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REMARKS ON THE CONDITIONS FOR MAGNETIC INSTABILITIES IN ACTINIDES; HARTREE-FOCK APPROACH

by

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Fock limit, the criterion for magnetic instabilities. The general idea is to calculate the response of the system to an external, wave vector dependent magnetic field. Once the response is known one searches for the poles of the static susceptibility, as a function of wave vector q, and this provides the criterion for a magnetic instability, of wave vector q. When this work was being finished, Jullien and Coqblin [3] pointed out to the authors that they succeed in discussing within the Hartree-Fock picture the magnetic properties of the actinide metals in terms of the band model. In particular they give a quite interesting model for the d-f hybridization and its k-dependence. In the light of these results, the calculation presented here seems to be a complementary approach for this problem. * The plan of this work is the following: firstly we compute the response to the external field [4] of a two band model (d and f) the electrons being treated within the Hartree-Fock approximation, the mixing matrix elements being considered as an open parameter. Then the condition for a magnetic instability of wave vector q is derived, and a Stoner like criterion with effective "exchange interaction" is obtained. Finally the details for numerical computation are briefly discussed, the numerical results being discussed in a following publication.

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* Since it presents the conditions for magnetic instabilities of arbitrary wave vector q.

I. FORMULATION OF THE PROBLEM

In this calculation, we consider for simplicity, only a static, wave number dependent external magnetic field. Since we are interested only in the magnetic instabilities, and these are determined by the poles of the susceptibility $\chi(q, \omega)$ at zero frequency, the response to a static field suffices for our purposes. The magnetic field contribution we consider here is:

$$\mathcal{H}_{ext} = h_o \sum_{i,\sigma} \sigma(n_{i\sigma}^{(d)} + n_{i\sigma}^{(f)}) e^{-iq\cdot R_i} \tag{1}$$

where q is the wave vector of the applied external magnetic field, and $n_{i\sigma}^{(d)}$, $n_{i\sigma}^{(f)}$ are the number of d and f electrons respectively (the field being applied parallel to the z-axis). We describe the actinide metals in terms of d and f bands, Coulomb repulsions and the d-f hybridization [1, 2, 3]. As discussed in ref. 3 we consider k-dependent d-f hybridization matrix elements. The Hamiltonian of the actinide metal is then (in the Wannier representation)

$$\mathcal{H} = \sum_{i,j,\sigma} T_{ij}^{(d)} d_{i\sigma}^{+} d_{j\sigma} + \sum_{i,j,} T_{ij}^{(f)} f_{i\sigma}^{+} f_{j\sigma} + \sum_{i,j,\sigma} \{V_{df}(R_i-R_j) d_{i\sigma}^{+} f_{j\sigma} +$$

$$+ V_{fd}(R_i-R_j) f_{i\sigma}^{+} d_{j\sigma}\} + U_d \sum_i n_{i\uparrow}^{(d)} n_{i\downarrow}^{(d)} + U_f \sum_i n_{i\uparrow}^{(f)} n_{i\downarrow}^{(f)} +$$

$$+ I_{df} \sum_i \{n_{i\uparrow}^{(d)} n_{j\downarrow}^{(f)} + n_{i\downarrow}^{(d)} n_{i\uparrow}^{(f)}\} \tag{2}$$

Then the Hamiltonian for the system is:

$$\mathcal{H} = \mathcal{H}_o + \mathcal{H}_{ext} \tag{3}$$

Now we calculate the one-electron propagators $g_{ij}^{dd}(\omega) = \langle\langle d_{i\sigma}; d_{j\sigma}^{+} \rangle\rangle_\omega$ and

$g_{ij}^{ff} = \langle\langle f_{i\sigma}; f_{j\sigma}^{+} \rangle\rangle_{\omega}$ to first order in the external magnetic field [4]. Since Coulomb correlations are present in the actinide metals, one needs some type of approximate treatment. Here we adopt the simplest one, namely the Hartree-Fock approximation, which supposes that Coulomb correlations are small relatively to band widths. An opposite limit (narrow bands), should to discussed within a Hubbard like approximation [5]. The first order correction to the one electron propagators as defined by:

$$g_{ij}^{\alpha\alpha}(\omega) = g_{ij}^{\alpha\alpha(o)}(\omega) + g_{ij}^{\alpha\alpha(1)}(\omega), \quad \alpha = d,f \tag{4}$$

