neq j \tag{26a}$$

and

$$\chi_i^{\alpha\alpha} = \frac{N_i + M_i + U_j^{(\alpha)}(N_A N_B - M_A M_B)}{1 - \left[U_A^{(\alpha)} M_A + U_B^{(\alpha)} M_B + U_A^{(\alpha)} U_B^{(\alpha)}(N_A N_B - M_A M_B\right]}, \quad i,j = A \text{ or } B; \quad i \neq j \tag{26b}$$

From (26) the condition for magnetic instability turns out to be

$$U_A^{(\alpha)} M_A + U_B^{(\alpha)} M_B + U_A^{(\alpha)} U_B^{(\alpha)}(N_A N_B - M_A M_B) = 1. \tag{27}$$

IV) APPLICATION TO SPECIFIC CASES.

i) Reduction to one band model

Here we recover the result obtained by Hasegawa and Kanamori[1] namely the condition for magnetic instabilities in a disordered binary alloy described by a single band. To do this we switch-off the mixing $|V_{\alpha\beta}|^2$ and the external magnetic field $h_o^{(\beta)}$ (which acts on the β states). So it remains only an α band with diagonal randomness and the external magnetic field $h_o^{(\alpha)}$. In this case equation (18a) reduces to

$$\delta\Sigma_{(\alpha)} = U_A^{(\alpha)} K_A(\omega)\, \delta n_A^{(\alpha)} + U_B^{(\alpha)} K_B(\omega)\, \delta n_B^{(\alpha)} + \left[K_A(\omega) + K_B(\omega)\right] h_o^{(\alpha)} \qquad (28)$$

and the terms which appear in the definitions of $K_A(\omega)$ and $K_B(\omega)$ become (cf. equations 17a, 17c)

$$F_p(\omega) = \int d\,\varepsilon\, \rho_o(\varepsilon)\, \frac{1}{\omega - \Sigma^p_{(\alpha)} - \varepsilon^{(\alpha)}} \qquad (29a)$$

and

$$H_p(\omega) = \int d\,\varepsilon \rho_o(\varepsilon)\, \frac{1}{\left[\omega - \Sigma^p_{(\alpha)} - \varepsilon^{(\alpha)}\right]^2} \qquad (29b)$$

Hence, our expression for $\delta\,\Sigma_{(\alpha)}$ agrees with that obtained in Ref. 1. On the other hand, in this special case, the terms involved in the condition for magnetic instability (see eqs. 25, 27 and the Appendix) turn out to be

$$N_i = \zeta_i^j - \lambda_i^j = -\mathcal{F}_\omega \left[\frac{\{H_p(\omega) - (F_p(\omega))^2\} K_j(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, F_p(\omega)\}^2} \right] =$$

$$= -\frac{1}{\pi} c_j \frac{1}{c_i\, c_j (\varepsilon_{Ap}^{(\alpha)} - \varepsilon_{Bp}^{(\alpha)})^2} \int_{-\infty}^{+\infty} f(\varepsilon) d\varepsilon \quad x$$

$$x \quad \mathrm{Im} \left\{ \frac{(\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^p) \left[H_p(\omega) - (F_p(\omega))^2 \right]}{1 - (\varepsilon_{Ap}^{(\alpha)} + \varepsilon_{Bp}^{(\alpha)} - 2\Sigma_{(\alpha)}^p)\, F_p(\omega) + (\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, H_p(\omega)} \right\}_{\omega = \varepsilon + i\delta}$$

$$\delta \to 0, \qquad i,j = A, B, \quad i \neq j \qquad (30a)$$

and

$$M_i = \zeta_i^i - \lambda_i^i + \xi_i = -\mathcal{F}_\omega \cdot \left[\frac{\{H_p(\omega) - (F_p(\omega))^2\} K_i(\omega) + (F_p(\omega))^2}{\left[1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, F_p(\omega)\right]^2} \right] =$$

$$= + \frac{1}{\pi} \int_{-\infty}^{+\infty} f(\varepsilon) d\varepsilon \quad \mathrm{Im} \left\{ \frac{\left[K_A(\omega) + K_B(\omega)\right]\left[H_p(\omega) - (F_p(\omega))^2\right] + (F_p(\omega))^2}{\left[1 - (\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^p)\, F_p(\omega)\right]^2} + \frac{1}{c_i (\varepsilon_{Ap}^{(\alpha)} - \varepsilon_{Bp}^{(\alpha)})^2} \right. x$$

cont.

