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by

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EFFECT OF ELECTRON CORRELATION AND s-d HYBRIDIZATION IN THE SPIN POLARIZATION

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I . INTRODUCTION

The problem of calculating the spin polarization associated to a localized spin in a metal has been the subject of much work. In particular the effect of electron correlations in such a problem is a quite interesting subject. If one intends to discuss rare earth systems, where the existence of d-band is now shown through band calculations, such effects should be included. In a previous work[1], correlation effects were introduced in a narrow d-band using Hubbard's picture, taking into account in a self-consistent way the effect of scattering on the correlated electron motion. It is the purpose of this work cf extend this treatment including the broad s-band and the hybridization between s and d-bands. We expect that, even in the simplified model adopted here, the main features of a transition metal host (s and d hybridized bands) are conserved and then a complete calculation of the spin polarizations ρ_s and ρ_d associated to these bands may be performed. We adopt here the treatment of hybridized s and d bands introduced by Kishore and Joshi[2] in discussing the stability of magnetic phases in transition metals. The hybridized s-d bands is then coupled to a localized spin S through exchange couplings J^s and J^d (this is an appropriate description of a localized f state in a transition host or rare earth metal or intermetallic). We recover the main results of reference 1 for the "feed-back" effects, although s-d renormalization is present everywhere, and the enhancement of the spin polarization is still present. In the general discussion we present possible applications of this calculation.

II . FORMULATION OF THE PROBLEM

We start defining the host metal hamiltonian which includes the s and d bands, intra d-band electron correlations and s-d mixing. In the Wannier representation this hamiltonians reads:

$$H_o = \sum_{i,j,\sigma} T^s_{ij} c^+_{i\sigma} c_{j\sigma} + \sum_{i,j,\sigma} T^d_{ij} d^+_{i\sigma} d_{j\sigma} + I \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{i,\sigma} (c^+_{i\sigma} d_{i\sigma} + d^+_{i\sigma} c_{i\sigma}) \qquad (1)$$

In expression (1) $c_{i\sigma}^{+}$ and $d_{i\sigma}^{+}$ create s and d electrons respectively and $n_{i\sigma} = d_{i\sigma}^{+} d_{i\sigma}$; the s-d mixing term is an Anderson type of mixing, the matrix elements of V_{sd} being assumed constant for simplicity sake.

There are now two types of exchange scattering involving s and d electrons, through the couplings of the localized spin $\vec{S}$ to conduction states, respectively J^{s} and J^{d}. In the Wannier representation[1]:

$$H_1 = \sum_{i,j,\sigma} J^{s}(R_i,R_j) S^{z} \sigma c_{i\sigma}^{+} c_{j\sigma} + \sum_{i,j,\sigma} J^{d}(R_i,R_j) S^{z} \sigma d_{i\sigma}^{+} d_{j\sigma} \tag{2}$$

The total hamiltonian is then

$$H = H_o + H_1 \tag{3}$$

One expects physically that in (3) to the separate scatterings (the d electron spin polarization being enhanced by the Coulomb repulsion) one adds the interference processes induced through s-d mixing.

The procedure to calculate the spin polarization is as usual to introduce the d and s propagators. We start discussing the equations of motion for d-propagators.

i) *EQUATIONS OF MOTION FOR d-PROPAGATORS*

Let us define the propagators $G^{11}_{ij} = \langle\langle d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}$, $G^{21}_{ij}(\omega) = \langle\langle n_{i-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}$ and $G^{s1}_{ij}(\omega) = \langle\langle c_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}$. These propagators satisfy the following equations of motion:

$$\omega\, G^{11}_{ij}(\omega) = \frac{1}{2\pi}\,\delta_{ij} + \sum_{\ell} T_{i\ell}{}^{d} G^{11}_{\ell j}(\omega) + I\, G^{21}_{ij}(\omega) + V\, G^{s1}_{ij}(\omega)$$

$$+ \sum_{\ell} J^{d}(r_i, R_{\ell}) S^{z} \sigma G^{11}_{\ell j}(\omega) \qquad \text{(4-a)}$$

$$\omega\, G^{s1}_{ij}(\omega) = \sum_{\ell} T_{i\ell}{}^{s} G^{s1}_{\ell j}(\omega) + V\, G^{11}_{ij}(\omega) + \sum_{\ell} J^{s}(R_i, R_{\ell}) S^{z} \sigma G^{s1}_{\ell j}(\omega) \qquad \text{(4-b)}$$

$$(\omega - I) G^{21}_{ij}(\omega) = \frac{1}{2\pi} \langle n_{i-\sigma}\rangle \delta_{ij} + \sum_{\ell} T_{i\ell}{}^{d} \big(\langle\langle n_{i-\sigma} d_{\ell\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}$$

$$+ \langle\langle d^{+}_{i-\sigma} d_{\ell-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega} - \langle\langle d^{+}_{\ell-\sigma} d_{i-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}\big)$$

$$+ \sum_{\ell} J^{d}(R_i, R_{\ell}) S^{z} \sigma \big(\langle\langle n_{i-\sigma} d_{\ell\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}$$

$$- \langle\langle d^{+}_{i-\sigma} d_{\ell-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega} + \langle\langle d^{+}_{\ell-\sigma} d_{i-\sigma} d_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega}\big)$$

$$+ V\, \langle\langle n_{i-\sigma} c_{i\sigma};\, d^{+}_{j\sigma}\rangle\rangle_{\omega} \qquad \text{(4-c)}$$

