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REMARKS ON THE STATIC MAGNETIC RESPONSES OF COUPLED METALLIC SYSTEMS: APPLICATION TO ACTINIDES AND TRANSITION METALS*

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ABSTRACT

The static magnetic responses of a general hybridized and coupled three-band metal are calculated within the framework of the Hartree-Fock approximation. The magnetic responses, which are obtained through "partial static susceptibilities", are discussed in general and applied to consider specific cases, namely, actinide metals and transition metal systems. Concerning actinide metals, we obtain the magnetic responses for these metals described by three - bands (s,d,f) and the case of spin-orbit splitted f-bands is reduced also to a three-band problem (which may be formally incorpora-

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ted in two coupled f_1, f_2 bands). Transition metals are considered including d-band degeneracy (Hund's coupling effects) together with s-d hybridization. One discusses briefly the role of s-d mixing in providing negative exchange couplings to magnetic rare earth moments (ESR experiments) in presence of s-d interband exchange effects.

In this work, we consider a class of coupled metallic systems which cover transition metal-like systems, actinides and intermetallic compounds. The term coupled originates in the fact that the above mentioned class of systems involve in general several bands (or sub-bands in degeneracy is taken into account). The nature of the coupling between these bands may be associated to host hybridizations (s-d, s-f, d-f) or more naturally to the Coulomb interaction terms (where one includes also intraband Coulomb terms, which in general play an important role in the magnetic properties). In what follows, the presence of impurities (magnetic or not) is excluded and consequently only translationally invariant systems will be considered.

The class of systems of interest here, three-band metals, is described by the following model Hamiltonian, which in the Wannier notation is

$$\mathcal{H}_{host} = \sum_{\lambda ij\sigma} T_{ij}^{(\lambda)} c_{\lambda i\sigma}^{+} c_{\lambda j\sigma} + \sum_{\lambda i} U_{\lambda} n_{i\uparrow}^{(\lambda)} n_{i\downarrow}^{(\lambda)} + \sum_{\substack{\lambda\mu i\sigma \\ \mu\neq\lambda}} (U_{\lambda\mu} - J_{\lambda\mu}) n_{i\sigma}^{(\lambda)} n_{i\sigma}^{(\mu)} +$$

$$+ \sum_{\substack{\lambda\mu i \\ \mu\neq\lambda}} U_{\lambda\mu} (n_{i\uparrow}^{(\lambda)} n_{i\downarrow}^{(\mu)} + n_{i\uparrow}^{(\mu)} n_{i\downarrow}^{(\lambda)}) + \sum_{\substack{\lambda\mu ij\sigma \\ \mu\neq\lambda}} \{V_{\lambda\mu}(\underset{\sim}{R}_i - \underset{\sim}{R}_j) c_{\lambda i\sigma}^{+} c_{\mu j\sigma} +$$

$$+V_{\mu\lambda}(\underset{\sim}{R}_i - \underset{\sim}{R}_j)c^{+}_{\mu i\sigma}\, c_{\lambda j\sigma}\} \qquad n^{(\lambda)}_{i\sigma} = c^{+}_{\lambda i\sigma}c_{\lambda i\sigma}. \qquad (1)$$

where $c^{+}_{\lambda i\sigma}(c_{\lambda i\sigma})$ are creation (annihilation) operators of electrons with spin σ ($\sigma = \uparrow$ or $\downarrow$) in the λ-band. $T^{(\mu)}_{ij}$ is the hopping amplitude defined in terms of the band energy as

$$T^{(\mu)}_{ij} = \sum_{\underset{\sim}{k}} \varepsilon^{(\mu)}_{\underset{\sim}{k}} \exp\left[i\underset{\sim}{k}.(\underset{\sim}{R}_i - \underset{\sim}{R}_j)\right]$$

where $\varepsilon^{(\mu)}_{\underset{\sim}{k}}$ is the Bloch dispersion relation for the μ' th band. The mixing matrix elements $V_{\lambda\mu}$ are assumed to be $\underset{\sim}{k}$-dependent, i.e.

$$V_{\lambda\mu}(\underset{\sim}{R}_i - \underset{\sim}{R}_j) = \sum_{\underset{\sim}{k}} V_{\lambda\mu}(k) \exp\left[i\underset{\sim}{k}.(\underset{\sim}{R}_i - \underset{\sim}{R}_j)\right] .$$

The interaction parameters are the following: U_λ denotes intra-atomic intraband Coulomb energy, $U_{\lambda\mu}$ and $J_{\lambda\mu}$ being intra-atomic interband Coulomb and exchange energies respectively. The Hamiltonian (1) is a generalization of previously discussed model Hamiltonians as applied to specific cases, namely, transition metals[1,2,3], actinide metals[4,5] and intermetallic compounds[6].

In the literature, two ways of dealing with this class of Hamiltonians (1) have been used[1,5], namely, the self-consistent determination of the $\langle n^{(\lambda)}_{\sigma}\rangle$ occupation numbers or the magnetic response method[2] (static in general, but in some cases extended to include frequency dependence).

As far the first method is concerned, the effect of s-d hybridization[1] (transition like metals) and d-f hybridization[5] (actinide metals) in the Hartree-Fock description of the magnetic behaviour of these metals was discussed in a quite de

tailed way.

The second approach[2] was used to discuss the possible connection between microscopic and macroscopic (phenomenological) description of the magnetic response of hybridized systems, and the criterion for magnetic (Hartree-Fock) instabilities in pure actinide metals[7]. Taking into account the frequency dependence of the external magnetic field, the evaluation of the Korringa relaxation[8] in s-p coupled systems is possible. A clear generalization of Yafet's work[8] for more complex sistems is to extend the computation of the T^2 term of the resistivity[9] in coupled systems, assuming as usually that conduction is mostly performed by the s-electrons. The study of g-shifts in pure metals or intermetallic compounds finds also an application (see ref. 2) of the method of the linear response function.

