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EFFECT OF s-d HYBRIDIZATION IN THE SPIN POLARIZATION: DOUBLY DEGENERATE d-band IN HARTREE-FOCK

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INTRODUCTION

The effect of the s-d hybridization in the problem of the spin polarization has been the subject of a recent calculation.[1] In that paper, the response of an s-d conduction band was calculated within the Hartree-Fock approximation for the d-d electron correlations, thus extending the previous work of Giovaninni et al.[2] The main result of this type of response problem is the possibility of defining effective exchange interactions, coupling the itinerant and localized electrons. It was shown that even in the s-d coupled systems the total induced magnetization is still the sum of the s and d responses provided effective exchanges and susceptibilities corrected for s-d mixing are used. Quite similar results are expected for an external magnetic field of wave vector q. It is the purpose of this paper to extend the previous calculation to include (at least within a simple model) the degeneracy of the d-band. The effects we want to see are firstly if the definition of effective exchange is still possible , and what is the role of exchange interaction among itinerant d-electrons. In pure hosts it is known that, when degeneracy is present, and for two identical sub-bands, the effect of exchange is to replace the Coulomb interaction in the Stoner factor by U + J.

The same effect persists in the present case, and also in the definition of the effective s-exchange one has this extra enhancement.

The plan of this paper is as follows: Firstly we formulate the problem and determine the equations of motion. Next the self consistency problem is solved and the effective exchange couplings of the s-states to the local spin is determined. Then the s-magnetization is evaluated, and the effective coupling of the s-states is determined.

Finally the previous case of a single d-band is recovered as a simple limit and the simplified expressions valid for identical sub-bands are derived.

II. FORMULATION OF THE PROBLEM

a) *Hamiltonian of the system*

We intend to simulate the degeneracy of the d-band, and the consequent existence of exchange interactions using a two band approximation introduced by Schneider et al [3]. The Hamiltonian for the non-interacting host is:

$$\mathcal{H}_o = \sum_{ij\sigma} T_{ij}^{(s)} C_{i\sigma}^{+} C_{j\sigma} + \sum_{ij\sigma} T_{ij}^{(\alpha)} \alpha_{i\sigma}^{+} \alpha_{j\sigma} + \sum_{ij\sigma} T_{ij}^{(\beta)} \beta_{i\sigma}^{+} \beta_{j\sigma} + \sum_{ij\sigma} \left\{ V_{sd}^{(\alpha)}(R_i - R_j) C_{i\sigma}^{+} \alpha_{j\sigma} + V_{ds}^{(\alpha)}(R_i - R_j) \alpha_{i\sigma}^{+} C_{j\sigma} \right\} + \sum_{ij\sigma} \left\{ V_{sd}^{(\beta)}(R_i - R_j) C_{i\sigma}^{+} \beta_{j\sigma} + V_{ds}^{(\beta)}(R_i - R_j) \beta_{i\sigma}^{+} C_{j\sigma} \right\} \quad (1)$$

We considered in (1) mixing matrix elements which are in general different for the two sub bands. The Coulomb interactions among d-electrons are described through the hamiltonian:

$$\mathcal{H}_c = U_\alpha \sum_i n_{i\uparrow}^{(\alpha)} n_{i\downarrow}^{(\alpha)} + U_\beta \sum_i n_{i\uparrow}^{(\beta)} n_{i\downarrow}^{(\beta)} + U_{\alpha\beta} \left\{ \sum_i n_{i\uparrow}^{(\alpha)} n_{i\downarrow}^{(\beta)} + \sum_i n_{i\downarrow}^{(\alpha)} n_{i\uparrow}^{(\beta)} \right\} + (U_{\alpha\beta} - J_{\alpha\beta}) \sum_i n_{i\sigma}^{(\alpha)} n_{i\sigma}^{(\beta)} \quad (2)$$

The last term of (2) describes Coulomb repulsions and exchange among parallel spin electrons and this is a clear feature of the degeneracy of the d-band. Finally the coupling to the localized spin is given by:

$$\mathcal{H}_{imp} = \sum_{i,j,\sigma} J_{(\alpha)}^{(d)}(R_i, R_j) \langle S^z \rangle \sigma \alpha_{i\sigma}^{+} \alpha_{j\sigma} + \sum_{i,j,\sigma} J_{(\beta)}^{(d)}(R_i, R_j) \langle S^z \rangle \sigma \beta_{i\sigma}^{+} \beta_{j\sigma} + \sum_{i,j,\sigma} J^{(s)}(R_i, R_j) \langle S^z \rangle \sigma C_{i\sigma}^{+} C_{j\sigma} \quad (3)$$

the complete hamiltonian is then:

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_c + \mathcal{H}_{imp} \quad (4)$$

b) *Determination of the equations of motion for the propagators $G^{\alpha\alpha}_{ij}$, $G^{\beta\beta}_{ij}$ and G^{ss}_{ij}*

i) Complete determination of the $G^{\alpha\alpha}_{ij}(\omega)$ propagator

Within the Hartree-Fock approximation one has:

$$\omega\, G^{\alpha\alpha}_{ij}(\omega) = \frac{1}{2\pi}\,\delta_{ij} + \sum_{\ell} T^{(\alpha)}_{i\ell} G^{\alpha\alpha}_{\ell j}(\omega) + \left\{ U_{\alpha} \langle n^{(\alpha)}_{i-\sigma}\rangle + U_{\alpha\beta} \langle n^{(\beta)}_{i-\sigma}\rangle + (U_{\alpha\beta} - J_{\alpha\beta}) \langle n^{(\beta)}_{i\sigma}\rangle \right\} G^{\alpha\alpha}_{ij}(\omega) + $$
$$+ \sum_{\ell} V^{(\alpha)}_{ds}(R_i - R_\ell) G^{s\alpha}_{\ell j}(\omega) + \sum_{\ell} J^{(d)}_{(\alpha)}(R_i, R_\ell) G^{\alpha\alpha}_{\ell j}(\omega) \qquad (5\text{-a})$$

$$\omega\quad G^{s\alpha}_{ij}(\omega) = \sum_{\ell} T^{(s)}_{i\ell}\, G^{s\alpha}_{\ell j}(\omega) + \sum_{\ell} V^{(\alpha)}_{sd}(R_i - R_\ell) G^{\alpha\alpha}_{\ell j}(\omega) + \sum_{\ell} V^{(\beta)}_{sd}(R_i - R_\ell) G^{\beta\alpha}_{\ell j}(\omega) + $$
$$+ \sum_{\ell} J^{(s)}(R_i, R_\ell)\, \langle S^z\rangle\, \sigma\, G^{s\alpha}_{\ell j}(\omega) \qquad (5\text{-b})$$

and finally:

$$\omega\, G^{\beta\alpha}_{ij}(\omega) = \sum_{\ell} T^{(\beta)}_{i\ell}\, G^{\beta\alpha}_{\ell j}(\omega) + \left\{ U_{\beta}\, \langle n^{(\beta)}_{i-\sigma}\rangle + U_{\alpha\beta}\, \langle n^{(\alpha)}_{i-\sigma}\rangle + (U_{\alpha\beta} - J_{\alpha\beta}) \langle n^{(\alpha)}_{i\sigma}\rangle \right\} G^{\beta\alpha}_{ij}(\omega) + $$
$$+ \sum_{\ell} V^{(\beta)}_{ds}(R_i - R_\ell) G^{s\alpha}_{\ell j}(\omega) + \sum_{\ell} J^{(d)}_{(\beta)}(R_i, R_\ell)\, \langle S^z\rangle\, \sigma\, G^{\beta\alpha}_{\ell j}(\omega) \qquad (5\text{-c})$$

The coupled system (5) completely determine the propagator $G^{\alpha\alpha}_{ij}(\omega)$.

ii) Determination of the propagator $G^{\beta\beta}_{ij}(\omega)$

One just needs to replace in equations (5), where it appears α by β and β by α.

iii) Complete determination of the propagator $G_{ij}^{ss}(\omega)$

Using again the Hartree-Fock approximation one gets:

$$\omega\, G_{ij}^{ss}(\omega)=\frac{1}{2\pi}\,\delta_{ij} + \sum_{\ell} T_{i\ell}^{(s)}\, G_{\ell j}^{ss}(\omega) + \sum_{\ell} V_{sd}^{(\alpha)}(R_i-R_\ell)G_{\ell j}^{\alpha s}(\omega)+\sum_{\ell} V_{sd}^{(\beta)}(R_i-R_\ell)G_{\ell j}^{\beta s}(\omega) + $$
$$+ \sum_{\ell} J^{(s)}(R_i,R_\ell)\langle S^z\rangle\, \sigma\, G_{\ell j}^{ss}(\omega) \qquad (6\text{-a})$$

$$\omega\, G_{ij}^{\alpha s}(\omega)= \sum_{\ell} T_{i\ell}^{(\alpha)}\, G_{\ell j}^{\alpha s}(\omega) + \left\{U_\alpha \langle n_{i-\sigma}^{(\alpha)}\rangle + U_{\alpha\beta}\, \langle n_{i-\sigma}^{(\beta)}\rangle+(U_{\alpha\beta}-J_{\alpha\beta})\langle n_{i\sigma}^{(\beta)}\rangle\right\}G_{ij}^{\alpha s}(\omega) +$$
$$+ \sum_{\ell} V_{ds}^{(\alpha)}(R_i-R_\ell)G_{\ell j}^{ss}(\omega) + \sum_{\ell} J_{(\alpha)}^{(d)}(R_i,R_\ell)\, \langle S^z\rangle\, \sigma\, G_{\ell j}^{\alpha s}(\omega) \qquad (6\text{-b})$$

$$\omega\, G_{ij}^{\beta s}(\omega)= \sum_{\ell} T_{i\ell}^{(\beta)}G_{\ell j}^{\beta s}(\omega)+\left\{U_\beta\langle n_{i-\sigma}^{(\beta)}\rangle+U_{\alpha\beta}\, \langle n_{i-\sigma}^{(\alpha)}\rangle + (U_{\alpha\beta}-J_{\alpha\beta})\langle n_{i\sigma}^{(\alpha)}\rangle\right\}G_{ij}^{\beta s}(\omega) +$$
$$+ \sum_{\ell} V_{ds}^{(\beta)}(R_i-R_\ell)G_{\ell j}^{ss}(\omega) + \sum_{\ell} J_{(\beta)}^{(d)}(R_i,R_\ell)\, \langle S^z\rangle\, \sigma\, G_{\ell j}^{\beta s}(\omega) \qquad (6\text{-c})$$

The coupled system (6) specifies the propagator $G_{ij}^{ss}(\omega)$. It should be noted that equations (5) and (6) are a clear generalization for a degenerate two d-band problem of the results obtained in [1].