Equations (4-a) and (4-b) are exact, and now one must adopt a decoupling scheme in order to deal with equation (4-c). The simplest approach possible is to use Hubbard's decoupling scheme. Following the same lines as in 1 one obtains for the equation (4-c):

$$(\omega-I)G^{21}_{ij}(\omega) = \frac{1}{2\pi} <n_{i-\sigma}>\delta_{ij} + <n_{i-\sigma}>\sum_{\ell} T_{i\ell}{}^{d} G^{11}_{\ell j}(\omega)$$

$$+ J^{d}(R_i,R_i)\left[G^{21}_{ij}(\omega)-<n_{i-\sigma}>G^{11}_{ij}(\omega)\right]S^{z}\sigma$$

$$+ <n_{i-\sigma}> \sum_{\ell} J^{d}(R_i,R_{\ell})S^{z}\sigma G^{11}_{\ell j}(\omega) + V <n_{i-\sigma}>G^{S1}_{ij}(\omega) \qquad (5)$$

Equations (4-a), (4-b) and (5) form a closed set which completely determines the propagator $G^{11}_{ij}(\omega)$

ii) EQUATIONS OF MOTION FOR THE s-PROPAGATORS

We define the following propagators: $G^{SS}_{ij}(\omega) = <<c_{i\sigma}; c^{+}_{j\sigma}>>_{\omega}$, $G^{1S}_{ij}(\omega) = <<d_{i\sigma}; c^{+}_{j\sigma}>>_{\omega}$ and $G^{2S}_{ij}(\omega) = <<n_{i-\sigma}d_{i\sigma}; c^{+}_{j\sigma}>>_{\omega}$. The propagators G^{SS}_{ij} and $G^{1S}_{ij}(\omega)$ satisfy the following exact equations of motion:

$$\omega\, G_{ij}^{ss}(\omega) = \frac{1}{2\pi}\,\delta_{ij} + \sum_\ell T_{i\ell}{}^{s} G_{\ell j}^{ss}(\omega) + V\, G_{ij}^{1s}(\omega)$$

$$+ \sum_\ell J^{s}(R_i,R_\ell) S^{z}\sigma G_{\ell j}^{ss}(\omega) \qquad (6\text{-a})$$

$$\omega\, G_{ij}^{1s}(\omega) = \sum_\ell T_{i\ell}{}^{d} G_{\ell j}^{1s}(\omega) + I\, G_{ij}^{2s}(\omega) + V\, G_{ij}^{ss}(\omega)$$

$$+ \sum_\ell J^{d}(R_i,R_\ell) S^{z}\sigma G_{\ell j}^{1s}(\omega) \qquad (6\text{-b})$$

The propagator $G_{ij}^{2s}(\omega)$ satisfy a equation quite similar to (4-c); performing the same type of decoupling as above one obtains;

$$(\omega-I)G_{ij}^{2s}(\omega) = \langle n_{i-\sigma}\rangle \sum_\ell T_{i\ell}{}^{d} G_{\ell j}^{1s}(\omega) + J^{d}(R_i,R_i)\left[G_{ij}^{2s}(\omega)\right.$$

$$\left. - \langle n_{i-\sigma}\rangle G_{ij}^{1s}(\omega)\right] S^{z}\sigma + \langle n_{i-\sigma}\rangle \sum_\ell J^{d}(R_i,R_\ell) S^{z}\sigma G_{\ell j}^{1s}(\omega)$$

$$+ V \langle n_{i-\sigma}\rangle G_{ij}^{ss}(\omega) \qquad (6\text{-c})$$

Again equations (6) form a closed set which determines the propagator $G_{ij}^{ss}(\omega)$

III. SOLUTION OF THE COUPLED EQUATIONS USING PERTURBATION THEORY

i) SOLUTION FOR THE $G^{dd}_{ij}(\omega)$ PROPAGATOR

We start Fourier transforming equations (4) and (5); introducing $\Delta n^{-\sigma}_{kk'}$ through the definition:

$$\Delta n^{-\sigma}_{kk'} = \sum_i \Delta n^{-\sigma}_i \, e^{i(k-k').R_i} \qquad (7)$$

and assuming that the exchange integrals $J^s(k,k')$ and $J^d(k,k')$ depend only on k-k' one obtains:

$$(\omega-\varepsilon_k{}^d)G^{11}_{kk'}(\omega) = \frac{1}{2\pi}\,\delta_{kk'} + I\,G^{21}_{kk'}(\omega) + V\,G^{s1}_{kk'}(\omega)$$

$$+ \sum_q J^d(q)S^z\sigma G_{k-q,k'}(\omega) \qquad (8\text{-a})$$

$$(\omega-\varepsilon_k{}^s)G^{s1}_{kk'}(\omega) = V\,G^{11}_{kk'}(\omega) + \sum_q J^s(q)S^z\sigma G^{s1}_{k-q,k'}(\omega) \qquad (8\text{-b})$$

$$(\omega-I)G^{21}_{kk'}(\omega) = \frac{1}{2\pi}\,\langle n_{-\sigma}\rangle\delta_{kk'} + \frac{1}{2\pi}\,\Delta n^{-\sigma}_{kk'} + \langle n_{-\sigma}\rangle\varepsilon_k{}^d G^{11}_{kk'}(\omega)$$

$$+ \sum_{k''}\varepsilon^d_{k''}\Delta n^{-\sigma}_{kk''}G^{11}_{k''k'}(\omega) + V\,\langle n_{-\sigma}\rangle G^{s1}_{kk'}(\omega)$$

$$+ V \sum_{k''} \Delta n^{-\sigma}_{kk''} G^{s1}_{k''k'}(\omega) + S^z\sigma \sum_q J^d(q) G^{21}_{k-q,k'}(\omega) \qquad (8\text{-c})$$

The perturbation solution of equations (8) to first order in J^s and J^d goes as follows: firstly one obtains the $G^{s1}_{kk'}(\omega)$ propagator as:

$$G^{s1}_{kk'}(\omega) = \frac{V}{\omega - \varepsilon^s_k} G^{11}_{kk'}(\omega) + \frac{VS^z\sigma}{\omega - \varepsilon^s_k} \sum_q J^s(q) \frac{1}{\omega - \varepsilon^s_{k-q}} G^{11\,(o)}_{k-q,k'}(\omega) \qquad (9)$$

Where $G^{11\,(o)}_{kk'}$ is the zeroth order d-d propagator (this propagator contains only correlation and hybridization effects of the pure host).