satisfy the following equations of motion:

$$\omega\, g_{ij}^{dd(1)}(\omega) = \sum_{\ell} T_{i\ell}^{(d)}\; g_{\ell j}^{dd(1)}(\omega) + (U_d \langle n_{-\sigma}^{d}\rangle + I_{df}\langle n_{-\sigma}^{f}\rangle) g_{ij}^{dd(1)}(\omega) +$$

$$+ \sum_{\ell} V_{df}(R_i - R_\ell) g_{\ell j}^{fd(1)}(\omega) + h_o\sigma\, e^{-iq\cdot R_i}\; g_{ij}^{dd(o)}(\omega) + (U_d\, \Delta n_{i-\sigma}^{(d)} + I_{df}\, \Delta n_{i-\sigma}^{(f)}) g_{ij}^{dd(o)}(\omega) \tag{5-a}$$

$$\omega\, g_{ij}^{fd(1)}(\omega) = \sum_{\ell} T_{i\ell}^{(f)}\; g_{\ell j}^{fd(1)}(\omega) + (U_f \langle n_{-\sigma}^{f}\rangle + I_{df}\langle n_{-\sigma}^{d}\rangle) g_{ij}^{fd(1)}(\omega) +$$

$$+ \sum_{\ell} V_{fd}(R_i - R_\ell) g_{\ell j}^{dd(1)}(\omega) + h_o\sigma\, e^{-iq\cdot R_i}\; g_{ij}^{fd(o)}(\omega) + (U_f\, \Delta n_{i-\sigma}^{(f)} + I_{df}\, \Delta n_{i-\sigma}^{(d)}) g_{ij}^{fd(o)}(\omega) \tag{5-b}$$

In equations (5) $\langle n_{-\sigma}^{d}\rangle$ and $\langle n_{-\sigma}^{f}\rangle$ are the d and f occupation numbers in the absence of the external magnetic field, and should be self-consistently determined from the zero-order one-electron propagators (cf. below). The fluctuations in occupation numbers ($\Delta n_{i-\sigma}^{(d)}$ and $\Delta n_{i-\sigma}^{(f)}$) are to be self-consistently calculated from the first order propagators [4].

II. SELF-CONSISTENCY PROBLEM: DETERMINATION OF THE SUSCEPTIBILITIES

Now we solve the coupled system [5] by Fourier transformation in the spatial variables; introducing the Hartree-Fock d and f energies:

$$E^{(d)}_{k\sigma} = \varepsilon^{(d)}_k + U_d \langle n^d_{-\sigma}\rangle + I_{df} \langle n^f_{-\sigma}\rangle$$

$$E^{(f)}_{k\sigma} = \varepsilon^{(f)}_k + U_f \langle n^f_{-\sigma}\rangle + I_{df} \langle n^d_{-\sigma}\rangle \qquad (6)$$

one gets the following equations of motion:

$$(\omega - E^{(d)}_{k\sigma}) g^{dd(1)}_{kk'}(\omega) = V_{df}(k) g^{fd(1)}_{kk'}(\omega) + h_o \sigma \delta_{k-q,k'} g^{dd(o)}_{k'}(\omega)$$

$$+ (U_d \Delta n^{-\sigma(d)}_{kk'} + I_{df} \Delta n^{-\sigma(f)}_{kk'}) g^{dd(o)}_{k'}(\omega) \qquad (7\text{-a})$$

and

$$(\omega - E^{(f)}_{k\sigma}) g^{fd(1)}_{kk'}(\omega) = V_{fd}(k) g^{dd(1)}_{kk'}(\omega) + h_o \sigma \delta_{k-q,\,k'} g^{fd(o)}_{k'}(\omega)$$

$$+ (U_f \Delta n^{-\sigma(f)}_{kk'} + I_{df} \Delta n^{-\sigma(d)}_{kk'}) g^{fd(o)}_{k'}(\omega). \qquad (7\text{-b})$$