III. SOLUTION OF THE PURE-HOST PROBLEM

In this situation one has translation symmetry, so one introduces renormalized energies:

$$E_{k\sigma}^{(\alpha)} = \varepsilon_k^{(\alpha)} + U_\alpha\, \langle n_{-\sigma}^{(\alpha)}\rangle + U_{\alpha\beta}\, \langle n_{-\sigma}^{(\beta)}\rangle + (U_{\alpha\beta} - J_{\alpha\beta})\, \langle n_\sigma^{(\beta)}\rangle \qquad (7\text{-a})$$

$$E_{k\sigma}^{(\beta)} = \varepsilon_k^{(\beta)} + U_\beta <n_{-\sigma}^{(\beta)}> + U_{\alpha\beta} <n_{-\sigma}^{(\alpha)}> + (U_{\alpha\beta} - J_{\alpha\beta}) <n_\sigma^{(\alpha)}> \qquad (7\text{-b})$$

i) Solution for the propagator $g_{k\sigma}^{\alpha\alpha}(\omega)$

Using equations (5)and dropping impurity terms:

$$(\omega - E_{k\sigma}^{(\alpha)})\, g_{k\sigma}^{\alpha\alpha}(\omega) = \frac{1}{2\pi} + V_{ds}^{(\alpha)}(k)\, g_{k\sigma}^{s\alpha}(\omega) \qquad (8\text{-a})$$

$$(\omega - \varepsilon_k^{(s)})g_{k\sigma}^{s\alpha}(\omega) = V_{sd}^{(\alpha)}(k)\, g_{k\sigma}^{\alpha\alpha}(\omega) + V_{sd}^{(\beta)}(k)\, g_{k\sigma}^{\beta\alpha}(\omega) \qquad (8\text{-b})$$

$$(\omega - E_{k\sigma}^{(\beta)})\, g_{k\sigma}^{\beta\alpha}(\omega) = V_{ds}^{(\beta)}(k)\, g_{k\sigma}^{s\alpha}(\omega) \qquad (8\text{-c})$$

In equation (8) we have used definitions (8) and the translation symmetry of the host (the propagators are diagonal in k, k'). The coupled system (8) is easily solved; introducing the definitions:

$$\varepsilon_{k\sigma}^{(s,\beta)} = \varepsilon_k^{(s)} + \frac{|V_{sd}^{(\beta)}(k)|^2}{\omega - E_{k\sigma}^{(\beta)}} \qquad (9\text{-a})$$

$$\tilde{E}_{k\sigma}^{(\alpha)}(\omega) = E_{k\sigma}^{(\alpha)} + \frac{|V_{sd}^{(\alpha)}(k)|^2}{\omega - \varepsilon_k^{(s,\beta)}(\omega)} \qquad (9\text{-b})$$

one gets for the $g_{k\sigma}^{\alpha\alpha}(\omega)$ propagator the result:

$$g_{k\sigma}^{\alpha\alpha}(\omega) = \frac{1}{2\pi}\, \frac{1}{\omega - \tilde{E}_{k\sigma}^{(\alpha)}(\omega)} \qquad (10\text{-a})$$

and the following intermediate propagators (useful for later calculations).

$$g_{k\sigma}^{s\alpha}(\omega) = \frac{V_{sd}^{(\alpha)}(k)}{\omega - \varepsilon_{k\sigma}^{(s,\beta)}(\omega)}\, g_{k\sigma}^{\alpha\alpha}(\omega) \qquad (10\text{-b})$$

and

$$g^{\beta\alpha}_{k\sigma}(\omega) = \frac{V^{(\beta)}_{ds}(k)}{\omega - E^{(\beta)}_{k\sigma}} \; \frac{V^{(\alpha)}_{sd}(k)}{\omega - \varepsilon^{(s,\beta)}_{k\sigma}(\omega)} \; g^{\alpha\alpha}_{k\sigma}(\omega) \tag{10-c}$$

Equations (10) complete the determination of the $g^{\alpha\alpha}_{k\sigma}$ propagator.

ii) **Determination of the $g^{ss}(\omega)$ propagator**

From equations (6) and using (7) one has:

$$(\omega - \varepsilon^{(s)}_{k}) g^{ss}_{k\sigma}(\omega) = \frac{1}{2\pi} + V^{(\alpha)}_{sd}\, g^{\alpha s}_{k\sigma}(\omega) + V^{(\beta)}_{sd}\, g^{\beta s}_{k\sigma}(\omega) \tag{11-a}$$

$$(\omega - E^{(\alpha)}_{k\sigma})\, g^{\alpha s}_{k\sigma}(\omega) = V^{(\alpha)}_{ds}(k)\, g^{ss}_{k\sigma}(\omega) \tag{11-b}$$

$$(\omega - E^{(\beta)}_{k\sigma}) g^{\beta s}_{k\sigma}(\omega) = V^{(\beta)}_{ds}(k)\, g^{ss}_{k\sigma}(\omega) \tag{11-c}$$

Now introducing the definition:

$$\tilde{\varepsilon}^{(s)}_{k\sigma}(\omega) = \varepsilon^{(s)}_{k} + \frac{|V^{(\alpha)}_{sd}(k)|^2}{\omega - E^{(\alpha)}_{k\sigma}} + \frac{|V^{(\beta)}_{sd}(k)|^2}{\omega - E^{(\beta)}_{k\sigma}} \tag{12}$$

one finally gets for the $g^{ss}_{k\sigma}(\omega)$ propagator:

$$g^{ss}_{k\sigma}(\omega) = \frac{1}{2\pi} \; \frac{1}{\omega - \tilde{\varepsilon}^{(s)}_{k\sigma}(\omega)} \tag{13-a}$$

and for the intermediate propagator:

$$g^{\alpha s}_{k\sigma}(\omega) = \frac{V^{(\alpha)}_{ds}(k)}{\omega - E^{(\alpha)}_{k\sigma}}\, g^{ss}_{k\sigma}(\omega); \quad g^{\beta s}_{k\sigma}(\omega) = \frac{V^{(\beta)}_{ds}(k)}{\omega - E^{(\beta)}_{k\sigma}}\, g^{ss}_{k\sigma}(\omega) \tag{13-b}$$

IV. FIRST ORDER SOLUTION FOR THE $G^{\alpha\alpha}_{kk'}$ AND $G^{\beta\beta}_{kk'}$ PROPAGATORS (PARAMAGNETIC PHASE)

From equations (5) one gets the following first order results:

$$(\omega-E_k^{(\alpha)})G^{\alpha\alpha(1)}_{kk'}(\omega) = V^{(\alpha)}_{ds}(k)\; G^{s\alpha(1)}_{kk'}(\omega) + J^{(d)}_{(\alpha)}(k,k')\langle S^z\rangle\;\sigma\; g^{\alpha\alpha}_{k'}(\omega) + \left\{ U_\alpha\,\Delta\, n^{-\sigma(\alpha)}_{kk'} + U_{\alpha\beta}\,\Delta\, n^{-\sigma(\beta)}_{kk'} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n^{\sigma(\beta)}_{kk'}\right\} g^{\alpha\alpha}_{k'}(\omega) \tag{14-a}$$

$$(\omega-\varepsilon_k^{(s)})G^{s\alpha(1)}_{kk'}(\omega) = V^{(\alpha)}_{sd}(k)\; G^{\alpha\alpha(1)}_{kk'}(\omega) + V^{(\beta)}_{sd}(k)G^{\beta\alpha(1)}_{kk'}(\omega)+J^{(s)}(k,k')\langle S^z\rangle\sigma g^{s\alpha}_{k'}(\omega) \tag{14-b}$$

$$(\omega-E_k^{(\beta)})G^{\beta\alpha(1)}_{kk'}(\omega) = V^{(\beta)}_{ds}(k)\; G^{s\alpha(1)}_{kk'}(\omega) + J^{(d)}_{(\beta)}(k,k')\langle S^z\rangle\;\sigma\; g^{\beta\alpha}_{k'}(\omega) + \left\{ U_\beta\,\Delta n^{-\sigma(\beta)}_{kk'} + U_{\alpha\beta}\,\Delta\, n^{-\sigma(\alpha)}_{kk'} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n^{\sigma(\alpha)}_{kk'}\right\} g^{\beta\alpha}_{k'}(\omega) \tag{14-c}$$

In deriving (14) we have used the fact that host metal propagators are diagonal in k-representation and also the definitions:

$$\Delta\, n^{(\lambda)\sigma}_{kk'} = \sum_i \Delta\, n^{\sigma(\lambda)}_i\, e^{i(k-k')\cdot R_i} = \Delta\, n^{(\lambda)\sigma}_{k-k'}\;;\qquad \lambda = s,d$$

Now combining equations (14-b), (14-c) and using the definition (9-a) one gets:

$$V^{(\alpha)}_{ds}(k)G^{s\alpha(1)}_{kk'}(\omega)= \frac{|V^{(\alpha)}_{sd}(k)|^2}{\omega-\varepsilon_k^{(s,\beta)}(\omega)}\; G^{\alpha\alpha(1)}_{kk'}(\omega) + \frac{V^{(\alpha)}_{ds}(k)}{\omega-\varepsilon_k^{(s,\beta)}(\omega)}\; J^{(s)}(k,k')\langle S^z\rangle\,\sigma\, g^{s\alpha}_{k'}(\omega) + \frac{V^{(\alpha)}_{ds}(k)}{\omega-\varepsilon_k^{(s,\beta)}(\omega)}\;\frac{V^{(\beta)}_{ds}(k)}{\omega-E_k^{(\beta)}}\left\{ J^{(d)}_{(\beta)}(k,k')\langle S^z\rangle\sigma + U_\beta\;\Delta n^{-\sigma(\beta)}_{kk'}+U_{\alpha\beta}\Delta\; n^{-\sigma(\alpha)}_{kk'} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n^{\sigma(\alpha)}_{kk'}\right\} g^{\beta\alpha}_{k'}(\omega) \tag{15}$$