Next step is to derive an approximate expression for the $G^{21}_{ij}(\omega)$ propagator; substituting (9) in (8-c) one gets:

$$I\, G^{21}_{kk'}(\omega) = \frac{1}{2\pi} \frac{I \langle n_{-\sigma}\rangle}{\omega - I} \delta_{kk'} + \frac{I \langle n_{d-\sigma}\rangle \varepsilon^d_k}{\omega - I} G^{11}_{kk'}(\omega)$$

$$+ \frac{IV^2 \langle n_{d-\sigma}\rangle}{(\omega - I)(\omega - \varepsilon_k{}^s)} G^{11}_{kk'}(\omega) + \frac{1}{2\pi} \frac{I\, \Delta n^{-\sigma}_{kk'}}{\omega - I}$$

$$+ \frac{I}{\omega - I} \sum_{k''} \varepsilon^d_{k''} \Delta n^{-\sigma}_{k,k''} G^{(o)}_{k''k'}(\omega) + \frac{V^2 \langle n_{d-\sigma}\rangle S^z \sigma I}{(\omega - I)(\omega - \varepsilon_k{}^s)} \sum_q \frac{J^s(q)}{\omega - \varepsilon^s_{k-q}}$$

$$\times G^{11\,(o)}_{k-q,k'}(\omega) + \frac{IV^2}{\omega - I} \sum_{k''} \Delta n^{-\sigma}_{kk''} \frac{1}{\omega - \varepsilon^s_{k''}} G^{11(o)}_{k''k'}$$

$$+ \frac{IS^z\sigma}{\omega - I} \sum_q J^d(q) G^{21\,(o)}_{k-q,k'}(\omega) \qquad (10)$$

Equation (11) becomes then:

$$G^{11}_{kk'}(\omega) = \frac{1}{2\pi}\frac{\delta_{kk'}}{\omega - \tilde{\varepsilon}_k^{\,d}} + \frac{1}{\omega - \tilde{\varepsilon}_k^{\,d}}\, I\, G^{21}_{kk'}(\omega)$$

$$+ \frac{V^2 S^z \sigma}{(\omega-\tilde{\varepsilon}_k^{\,d})\,(\omega-\varepsilon_k^{\,s})} \sum_q \frac{J^s(q)}{\omega - \varepsilon^s_{k-q}}\, G^{11\,(o)}_{k-q,k'}$$

$$+ \frac{1}{\omega - \tilde{\varepsilon}_k^{\,d}} \sum_q J^d(q) S^z \sigma G^{11\,(o)}_{k-q,k'}(\omega) \qquad (13)$$

From equations (10) and (13) one sees that the complete solution is obtained when $G^{11(o)}_{kk'}(\omega)$ and $G^{21(o)}_{kk'}(\omega)$ are known; in order to get them we calculate explicitly:

$$I\, G^{21(o)}_{kk'}(\omega) = \frac{1}{2\pi}\frac{I\langle n_{d-\sigma}\rangle}{\omega - I}\,\delta_{kk'} + \frac{I\langle n_{d-\sigma}\rangle\, \tilde{\varepsilon}_k^{\,d}}{\omega - I}\, G^{11(o)}_{kk'}(\omega) \qquad (14\text{-a})$$

and

$$G^{11(o)}_{kk'} = \frac{1}{2\pi}\frac{\delta_{kk'}}{\omega - \tilde{\varepsilon}_k^{\,d}} + \frac{1}{\omega - \tilde{\varepsilon}_k^{\,d}}\, I\, G^{21(o)}_{kk'}(\omega) \qquad (14\text{-b})$$

The solution of equations (14) is the usual s-d renormalized Hubbard propagator;

$$G^{11(o)}_{kk'}(\omega) = \frac{1}{2\pi}\,\delta_{kk'}\,\frac{1+\dfrac{I\langle n_{d-\sigma}\rangle}{\omega - I}}{\omega - \tilde{\varepsilon}_k^{\,d}\left(1+\dfrac{I\langle n_{d-\sigma}\rangle}{\omega - I}\right)} \tag{15}$$

Which is expected in the absence of the localized spin.

Introduce now the notation: $G^{11\,(o)}_{kk'} = g_k^{\,d}(\omega)\delta_{kk'}$; one expects then for the propagator $G^{11}_{kk'}(\omega)$:

$$G^{11}_{kk'}(\omega) = g_k^{\,d}(\omega)\delta_{kk'} + G^{11(1)}_{kk'}(\omega) \tag{16}$$