$$\times \left. \frac{(\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^{p})(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^{p}) \cdot [H_p(\omega) - (F_p(\omega))^2]}{1-(\varepsilon_{Ap}^{(\alpha)} + \varepsilon_{Bp}^{(\alpha)} - 2\,\Sigma_{(\alpha)}^{p})\, F_p(\omega) + (\varepsilon_{Ap}^{(\alpha)} - \Sigma_{(\alpha)}^{p})(\varepsilon_{Bp}^{(\alpha)} - \Sigma_{(\alpha)}^{p})\, H_p(\omega)} \right]\Bigg\}_{\omega=\varepsilon+i\delta} \tag{30b}$$

$\delta \to 0, \quad i = A, B.$

Then, the condition (27) for magnetic instability in the case of a single band reduces to the previous result obtained in Ref. 1.

ii) Transition metal alloys

Now the α and β bands are the d and s bands respectively. In this situation, except for the approximate Hartree-Fock treatment of the d-d Coulomb correlations, our procedure is exact within the framework of CPA. This follows from the fact that $U_i^{(\alpha)} = U_i^{(d)}$ and $U^{(\beta)} = 0$ since Coulomb interactions are completely neglected within the s band, which is commonly described in OPW (orthogonalized plane waves). Consequently our drastic approximation $\langle n_{i-\sigma}^{(s)} \rangle = \langle n_{-\sigma}^{(s)} \rangle_{alloy}$ is no longer present and randomness is completely removed from the s band. It should also be noted that no exchange enhancement associated to the s band is present (cf. eq. 22), as expected. Hence, we recover the same model adopted by Brouers et al.[9, 11] to describe transition metal alloys, although the spirit of our formulation of the problem is to obtain a criterion for magnetic instabilitities. The role of s-d mixing in this criterion is to modify the functions $F_p(\omega)$ and $H_p(\omega)$ which appear explicitly in the result of Ref. 1, so introducing a departure from their result but conserving the formal equivalence to the one band problem. Another feature, intrinsic to a two-band problem is to introduce cross partial static susceptibilities as $\chi_i^{\alpha\beta} = f(n_i, \Pi_i, \Gamma_i) = f(F_p, H_p, H_1)$; $i = A, B$, (see eq. 26a) where new functions $H_1(\omega)$, n_i , Π_i and Γ_i appear (cf. eq. 17b and the Appendix) which are completely absent in the result obtained by Ref. 1.

iii) Actinide alloys

In this situation the α and β bands are the f and d bands respectively. As discussed in the introduction, we have assumed that disorder exists only within the f band, the d band acting as a source of hybridization. However, through the approximation $\langle n_{i-\sigma}^{(d)}\rangle = \langle n_{-\sigma}^{(d)}\rangle_{alloy}$ and since $U^{(d)} \neq 0$ in actinide metals, the d band influences the criterion for magnetic instabilities explicitly. In fact, recalling the definitions of the functions M_i, N_i appearing in the criterion for magnetic instabilities, one obtains

$$M_i = \zeta_i^i - \lambda_i^i + \xi_i + |V_{df}|^4 \frac{U^{(d)}\ \phi_2^{(i)}(n_i - \pi_i + \Gamma_i)}{1 - U^{(d)}(\phi_1 - |V_{df}|^4\ \phi_3)} = M_i^{(k)} + |V_{df}|^4\ \ U^{(d)}\delta M_i, \tag{31a}$$

and

$$N_i = \zeta_i^j - \lambda_i^j + |V_{df}|^4 \frac{U^{(d)} \phi_2^{(j)}(\eta_i - \pi_i + \Gamma_i)}{1 - U^{(d)}(\phi_1 - |V_{df}|^4 \phi_3)} = N_i^{(k)} + |V_{df}|^4 U^{(d)} \delta N_i \quad , \tag{31b}$$