Next step is to substitute equation (15) into equation (14-a); this procedure explicitates $G^{\alpha\alpha}_{kk'}(\omega)$ in terms of zero order propagators and the fluctuation numbers: Using the expression (10) for zero-order propagators one gets the final result:

$$G^{\alpha\alpha(1)}_{k+q,k}(\omega) = \frac{1}{2\pi}\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k+q}(\omega)} J^{(d)}_{(\alpha)}(k+q,k) <S^z> \sigma \frac{1}{\omega-\tilde{E}^{(\alpha)}_{k}(\omega)} +$$

$$+\frac{1}{2\pi}\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k+q}(\omega)}\left\{U_\alpha\ \Delta n_q^{-\sigma(\alpha)} + U_{\alpha\beta}\ \Delta n_q^{-\sigma(\beta)} + (U_{\alpha\beta}-J_{\alpha\beta})\ \Delta n_q^{\sigma(\beta)}\right\}\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k}(\omega)}$$

$$+\frac{1}{2\pi}\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k+q}(\omega)}V^{(\alpha)}_{ds}(k+q)\frac{1}{\omega-\varepsilon^{(s,\beta)}_{k+q}(\omega)}J^{(s)}(k+q,k)<S^z>\sigma\frac{1}{\omega-\varepsilon^{(s,\beta)}_{k}(\omega)}V^{(\alpha)}_{sd}(k)\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k}(\omega)}+$$

$$+\frac{1}{2\pi}\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k+q}(\omega)}V^{(\alpha)}_{ds}(k+q)\frac{1}{\omega-\varepsilon^{(s,\beta)}_{k+q}(\omega)}V^{(\beta)}_{sd}(k+q)\frac{1}{\omega-E^{(\beta)}_{k+q}}\left\{J^{(d)}_{(\beta)}(k+q,k)\ <S^z>\ \sigma\ +\right.$$

$$\left.+\ U_\beta\Delta n_q^{-\sigma(\beta)}+U_{\alpha\beta}\Delta n_q^{-\sigma(\alpha)}+(U_{\alpha\beta}-J_{\alpha\beta})\Delta n_q^{\sigma(\alpha)}\right\}\frac{1}{\omega-E^{(\beta)}_{k}}V^{(\beta)}_{ds}(k)\frac{1}{\omega-\varepsilon^{(s,\beta)}_{k}(\omega)}V^{(\alpha)}_{sd}(k)\frac{1}{\omega-\tilde{E}^{(\alpha)}_{k}(\omega)} \tag{16}$$

The physical interpretation of equation (16) is quite clear; the first term describes a renormalized α electron which scatters from k to k+q due to the impurity exchange potential. The second term is quite similar except that the source of scattering are the fluctuations in occupation numbers, the coupling constants being the Coulomb and exchange interactions. The third and fourth terms describe the role of mixing; the third term corresponds to a process where an α electron is admixed into the renormalized s-band then scattered through the exchange interaction associated to the impurity. Finally the fourth term describes how the β band couples to the α band through mixing; an α electron is admixed into the s-band and then into the β band being then scattered by $J_{\beta}^{(d)}$ and by the fluctuations associated to the β band.

Equation (16) formally solves the problem of determining the $G_{k+q,k}^{\alpha\alpha(1)}(\omega)$ propagator; it remains only the self-consistent determination of the occupation number fluctuations. The $G_{k+q,k}^{\beta\beta(1)}(\omega)$ propagator can be easily derived from (16) just by replacing α by β and β by α where they appear.

V. SELF-CONSISTENCY PROBLEM IN THE ABSENCE OF MIXING

In this paragraph we consider the simpler case where mixing vanishes in order to clearly separate the effects of the degeneracy of the d-band. These results can then be compared to Giovaninni's work [2]. In the absence of mixing, equation (16) reduces to:

$$G_{k+q,k}^{\alpha\alpha(1)}(\omega) = \frac{1}{2\pi}\frac{1}{\omega-E_{k+q}^{(\alpha)}}\left\{J_{(\alpha)}^{(d)}(k+q,k)\langle S^z\rangle\sigma + U_{\alpha}\,\Delta n_q^{-\sigma(\beta)} + U_{\alpha\beta}\Delta n_q^{-\sigma(\beta)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n_q^{\sigma(\beta)}\right\}\frac{1}{\omega-E_k^{(\alpha)}} \tag{17-a}$$

and quite similarly:

$$G_{k+q,k}^{\beta\beta(1)}(\omega) = \frac{1}{2\pi}\frac{1}{\omega-E_{k+q}^{(\beta)}}\left\{J_{(\beta)}^{(d)}(k+q,k)\langle S^z\rangle\sigma + U_{\beta}\Delta n_q^{-\alpha(\beta)} + U_{\alpha\beta}\Delta n_q^{-\sigma(\alpha)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n_q^{\alpha(\beta)}\right\}\frac{1}{\omega-E_k^{(\beta)}} \tag{17-b}$$

Now remembering the definition:

$$\Delta n_q^{\sigma(\lambda)} = \Sigma_k \; F_\omega \left[G_{k+q,k}^{\lambda\lambda(\sigma)}\right] \quad , \qquad \lambda = \alpha,\beta \tag{18-a}$$

and defining the susceptibilities (in the absence of mixing):

$$\chi_{(p)}^{(\lambda)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega - E_{k+q}^{(\lambda)}} \; \frac{1}{\omega - E_k^{(\lambda)}} \right\}$$

$$= \frac{f(E_{k+q}^{(\lambda)}) - f(E_k^{(\lambda)})}{E_{k+q}^{(\lambda)} - E_k^{(\lambda)}} \tag{18-b}$$

and

$$\chi_{(p)}^{(\lambda)}(q) = \Sigma_k \; \chi_{(p)}^{(\lambda)}(k,q) \tag{18-c}$$

one obtains from equations (17):

$$\Delta n_q^{\sigma(\alpha)} = \sum_k J_{(\alpha)}^{(d)}(k+q,k) \langle S^z \rangle \sigma \; \chi_{(p)}^{(\alpha)}(k,q) + \left\{ U_\alpha \Delta n_q^{-\sigma(\alpha)} + U_{\alpha\beta} \Delta n_q^{-\sigma(\beta)} + \right.$$

$$\left. + (U_{\alpha\beta} - J_{\alpha\beta}) \Delta n_q^{\sigma(\beta)} \right\} \chi_{(p)}^{(\alpha)}(q) \tag{19-a}$$

and

$$\Delta n_q^{\sigma(\beta)} = \sum_k J_{(\beta)}^{(d)}(k+q,k) \langle S^z \rangle \sigma \; \chi_{(p)}^{(\beta)}(k,q) + \left\{ U_\beta \Delta n_q^{-\sigma(\beta)} + U_{\alpha\beta} \; \Delta n_q^{-\sigma(\alpha)} + \right.$$

$$\left. + (U_{\alpha\beta} - J_{\alpha\beta}) \Delta n_q^{\sigma(\alpha)} \right\} \chi_{(p)}^{(\beta)}(q) \tag{19-b}$$

This is a coupled linear system determining the occupation numbers; by inspection one verifies that the solutions must be proportional to σ so in general:

$$\Delta n_q^{\sigma(\lambda)} = - \Delta n_q^{-\sigma(\lambda)}; \qquad \lambda = \alpha,\beta \tag{19-c}$$

So introducing the definitions:

$$x^{\alpha}(q) = \sum_k J\begin{Bmatrix}d\\ \alpha\end{Bmatrix}(k+q,k)\ \chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(k,q) \qquad (19\text{-d})$$

and

$$x^{\beta}(q) = \sum_k J\begin{Bmatrix}d\\ \beta\end{Bmatrix}(k+q,k)\chi^{(\beta)}_{(p)}(k,q)$$

equations (19) become:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle\sigma\ x^{\alpha}(q) - \left\{U_\alpha\ \Delta n_q^{\sigma(\alpha)} + J_{\alpha\beta}\ \Delta\ n_q^{\sigma(\beta)}\right\}\chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(q)$$

$$\Delta n_q^{\sigma(\beta)} = \langle S^z\rangle\sigma\ x^{\beta}(q) - \left\{U_\beta\ \Delta n_q^{\sigma(\beta)} + J_{\alpha\beta}\ \Delta\ n_q^{\sigma(\alpha)}\right\}\chi\begin{Bmatrix}\beta\\ p\end{Bmatrix}(q) \qquad (20)$$

The solution of (20) is easily obtained to give:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle\ \sigma\ \frac{(1+U_\beta\ \chi\begin{Bmatrix}\beta\\ p\end{Bmatrix}(q))\ x^{(\alpha)}(q) - J_{\alpha\beta}\ \ \chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(q)\ x^{(\beta)}(q)}{(1+U_\alpha\ \chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(q))(1+U_\beta\ \chi\begin{Bmatrix}\beta\\ p\end{Bmatrix}(q)) - J^2_{\alpha\beta}\ \ \chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(q)\ \chi\begin{Bmatrix}\beta\\ p\end{Bmatrix}(q)} \qquad (21)$$

and a quite similar expression for $\Delta n_q^{\sigma(\beta)}$ (it should be noted that denominators are identical). A very interesting expression can be obtained from (21) in the case of identical susceptibilities and interactions. If we assume:

$$\chi\begin{Bmatrix}\alpha\\ p\end{Bmatrix}(k,q) = \chi\begin{Bmatrix}\beta\\ p\end{Bmatrix}(k,q) = \chi\begin{Bmatrix}d\\ p\end{Bmatrix}(k,q)$$

$$U_\alpha = U_\beta = U \text{ and } J_{\alpha\beta} = J$$

$$J\begin{Bmatrix}d\\ \alpha\end{Bmatrix}(k+q,k) = J\begin{Bmatrix}d\\ \beta\end{Bmatrix}(k+q,k) = J^{(d)}(k+q,k) \qquad (22)$$

one gets:

$$x^{\alpha}(q) = x^{\beta}(q) = \Sigma_k\ J^{(d)}(k+q,k)\ \chi\begin{Bmatrix}d\\ p\end{Bmatrix}(k,q)$$

so:

$$m_q^{(\alpha)} = m_q^{(\beta)} = 2 \langle S^z \rangle \; \Sigma_k \; \frac{J^{(d)}(k+q,k)\, \chi_{(p)}^{(d)}(k,q)}{1+(U+J)\chi_{(p)}^{(d)}(k,q)} \tag{23}$$

Expression (23) is a clear generalization of Giovaninni's result [2] for k,k' dependent exchange interactions and doubly degenerate d-band. Comparing to ref. 1 one sees that the effect of the degeneracy is as expected to modify Stoner's, replacing in ref. 1 U by U+J.