Where $G^{11(1)}_{kk'}(\omega)$ is the first order correction to the d-d propagator due to the scattering by the localized spin. The equation for it is obtained retaining the first order terms in equations (10) and (13) and using equations (14) to connect $G^{21(o)}_{kk'}$ to $g_k^{\,d}(\omega)$. The result is:

$$G^{11(1)}_{kk'}(\omega) = \frac{1}{\omega-\tilde{\varepsilon}_k^{\,d}}\, I\, G^{21(1)}_{kk'}(\omega) + \frac{V^2 S^z \sigma J^s(k-k')}{(\omega-\tilde{\varepsilon}_k^{\,d})\,(\omega-\varepsilon_k^{\,s})\,(\omega-\varepsilon_{k'}^{\,s})}\, g_{k'}^{\,d}(\omega)$$

$$+ \frac{J^d(k-k')S^z\sigma}{\omega - \tilde{\varepsilon}_k^{\,d}}\, g_{k'}^{\,d}(\omega) \tag{17-a}$$

and

$$I\, G^{21(1)}_{kk'}(\omega) = \frac{1}{2\pi}\,\frac{I\,\Delta n^{-\sigma}_{kk'}}{\omega - I} + \frac{I\langle n_{d-\sigma}\rangle\,\tilde{\varepsilon}_k^{\,d}}{\omega - I}\, G^{11(1)}_{kk'}(\omega)$$

$$+ \frac{I}{\omega - I} \varepsilon_{k'}^{d} \Delta n_{kk'}^{-\sigma} g_{k'}^{d}(\omega)$$

$$+ \frac{V^2 <n_{d-\sigma}> S^z \sigma I J^s(k-k')}{(\omega-I)(\omega-\varepsilon_k^s)(\omega-\varepsilon_{k'}^s)} g_{k'}^{d}(\omega)$$

$$+ \frac{IV^2 \Delta n_{kk'}^{-\sigma}}{(\omega-I)(\omega-\varepsilon_{k'}^s)} g_{k'}^{d}(\omega) + \frac{S^z \sigma J^d(k-k')}{\omega - I} [\frac{1}{2\pi} \frac{I<n_{d-\sigma}>}{\omega - I}$$

$$+ \frac{I<n_{d-\sigma}> \tilde{\varepsilon}_{k'}^{d}}{\omega - I} g_{k'}^{d}(\omega)] \qquad (17\text{-b})$$

It is clear that substituing (17-b) into (17-a) one obtains the complete solution $G_{kk'}^{11}(\omega)$ in terms of known propagators.

At this point it is useful to introduce the simplifying approximation of infinite repulsion ($I\to\infty$). We calculate then $\lim_{I\to\infty} I\, G_{kk'}^{21}(\omega)$ and substitute the result into (17-a). One finds for (17-b) in this limit:

$$\lim_{I\to\infty} I\, G_{kk'}^{21(1)}(\omega) = -\frac{1}{2\pi} \Delta n_{kk'}^{-\sigma} - <n_{d-\sigma}>\tilde{\varepsilon}_k^{d}\, G_{kk'}^{11(1)}(\omega)$$

$$- \varepsilon_k^{d} \Delta n_{kk'}^{-\sigma} g_{k'}^{d}(\omega) - \frac{V^2 <n_{d-\sigma}> S^z \sigma J^s(k-k')}{(\omega-\varepsilon_k^s)(\omega-\varepsilon_{k'}^s)} g_{k'}^{d}(\omega)$$

$$- \frac{V^2 \Delta n_{kk'}^{-\sigma}}{\omega-\varepsilon_{k'}^s} g_{k'}^{d}(\omega) \qquad (18)$$

Using (18) one easily obtains the final result for the $G^{11}_{kk'}(\omega)$ propagator. In order to put things in a simpler and more visible way we define the propagator:

$$\bar{g}_k^{\,d}(\omega) = \frac{1}{\omega - \tilde{\varepsilon}_k^{\,d}\,(1-\langle n_{d-\sigma}\rangle)}$$

The propagator $\bar{g}_k^{\,d}(\omega)$ should be compared to equation (15) in the limit of $I\to\infty$. They differ only in the $1-\langle n_{d-\sigma}\rangle$ factor that appears in the numerator, the poles being identical. Physically the poles correspond to a Hubbard narrowed s-d hybridized d-band.

In terms of this propagator the final solution for $G^{11}_{kk'}(\omega)$ reads:

$$G^{11}_{kk'}(\omega) = g_k^{\,d}(\omega)\,\delta_{kk'} + \bar{g}_k^{\,d}(\omega)\,J^d(k-k')\hat{S}^z\sigma(1-\langle n_{d-\sigma}\rangle)\,\bar{g}_{k'}^{\,d}(\omega)$$

$$-\frac{1}{2\pi}\,\bar{g}_k^{\,d}(\omega)\,\Delta n^{-\sigma}_{kk'} - \bar{g}_k^{\,d}(\omega)\,\tilde{\varepsilon}_{k'}^{\,d}\,\Delta n^{-\sigma}_{kk'}(1-\langle n_{d-\sigma}\rangle)\,\bar{g}_{k'}^{\,d}(\omega)$$

$$+\,\bar{g}_k^{\,d}(\omega)\,\frac{V^2S^z\sigma J^s(k-k')\,(1-\langle n_{d-\sigma}\rangle)^2}{(\omega-\varepsilon_k^{\,s})\,(\omega-\varepsilon_{k'}^{\,s})}\,\bar{g}_{k'}^{\,d}(\omega) \qquad (19)$$

Written in this way the propagator $G^{11}_{kk'}(\omega)$ is shown to be the sum of three main contributions. Firstly one has the pure host propagator $g_k^d(\omega)\,\delta_{kk'}$ which is (15) in the infinite repulsion limit. The next three terms correspond respectively to the first Born approximation for direct d-d scattering associated to J^d and the "feed-back effects"[1]. The expression for these d-d terms is formally identical to that obtained in reference 1 for the non-hybridized band. The only difference introduced by the existence of hybridization is that the involved d-electron energies (explicitly or implicitly in the $\bar{g}_k^d(\omega)$) are now s-d renormalized d-electron energies as defined in (12). Finally the last term is a new one which describes a process where a d electron of wave vector k' is s-d admixed into the s-band, scattered into wave vector k through J^s and then admixed into the final d-state.