In this work, we intend, discussing the general Hamiltonian (1), within the framework of the linear response method, to generalize some previously obtained results of magnetic instability, thus connecting this method to previously developped numerical analysis of the density of states of an hybridized three-band model[10]. This work[10] in particular, suggests, as is included in the Hamiltonian (1), the possibility of studying the low temperature band description of actinide metals in presence of spin-orbit coupling. (To do this we consider in (1), two f-character bands f_1 and f_2 and one d-character band, i. e. $\lambda = f_1, f_2, d$, see below). This program faces with the usual difficulty of how to deal with the electron-electron correlation included in (1). We will assume, throughout this work, that the bands are large enough and that the correlations are

not so strong. So, we assume that the approximate validity of the Hartree-Fock scheme is fulfilled.

We recall briefly the method used in previous publications[2,3]: Let $h_o^{(\lambda)} \exp(-i\underset{\sim}{q}.\underset{\sim}{R}_i)$, be the static, $\underset{\sim}{q}$-dependent, external magnetic field acting on the λ-electrons; the magnetic interaction may be written as

$$\mathcal{H}_{mag} = -\frac{1}{2} \sum_{\lambda i \sigma} \sigma h_o^{(\lambda)} n_{i\sigma}^{(\lambda)} \exp(-i\underset{\sim}{q}.\underset{\sim}{R}_i) \qquad (2)$$

The complete Hamiltonian of interest is then

$$\mathcal{H} = \mathcal{H}_{host} + \mathcal{H}_{mag} \qquad (3)$$

One must calculate the one-electron propagators $G_{ij\sigma}^{\lambda\lambda}(\omega) = \langle\langle c_{\lambda i\sigma}; c_{\lambda j\sigma}^{+} \rangle\rangle_{\omega}$ to first order in the external magnetic field (linear response), Coulomb correlations being treated in the Hartree-Fock approximation. The first order correction to the one-electron propagators is defined as

$$G_{ij\sigma}^{\lambda\lambda}(\omega) = g_{ij\sigma}^{\lambda\lambda}(\omega) + G_{ij\sigma}^{\lambda\lambda(1)}(\omega) \quad .$$

The zero order λ-λ propagators ($h_o^{(\lambda)}=0$) are easily obtained in the Bloch representation, and read

$$g_{\underset{\sim}{k}\underset{\sim}{k}'\sigma}^{\lambda\lambda}(\omega) = \frac{1}{2\pi} \delta_{\underset{\sim}{k}\underset{\sim}{k}'} \frac{1}{\omega - E_{\underset{\sim}{k}\sigma}^{(\lambda)} - \sum_{\mu\neq\lambda} \frac{|V_{\lambda\mu}(\underset{\sim}{k})|^2}{\omega - E_{\underset{\sim}{k}\sigma}^{(\mu,\beta)}}} = \frac{1}{2\pi} g_{\underset{\sim}{k}\sigma}^{\lambda\lambda}(\omega) \quad , (\beta\neq\lambda,\mu) \qquad (4.a)$$

while the cross μ-λ propagators turn out to be

$$g^{\mu\lambda}_{\underset{\sim}{k}\underset{\sim}{k}'\sigma}(\omega)= \frac{V_{\mu\lambda}(\underset{\sim}{k})}{\omega-E^{(\mu,\beta)}_{\underset{\sim}{k}\sigma}}\, g^{\lambda\lambda}_{\underset{\sim}{k}\underset{\sim}{k}'\sigma}(\omega)+ \frac{V_{\mu\beta}(\underset{\sim}{k})V_{\beta\lambda}(\underset{\sim}{k})}{(\omega-E^{(\mu,\beta)}_{\underset{\sim}{k}\sigma})(\omega-E^{(\beta)}_{\underset{\sim}{k}\sigma})}\, g^{\lambda\lambda}_{\underset{\sim}{k}\underset{\sim}{k}'\sigma}(\omega) \quad , \qquad (\beta\neq\lambda,\mu). \tag{4.b}$$

In equations (4)we have introduced the renormalized Hartree-Fock energies,

$$E^{(\lambda)}_{\underset{\sim}{k}\sigma}=\varepsilon^{(\lambda)}_{k}+U_\lambda\langle n^{(\lambda)}_{-\sigma}\rangle+ \sum_{\mu\neq\lambda}\{U_{\lambda\mu}\langle n^{(\mu)}_{-\sigma}\rangle+ (U_{\lambda\mu}-J_{\lambda\mu})\langle n^{(\mu)}_{\sigma}\rangle\} \tag{5.a}$$

and we have defined

$$E^{(\mu,\beta)}_{\underset{\sim}{k}\sigma} = E^{(\mu)}_{\underset{\sim}{k}\sigma} + \frac{|V_{\mu\beta}(\underset{\sim}{k})|^2}{\omega - E^{(\beta)}_{\underset{\sim}{k}\sigma}} \quad . \tag{5.b}$$

(Note that we have used in equation (5.a) the fact that the host is translationally invariant ($h^{(\lambda)}_{o}=0$) and so $n^{(\lambda)}_{i\sigma} = \langle n^{(\lambda)}_{\sigma}\rangle$).

To obtain the first order correction, one retains,from the general equation of motion for the propagator $G^{\lambda\lambda}_{ij\sigma}(\omega)$, only the terms proportional (directly or implicity) to the external fields. One gets, in the Bloch representation and assuming a paramagnetic host,

$$G^{\lambda\lambda(1)}_{\underset{\sim}{k}+\underset{\sim}{q},\underset{\sim}{k};\sigma}(\omega)= - \frac{1}{2\pi}\,\bar{g}^{\lambda\lambda}_{\underset{\sim}{k}+\underset{\sim}{q}}(\omega)\,\frac{1}{2}\,h^{(\lambda)}_{o}\sigma\bar{g}^{\lambda\lambda}_{\underset{\sim}{k}}(\omega)+ \frac{1}{2\pi}\,\bar{g}^{\lambda\lambda}_{\underset{\sim}{k}+\underset{\sim}{q}}(\omega)\left\{U_\lambda\Delta n^{-\sigma(\lambda)}_{\underset{\sim}{q}} + \sum_{\mu\neq\lambda}\left[U_{\lambda\mu}\Delta n^{-\sigma(\mu)}_{\underset{\sim}{q}}+ (U_{\lambda\mu}-J_{\lambda\mu})\Delta n^{\sigma(\mu)}_{\underset{\sim}{q}}\right]\right\}\bar{g}^{\lambda\lambda}_{\underset{\sim}{k}}(\omega) +$$