VI. GENERAL SELF-CONSISTENCY PROBLEM FOR THE α AND β MAGNETIZATIONS

Now we return to equation (16) and define the following susceptibilities:

$$\chi_{(o)}^{(\lambda)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega-\tilde{E}_{k+q}^{(\lambda)}(\omega)} \; \frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} \right\} ; \; \chi_{(o)}^{(\lambda)}(q) = \Sigma_k \, \chi_{(o)}^{(\lambda)}(k,q) \tag{24-a}$$

$$\chi_{(1)}^{(\lambda\delta)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega-\tilde{E}_{k+q}^{(\lambda)}(\omega)} \; \frac{1}{\omega-\varepsilon_{k+q}^{(s,\delta)}(\omega)} \; \frac{1}{\omega-\varepsilon_k^{(s,\delta)}(\omega)} \; \frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} \right\} ;$$

$$\chi_{(1)}^{(\lambda\delta)}(q) = \sum_k \chi_1^{(\lambda\delta)}(k,q) \tag{24-b}$$

$$\chi_{(2)}^{(\lambda\delta)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega-\tilde{E}_{k+q}^{(\lambda)}(\omega)} \; \frac{1}{\omega-\varepsilon_{k+q}^{(s,\delta)}(\omega)} \; \frac{1}{\omega-E_{k+q}^{(\delta)}} \; \frac{1}{\omega-E_k^{(\delta)}} \; \frac{1}{\omega-\varepsilon_k^{(s,\delta)}(\omega)} \; \frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} \right\} ;$$

$$\chi_{(2)}^{(\lambda\delta)}(q) = \sum_k \chi_{(2)}^{(\lambda,\delta)}(k,q) \tag{24-c}$$

In expression (24-b), (24-c) one has:

$$\lambda,\delta = \alpha,\beta; \quad \lambda \neq \delta$$

Explicit expressions for the susceptibilities, ready for numerical calculation are given in Appendix I. It is shown in this Appendix that $\chi^{\alpha\beta}_{(2)}(k,q) = \chi^{\beta\alpha}_{(2)}(k,q) = \chi_{(o)}(k,q)$.

Using (18-a) and the definitions (24) one has:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle\, \sigma \Big\{ \sum_k J^{(d)}_{(\alpha)}(k+q,k)\chi^{(\alpha)}_{(o)}(k,q) + \sum_k J^{(s)}(k+q,k)V^{(\alpha)}_{ds}(k+q)V^{(\alpha)}_{sd}(k)\chi^{\alpha\beta}_{(1)}(k,q)$$

$$+ \sum_k J^{(d)}_{(\beta)}(k+q,k)V^{(\alpha)}_{ds}(k+q)V^{(\alpha)}_{sd}(k)V^{(\beta)}_{sd}(k+q)V^{(\beta)}_{ds}(k)\chi_{(o)}(k,q)\Big\}$$

$$+ \Big\{U_\alpha\, \Delta n_q^{-\sigma(\alpha)} + U_{\alpha\beta}\, \Delta n_q^{-\sigma(\beta)} + (U_{\alpha\beta} - J_{\alpha\beta})\, \Delta n_q^{\sigma(\beta)}\Big\} \chi^{(\alpha)}_{(o)}(q)$$

$$+ \Big\{U_\beta\, \Delta n_q^{-\sigma(\beta)} + U_{\alpha\beta}\, \Delta n_q^{-\sigma(\alpha)} + (U_{\alpha\beta} - J_{\alpha\beta})\, \Delta n_q^{\sigma(\beta)}\Big\} \chi^{\alpha\beta}_{mix}(q) \qquad (25\text{-a})$$

where we have defined:

$$\chi^{\alpha\beta}_{mix}(q) = \sum_k V^{(\alpha)}_{ds}(k+q)V^{(\alpha)}_{sd}(k)V^{(\beta)}_{sd}(k+q)V^{(\beta)}_{ds}(k)\chi_{(o)}(k,q) \qquad (25\text{-b})$$

Introduce now the generalization of (19-d):

$$\chi^{\alpha\beta}(q) = \sum_k J^{(d)}_{(\alpha)}(k+q,k)\chi^{(\alpha)}_{(o)}(k,q) + \sum_k J^{(s)}(k+q,k)V^{(\alpha)}_{ds}(k+q)V^{(\alpha)}_{sd}(k)\chi^{\alpha\beta}_{(1)}(k,q) +$$

$$+ \sum_k J^{(d)}_{(\beta)}(k+q,k)\, V^{(\alpha)}_{ds}(k+q)\, V^{(\alpha)}_{sd}(k)\, V^{(\beta)}_{sd}(k+q)V^{(\beta)}_{ds}(k)\chi_{(o)}(k,q) \qquad (26)$$

Equation (25) together with a similar one for $\Delta n_q^{\sigma(\beta)}$ solve completely the self-consistency problem; again equation (19-c) holds and one gets the following coupled system:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle\,\sigma\,\chi^{\alpha\beta}(q) - \left\{U_\alpha\,\chi_{(o)}^{(\alpha)}(q) + J_{\alpha\beta}\,\chi_{mix}^{\alpha\beta}(q)\right\}\Delta n_q^{\sigma(\alpha)}$$

$$- \left\{J_{\alpha\beta}\,\chi_{(o)}^{(\alpha)}(q) + U_\beta\chi_{mix}^{\alpha\beta}(q)\right\}\Delta n_q^{\sigma(\beta)} \qquad (27\text{-a})$$

and similarly:

$$\Delta n_q^{\sigma(\beta)} = \langle S^z\rangle\,\sigma\,\chi^{\beta\alpha}(q) - \left\{U_\beta\,\chi_{(o)}^{(\beta)}(q) + J_{\alpha\beta}\,\chi_{mix}^{\beta\alpha}(q)\right\}\Delta n_q^{\sigma(\beta)}$$

$$- \left\{J_{\alpha\beta}\chi_{(o)}^{(\beta)}(q) + U_\alpha\,\chi_{mix}^{\beta\alpha}(q)\right\}\Delta n_q^{\sigma(\alpha)} \qquad (27\text{-b})$$

The coupled system (27) can now be easily solved; introduce the following effective Coulomb and exchange interactions:

$$U_{eff}^{(\alpha)}(q) = U_\alpha\left\{1 + \frac{J_{\alpha\beta}}{U_\alpha}\,\frac{\chi_{mix}^{\alpha\beta}(q)}{\chi_{(o)}^{(\alpha)}(q)}\right\}$$

$$U_{eff}^{(\beta)}(q) = U_\beta\left\{1 + \frac{J_{\alpha\beta}}{U_\beta}\,\frac{\chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\beta)}(q)}\right\} \qquad (28)$$

$$J_{\alpha\beta}^{(\alpha)}(q) = J_{\alpha\beta}\left\{1 + \frac{U_\beta}{J_{\alpha\beta}}\,\frac{\chi_{mix}^{\alpha\beta}(q)}{\chi_{(o)}^{(\alpha)}(q)}\right\}$$

$$J_{\alpha\beta}^{(\beta)}(q) = J_{\alpha\beta}\left\{1 + \frac{U_\alpha}{J_{\alpha\beta}}\,\frac{\chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\beta)}(q)}\right\}$$

Using definitions (28), the solution of the coupled system (27) reads:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z \rangle \, \sigma \, \chi^{\alpha\beta}(q) - \left\{ U_\alpha \, \chi_{(o)}^{(\alpha)}(q) + J_{\alpha\beta} \, \chi_{mix}^{\alpha\beta}(q) \right\} \Delta n_q^{\sigma(\alpha)}$$
$$- \left\{ J_{\alpha\beta} \, \chi_{(o)}^{(\alpha)}(q) + U_\beta \chi_{mix}^{\alpha\beta}(q) \right\} \Delta n_q^{\sigma(\beta)} \qquad (27\text{-a})$$

and similarly:

$$\Delta n_q^{\sigma(\beta)} = \langle S^z \rangle \, \sigma \, \chi^{\beta\alpha}(q) - \left\{ U_\beta \, \chi_{(o)}^{(\beta)}(q) + J_{\alpha\beta} \, \chi_{mix}^{\beta\alpha}(q) \right\} \Delta n_q^{\sigma(\beta)}$$
$$- \left\{ J_{\alpha\beta} \chi_{(o)}^{(\beta)}(q) + U_\alpha \, \chi_{mix}^{\beta\alpha}(q) \right\} \Delta n_q^{\sigma(\alpha)} \qquad (27\text{-b})$$

The coupled system (27) can now be easily solved; introduce the following effective Coulomb and exchange interactions:

$$U_{eff}^{(\alpha)}(q) = U_\alpha \left\{ 1 + \frac{J_{\alpha\beta}}{U_\alpha} \, \frac{\chi_{mix}^{\alpha\beta}(q)}{\chi_{(o)}^{(\alpha)}(q)} \right\}$$

$$U_{eff}^{(\beta)}(q) = U_\beta \left\{ 1 + \frac{J_{\alpha\beta}}{U_\beta} \, \frac{\chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\beta)}(q)} \right\} \qquad (28)$$

$$J_{\alpha\beta}^{(\alpha)}(q) = J_{\alpha\beta} \left\{ 1 + \frac{U_\beta}{J_{\alpha\beta}} \, \frac{\chi_{mix}^{\alpha\beta}(q)}{\chi_{(o)}^{(\alpha)}(q)} \right\}$$

$$J_{\alpha\beta}^{(\beta)}(q) = J_{\alpha\beta} \left\{ 1 + \frac{U_\alpha}{J_{\alpha\beta}} \, \frac{\chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\beta)}(q)} \right\}$$

Using definitions (28), the solution of the coupled system (27) reads:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z \rangle \sigma \frac{(1+U_{eff}^{(\beta)}(q)\ \chi_{(o)}^{(\beta)}(q))\ \chi^{\alpha\beta}(q) - J_{\alpha\beta}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)\ \chi^{\beta\alpha}(q)}{(1+U_{eff}^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q))(1+U_{eff}^{(\beta)}(q)\chi_{(o)}^{(\beta)}(q)) - J_{\alpha\beta}^{(\alpha)}(q) J_{\alpha\beta}^{(\beta)}(q)\chi_{(o)}^{(\alpha)}(q)\chi_{(o)}^{(\beta)}(q)} \tag{29}$$

The result (29) solves completely for the localized spin induced magnetization in the α band. We want to emphasize that this result shows a great formal similarity to the susceptibility of an actinide metal within the Hartree-Fock approximation [4]. This similarity just reflects the common feature of a coupled two band problem. Now following the procedure used in [4] we rewrite the denominator of (29) in terms of an "effective exchange interaction".