ii) SOLUTION FOR THE $G^{ss}_{ij}(\omega)$ PROPAGATOR

Again one starts Fourier transforming equations (6) to get:

$$(\omega-\varepsilon_k^{\ s})\, G^{ss}_{kk'}(\omega) = \frac{1}{2\pi}\,\delta_{kk'} + V\, G^{1s}_{kk'}(\omega) + \sum_{k''} J^s(k,k'')S^z\sigma G^{ss}_{k''k'}(\omega) \qquad (20\text{-a})$$

$$(\omega-\varepsilon_k^{\ d})\, G^{1s}_{kk'}(\omega) = I\, G^{2s}_{kk'}(\omega) + V\, G^{ss}_{kk'}(\omega) + \sum_{k''} J^d(k,k'')S^z\sigma G^{1s}_{k''k'}(\omega) \qquad (20\text{-b})$$

$$(\omega - I)\, G^{2s}_{kk'}(\omega) = \langle n_{d-\sigma}\rangle \varepsilon_k^{\ d} G^{1s}_{kk'}(\omega) + \sum_{k''} \varepsilon_{k''}^{\ d}\, \Delta n^{-\sigma}_{kk''} G^{1s}_{k''k'}(\omega)$$

$$+ V \langle n_{d-\sigma}\rangle G^{ss}_{kk'}(\omega) + V \sum_{k''} \Delta n^{-\sigma}_{kk''} G^{ss}_{k''k'}(\omega)$$

$$+ \sum_{k''} J^{d}(k,k'') S^{z}\sigma G^{2s}_{k''k'}(\omega) \qquad (20\text{-c})$$

Following the perturbation scheme we first calculate the zero order propagators. From (20-b) and (20-c) one gets:

$$(\omega - I) G^{2s(o)}_{kk'}(\omega) = \langle n_{d-\sigma}\rangle \varepsilon_k{}^{d} G^{1s(o)}_{kk'}(\omega) + V \langle n_{d-\sigma}\rangle G^{ss(o)}_{kk'}(\omega) \qquad (21\text{-a})$$

and

$$(\omega - \varepsilon_k{}^{d}) G^{1s(o)}_{kk'}(\omega) = I\, G^{2s(o)}_{kk'}(\omega) + V\, G^{ss(o)}_{kk'}(\omega) \qquad (21\text{-b})$$

From which one gets for $G^{1s(o)}_{kk'}(\omega)$:

$$G^{1s(o)}_{kk'}(\omega) = V\, G^{H}_{k}(\omega)\, G^{ss(o)}_{kk'}(\omega) \qquad (21\text{-c})$$

the Hubbard propagator being defined as:

$$G^{H}_{k}(\omega) = \frac{1 + \dfrac{I\langle n_{d-\sigma}\rangle}{\omega - I}}{\omega - \varepsilon_k{}^{d}\left(1 + \dfrac{I\langle n_{d-\sigma}\rangle}{\omega - I}\right)}$$

To complete the zero order solution we substitute (21-c) in the zero order equation for $G^{ss(o)}_{kk'}$, namely:

$$(\omega-\varepsilon_k{}^s)G^{ss(o)}_{kk'}(\omega) = \frac{1}{2\pi}\,\delta_{kk'} + V\,G^{1s(o)}_{kk'}(\omega) \tag{21-d}$$

to obtain the final solution:

$$G^{ss(o)}_{kk'}(\omega) = \frac{1}{2\pi}\,\delta_{kk'}\,\frac{1}{\omega-\varepsilon_k{}^s - V^2G^H_k(\omega)} \tag{22}$$

This represents an s-electron which can be admixed into a Hubbard correlated d-band. Again we search for solutions $G^{ss}_{kk'}(\omega)$ in the form:

$$G^{ss}_{kk'}(\omega) = G^{ss(o)}_{kk'}(\omega) + G^{ss(1)}_{kk'}(\omega)$$

and write down first order equations associated to the system (20). These equations are:

$$(\omega-\varepsilon_k{}^s)G^{ss(1)}_{kk'}(\omega) = V\,G^{1s(1)}_{kk'}(\omega) + \sum_{k''}J^s(k,k'')S^z\sigma G^{ss(o)}_{k''k'}(\omega) \tag{23-a}$$

$$(\omega-\varepsilon_k{}^d)G^{1s(1)}_{kk'}(\omega) = I\,G^{2s(1)}_{kk'}(\omega) + V\,G^{ss(1)}_{kk'}(\omega)$$

$$+ \sum_{k''}J^d(k,k'')S^z\sigma G^{1s(o)}_{k''k'}(\omega) \tag{23-b}$$

$$(\omega-I)G^{2s(1)}_{kk'}(\omega) = \langle n_{d-\sigma}\rangle \varepsilon_k^d G^{1s(1)}_{kk'}(\omega) + \sum_{k''} \varepsilon_{k''}^d \Delta n^{-\sigma}_{kk''} G^{1s(o)}_{k''k'}(\omega)$$

$$+ V \langle n_{d-\sigma}\rangle G^{ss(1)}_{kk'}(\omega) + V \sum_{k''} \Delta n^{-\sigma}_{kk''} G^{ss(o)}_{k''k'}(\omega)$$

$$+ \sum_{k''} J^d(k,k'') S^z \sigma G^{2s(o)}_{k''k'}(\omega) \qquad (23\text{-c})$$