$$+\frac{1}{2\pi}\,\bar{g}^{\lambda\lambda}_{\underset{\sim}{k}+\underset{\sim}{q}}(\omega)\left\{\sum_{\mu\neq\lambda}\left[V_{\lambda\mu}(\underset{\sim}{k}+\underset{\sim}{q})\frac{1}{\omega-E^{(\mu,\beta)}_{\underset{\sim}{k}+\underset{\sim}{q}}}\left(-\frac{1}{2}\,h^{(\mu)}_{o}\sigma+U_\mu\Delta n^{-\sigma(\mu)}_{\underset{\sim}{q}}+U_{\lambda\mu}\Delta n^{-\sigma(\lambda)}_{\underset{\sim}{q}}+\right.\right.\right.$$

$$+(U_{\lambda\mu}-J_{\lambda\mu})\,\Delta\eta_{\underline{q}}^{\sigma(\lambda)}\Big)\,\frac{1}{\omega-E_{\underline{k}}^{(\mu,\beta)}}\,V_{\mu\lambda}(\underline{k})\Big]\Big\}\,\bar{g}_{\underline{k}}^{\lambda\lambda}(\omega) \;+$$

$$+\,\frac{1}{2\pi}\,\bar{g}_{\underline{k}+\underline{q}}^{\lambda\lambda}(\omega)\,\Big\{\sum_{\mu\neq\lambda}\Big[V_{\lambda\mu}(\underline{k}+\underline{q})\,\frac{1}{\omega-E_{\underline{k}+\underline{q}}^{(\mu,\beta)}}\,V_{\mu\beta}(\underline{k}+\underline{q})\,\frac{1}{\omega-E_{\underline{k}+\underline{q}}^{(\beta)}}\quad x$$

$$x\,\Big(-\frac{1}{2}\,h_o^{(\beta)}{}_\sigma+U_\beta\Delta\eta_{\underline{q}}^{-\sigma(\beta)}+U_{\lambda\beta}\Delta\eta_{\underline{q}}^{-\sigma(\lambda)}+(U_{\lambda\beta}-J_{\lambda\beta})\Delta\eta_{\underline{q}}^{\sigma(\lambda)}\Big)\frac{1}{\omega-E_{\underline{k}}^{(\beta)}}\quad x$$

$$x\,V_{\beta\mu}(\underline{k})\,\frac{1}{\omega-E_{\underline{k}}^{(\mu,\beta)}}\,V_{\mu\lambda}(\underline{k})\Big]\Big\}\,\bar{g}_{\underline{k}}^{\lambda\lambda}(\omega)\quad,\qquad(\beta\neq\mu,\lambda)\,,\qquad(6)$$

where we have introduced the fluctuation numbers

$$\Delta\eta_{\underline{q}}^{\sigma(\lambda)}=\sum_i\Delta\eta_i^{\sigma(\lambda)}\,\exp\left|i(\underline{k}-\underline{k}').\underline{R}_i\right|=\Delta\eta_{\underline{k}-\underline{k}'}^{\sigma(\lambda)}\quad,$$

$\Delta\eta_i^{\sigma(\lambda)}$ being the first order correction in the occupation numbers, namely, $\Delta\eta_i^{\sigma(\lambda)}=\langle\eta_{i\sigma}^{(\lambda)}\rangle^{(1)}-\langle\eta^{(\lambda)}\rangle$.

Equation (6) defines a self-consistency problem which must be solved using a classical prescription[11]

$$\langle BA\rangle=\mathcal{F}_\omega\left[\langle\langle A;B\rangle\rangle_\omega\right]=i\int_{-\infty}^{+\infty}d\omega f(\omega)\left[\langle\langle A;B\rangle\rangle_{\omega+i\delta}-\langle\langle A;B\rangle\rangle_{\omega-i\delta}\right]\,,\ \delta\to o\,,$$

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

We refer the reader to refs. 2 and 3, where this kind of self-consistency problem has been solved in detail, for more particular situations. Once the calculations are performed and remembering that $\Delta\eta_{\underline{q}}^{\sigma(\lambda)}=\sum_{\underline{k}}\mathcal{F}_\omega\left[G_{\underline{k}+\underline{q},\underline{k};\sigma}^{\lambda\lambda(1)}(\omega)\right]$, the total λ-magnetization is

given by

$$m^{\lambda}(\underline{q}) = \chi^{\lambda\lambda}(\underline{q})\, h_o^{(\lambda)} + \sum_{\mu\neq\lambda} \chi^{\lambda\mu}(\underline{q})\, h_o^{(\mu)} \quad , \qquad (7.a)$$

the Hartree-Fock "partial static susceptibilities" (response functions) being defined as

$$\chi^{\lambda\mu}(\underline{q}) = \frac{m^{\lambda}(\mu)}{h_o^{(\mu)}} \quad , \quad m^{\lambda}(\mu) = \Delta n_{\uparrow}^{\lambda}(\omega) - \Delta n_{\downarrow}^{\lambda}(\mu) \qquad (7.b)$$

In equation (7.b), $m^{\lambda}(\mu)$ is the magnetization induced on λ-states by a magnetic field acting on μ-states.

One should not that the response functions show a general characteristic of coupled systems: although starting from constant "bare" coupling interactions, they acquire an explicit $\underline{q}$-dependence associated to the susceptibilities involved in their definitions (see below).