Define:

$$1 + J_{eff}^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q) = (1+U_{eff}^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q))(1+U_{eff}^{(\beta)}(q)\chi_{(o)}^{(\beta)}(q)) - J_{\alpha\beta}^{(\alpha)}(q)\ J_{\alpha\beta}^{(\beta)}(q)\ \chi_{(o)}^{(\alpha)}(q)\ \chi_{(o)}^{(\beta)}(q) \tag{30-a}$$

From (30-a) it terms out for $J_{eff}^{(\alpha)}(q)$ the following result:

$$J_{eff}^{(\alpha)}(q) = U_\alpha + U_\beta \frac{\chi_{(o)}^{(\beta)}(q)}{\chi_{(o)}^{(\alpha)}(q)} - (J_{\alpha\beta}^2 - U_\alpha U_\beta)\left[\chi_{(o)}^{(\beta)}(q) - \frac{\chi_{mix}^{\alpha\beta}(q)\ \chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\alpha)}(q)}\right] + J_{\alpha\beta}\frac{\chi_{mix}^{\alpha\beta}(q) + \chi_{mix}^{\beta\alpha}(q)}{\chi_{(o)}^{(\alpha)}(q)} \tag{30-b}$$

which is formally identical to the effective exchange obtained for actinide metals in [4].

VII. DETERMINATION OF THE EFFECTIVE d-EXCHANGE COUPLING TO THE LOCAL SPIN

Using equations (30) we rewrite (29) as:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle\sigma \left\{ \frac{1+U_{eff}^{(\beta)}(q)\ \chi_{(o)}^{(\beta)}(q)}{1+J_{eff}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)}\ x^{\alpha\beta}(q) - \frac{J_{\alpha\beta}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)}{1+J_{eff}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)}\ x^{\beta\alpha}(q) \right\} \quad (31)$$

Now using definition (26) one gets for the first term of (31):

$$\frac{1+U_{eff}^{(\beta)}(q)\chi_{(o)}^{(\beta)}(q)}{1+J_{eff}^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q)}\ x^{\alpha\beta}(q) = \sum_k \left\{ J_{(\alpha)}^{(d)}(k+q,k) + J^{(s)}(k+q,k)V_{ds}^{(\alpha)}(k+q)V_{sd}^{(\alpha)}(k)\frac{\chi_{(1)}^{\alpha\beta}(k,q)}{\chi_{(o)}^{(\alpha)}(k,q)} \right.$$

$$\left. + J_{(\beta)}^{(d)}(k+q,k)V_{ds}^{(\alpha)}(k+q)V_{sd}^{(\alpha)}(k)V_{sd}^{(\beta)}(k+q)V_{ds}^{(\beta)}(k)\frac{\chi_{(o)}(k,q)}{\chi_{(o)}^{(\alpha)}(k,q)} \right\} \frac{(1+U_{eff}^{(\beta)}(q)\ \chi_{(o)}^{(\beta)}(q))\chi_{(o)}^{(\alpha)}(k,q)}{1+J_{eff}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)} \quad (32)$$

The second term of (31) becomes:

$$\frac{J_{\alpha\beta}^{(\alpha)}(q)\ \chi_{(o)}^{(\alpha)}(q)}{1+J_{eff}^{(\alpha)}\ \chi_{(o)}^{(\alpha)}(q)}\ x^{\beta\alpha}(q) = \sum_k \left\{ J_{(\beta)}^{(d)}(k+q,k) + J^{(s)}(k+q,k)V_{ds}^{(\beta)}(k+q)\ V_{sd}^{(\beta)}(k)\frac{\chi_{(1)}^{\beta\alpha}(k,q)}{\chi_{(o)}^{(\beta)}(k,q)} \right.$$

$$\left. + J_{(\alpha)}^{(d)}(k+q,k)V_{ds}^{(\beta)}(k+q)V_{sd}^{(\beta)}(k)V_{sd}^{(\alpha)}(k+q)V_{ds}^{(\alpha)}(k)\frac{\chi_{(o)}(k,q)}{\chi_{(o)}^{(\beta)}(k,q)} \right\} \frac{J^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q)\chi_{(o)}^{(\beta)}(k,q)}{1+J_{eff}^{(\alpha)}(q)\chi_{(o)}^{(\alpha)}(q)} \quad (33)$$

Now we assume that the impurity exchange satisfies:

$$J_{(\alpha)}^{(d)}(k+q,k) = J_{(\beta)}^{(d)}(k+q,k) = J^{(d)}(k+q,k)$$

Introduce the definitions:

$$\tilde{J}^{(d)}_{(\alpha)}(k+q,k)=J^{(d)}(k+q,k)\left\{1+V^{(\alpha)}_{ds}(k+q)\ V^{(\alpha)}_{sd}(k)\ V^{(\beta)}_{sd}(k+q)\ V^{(\beta)}_{ds}(k)\ \frac{\chi_{(o)}(k,q)}{\chi^{(\alpha)}_{(o)}(k,q)}\right\} \tag{34-a}$$

$$\tilde{J}^{(d)}_{(\beta)}(k+q,k)=J^{(d)}(k+q,k)\left\{1+V^{(\beta)}_{ds}(k+q)V^{(\beta)}_{sd}(k)V^{(\alpha)}_{sd}(k+q)V^{(\alpha)}_{ds}(k)\ \frac{\chi_{(o)}(k,q)}{\chi^{(\beta)}_{(o)}(k,q)}\right\} \tag{34-b}$$

$$\frac{1+U^{(\beta)}_{eff}\ \chi^{(\beta)}_{(o)}(q)}{1+J^{(\alpha)}_{eff}\ \chi^{(\alpha)}_{(o)}(q)}\ \chi^{\alpha\beta}(q) = \sum_k\left\{\tilde{J}^{(d)}_{(\alpha)}(k+q,k)\ -\right.$$

$$\left. -\ J^{(s)}(k+q,k)V^{(\alpha)}_{ds}(k+q)\ V^{(\alpha)}_{sd}(k)\ \frac{\chi^{\alpha\beta}_{(1)}(k,q)}{\chi^{(\alpha)}_{(o)}(k,q)}\right\}\ \frac{(1+U^{(\beta)}_{eff}(q)\ \chi^{(\beta)}_{(o)}(q)\chi^{(\alpha)}_{(o)}(k,q)}{1\ +\ J^{(\alpha)}_{eff}(q)\quad {}^{(\alpha)}_{(o)}(q)} \tag{35-a}$$

and

$$\frac{J^{(\alpha)}_{\alpha\beta}(q)\ \chi^{(\alpha)}_{(o)}(q)}{1+J^{(\alpha)}_{eff}(q)\chi^{(\alpha)}_{(o)}(q)}\ \chi^{\beta\alpha}(q)\ =\ \sum_k\left\{\tilde{J}^{(d)}_{(\beta)}(k+q,k)\ +\right.$$

$$\left. +\ J^{(s)}(k+q,k)V^{(\beta)}_{ds}(k+q)V^{(\beta)}_{sd}(k)\ \frac{\chi^{\beta\alpha}_{(1)}(k,q)}{\chi^{(\beta)}_{(o)}(k,q)}\right\}\ \frac{J^{(\alpha)}_{\alpha\beta}(q)\chi^{(\alpha)}_{(o)}(q)\chi^{(\beta)}_{(o)}(k,q)}{1+J^{(\alpha)}_{eff}(q)\chi^{(\alpha)}_{(o)}(q)} \tag{35-b}$$

Now in order to get a result easily comparable to that obtained without degeneracy introduce the effective couplings:

$$\tilde{\tilde{J}}^{(d)}_{(\alpha)}(k+q,k)=\tilde{J}^{(d)}_{(\alpha)}(k+q,k)\left\{1\ +\ \frac{J^{(s)}(k+q,k)}{\tilde{J}^{(d)}_{(\alpha)}(k+q,k)}\ V^{(\alpha)}_{ds}(k+q)V^{(\alpha)}_{sd}(k)\ \frac{\chi^{\alpha\beta}_{(1)}(k,q)}{\chi^{(\alpha)}_{(o)}(k,q)}\right\}$$

$$\tilde{\tilde{J}}^{(d)}_{(\beta)}(k+q,k)=\tilde{J}^{(d)}_{(\beta)}(k+q,k)\left\{1\ +\ \frac{J^{(d)}(k+q,k)}{\tilde{J}^{(d)}_{(\beta)}(k+q,k)}\ V^{(\beta)}_{ds}(k+q)V^{(\beta)}_{sd}(k)\ \frac{\chi^{\beta\alpha}_{(1)}(k,q)}{\chi^{(\beta)}_{(o)}(k,q)}\right\} \tag{36}$$

Using these results and (31) one gets:

$$\Delta n_q^{\sigma(\alpha)} = \langle S^z\rangle \sigma \sum_k \left\{ \tilde{\tilde{J}}^{(d)}_{(\alpha)}(k+q,k) \frac{(1+U^{(\beta)}_{eff}(q)\ \chi^{(\beta)}_{(o)}(q))\ \chi^{(\alpha)}_{(o)}(k,q)}{1+J^{(\alpha)}_{eff}(q)\ \ \chi^{(\alpha)}_{(o)}\ (q)} - \tilde{\tilde{J}}^{(d)}_{(\beta)}(k+q,k) \frac{J^{(\alpha)}_{\alpha\beta}(q)\ \chi^{(\alpha)}_{(o)}(q)\ \chi^{(\beta)}_{(o)}(k,q)}{1+J^{(\alpha)}_{eff}(q)\ \ \chi^{(\alpha)}_{(o)}\ (q)} \right\} \tag{37}$$

Finally introducing:

$$v^{(d)}_{(\alpha)}(k,q) = \frac{\tilde{\tilde{J}}^{(d)}_{(\beta)}(k+q,k)}{\tilde{\tilde{J}}^{(d)}_{(\alpha)}(k+q,k)} \tag{38-a}$$

one obtains the final result:

$$m_q^{(\alpha)} = 2\ \langle S^z\rangle \sum_k \tilde{\tilde{J}}^{(d)}_{(\alpha)}(k+q,k)\ \chi^{(\alpha)}_{(J)}(k,q) \tag{38-b}$$

where:

$$\chi^{(\alpha)}_{(J)}(k,q) = \frac{(1+U^{(\beta)}_{eff}(q)\chi^{(\beta)}_{(o)}(q))\chi^{(\alpha)}_{(o)}(k,q) - v^{(d)}_{(\alpha)}(k,q)J^{(\alpha)}_{\alpha\beta}(q)\chi^{(\alpha)}_{(o)}(q)\chi^{(\beta)}_{(o)}(k,q)}{1+J^{(\alpha)}_{eff}(q)\ \chi^{(\alpha)}_{(o)}(q)} \tag{38-c}$$

Quite similar expressions hold for the effective β exchange coupling.