Substituing in (23) the values of the zero order propagators obtained above and performing a straightforward algebra one finally gets (in the limit $I\to\infty$):

$$G^{ss}_{kk'}(\omega) = g_k^{\ s}(\omega)\ \delta_{kk'} + g_k^{\ s}(\omega)\ J^s(k,k') S^z \sigma g_{k'}^{\ s}(\omega)$$

$$+ g_k^{\ s}(\omega)\ V\ [\bar{g}_k^{\ d}(\omega)\ J^d(k,k') S^z \sigma (1-\langle n_{d-\sigma}\rangle)\bar{g}_{k'}^{\ d}(\omega)]\ V\ g_{k'}^{\ s}(\omega)$$

$$- g_k^{\ s}(\omega)\ V\ [\bar{g}_k^{\ d}\ \Delta n^{-\sigma}_{kk'} + \varepsilon_{k'}^d \bar{g}_k^{\ d}\ \Delta n^{-\sigma}_{kk'}(1-\langle n_{d-\sigma}\rangle)\bar{g}_{k'}^{\ d}]\ V\ g_{k'}^{\ s}(\omega) \qquad (24)$$

Equation (24) shows clearly the effects of exchange scattering and hybridization in the s-states. The first and second terms are respectively the host metal s-propagator and the Born approximation for the scattering through J^s. The third and fourth term show respectively how direct d-d scattering and feed back effects present in the d-band affect through the s-d mixing the s-electron propagator.

IV . SELF-CONSISTENCY PROBLEM FOR THE d-PROPAGATOR

In expression (19) the d-propagator is related to known quantities and to $\Delta n_{kk'}^{-\sigma}$, thus implying in a self-consistency problem. From the standard procedure to calculate thermal averages from Green's functions one needs to calculate:

$$\delta\langle c_{k'\sigma}^{+} c_{k\sigma}\rangle = F_{\omega}\left[\delta G_{kk'}^{11}(\omega)\right] \tag{25}$$

Where $\delta G_{kk'}^{11}(\omega)$ is just equation (19) without the first term. In (25) the notation for F_{ω} is just Bloomfield's one[2]. Since we are interested in calculating $\Delta n_{q}^{-\sigma}$, the involved thermal average[1] is $\delta\langle c_{k+q\sigma}^{+} c_{k\sigma}\rangle = F_{\omega}\left[\delta G_{k,k+q}(\omega)\right]$. From equation (19) one gets:

$$\begin{aligned}\sum_k \delta\langle c_{k+q\sigma}^{+} c_{k\sigma}\rangle = {} & J^{d}(q) S^{z}\sigma(1-\langle n_{d-\sigma}\rangle) \sum_k F_{\omega}\left[\bar{g}_k^{d}(\omega)\, \bar{g}_{k+q}^{d}(\omega)\right] \\ & - \frac{1}{2\pi}\, \Delta n_q^{-\sigma} \sum_k F_{\omega}\left[\bar{g}_k^{d}(\omega)\right] \\ & - \Delta n_q^{-\sigma}(1-\langle n_{d-\sigma}\rangle) \sum_k \varepsilon_{k+q}^{d}\, F_{\omega}\left[\bar{g}_k^{d}(\omega)\, \bar{g}_{k+q}^{d}(\omega)\right] \\ & - \Delta n_q^{-\sigma}\, V^2 (1-\langle n_{d-\sigma}\rangle) \sum_k F_{\omega}\left[\bar{g}_k^{d} \frac{1}{\omega-\varepsilon_{k+q}^{s}} \bar{g}_{k+q}^{d}\right] \\ & + V^2 S^z \sigma J^{s}(q)(1-\langle n_{d-\sigma}\rangle)^2 \sum_k F_{\omega}\left[\bar{g}_k^{d} \frac{1}{\omega-\varepsilon_k^{s}} \frac{1}{\omega-\varepsilon_{k+q}^{s}} \bar{g}_{k+q}^{d}\right]\end{aligned} \tag{26}$$

Since $\Delta n_q^\sigma = \sum_k \delta\langle c_{k+q}^+ c_k\rangle$ it follows from (26) that the self-consistency is readly obtained if one evaluates the F_ω symbols. We do that in such a way to introduce some kind of generalized susceptibilities. Firstly consider the propagator $\bar{g}_k^d(\omega)$:

$$\bar{g}_k^d(\omega) = \frac{1}{\omega - (1-\langle n_{d-\sigma}\rangle)(\varepsilon_k^d + \frac{V^2}{\omega-\varepsilon_k^s})} = \frac{\omega - \varepsilon_k^s}{(\omega-E_{k\sigma}^1)\ (\omega-E_{k\sigma}^2)} \qquad (27\text{-a})$$

In (27) E_k^1 and E_k^2 are the roots of:

$$\omega^2-\omega\left[\varepsilon_k^s + (1-\langle n_{d-\sigma}\rangle)\varepsilon_k^d\right] + (1-\langle n_{d-\sigma}\rangle)\left(\varepsilon_k^s\varepsilon_k^d - V^2\right) = 0 \qquad (27\text{-b})$$

For further calculation we separate (27-a) as:

$$\bar{g}_k^d(\omega) = \frac{\omega - \varepsilon_k^s}{E_{k\sigma}^1 - E_{k\sigma}^2}\left(\frac{1}{\omega-E_{k\sigma}^1} - \frac{1}{\omega-E_{k\sigma}^2}\right) \qquad (28)$$

Using the form (28) for the propagator $\bar{g}_k^d(\omega)$ now it is easy to evaluate the F_ω symbols in (26). Using (28) one gets for:

$$F_\omega\left[\varepsilon_k^d \frac{1}{(\omega-\varepsilon_k^s)(\omega-\varepsilon_{k+q}^s)}\bar{g}_{k+q}^d\right]:$$

$$F_\omega\left[\bar{g}_k^{\,d}\frac{1}{(\omega-E_k^{\,s})(\omega-E_{k+q}^{\,s})}\bar{g}_{k'}^{\,d}\right] = \frac{1}{(E_{k\sigma}^{1}-E_{k\sigma}^{2})(E_{k'\sigma}^{1}-E_{k'\sigma}^{2})}\{F_\omega\left[\frac{1}{(\omega-E_{k\sigma}^{1})(\omega-E_{k+q\sigma}^{1})}\right]$$

$$+ F_\omega\left[\frac{1}{(\omega-E_{k\sigma}^{2})(\omega-E_{k+q\sigma}^{2})}\right]$$

$$- F_\omega\left[\frac{1}{(\omega-E_{k\sigma}^{1})(\omega-E_{k+q,\sigma}^{2})}\right]$$

$$- F_\omega\left[\frac{1}{(\omega-E_{k\sigma}^{2})(\omega-E_{k\sigma}^{1})}\right]\} \qquad (29)$$