For the general Hamiltonian (1), the Hartree-Fock condition for a magnetic instability of wave-vector $\underline{q}$ is given by the poles of the denominator

$$D(\underline{q}) = \left[1-U_{eff}^{(\lambda)}(\underline{q})\chi_{\lambda}(\underline{q})\right]\left[1-U_{eff}^{(\mu)}(\underline{q})\chi_{\mu}(\underline{q})\right]\left[1-U_{eff}^{(\beta)}(\underline{q})\chi_{\beta}(\underline{q})\right] -$$

$$- \sum_{\mu}\left\{\left[1-U_{eff}^{(\mu)}(\underline{q})\chi_{\mu}(\underline{q})\right] J_{\beta\lambda}(\underline{q})\, J_{\lambda\beta}(\underline{q})\chi_{\beta}(\underline{q})\chi_{\lambda}(\underline{q})\right\} -$$

$$- \sum_{\lambda\neq\mu} J_{\mu\lambda}(\underline{q})J_{\lambda\beta}(\underline{q})J_{\beta\mu}(\underline{q})\chi_{\mu}(\underline{q})\chi_{\lambda}(\underline{q})\chi_{\beta}(\underline{q}) \quad , \qquad (8)$$

where in the last term the sum is performed for a fixed μ; and $\lambda \neq \mu, \beta$, $\mu \neq \beta$. The "susceptibilities" and the effective couplings which appear in equation (8) are defined explicitly in

the Appendix. This denominator is common to all "partial static susceptibilities" (cf. equations 9a-9b).

The static responses, i.e. the "partial static susceptibilities" for our general three-band problem (see equations 7a-7b) are given by

$$\chi^{\lambda\lambda}(\underline{q}) = \frac{1}{D(\underline{q})} \left\{ \left[1 - U^{(\mu)}_{eff}(\underline{q})\chi_\mu(\underline{q})\right]\left[1 - U^{(\beta)}_{eff}(\underline{q})\chi_\beta(\underline{q})\right] - \right.$$

$$\left. - J_{\mu\beta}(\underline{q})J_{\beta\mu}(\underline{q})\chi_\mu(\underline{q})\chi_\beta(\underline{q}) \right\} \chi_\lambda(\underline{q}) +$$

$$+ \frac{1}{D(\underline{q})} \left\{ \left[\chi^{(1)}_{\beta\lambda}(\underline{q}) + \chi^{(2)}_{\beta\mu}(\underline{q})\right]\left[1 - U^{(\mu)}_{eff}\,\chi_\mu(\underline{q})\right] J_{\lambda\beta}(\underline{q}) + \right.$$

$$\left. + J_{\lambda\mu}(\underline{q})\, J_{\mu\beta}(\underline{q})\chi_\mu(\underline{q}) \right\} \chi_\lambda(\underline{q}) +$$

$$+ \frac{1}{D(\underline{q})} \left\{ \left[\chi^{(1)}_{\mu\lambda}(\underline{q}) + \chi^{(2)}_{\mu\beta}(\underline{q})\right]\left[1 - U^{(\beta)}_{eff}(\underline{q})\chi_\beta(\underline{q})\right] J_{\lambda\mu}(\underline{q}) + \right.$$

$$\left. + J_{\lambda\beta}(\underline{q})J_{\beta\mu}(\underline{q})\chi_\mu(\underline{q}) \right\} \chi_\lambda(\underline{q}) \qquad (9.a)$$

$$\chi^{\lambda\mu}(\underline{q}) = \frac{1}{d(\underline{q})} \left\{ \left[1 - U^{(\beta)}_{eff}(\underline{q})\chi_\beta(\underline{q})\right] J_{\lambda\mu}(\underline{q})\chi_\lambda(\underline{q}) + \right.$$

$$\left. + J_{\lambda\beta}(\underline{q})\, J_{\beta\mu}(\underline{q})\chi_\lambda(\underline{q})\chi_\beta(\underline{q}) \right\} \chi_\mu(\underline{q}) +$$

$$+ \frac{1}{D(\underline{q})} \left\{ \left[1 - U^{(\mu)}_{eff}(\underline{q})\chi_\mu(\underline{q})\right] J_{\lambda\mu}(\underline{q})\chi_\lambda(\underline{q}) + \right.$$

$$\left. + J_{\lambda\beta}(\underline{q})J_{\mu\beta}(\underline{q})\chi_\lambda(\underline{q})\chi_\mu(\underline{q}) \right\} \left[\chi^{(1)}_{\beta\mu}(\underline{q}) + \chi^{(2)}_{\beta\lambda}(\underline{q})\right] +$$

$$+\frac{1}{D(\underline{q})}\left\{\left[1-U_{eff}^{(\mu)}(\underline{q})\chi_{\mu}(\underline{q})\right]\left[1-U_{eff}^{(\beta)}(\underline{q})\chi_{\beta}(\underline{q})\right] -\right.$$

$$\left. - J_{\mu\beta}(\underline{q})J_{\beta\mu}(\underline{q})\chi_{\mu}(\underline{q})\chi_{\beta}(\underline{q})\right\}\left[\chi_{\lambda\mu}^{(1)}(\underline{q})+\chi_{\lambda\beta}^{(2)}(\underline{q})\right] \quad . \tag{9.b}$$

$$(\lambda\neq\mu\neq\beta).$$

In what follows, depending on the particular problem which will be considered bellow, some comments and discussions about these "partial static susceptibilities" will be done.

At this point we recover some previously obtained results[7]. We recall that in ref. 7, actinide metals are described by a two-band model in terms of d and f non-degenerate bands, where Coulomb repulsions (through the interactions $U_d \sum_i n_{i\uparrow}^{(d)} n_{i\downarrow}^{(d)}$, $U_f \sum_i n_{i\uparrow}^{(f)} n_{i\downarrow}^{(f)}$, $U_{df} \sum_i \{n_{i\uparrow}^{(f)} n_{i\downarrow}^{(d)} + n_{i\downarrow}^{(f)} n_{i\uparrow}^{(d)}\}$) and $\underline{k}$-dependent d-f hybridization are taken into account.