VIII. DETERMINATION OF THE s-MAGNETIZATION

i) Determination of the propagator

From equations (6) one gets:

$$(\omega-\varepsilon_k^{(s)})G^{ss(1)}_{kk'}(\omega) = V^{(\alpha)}_{sd}(k)G^{\alpha s(1)}_{kk'}(\omega)+V^{(\beta)}_{sd}(k)G^{\beta s(1)}_{kk'}(\omega)+J^{(s)}(k,k')\langle S^z\rangle\sigma g^{ss}_{k'}(\omega) \tag{39-a}$$

$$(\omega-E_k^{(\alpha)})G_{kk'}^{\alpha s(1)}(\omega) = V_{ds}^{(\alpha)}(k)\ G_{kk'}^{ss(1)}(\omega) + J_{(\alpha)}^{(d)}(k,k')\ \langle S^z\rangle\ \sigma\ g_{k'}^{\alpha s}(\omega) +$$

$$+ \left\{U_\alpha \Delta n_{kk'}^{-\sigma(\beta)} + U_{\alpha\beta}\Delta n_{kk'}^{-\sigma(\alpha)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n_{kk'}^{\sigma(\alpha)}\right\} g_{k'}^{\beta s}(\omega) \qquad (39\text{-b})$$

$$(\omega-E_k^{(\beta)})G_{kk'}^{\beta s(1)}(\omega)=V_{ds}^{(\beta)}(k)G_{kk'}^{ss(1)}(\omega) + J_{(\beta)}^{(\alpha)}(k,k')\ \langle S^z\rangle\ \sigma\ g_{k'}^{\beta s}(\omega) +$$

$$+\left\{U_\beta\ \Delta n_{kk'}^{-\sigma(\beta)} + U_{\alpha\beta}\ \Delta n_{kk'}^{-\sigma(\alpha)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n_{kk'}^{\sigma(\alpha)}\right\} g_{k'}^{\beta s}(\omega) \qquad (39\text{-c})$$

Substituting equations (39-c) and (39-b) in equation (39-a) one gets:

$$\left\{\omega-\varepsilon_k^{(s)} - \frac{|V_{sd}^{(\alpha)}(k)|^2}{\omega-E_k^{(\alpha)}} - \frac{|V_{sd}^{(\beta)}(k)|^2}{\omega-E_k^{(\beta)}}\right\} G_{kk'}^{ss(1)}(\omega) =$$

$$= \langle S^z\rangle\sigma\left\{J^{(s)}(k,k')g_{k'}^{ss}(\omega) + \frac{V_{sd}^{(\alpha)}(k)}{\omega-E_k^{(\alpha)}}\ J_{(\alpha)}^{(d)}(k,k')g_{k'}^{\alpha s}(\omega) + \frac{V_{sd}^{(\beta)}(k)}{\omega-E_k^{(\beta)}}\ J_{(\beta)}^{(d)}(k,k')g_{k'}^{\beta s}(\omega)\right\} +$$

$$+ \frac{V_{sd}^{(\alpha)}(k)}{\omega-E_k^{(\alpha)}} \left\{U_\alpha\ \Delta n_{kk'}^{-\sigma(\alpha)} + U_{\alpha\beta}\ \Delta n_{kk'}^{-\sigma(\beta)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta\ n_{kk'}^{\sigma(\beta)}\right\} g_{k'}^{\alpha s}\ (\omega)$$

$$+ \frac{V_{sd}^{(\beta)}(k)}{\omega-E_k^{(\beta)}} \left\{U_\beta\ \Delta n_{kk'}^{-\alpha(\beta)} + U_{\alpha\beta}\ \Delta n_{kk'}^{-\sigma(\alpha)} + (U_{\alpha\beta}-J_{\alpha\beta})\Delta n_{kk'}^{\sigma(\alpha)}\right\}\ g_{k'}^{\beta s}(\omega) \qquad (40)$$

Now using (12), (13-a) and (13-b) one finally obtains:

$$G^{ss(1)}_{k+q,k}(\omega) = \frac{1}{2\pi} \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)} J^{(s)}(k+q,k)\langle S^z\rangle \sigma \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)} V^{(\alpha)}_{sd}(k+q) \frac{1}{\omega-E^{(\alpha)}_{k+q}} \left\{ J^{(d)}_{(\alpha)}(k+q,k)\langle S^z\rangle\sigma + U_\alpha \Delta n^{-\sigma(\alpha)}_q + U_{\alpha\beta}\, \Delta n^{-\sigma(\beta)}_q + \right.$$

$$\left. + (U_{\alpha\beta} - J_{\alpha\beta})\Delta n^{\sigma(\beta)}_q \right\} \frac{1}{\omega-E^{(\alpha)}_k} V^{(\alpha)}_{ds}(k) \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)} +$$

$$+ \frac{1}{2\pi} \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)} V^{(\beta)}_{sd}(k+q) \frac{1}{\omega-E^{(\beta)}_{k+q}} \left\{ J^{(d)}_{(\beta)}(k+q,k)\langle S^z\rangle\sigma + U_\beta \Delta n^{-\sigma(\alpha)}_q + U_{\alpha\beta}\, \Delta n^{-\sigma(\alpha)}_q + \right.$$

$$\left. + (U_{\alpha\beta} - J_{\alpha\beta})\Delta\, n^{\sigma(\alpha)}_q \right\} \frac{1}{\omega-E^{(\beta)}_k} V^{(\beta)}_{ds} \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)} \qquad (41)$$

In equation (41) the first term describes scattering of hybridized s-electrons by the impurity spin. The second term show how an s-electron is admixed into the α band and then scattered by the impurity and by the fluctuations in occupation numbers last term describes the correspondent process involving the β band.

ii) Self-consistent determination of the s-magnetization

Introduce the following susceptibilities:

$$\chi^{(s)}_{(o)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)} \frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)} \right\} \qquad (42\text{-a})$$

$$\chi^{s\alpha}_{(1)}(k,q)=\frac{1}{2\pi}F_{\omega}\left\{\frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)}\;\frac{1}{\omega-E^{(\alpha)}_{k+q}}\;\frac{1}{\omega-E^{(\alpha)}_{k}}\;\frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)}\right\};$$

$$\chi^{s\alpha}_{(1)}(q)=\sum_k \chi^{s\alpha}_{(1)}(k,q) \qquad (42\text{-b})$$

$$\chi^{s\beta}_{(2)}(k,q)=\frac{1}{2\pi}F_{\omega}\left\{\frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k+q}(\omega)}\;\frac{1}{\omega-E^{(\beta)}_{k+q}}\;\frac{1}{\omega-E^{(\beta)}_{k}}\;\frac{1}{\omega-\tilde{\varepsilon}^{(s)}_{k}(\omega)}\right\};$$

$$\chi^{s\beta}_{(2)}(q)=\sum_k \chi^{s\beta}_{(2)}(k,q) \qquad (42\text{-c})$$

Using the definitions and equation (41) one gets:

$$\Delta n^{\sigma(s)}_{q}=\langle S^{z}\rangle\sigma x^{s}(q)-\left\{U_{\alpha}\,\Delta n^{\sigma(\alpha)}_{q}+J_{\alpha\beta}\,\Delta\, n^{\sigma(\beta)}_{q}\right\}x^{s\alpha}(q)$$
$$\left\{U_{\beta}\,\Delta n^{\sigma(\beta)}_{q}+J_{\alpha\beta}\,\Delta\, n^{\sigma(\alpha)}_{q}\right\}x^{s\beta}(q) \qquad (43\text{-a})$$

Where we have defined:

$$x^{s}(q)=\sum_k\left\{J^{(s)}(k+q,k)\chi^{(s)}_{(o)}(k,q)+V^{(\alpha)}_{sd}(k+q)V^{(\alpha)}_{ds}(k)J^{(d)}_{(\alpha)}(k+q,k)\chi^{s\alpha}_{(1)}(k,q)\right.$$
$$\left.+\,V^{(\beta)}_{sd}(k+q)\;V^{(\beta)}_{ds}(k)J^{(d)}_{(\beta)}(k+q,k)\chi^{s\beta}_{(2)}(k,q)\right\} \qquad (43\text{-b})$$

$$x^{s\alpha}(q)=\sum_k\;V^{(\alpha)}_{sd}(k+q)\;V^{(\alpha)}_{ds}(k)\;\chi^{s\alpha}_{(1)}(k,q)$$

$$x^{s\beta}(q)=\sum_k\;V^{(\beta)}_{sd}(k+q)\;V^{(\beta)}_{ds}(k)\;\chi^{s\beta}_{(2)}(k,q) \qquad (43\text{-c})$$

An alternative form of (43-a) more useful for defining effective couplings is:

$$\Delta n_q^{\sigma(s)} = \langle S^z \rangle \sigma\, x^s(q) - \left\{ U_\alpha\, x^{s\alpha}(q) + J_{\alpha\beta}\, x^{s\beta}(q) \right\} \Delta n_q^{\sigma(\alpha)} - \left\{ U_\beta\, x^{s\beta}(q) + J_{\alpha\beta}\, x^{s\alpha}(q) \right\} \Delta n_q^{\sigma(\beta)} \quad (44)$$

iii) Determination of the effective coupling

Using the result (38-b) one gets for the magnetization:

$$m_q^{(s)} = 2\langle S^z \rangle \left\{ x^{(s)}(q) - \sum_{k'} \tilde{\tilde{J}}{}^{(d)}_{(\alpha)}(k'+q,k') \left[U_\alpha\, x^{s\alpha}(q) + J_{\alpha\beta}\, x^{s\beta}(q) \right] \chi^{(\alpha)}_{(J)}(k',q) - \sum_{k'} \tilde{\tilde{J}}{}^{(d)}_{(\beta)}(k'+q,k') \left[U_\beta\, x^{s\beta}(q) + J_{\alpha\beta}\, x^{s\alpha}(q) \right] \chi^{(\beta)}_{(J)}(k',q) \right\} \quad (45)$$