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

The quantities $M_i^{(k)}$ and $N_i^{(k)}$ emphasize the fact that the functions involved are simply corrected by hybridization effects (namely V_{df} mixing). Another remark refers to the enhancement factor which appears in the denominators of δN_i and δM_i. It is assumed throughout this work that the d band does not sustain magnetism independently of the f band. Then the zeros of $1 - U^{(d)}(\phi_1 - |V_{df}|^4 \phi_3)$ do not exist although this quantity may assume small values giving rise to exchange enhancements that may attain the order of 10 in favourable cases. Consequently the corrections associated to the quantities δN_i and δM_i may be of critical importance in the magnetic instabilities. Substituting (31a) and (31b) in the general instability condition (27), one gets

$$U_A^{(f)} M_A^{(k)} + U_B^{(f)} M_B^{(k)} + U_A^{(f)} U_B^{(f)} \left[N_A^{(k)} N_B^{(k)} - M_A^{(k)} M_B^{(k)}\right] +$$

$$+ |V_{df}|^4 U^{(d)} \left\{U_A^{(f)} \delta M_A + U_B^{(f)} \delta M_B + U_A^{(f)} U_B^{(f)} \left[\delta N_A N_B^{(k)} + \delta N_B N_A^{(k)} - \right.\right.$$

$$\left.\left. - (\delta M_A M_B^{(k)} + \delta M_B M_A^{(k)})\right]\right\} + \phi(|V_{df}|^8) = 1 \tag{32}$$

Hence one sees from (32) that the first term including only hibridization effects behaves like a transition metal in presence of hybridization and for similar values of hybridization parameters one gets identical results. The essential characteristic of actinide metals lying in the existence of correlated d bands which hybridize with the "magnetic band" is then clearly incorporated in the second term of (32) and it may act as a decisive term in the occurrence of magnetism.

APPENDIX

i) Definition of the functions ζ_i^j, λ_i^j, ξ_i, π_i, Γ_i and η_i.

These functions are defined as follows

$$\zeta_i^j = -\mathcal{F}_\omega\left[\frac{H_p(\omega)\ K_j(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^p)\ F_p(\omega)\}^2}\right] , \qquad i,j = A,B\ ;\quad i \neq j \tag{A.1}$$

$$\lambda_i^j = -\mathcal{F}_\omega\left[\frac{(F_p(\omega))^2 K_j(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^p)\ F_p(\omega)\}^2}\right] , \tag{A.2}$$

$$\xi_i = \mathcal{F}_\omega\left[\frac{(F_p(\omega))^2}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^p)\ F_p(\omega)\}^2}\right] , \tag{A.3}$$

$$\pi_i = -\mathcal{F}_\omega\left[\frac{H_p(\omega)\ K(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^{p})\ F_p(\omega)\}^2}\right], \quad (A.4)$$

$$\Gamma_i = -\mathcal{F}_\omega\left[\frac{(F_p(\omega))^2 K(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^{p}) F_p(\omega)\}^2}\right] \quad (A.5)$$

and finally

$$\eta_i = -\mathcal{F}_\omega\left[\frac{H_1(\omega)}{\{1 - (\varepsilon_{ip}^{(\alpha)} - \Sigma_{(\alpha)}^{p})\ F_p(\omega)\}^2}\right] \quad (A.6)$$

ii) Definition of the functions ϕ_i , i = 1,2,3.

$$\phi_1 = -\mathcal{F}_\omega\left[\sum_k \frac{(\omega - \varepsilon_k^{(\alpha)} - \Sigma_{(\alpha)}^{p})^2}{\{(\omega - \varepsilon_{kp}^{(\beta)})(\omega - \varepsilon_k^{(\alpha)} - \Sigma_{(\alpha)}^{p}) - |V_{\alpha\beta}|^2\}^2}\right], \quad (A.7)$$

It should be noted that in the absence of $V_{\alpha\beta}$ mixing (A.7) reduces to the pure β band susceptibility.

$$\phi_2^{(j)} = -\mathcal{F}_\omega \left[\sum_k \frac{K_j(\omega)}{\{(\omega - \varepsilon_{kp}^{(\beta)})(\omega - \varepsilon_k^{(\alpha)} - \Sigma_{(\alpha)}^p) - |V_{\alpha\beta}|^2\}^2} \right], \quad j = A, B . \tag{A.8}$$

and

$$\phi_3 = -\mathcal{F}_\omega \left[\sum_k \frac{K(\omega)}{\{(\omega - \varepsilon_{kp}^{(\beta)})(\omega - \varepsilon_k^{(\alpha)} - \Sigma_{(\alpha)}^p) - |V_{\alpha\beta}|^2\}^2} \right]. \tag{A.9}$$

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