Now one uses the usual formula:

$$F_\omega\left[\frac{1}{(\omega-E_1)(\omega-E_2)}\right] = \frac{f(E_1)-f(E_2)}{E_1-E_2}$$

Where f(E) is the Fermi-function to obtain:

$$\sum_k F_\omega\left[\bar{g}_k^{\,d}(\omega)\frac{1}{(\omega-E_k^{\,s})(\omega-E_{k+q}^{\,s})}\bar{g}_{k'}^{\,d}(\omega)\right] = \sum_{\mu,\nu=1}^{2}(-1)^{\mu+\nu}\sum_k \frac{1}{(E_{k\sigma}^{1}-E_{k\sigma}^{2})}\frac{1}{(E_{k+q,\sigma}^{1}-E_{k+q\sigma}^{2})}$$

$$\times \frac{f(E_{k\sigma}^{\mu})-f(E_{k+q\sigma}^{\nu})}{(E_{k\sigma}^{\mu}-E_{k+q\sigma}^{\nu})} \qquad (30)$$

Introducing the generalized susceptibility

$$\overline{\chi}^{\mu\nu}(q) = \sum_k \frac{1}{(E^1_{k\sigma}-E^2_{k\sigma})(E^1_{k+q\sigma}-E^2_{k+q\sigma})} \; \frac{f(E^\mu_{k\sigma}) - f(E^\nu_{k+q\sigma})}{E^\mu_{k\sigma} - E^\nu_{k+q\sigma}}$$

one obtains finally:

$$\sum_k F_\omega \left(\overline{g}_k^{\,d} \frac{1}{\omega-\varepsilon^s_k} \cdot \frac{1}{\omega-\varepsilon^s_{k+q}} \overline{g}^{\,d}_{k'}\right) = \sum_{\mu,\nu} (-1)^{\mu+\nu}\overline{\chi}^{\mu\nu}(q) = \overline{\chi}(q) \qquad (31)$$

Using a quite similar procedure for the other terms involving products of $\overline{g}_k^{\,d}$ one gets:

$$\sum_k F_\omega \left[\overline{g}^{\,d}_{k+q}(\omega)\, \overline{g}^{\,d}_{k+q}(\omega)\right] = \sum_{\mu,\nu} (-1)^{\mu+\nu}\chi_1^{\mu\nu}(q) = \chi_1(q) \qquad (32\text{-a})$$

Where the "generalized susceptibility" $\chi_1(q)$ is defined as:

$$\chi_1^{\mu\nu}(q) = \sum_k \frac{(E^\mu_{k\sigma}-\varepsilon^s_k)(E^\mu_{k\sigma}-\varepsilon_{k+q\sigma})f(E^\mu_{k\sigma}) - (E^\nu_{k+q,\sigma}-\varepsilon^s_k)(E_{k+q,\sigma}-\varepsilon_{k+q})f(E_{k+q\sigma})}{(E^1_{k\sigma}-E^2_{k\sigma})(E_{k+q\sigma}-E^2_{k+q\sigma})(E^\mu_{k\sigma}-E^\nu_{k+q\sigma})} \qquad (32\text{-b})$$

Similarly for the feed-back term:

$$\sum_k F_\omega \left[\overline{g}_k^{\,d}(\omega)\varepsilon^d_{k+q}\, \overline{g}^{\,d}_{k+q}(\omega)\right] = \sum_{\mu,\nu} (-1)^{\mu+\nu}\overline{\chi}_1^{\,\mu\nu}(q) = \overline{\chi}_1(q) \qquad (32\text{-c})$$

Where

$$\bar{\chi}_1^{\mu\nu}(q)=\sum_k \varepsilon_{k+q}^{d}\frac{(E_{k\sigma}^{\mu}-\varepsilon_k^{s})(E_{k\sigma}^{\mu}-\varepsilon_{k+q}^{s})f(E_{k\sigma}^{\mu})-(E_{k+q}^{\nu}-\varepsilon_k^{s})(E_{k+q\sigma}^{\nu}-\varepsilon_{k+q}^{s})f(E_{k+q\sigma}^{\nu})}{(E_{k\sigma}^{1}-E_{k\sigma}^{2})(E_{k+q\sigma}^{1}-E_{k+q\sigma}^{2})(E_{k\sigma}^{\mu}-E_{k+q\sigma}^{\nu})} \quad (32\text{-d})$$

The last "susceptibility" appears in

$$\sum_k F_\omega[\bar{g}_k^{d}(\omega)\frac{1}{\omega-\varepsilon_{k+q}^{s}}\bar{g}_{k+q}^{d}(\omega)] = \sum_{\mu,\nu}(-1)^{\mu+\nu}\chi_2^{\mu\nu}(q) = \chi_2(q) \quad (32\text{-e})$$

Where

$$\chi_2^{\mu\nu}(q) = \sum_k \frac{(E_{k\sigma}^{\mu}-\varepsilon_k^{s})f(E_{k\sigma}^{\mu})-(E_{k+q\sigma}^{\nu}-\varepsilon_{k+q}^{s})f(E_{k+q\sigma}^{\nu})}{(E_{k\sigma}^{1}-E_{k\sigma}^{2})(E_{k+q\sigma}^{1}-E_{k+q\sigma}^{2})(E_{k\sigma}^{\mu}-E_{k+q\sigma}^{\nu})} \quad (32\text{-f})$$