As far the denominator $D(\underline{q})$ is concerned, one has in this particular case

$$D(\underline{q})=\left[1-U_{eff}^{(f)}(\underline{q})\chi_f(\underline{q})\right]\left[1-U_{eff}^{(d)}(\underline{q})\chi_d(\underline{q})\right] - J_{df}(\underline{q})J_{fd}(\underline{q})\chi_d(\underline{q})\chi_f(\underline{q}) =$$

$$= 1 - J_{eff}^{(f)}(\underline{q})\chi_f(\underline{q}) \tag{10}$$

where

$$U_{eff}^{(f)}(\underline{q}) = U_f\left\{1+\frac{U_{df}\chi_{fd}^{(1)}(\underline{q})}{U_f\chi_f(\underline{q})}\right\};\quad U_{eff}^{(d)}(\underline{q}) = U_d\left\{1+\frac{U_{df}\chi_{df}^{(1)}(\underline{q})}{U_d\chi_d(\underline{q})}\right\} \tag{11.a}$$

$$J_{fd}(\underline{q})=U_{df}\left\{1+\frac{U_d\chi^{(1)}_{fd}(\underline{q})}{U_{df}\chi_f(\underline{q})}\right\}\ ;\quad J_{df}(\underline{q})=U_{df}\left\{1+\frac{U_f\chi^{(1)}_{df}(\underline{q})}{U_{df}\chi_d(\underline{q})}\right\} \qquad (11.b)$$

and

$$J^{(f)}_{eff}(\underline{q})=U_f+U_d\,\frac{\chi_d(\underline{q})}{\chi_f(\underline{q})}-(U_dU_f-U^2_{df})\chi_d(\underline{q})\left[1-\frac{\chi^{(1)}_{fd}(\underline{q})\chi^{(1)}_{df}(\underline{q})}{\chi_f(\underline{q})\ \chi_d(\underline{q})}\right]+$$

$$+\ U_{df}\,\frac{\chi^{(1)}_{fd}(\underline{q})+\chi^{(1)}_{df}(\underline{q})}{\chi_f(\underline{q})} \qquad (12)$$

Again we stress, and this is a common feature of coupled and hybridized band problems, that, although we start with "bare" constant couplings (cf. equation (1)), we obtain $\underline{q}$-dependent effective couplings in the final expressions.

The Hartree-Fock criterion for a magnetic instability of wave-vector $\underline{q}$ is

$$D(\underline{q}) = 1 - J^{(f)}_{eff}(\underline{q})\chi_f(\underline{q}) = 0 \qquad (13)$$

Two interesting limiting situations, concerning the condition for occurrence for magnetic instabilities, may be mentioned, viz.

(i) If d-f hybridization is absent, the bands remaining coupled through the correlation interband term U_{df}, $D(\underline{q})$turns out to be

$$D(\underline{q}) = \left[1-U_f\chi_f(\underline{q})\right]\left[1-U_d\chi_d(\underline{q})\right]\ U^2_{df}\ \chi_d(\underline{q})\chi_f(\underline{q}) \qquad (14.a)$$

(ii) On the other hand, if $U_{df} = 0$, but $V_{df} \neq 0$, one has

$$D(\underline{q}) = \left[1 - U_f \chi_f(\underline{q})\right] \left[1 - U_d \chi_d(\underline{q})\right] - U_d\, U_f \chi_{df}^{(1)}(\underline{q})\, \chi_{fd}^{(1)}(\underline{q}) \quad , \quad (14.b)$$

where two-band effects appear due to d-f mixing associated to the simultaneous existence of Coulomb intraband repulsions.

This model[7] can be refined in order to describe the role of spin-orbit coupling in pure actinide metals at low temperatures. So, we adopt now our three-band model* (cf. equation (1)), specialized to describe a metallic system consisting of a single d band and f bands, where spin-orbit coupling splits them into two f-character bands f_1 and f_2†.

Recall that in the two band simple situation of two non-hybridized bands f_1 and f_2 ($V_{f_1 f_2} = o$ but $U_{f_1} \neq 0$, $U_{f_2} \neq 0$, $U_{f_1 f_2} \neq 0$), the denominator of the magnetic response is given by, (cf. equation 14.a)

$$D(q) = \left[1 - U_{f_1} \chi_{f_1}(q)\right] \left[1 - U_{f_2} \chi_{f_2}(q)\right] - U_{f_1 f_2}^2 \chi_{f_1}(q) \chi_{f_2}(q) \quad (14.c)$$

Now, if in our spin-orbit splitted case, and within the framework of a three-band problem, we persist in keeping a formally result to the above (14.c) one may obtain, after some algebra, an expression of the form

$$D(\underline{q}) = \left(1 - J_{eff}^{(f_1)}(\underline{q}) \chi_{f_1}(\underline{q})\right)\left(1 - \bar{J}_{eff}^{(f_2)}(\underline{q}) \chi_{f_2}(\underline{q}) - \tilde{J}_{f_1 f_2}(\underline{q}) \chi_{f_1}(\underline{q}) \chi_{f_2}(\underline{q})\right) \quad (15)$$

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* In this particular case, we disregard, for simplicity, interband Coulomb and exchange interactions among electrons with same spin.

† The case of actinide impurities dissolved in transition metals, in presence of spin-orbit coupling of the f-level is discussed in ref. 29.

In equation (15), we have arbitrarily chosen $J_{eff}^{(f_1)}$ to have exactly the same form as in (12), whereas it turns out that in the definition of $J_{eff}^{(f_2)}$ a term of the form $U_d\chi_d(q)/\chi_{f_2}(q)$ is absent. $\tilde{J}_{f_1f_2}(\underline{q})$ is a rather complicated expression describing an effective interband interaction between f_1 and f_2 bands.