Now we rewrite (45) collecting terms proportional to $x^{s\alpha}$ and $x^{s\beta}$; taking the explicit form of $x^{(s)}(q)$

One gets:

$$m_q^{(s)} = 2\langle S^z \rangle \sum_k \left\{ J^{(s)}(k+q,k)\chi^{(s)}_{(o)}(k,q) + J^{(d)}(k+q,k) V^{(\alpha)}_{sd}(k+q) V^{(\alpha)}_{ds}(k) \chi^{s\alpha}_{(1)}(k,q) + J^{(d)}(k+q,k) V^{(\beta)}_{sd}(k+q) V^{(\beta)}_{ds}(k) \chi^{s\beta}_{(2)}(k,q) - x_1(q) V^{(\alpha)}_{sd}(k+q) V^{(\alpha)}_{ds}(k)\, \chi^{s\alpha}_{(1)}(k,q) - x_2(q)\, V^{(\beta)}_{sd}(k+q)\, V^{(\beta)}_{ds}(k)\, \chi^{s\beta}_{(2)}(k,q) \right\} \quad (46\text{-a})$$

Where we have defined:

$$x_1(q) = \sum_{k'} \left\{ \tilde{\tilde{J}}{}^{(d)}_{(\alpha)}(k'+q,k')\, U_\alpha\, \chi^{(\alpha)}_{(J)}(k',q) + \tilde{\tilde{J}}{}^{(d)}_{(\beta)}(k'+q,k') J_{\alpha\beta}\, \chi^{(\beta)}_{(J)}(k',q) \right\} \quad (46\text{-b})$$

$$x_2(q) = \sum_{k'} \left\{ \tilde{\tilde{J}}{}^{(d)}_{(\beta)}(k'+q,k') U_\beta\, \chi^{(\beta)}_{(J)}(k',q) + \tilde{\tilde{J}}{}^{(d)}_{(\alpha)}(k'+q,k') J_{\alpha\beta}\, \chi^{(\alpha)}_{(J)}(k',q) \right\} \quad (46\text{-c})$$

Equations (46) enable us to define an effective exchange coupling of s-states; define:

$$\bar{J}^{(d)}_{(\alpha)}(k+q,k) = J^{(d)}(k+q,k)\left\{1-\sum_{k'}\left[\frac{\tilde{\tilde{J}}^{(d)}_{(\alpha)}(k'+q,k')}{J^{(d)}(k+q,k)} U_\alpha \chi^{(\alpha)}_{(J)}(k',q) + \frac{\tilde{\tilde{J}}^{(d)}_{(\beta)}(k'+q,k')}{J^{(d)}(k+q,k)} J_{\alpha\beta} \chi^{(\beta)}_{(J)}(k',q)\right]\right\} \qquad (47\text{-a})$$

$$\bar{J}^{(d)}_{(\beta)}(k+q,k) = J^{(d)}(k+q,k)\left\{1-\sum_{k'}\left[\frac{\tilde{\tilde{J}}^{(d)}_{(\beta)}(k'+q,k')}{J^{(d)}(k+q,k)} U_\beta \chi^{(\beta)}_{(J)}(k',q) + \frac{\tilde{\tilde{J}}^{(d)}_{(\alpha)}(k'+q,k')}{J^{(d)}(k+q,k)} J_{\alpha\beta} \chi^{(\alpha)}_{(J)}(k',q)\right]\right\} \qquad (47\text{-b})$$

The s-magnetization becomes:

$$m^{(s)}_q = 2\langle S^z\rangle \sum_k \left\{J^{(s)}(k+q,k)\chi^{(s)}_{(o)}(k,q) + \bar{J}^{(d)}_{(\alpha)}(k+q,k)V^{(\alpha)}_{sd}(k+q)V^{(\alpha)}_{ds}(k)\chi^{s\alpha}_{(1)}(k,q) + \bar{J}^{(d)}_{(\beta)}(k+q,k)\, V^{(\beta)}_{sd}(k+q)\, V^{(\beta)}_{ds}(k)\, \chi^{s\beta}_{(2)}(k,q)\right\} \qquad (48)$$

Then the natural definition of an effective s exchange is:

$$J^{(s)}_{eff}(k+q,k)=J^{(s)}(k+q,k)\left\{1+\frac{\bar{J}^{(d)}_{(\alpha)}(k+q,k)}{J^{(s)}(k+q,k)} V^{(\alpha)}_{sd}(k+q)V^{(\alpha)}_{ds}(k)\frac{\chi^{s\alpha}_{(1)}(k,q)}{\chi^{(s)}_{(o)}(k,q)} + \frac{\bar{J}^{(d)}_{(\beta)}(k+q,k)}{J^{(s)}(k+q,k)} V^{(\beta)}_{sd}(k+q)V^{(\beta)}_{ds}(k)\frac{\chi^{s\beta}_{(1)}(k,q)}{\chi^{(s)}_{(o)}(k,q)}\right\} \qquad (49)$$

So the final result for the s-magnetization is:

$$m_q^{(s)} = 2 \langle S^z \rangle \sum_k J_{eff}^{(s)}(k+q,k)\, \chi_{(o)}^{(s)}(k,q) \tag{50}$$

IX. LIMITING CASE AND APPROXIMATE RESULTS

i) Non degenerate case

In this paragraph we firstly recover the case of a non-degenerate d-band hybridized with an s band [1]. To that we switch-off the mixing of the s-band to the β band, and also the exchange coupling; this procedure isolates the β band from the rest. Then we put:

$$V_{sd}^{(\beta)}(k) = 0; \qquad J_{\alpha\beta} = 0 \tag{51}$$

Equation (51) implies that $\tilde{J}_{(\alpha)}^{(d)}(k+q,k) = \tilde{J}_{(\beta)}^{(d)}(k+q,k) = J^{(d)}(k+q,k)$; consequently the effective exchange (36) reduce to:

$$\tilde{\tilde{J}}_{(\alpha)}^{(d)}(k+q,k) = J^{(d)}(k+q,k)\left\{1 + \frac{J^{(s)}(k+q,k)}{J^{(d)}(k+q,k)}\, V_{ds}^{(\alpha)}(k+q)\, V_{sd}^{(\alpha)}(k)\, \frac{\overline{\chi}_{(o)}(k,q)}{\chi_{(o)}^{(\alpha)}(k,q)}\right\} \tag{52-a}$$

$$\tilde{\tilde{J}}_{(\beta)}^{(d)}(k+q,k) = J^{(d)}(k+q,k) \tag{52-b}$$

Where $\overline{\chi}_{(o)}(k,q)$ can be seen from (24-b) to be:

$$\overline{\chi}_{(o)}(k,q) = \frac{1}{2\pi} F_\omega \left\{ \frac{1}{\omega-\tilde{E}_{k+q}^{(\alpha)}(\omega)}\; \frac{1}{\omega-\varepsilon_{k+q}^{(s)}}\; \frac{1}{\omega-\varepsilon_k^{(s)}}\; \frac{1}{\omega-\tilde{E}_k^{(\alpha)}(\omega)} \right\} \tag{52-c}$$

The energies $\tilde{\varepsilon}^{(\alpha)}(\omega)$ being defined now by $\tilde{\varepsilon}_k^{(\alpha)}(\omega) = \varepsilon_{k'}^{(\alpha)} +$ $+ \; V_{sd}^{(\alpha)}(k)^2/(\omega - E_k^{(s)})$. Consequently from (52-a) and (52-c) one sees that $\tilde{\tilde{J}}_{(\alpha)}^{(d)}(k+q,k)$ reduces to the value previously obtained [1]. Next one has from (25-b) that $\chi_{mix}^{\beta\alpha}(q) = 0$ in this limit, so from definitions (28) one gets the result:

$$J_{\alpha\beta}^{(\alpha)} \; \chi_{(o)}^{(\alpha)} = J_{\alpha\beta}^{(\beta)} \; \chi_{(o)}^{(\beta)} = 0$$

and

$$U_{eff}^{(\alpha)} = U_\alpha \; ; \qquad U_{eff}^{(\beta)} = U_\beta \tag{53}$$

The equation (38-c) reduces to:

$$\chi_J^{(\alpha)}(k,q) = \frac{\chi_{(o)}^{(\alpha)}(k,q)}{1 + U_\alpha \, \chi_{(o)}^{(\alpha)}(q)} \tag{54}$$

Equations (54), (52-a) and (38-b) show that the magnetization reduces exactly to the previous result [1] as expected. Now we briefly discuss the behaviour of the s-magnetization. From (49) one gets in this limit:

$$J_{eff}^{(s)}(k+q,k) = J^{(s)}(k+q,k) \left\{ 1 + \frac{\bar{J}_{(\alpha)}^{(d)}(k+q,k)}{J^{(s)}(k+q,k)} \, V_{sd}^{(\alpha)}(k+q) V_{ds}^{(\alpha)}(k) \, \frac{\bar{\chi}_{(o)}(k,q)}{\chi_{(o)}^{(s)}(k,q)} \right\} \tag{55-a}$$

where now $\bar{J}_{(\alpha)}^{(d)}(k+q,k)$ reads:

$$\bar{J}_{(\alpha)}^{(d)}(k+q,k) = J^{(d)}(k+q,k) \left\{ 1 - U_\alpha \sum_{k'} \left[\frac{J^{(d)}(k'+q,k')}{J^{(d)}(k+q,k)} \left(1 + \frac{J^{(s)}(k'+q,k')}{J^{(d)}(k'+q,k')} \, V_{ds}^{(\alpha)}(k'+q) V_{sd}^{(\alpha)}(k') \, \frac{\bar{\chi}_{(o)}(k',q)}{\chi_{(o)}^{(d)}(k',q)} \right) \right] \chi_{(J)}^{(\alpha)}(k',q) \right\} \tag{55-b}$$

These are exactly the results obtained in the non-degenerate case [1] .

ii) Identical sub-bands

We now considers two identical sub-bands, one gets the following results:

$$\chi^{(\alpha)}_{(o)}(k,q) = \chi^{(\beta)}_{(o)}(k,q) = \chi^{(d)}_{(o)}(k,q)$$

$$\chi^{\alpha\beta}_{(1)}(k,q) = \chi^{\beta\alpha}_{(1)}(k,q) = \chi_{(1)}(k,q) \qquad (56)$$

$$U_\alpha = U_\beta = U \qquad \text{and} \qquad V^{(\alpha)}_{sd}(k) = V^{(\beta)}_{sd}(k)$$

The results (55) imply that: $\tilde{\tilde{J}}_{(\alpha)}{}^{(d)}(k+q,k) = J_{(\beta)}{}^{(d)}(k+q,k)$ and consequently $v^{(d)}_{(\alpha)}(k,q) = 1$.