Finally for $\sum_k F_\omega[\bar{g}_k^{d}(\omega)]$ one obtains:

$$N = \sum_k F_\omega[g_k^{d}(\omega)] = \sum_k \left[\frac{E_{k\sigma}^{1}-\varepsilon_k^{s}}{E_{k\sigma}^{1}-E_{k\sigma}^{2}} f(E_{k\sigma}^{1}) - \frac{E_{k\sigma}^{2}-\varepsilon_k^{s}}{E_{k\sigma}^{1}-E_{k\sigma}^{2}} f(E_{k\sigma}^{2})\right] \quad (33)$$

Now substituing equations (31), (32) and (33) into (26) one obtains for a <u>paramagnetic</u> host ($\langle n\uparrow\rangle=\langle n\downarrow\rangle$):

$$\Delta n_q^{\sigma} = J^d(q)S^z\sigma(1-\langle n\rangle)\chi_1(q) + J^s(q)S^z\sigma V^2(1-\langle n\rangle)^2\bar{\chi}(q)$$

$$- \Delta n_q^{-\sigma} \left[\frac{1}{2\pi} N + (1-\langle n\rangle)\,\bar{\chi}_1(q) + V^2\,(1-\langle n\rangle)\chi_2(q)\right] \qquad (34)$$

Changing the spins σ into $-\sigma$ one obtains a similar equation for $\Delta n_q^{-\sigma}$; solving this system of equation one gets for the self-consistent Δn_q^{σ} :

$$\Delta n_q^{\sigma} = \frac{J^d(q)S^z\sigma(1-\langle n\rangle)\chi_1(q) + J^s(q)S^z\sigma V^2(1-\langle n\rangle)^2\bar{\chi}(q)}{1 - \left[\frac{1}{2\pi} N + (1-\langle n\rangle)\bar{\chi}_1(q) + V^2(1- n)\chi_2(q)\right]} \qquad (35)$$

DISCUSSION

The self-consistent solution obtained in (IV) is now discussed. Firstly one notes that a quite similar procedure may be developed for the s-like spin polarization. From equation (24) one sees that using the self-consistent Δn_q^{σ} obtained in (35) the s-spin polarization is uniquely determined in terms of host metal propagators and Δn_q^{σ}. The complete self-consistency is then solved exactly for this simple picture of the problem. Now it should be noted that in the absence of sd mixing (V=0) one recovers for the d-like part the result obtained in 1 . To see that, one notes that in this limit equation (35) reduces to:

$$\Delta n_q^{\sigma} = \frac{J^d(q)S^z\sigma(1-\langle n\rangle)\chi_1(q)}{1 - \left|\frac{1}{2\pi} N + (1-\langle n\rangle)\overline{\chi}_1(q)\right|} \qquad (36)$$

From definitions (32-a) and (32-c) and using the fact that the roots E_k^{μ} for $V = 0$ are respectively $E_{k\sigma}^d$ and E_k^s one finds that:

$$\chi_1(q) \underset{V=0}{=} \sum_k \frac{f(E_{k+q\sigma}^d) - f(E_{k\sigma}^d)}{E_{k+q\sigma}^d - E_{k\sigma}^d}$$

and

$$\overline{\chi}_1(q) \underset{V=0}{=} \sum_k E_{k\sigma}^d \frac{f(E_{k+q\sigma}^d) - f(E_{k\sigma}^d)}{E_{k+q\sigma}^d - E_{k\sigma}^d}$$

Then equation (36) is precisely the result obtained for the pure d-band case. In this limit the s-like propagator reads:

$$G_{kk'}^{ss}(\omega) = g_k^s(\omega)\delta_{kk'} + g_k^s(\omega)J^s(k,k')S^z\sigma g_{k'}^s(\omega)$$

Which is precisely Watson's[3] result for the spin polarization in a independent particle model.

Comparison between the general solution (35) for the changes in d-occupation numbers in the hybridized form and the pure d case shows that a formal similarity is conserved. In the pure d-case the numerator involves (in equation 36) the puré Watson's result, proportional to the band susceptibility,and feed back effects introduce the enhancement factor appearing in the denominator. In the hybridized version two driving contributions appear, namely the direct one $J^dS^z\sigma(1-<n>)\chi_1(q)$ where $\chi_1(q)$ is some kind of s-d renormalized d-susceptibility and a term describing a scattering of a s-electron admixed into the d-band.

The enhancement factor occuring in (35) still envolves as in its pure d-counterpart a term involving the renormalized d-susceptibility, but now a pure mixing term proportional to V^2 also appears. Since the enhancement factor may be understood as a kinetic effect (the exchange scattering acting as a change in hopping motion) it is natural that mixing acts as a reduction factor for hopping motion. A possible application of this calculation is the case of intermetallic compounds of rare earths with a localized f-moment. In particular for some intermetallics it is thought that the d-bands originate from transition atoms only, the s-band being associated both to the transition and rare earth atoms. An example of such a situation could be the case of $LuCo_2$ intermetallics with Gd impurities. For such systems the coupling between the 4f local moment and the 3d states is very weak since d-states are almost concentrated on the transition metal sites, then one takes $J^d(q) \cong 0$. In such a situation equation (35) involves only as driving term $J^S(q)S^z\sigma V^2(1-<n>)^2\bar{\chi}(q)$ which shows that the d-polarization originates only through s-d mixing. Similarly all terms in (24) involving J^d are dropped and only indirect terms are present as far as the d-band is concerned.

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