An interesting remark at this point is that, if intra-d-band correlation U_d is neglected, i.e. if the d-band acts only as a source of d-f hybridization, the effective intra-band couplings $J_{eff}^{(f_1)}(\underline{q})$ and $J_{eff}^{(f_2)}(\underline{q})$ become symmetrical, namely

$$J_{eff}^{(f_i)}(\underline{q}) = U_{f_i} + U_{df_i}^2\chi_d(\underline{q})\left\{1 - \frac{\chi_{fd_i}^{(1)}(\underline{q})\chi_{df_i}^{(1)}(\underline{q})}{\chi_{f_i}(\underline{q})\chi_d(\underline{q})}\right\} +$$

$$+ U_{df_i}\frac{\chi_{f_id}^{(1)}(\underline{q}) + \chi_{df_i}^{(1)}(\underline{q})}{\chi_{f_i}(\underline{q})}, \quad i=1,2. \qquad (16)$$

We stress that in the general case, where $U_d \neq 0$, (cf. equations (14.c), (15)), we have arbitrarily chosen one of the f-character bands, say f_1 band, to be the one where $J_{eff}^{(f_1)}$ is defined via equation (12). Automatically, the symmetry between the two definitions of $J_{eff}^{(f_1)}(\underline{q})$ and $J_{eff}^{(f_2)}(\underline{q})$ associated to the previous correlated two-band description of an actinide metal is broken, which is expected because of the intrinsic three-band nature of the problem in presence of correlations within the d band.

Let's consider now transition like metals, described in a simplified way by two non-degenerate s and d coupled bands. In a previous work[2], "partial static susceptibilities" were derived either from a microscopic or from a macroscopic (molecu-

lar field approach) point of view, and a comparison between these approaches was obtained. In what follows, and in the same spirit as in[2], we intend to give an improved version of such an analysis[2,15].

In fact, some experimental evidence (through ESR measurements of Gd and Eu)[12,13] of the validity of the previous explanations[14,6,2] may be contested by the argument that s-d exchange interaction was neglected in the comparison between the microscopic and macroscopic approaches as performed in ref.2. This stems from the fact that exchange interaction tends to align s and d magnetizations parallel, contrary to s-d hybridization. In this case, since competitive mechanisms do operate, a criterion of validity of the discussion contained in ref. 2 must be given.

We intend to include the effect of interband exchange J_{sd} and verify in which conditions and for pure hosts s-d mixing acts to provide antiparallel alignements of s and d magnetizations as suggested in ref. 14 and required in the model developped in [6].

Considering explicitly, in the model Hamiltonian which describes the transition metal like host, s-d interband exchange (through the interaction term $-J_{sd} \sum_{i\sigma} n_{i\sigma}^{(d)} n_{i\sigma}^{(s)}$) the partial static susceptibilities obtained via the microscopic approach, as a particular case from expressions (8) and (9), are

$$\chi^{dd}(\underline{q}) = S_{micro}(\underline{q})\, \chi_d(\underline{q}) \qquad (17.a)$$

$$\chi^{ss}(\underline{q}) = \left[1 - U_d \chi_d(\underline{q})\right] S_{micro}(\underline{q}) \chi_s(\underline{q}) \qquad (17.b)$$

$$\chi^{ds}(\underline{q}) = \left\{1+J_{sd}\,\frac{\chi_d(\underline{q})\,\chi_s(\underline{q})}{\chi^{(1)}_{ds}(\underline{q})}\right\}\chi^{(1)}_{ds}(\underline{q})\;S_{micro}(\underline{q}) \qquad (17.c)$$

$$\chi^{sd}(\underline{q}) = \left\{1+J_{sd}\,\frac{\chi_d(\underline{q})\,\chi_s(\underline{q})}{\chi^{(1)}_{sd}(\underline{q})}\right\}\chi^{(1)}_{sd}(\underline{q})\;S_{micro}(\underline{q}) \qquad (17.d)$$

where

$$S^{-1}_{micro}(\underline{q}) = 1-U_d\chi_d(\underline{q})-J_{sd}\left\{\left[\chi^{(1)}_{ds}(\underline{q})+\chi^{(1)}_{sd}(\underline{q})\right]+J_{sd}\left[\chi_s(\underline{q})\chi_d(\underline{q}) - \chi^{(1)}_{ds}(\underline{q})\,\chi^{(1)}_{sd}(\underline{q})\right]\right\} \qquad (18)$$

In the above expressions we have neglected terms in fourth order in mixing.

On the other hand, the partial static susceptibilities obtained via the macroscopic approach[2,15] are

$$\chi^{dd}(\underline{q}) = \chi^{(o)}_{d}(\underline{q})\;\;S_{macro}(\underline{q}) \qquad (19.a)$$

$$\chi^{ss}(\underline{q}) = \chi^{(o)}_{s}(\underline{q})\left\{1+\bar{\alpha}_{sd}(\underline{q})\bar{\alpha}_{ds}(\underline{q})\;S_{macro}(\underline{q})\right\} \qquad (19.b)$$

$$\chi^{ds}(\underline{q}) = -\,\bar{\alpha}_{ds}(\underline{q})\chi^{(o)}_{s}(\underline{q})\;S_{macro}(\underline{q}) \qquad (19.c)$$

$$\chi^{sd}(\underline{q}) = -\,\bar{\alpha}_{sd}(\underline{q})\chi^{(o)}_{d}(\underline{q})\;S_{macro}(\underline{q}) \qquad (19.d)$$

where

$$S^{-1}_{macro}(\underline{q}) = 1 - \lambda_{dd}\chi^{(o)}_{d}(\underline{q})-\bar{\alpha}_{sd}(\underline{q})-\bar{\alpha}_{ds}(\underline{q})\;; \qquad (20.a)$$

$$\bar{\alpha}_{ds}(\underline{q}) = \alpha_{ds} - \lambda_{ds}\chi_d^{(o)}(\underline{q}) \ , \qquad (20.b)$$

$$\bar{\alpha}_{sd}(\underline{q}) = \alpha_{sd} - \lambda_{sd}\chi_s^{(o)}(\underline{q}) \qquad (20.c)$$

In equations (19-20), $\lambda_{dd} = (g_e\mu_B^2)^{-1}\ U_d$ is the molecular field coefficient associated to intra-d-band correlations, $\lambda_{ds}=\lambda_{sd}=(g_e\mu_B^2)^{-1}$ J_{sd} describes interband exchange, where as α_{sd} and α_{ds} (both of them > 0) are phenomenological coefficients associated to s-d mixing.