The susceptibility $\chi^{(\alpha)}_{(J)} = \chi^{(\beta)}_{(J)}$ assume a particularly interesting form, namely:

$$\chi_{(J)}(k,q) = \frac{\chi^{(d)}_{(o)}(k,q)}{1+(U^{(d)}_{eff}(q) + \bar{J}_{\alpha\beta}(q))\chi^{(d)}_{(o)}(q)} \qquad (57\text{-a})$$

where the effective interactions are defined by:

$$U^{(d)}_{eff}(q) = U\left\{1 + \frac{J_{\alpha\beta}}{U}\,\frac{\chi_{mix}(q)}{\chi^{(d)}_{(o)}(q)}\right\} \qquad (57\text{-b})$$

$$\bar{J}_{\alpha\beta}(q) = J_{\alpha\beta}\left\{1 + \frac{U}{J_{\alpha\beta}}\,\frac{\chi_{mix}(q)}{\chi^{(d)}_{(o)}(q)}\right\}$$

As for the s-electrons are concerned, since $\bar{J}^{(d)}_{(\alpha)} = \bar{J}^{(d)}_{(\beta)}$ the effective exchange is given by:

$$J_{eff}^{(s)}(k+q,k) = J^{(s)}(k+q,k) \left\{ 1 + 2 \frac{\bar{J}^{(d)}(k+q,k)}{J^{(s)}(k+q,k)} V_{sd}(k+q) V_{ds}(k) \frac{\chi_{(1)}^{s\alpha}(k,q)}{\chi_{(o)}^{(s)}(k,q)} \right\} \quad (58)$$

CONCLUSIONS AND DISCUSSION

In the above paragraphs explicit expressions were obtained for the induced s and d polarizations in terms of the s-d corrected susceptibilities and effective exchanges. The results are clear generalizations of those obtained for the non-degenerate d-band. Again one expects greater corrections for the s effective exchange than for the correspondent to the d-one.

In order to perform numerical calculations, explicit expressions for the susceptibilities are given in the appendix. One needs to adopt explicit dispersion relations for the s and the two d-sub-bands, and also the k-dependent V_{sd} mixing matrix elements.

A simplifying approximation consists, as discussed in the text, to assume identical sub-bands. Finally it should be noted that similar results can be obtained to an external q-dependent magnetic field, and consequently to obtain the criterion of magnetism for s-d hybridized bands.

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APPENDIX I

EXPLICIT EXPRESSIONS FOR THE SUSCEPTIBILITIES

We firstly derive our expression for $\chi_{(o)}^{(\lambda)}(k,q)$ defined by equation (24-a). To do that we firstly write:

$$\frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} = \cfrac{1}{\omega-E_k^{(\lambda)} + \cfrac{|V_{sd}^{(\lambda)}(k)|^2}{\omega-\varepsilon_k^{(s)} - \cfrac{|V_{sd}^{(\delta)}(k)|^2}{\omega-E_k^{(s)}}}}$$

$$= \frac{(\omega-\varepsilon_k^{(s)})(\omega-E_k^{(\delta)}) - \left|V_{sd}^{(\delta)}(k)\right|^2}{(\omega-E_k^{(\lambda)})(\omega-E_k^{(\delta)})(\omega-\varepsilon_k^{(s)})-|V_{sd}^{(\lambda)}(k)|^2(\omega-E_k^{(\delta)})-|V_{sd}^{(\delta)}(k)|^2(\omega-E_k^{(\lambda)})} \; ; \quad \lambda\neq\delta \quad \text{(A-1)}$$

Introduce now the energies $E_k^{(1)}$, $E_k^{(2)}$, $E_k^{(3)}$ which are the roots of the third degree equation:

$$(\omega-E_k^{(\lambda)})(\omega-E_k^{(\delta)})(\omega-\varepsilon_k^{(s)})-\left|V_{sd}^{(\lambda)}(k)\right|^2(\omega-E_k^{(\delta)})-\left|V_{sd}^{(\delta)}(k)\right|^2(\omega-E_k^{(\lambda)}) = 0$$

Equation (A-1) can be rewritten as:

$$\frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} \quad \frac{(\omega-E_k^{(s)})(\omega-E_k^{(\delta)})-\left|V_{sd}^{(\delta)}(k)\right|^2}{(\omega-E_k^{(1)})(\omega-E_k^{(2)})(\omega-E_k^{(3)})} \qquad \text{(A-2)}$$

Now introduce the function:

$$g_\lambda(\omega, k) = (\omega-\varepsilon_k^{(s)})(\omega-E_k^{(\delta)}) - \left|V_{sd}^{(\delta)}(k)\right|^2, \quad \lambda\neq\delta \qquad \text{(A-3)}$$

and rewrite (A-2) in terms of simple fractions; one gets:

$$\frac{1}{\omega-\tilde{E}_k^{(\lambda)}(\omega)} = \sum_{\alpha,\beta,\gamma=1}^{3} \varepsilon_{\alpha\beta\gamma} \frac{g_\lambda(\omega,k)}{E_k^{(\alpha)}-E_k^{(\beta)}} \frac{1}{E_k^{(\alpha)}-E_k^{(\gamma)}} \frac{1}{\omega-E_k^{(\alpha)}} \tag{A-4}$$

where the symbol $\varepsilon_{\alpha\beta\gamma}$ is defined as:

$$\varepsilon_{\alpha\beta\gamma} = \begin{cases} 1, \text{ if } \alpha\neq\beta \ ; \ \alpha\neq\gamma \ ; \ \beta\neq\gamma \\ 0 \ \text{ otherwise} \end{cases} \tag{A-5}$$

Now using (A-4) and the definition (24-a) one gets for the susceptibility:

$$\chi_{(o)}^{(\lambda)}(k,q) = \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} \varepsilon_{\alpha\beta\gamma}\, \varepsilon_{\alpha'\beta'\gamma'}$$

$$\frac{g_\lambda(E_{k+q}^{(\alpha)},k+q)\ g_\lambda(E_{k+q}^{(\alpha)},k)\ f(E_{k+q}^{(\alpha)})-g_\lambda(E_k^{(\alpha)},k+q)\ g_\lambda(E_k^{(\alpha')},k)\ f(E_k^{(\alpha')})}{(E_{k+q}^{(\alpha)}-E_{k+q}^{(\beta)})(E_{k+q}^{(\alpha)}-E_{k+q}^{(\gamma)})(E_k^{(\alpha')}-E_k^{(\beta')})(E_k^{(\alpha')}-E_k^{(\gamma')})(E_{k+q}^{(\alpha)}-E_k^{(\alpha')})} \tag{A-6}$$

Next we calculate the susceptibility $\chi_{(1)}^{(\lambda\delta)}(k,q)$, to do that we firstly evaluate:

$$\frac{1}{\left[\omega-\tilde{E}_k^{(\lambda)}(\omega)\right]\left[\omega-\tilde{\varepsilon}_k^{(s,\delta)}(\omega)\right]} =$$

$$= \frac{\omega-E_k^{(\delta)}}{(\omega-E_k^{(\lambda)})(\omega-E_k^{(\delta)})(\omega-\varepsilon_k^{(s)})-|V_{sd}^{(\lambda)}(k)|^2(\omega-E_k^{(\delta)})-|V_{sd}^{(\delta)}(k)|^2(\omega-E_k^{(\lambda)})} =$$

$$= \frac{\omega - E_k^{(\delta)}}{(\omega - E_k^{(1)})(\omega - E_k^{(2)})(\omega - E_k^{(3)})} \tag{A-7}$$

Using (A-7) and definition (A-5) one gets:

$$\chi_{(1)}^{(\lambda\delta)}(k,q) = \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} \varepsilon_{\alpha\beta\gamma}\, \varepsilon_{\alpha'\beta'\gamma'}$$

$$\frac{(E_{k+q}^{(\alpha)}-E_{k+q}^{(\delta)})(E_{k+q}^{(\alpha)}-E_k^{(s)})\; f(E_{k+q}^{(\alpha)}) - (E_k^{(\alpha')}-E_{k+q}^{(\delta)})(E_k^{(\alpha')}-E_k^{(\delta)})\; f(E_k^{(\alpha')})}{(E_{k+q}^{(\alpha)}-E_{k+q}^{(\beta)})(E_{k+q}^{(\alpha)}-E_{k+q}^{(\gamma)})(E_k^{(\alpha')}-E_k^{(\beta')})(E_k^{(\beta')}-E_k^{(\gamma')})(E_{k+q}^{(\alpha)}-E_k^{(\alpha')})} \tag{A-8}$$

Finally one gets for $\chi_{(2)}^{(\alpha\delta)} = \chi_{(2)}^{(\delta\lambda)}$ the result:

$$\chi_{(1)}^{(\lambda\delta)}(k,q) = \sum_{\substack{\alpha,\beta,\gamma \\ \alpha',\beta',\gamma'}} \varepsilon_{\alpha\beta\gamma}\, \varepsilon_{\alpha'\beta'\gamma'}$$

$$\frac{f(E_{k+q}^{(\alpha)}) - f(E_k^{(\alpha')})}{(E_{k+q}^{(\alpha)}-E_{k+q}^{(\beta)})(E_{k+q}^{(\alpha)}-E_{k+q}^{(\gamma)})(E_k^{(\alpha')}-E_k^{(\beta')})(E_k^{(\alpha')}-E_k^{(\gamma')})(E_{k+q}^{(\alpha)}-E_k^{(\alpha')})} \tag{A-9}$$

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