By equating the macroscopic and microscopic crossed susceptibilities, assuming $S_{micro} = S_{macro}$ and using definitions (20.b-20.c) we arrive at

$$\frac{\bar{\alpha}_{ds}(\underline{q})}{\bar{\alpha}_{sd}(\underline{q})} = \frac{\chi_d^{(o)}(\underline{q})}{\chi_s^{(o)}(\underline{q})} \qquad (21)$$

where we have neglected mixing corrections in the susceptibilities $\chi_\lambda(\underline{q})$, (λ = s, d) thus originating the susceptibilities $\chi_\lambda^{(o)}(\underline{q})$.

From (21) one sees that the signs of $\bar{\alpha}_{ds}$ and $\bar{\alpha}_{sd}$ are the same; thus one needs to discuss only one of them.

The condition for positive coupling ($\bar{\alpha}_{sd} > 0$) can be derived using the definitions (20.b-20.c). From (20.c) one has , for $\underline{q} = 0$ (g-shift measurements)

$$\alpha_{sd} > \lambda_{sd}\ \chi_s^{(o)}(0) \qquad (22)$$

Since $\chi_s^{(o)}(0) = g_e\mu_B^2 n^{(s)}(\varepsilon_F)$, $n^{(s)}(\varepsilon_F)$ being the density of sta

tes associated to s-electrons, the condition reads

$$\alpha_{sd} > J_{sd}\, n^{(s)}(\varepsilon_F) \qquad (23)$$

From the study of transition metals, the α_{sd} coefficient is known to be of the order of 0.1. Thus, in order to have positive coefficients (and so antiparallel s and d magnetizations), we must have

$$J_{sd} n^{(s)}(\varepsilon_F) < 0.1 \qquad (24)$$

Now, we summarize our conclusions and make some final comments.

The general static magnetic responses ("partial susceptibilities") obtained in this paper (cf. equations 8 and 9), assuming the Hartree-Fock approximation, enable us to recover some previously obtained results for pure metallic systems described by a two band model (e.g. transition like metals[2], actinide metals[7]) as far magnetic instabilities are concerned. The general approach developped in this work may be used also to discuss the influence of hybridization on hyperfine properties like Knight shift experiments.

A similar three-band problem was discussed previously[3]. However, in that paper[3], emphasis was given on the spin polarization induced by a magnetic rare earth impurity embedded in a transition like metal. The host was described by a single s band hybridized with two d-character sub-bands, thus emphasizing both s-d hybridization and d-degeneracy on the spin polarization. Moreover, the full k,k' dependence of the exchange interaction[16] bet-

ween rare earth spin moment and conduction states was taken into account. In the model Hamiltonian for the host adopted in[3], Coulomb and exchange interactions (Hund's coupling) among conduction states was considered, thus exhibiting a clear feature of the degeneracy of the d band.

Recent calculations[17] show the importance of Hund's coupling in the magnetic solution of degenerate d band metals . So, our present work may be regarded also as a complementation of a previous one[3] in two aspects, namely

(i) one may obtain a q-dependent magnetic instability criterion for the pure transition metal, where s-d mixing effects and Hund's coupling role are simultaneously considered;

(ii) one may derive "partial static susceptibilities" which include this coupling and to discuss its importance on physical quantities like Knight shifts.

We recall that previous discussions about ESR experiments in pure metals and intermetallics[2,6], together with some experimental results[12,13] suggest the importance of s-d hybridization in analyzing effective exchange interactions among conduction (s,d) electrons and rare earth spins. Recent band calculations for Gd metal[18], suggest that Anderson-Wolff-Schrieffer transformation is irrelevant as far the sign of the effective interactions are concerned. This remark[18], reforcing the idea of the role of s-d mixing in providing negative exchange couplings, seems to be important in pure metals. The case of dilute alloys constitute, however, a different and delicate problem.

One of the questions that may be raised with respect

to this approach for the description of these ESR experiments[12,13], is the existence of s-d exchange couplings which provide parallel coupling between s and d magnetizations[19] (See our discussion throughout this work). One of the particular results which we obtain from our general formulation is to provide a criterion for the antiparallel alignement between s and d magnetizations, (cf. equation 24), together with a more detailed justification of a previous microscopic - macroscopic comparative calculation concerning coupled s-d hybridized systems[2]. In particular the proof of the validity of the ratio $\bar{\alpha}_{ds}/\bar{\alpha}_{sd} = \chi_d/\chi_s$ in presence of s-d interband exchange (cf. equation 21) may provide also a more refined answer to these questions. (For a detailed description of the phenomenological approach see also ref. 15).

The case of actinide metals, as another particular application of our general problem, complements a discussion[10] of the one-electron properties like density of states. In ref. 10, homothetic bands[1] and model density of states in presence of s-f, d-f, s-d hybridizations were used. The final result[10] shows the role of hybridization in deforming initial non-hybridized s, d and f bands. The conclusions of that calculation[10] although qualitative and without any attempt to self-consistency, confirm (within a Stoner-like criterion) the previous self-consistent calculation performed in[5].

We want to stress that one of the advantages of the method employed throughout this paper is that it provides magnetic instability criterions for general wave-vector $\underline{q}$. Beside this, equation (8), generalizes this criterion, previously ob-

tained for a two band problem[7] and shows the role of s-d, s-f and d-f hybridizations in modifying the susceptibilities involved (cf. the Appendix).

For paramagnetic actinide metals, and including the frequency dependence, a refined version of the calculation performed in[9] for the resistivity at low temperatures could be made. In that calculation, conduction is mostly performed by s electrons and the scattering by spin fluctuations, (contrary to the case discussed in[20,21] where only d states are present), would be provided by coupled and interacting d-f electrons through "partial dynamical susceptibilities".

If NMR results are available, Korringa relaxation may be computed in the same spirit of Yafet's work[8] suitably adapted to discuss actinide metals.

Returning back to our "static problem": another possible application in actinides would be the calculation of the Knight shift, if hyperfine coupling parameters A(z) and A_{cp} available[22] are adequate.

Concerning the role of spin-orbit coupling in splitting the f band into two f_1 and f_2 bands, the general formulation presented in this work provides a natural way to deal with the magnetic responses in this situation. Although this specific problem exhibit clear features of a three correlated (Hartree-Fock) band problem, it is possible, by suitable redefining the quantities involved (cf. equations 15-16), to reduce it to a two band one.

It is obvious that all the conclusions which we arrived throughout this work are based on the assumption of the va-

lidity of the Hartree-Fock approach. The present article has the intention to explore a more general situation supplied by this simplest approximation. We stress that a numerical effort would be profitable (following the same homothetic band scheme used in[10]) to get conclusive numerical results in all cases which were discussed here.

The narrow band limit must be discussed separately, and in this situation more complex algebraic problems are involved[23]. In this case, the methods to be used to deal with electron correlations must be or the classical Hubbard[24] approximation or the most refined Roth[25] linearization approach. The last method[25], however, present some difficulties[26] which could be circumvented.

Finally, we would like to make some remarks concerning the validity of the Hartree-Fock approach (molecular field approximation) adopted here. Besides well established criterions of validity, (large bands, small Coulomb correlations), recent progress in the Renormalization Group Theory restrict the validity of mean field approaches. More particularly, recent developments concerning the phase-transition character of the Mott-Anderson localization problem have appeared[28]. In this context, the high temperature behaviour of actinide metals[27] has been the subject of studies, involving the simultaneous presence of temperature induced disorder and Coulomb correlations.

As emphasized in 28, the localization problem, usually viewed as an one-electron problem, must be complemented by introducing correlations among electrons, with implications

on the magnetic response behaviour, which is the main subject of this work.

The role of "details" like hybridization, degeneracy , etc., perhaps may be conjectured as a source of "marginal behaviour" as viewed within the framework of Renormalization Group Theory.

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APPENDIX

i) DEFINITION OF THE "SUSCEPTIBILITIES" (cf. equations (8),(9)).

$$\chi_\lambda(\underline{k},\underline{q}) = -\frac{1}{2\pi}\mathcal{J}_\omega\left\{\bar{g}^{\lambda\lambda}_{\underline{k}+\underline{q}}(\omega)\ \bar{g}^{\lambda\lambda}_{\underline{k}}(\omega)\right\} \tag{A-1}$$

$$\chi^{(1)}_{\lambda\mu}(\underline{k},\underline{q}) = -\frac{1}{2\pi}\mathcal{J}_\omega\left\{\bar{g}^{\lambda\lambda}_{\underline{k}+\underline{q}}(\omega)\ \frac{1}{\omega-E^{(\mu,\beta)}_{\underline{k}+\underline{q}}}\ \frac{1}{\omega-E^{(\mu,\beta)}_{\underline{k}}}\ \bar{g}^{\lambda\lambda}_{\underline{k}}(\omega)\right\} \tag{A-2}$$

$$\chi^{(2)}_{\lambda\mu}(\underline{k},\underline{q}) = -\frac{1}{2\pi}\mathcal{J}_\omega\left\{\bar{g}^{\lambda\lambda}_{k+q}(\omega)\ \frac{1}{\omega-E^{(\mu,\beta)}_{\underline{k}+\underline{q}}}\ \frac{1}{\omega-E^{(\beta)}_{\underline{k}+\underline{q}}}\ \frac{1}{\omega-E^{(\beta)}_{\underline{k}}}\ \frac{1}{\omega-E^{(\mu,\beta)}_{\underline{k}}}\ \bar{g}^{\lambda\lambda}_{\underline{k}}(\omega)\right\} \tag{A-3}$$

$$\chi_\lambda(\underline{q}) = \sum_{\underline{k}}\chi_\lambda(\underline{k},\underline{q}) \tag{A-4}$$

$$\chi^{(1)}_{\lambda\mu}(\underline{q}) = \sum_{\underline{k}} V_{\lambda\mu}(\underline{k}+\underline{q})\ V_{\mu\lambda}(\underline{k})\ \chi^{(1)}_{\lambda\mu}(\underline{k},\underline{q}) \tag{A-5}$$

$$\chi^{(2)}_{\lambda\mu}(\underline{q}) = \sum_{\underline{k}} V_{\lambda\mu}(\underline{k}+\underline{q})\ V_{\mu\beta}(\underline{k}+\underline{q})\ V_{\beta\mu}(\underline{k})\ V_{\mu\lambda}(\underline{k})\ \chi^{(2)}_{\lambda\mu}(\underline{k},\underline{q}) \tag{A-6}$$

$$(\lambda \neq \mu \neq \beta)$$

ii) DEFINITION OF THE GENERAL $\underline{q}$-DEPENDENT EFFECTIVE COUPLINGS (cf. equations (8),(9)).

$$U^{(\lambda)}_{\text{eff}}(\underline{q}) = U_\lambda\left\{1+\frac{1}{U_\lambda\chi_\lambda(\underline{q})}\sum_{\mu\neq\lambda}\left[(U_{\lambda\mu}-J_{\lambda\mu})\chi^{(1)}_{\lambda\mu}(\underline{q})+(U_{\lambda\mu}-J_{\lambda\beta})\chi^{(2)}_{\lambda\mu}(\underline{q})\right]\right\} \tag{A-7}$$

$$J_{\lambda\mu}(\underline{q}) = (U_{\lambda\mu} - \bar{J}_{\lambda\mu}) \left\{ 1 + \frac{U_{\mu}\left[\chi^{(1)}_{\lambda\mu}(\underline{q}) + \chi^{(2)}_{\lambda\mu}(\underline{q})\right]}{(U_{\lambda\mu} - \bar{J}_{\lambda\mu})\chi_{\lambda}(\underline{q})} \right\} \qquad \text{(A-8)}$$

$$(\lambda \neq \mu \neq \beta)$$

where

$$\bar{J}_{\lambda\mu} = U_{\lambda\mu} - J_{\lambda\mu}$$

Note that when both intra-atomic interband Coulomb and exchange interactions are present, the contribution to the interband Coulomb repulsion coming from electrons with the same spin cancels out that one from opposite spins.

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