Combining equations (7) one gets for the d-propagator:

$$\left\{\omega - E^{(d)}_{k\sigma} - \frac{|V_{df}(k)|^2}{\omega - E^{(f)}_{k\sigma}}\right\} g^{dd(1)}_{kk'}(\omega) = (h_o \sigma \delta_{k-q,k'} + U_d \Delta n^{-\sigma(d)}_{kk'} + I_{df} \Delta n^{-\sigma(f)}_{kk'}) g^{dd(o)}_{k'}(\omega)$$

$$+ \frac{1}{\omega - E^{(f)}_{k\sigma}} (h_o \sigma \delta_{k-q,k'} + U_f \Delta n^{-\sigma(f)}_{kk'} + I_{df} \Delta n^{-\sigma(d)}_{kk'}) V_{df}(k) g^{fd(o)}_{k'}(\omega) \qquad (8)$$

Now one needs the zero order propagators in order that (8) provide the full answer for the first order correction. The equations of motion for zero-order propagators are:

$$\omega\, g_{ij}^{dd(o)}(\omega) = \frac{1}{2\pi}\delta_{ij} + \sum_{\ell} T_{i\ell}^{(d)}\, g_{\ell j}^{dd(o)}(\omega) + (U_d\langle n_{-\sigma}^{d}\rangle + I_{df}\langle n_{-\sigma}^{f}\rangle) g_{ij}^{dd(o)}(\omega)$$

$$+ \sum_{\ell} V_{df}(R_i - R_\ell) g_{\ell j}^{fd(o)}(\omega) \qquad (9\text{-a})$$

$$\omega\, g_{ij}^{fd(o)}(\omega) = \sum_{\ell} T_{i\ell}^{(f)}\, g_{\ell j}^{fd(o)}(\omega) + (U_f\langle n_{-\sigma}^{f}\rangle + I_{df}\langle n_{-\sigma}^{d}\rangle) g_{ij}^{fd(o)}(\omega)$$

$$+ \sum_{\ell} V_{fd}(R_i - R_\ell) g_{\ell j}^{dd(o)}(\omega) \qquad (9\text{-b})$$

Fourier transforming (9) one has:

$$(\omega - E_{k\sigma}^{(d)}) g_{kk'}^{dd(o)}(\omega) = \frac{1}{2\pi}\delta_{kk'} + V_{df}(k)\, g_{kk'}^{fd(o)}(\omega)$$

$$(\omega - E_{k\sigma}^{(f)}) g_{kk'}^{fd(o)}(\omega) = V_{fd}(k) g_{kk'}^{dd(o)}(\omega) \qquad (10)$$

Then:

$$g_{k'}^{fd(o)}(\omega) = \frac{V_{fd}(k')}{\omega - E_{k'\sigma}^{(f)}}\, g_{k'}^{dd(o)}(\omega) = \frac{1}{2\pi} V_{fd}(k')\bar{g}_{k'}^{dd}(\omega)$$

$$g_{k'}^{dd(o)}(\omega) = \frac{1}{2\pi}\, \frac{\omega - E_{k'\sigma}^{(f)}}{(\omega - E_{k'\sigma}^{(d)})(\omega - E_{k'\sigma}^{(f)}) - |V_{df}(k)|^2} = \frac{1}{2\pi}(\omega - E_{k'\sigma}^{(f)})\bar{g}_{k'}^{dd}(\omega) \qquad (11)$$

Putting (11) into (8) one gets:

$$g_{kk'}^{dd(1)}(\omega) = 2\pi\, g_{k}^{dd}(\omega)(h_{o\sigma}\,\delta_{k-q,k'} + U_d\,\Delta n_{kk'}^{-\sigma(d)} + I_{df}\,\Delta n_{kk'}^{-\sigma(f)})\, g_{k'}^{dd(o)}(\omega)$$

$$+ \frac{1}{2\pi}\bar{g}_{k}^{dd}(\omega)(h_{o\sigma}\,\delta_{k-q,k'} + U_f\,\Delta n_{kk'}^{-\sigma(f)} + I_{df}\,\Delta n_{kk'}^{-\sigma(d)}) V_{df}(k) V_{fd}(k')\bar{g}_{k'}^{dd}(\omega) \qquad (12\text{-a})$$

or introducing $k \to k+q$, $k' \to k$ and remembering that $\Delta n_{kk'}^{-\sigma(\alpha)} = \Delta n_{k-k'}^{-\sigma(\alpha)}$, $\alpha = d,f$ one gets:

$$g^{dd(1)}_{k+q,k}(\omega) = 2\pi\, g^{dd(o)}_{k+q}(\omega)\left\{h_o\sigma + U_d\,\Delta\bar{n}^{\sigma(d)}_q + I_{df}\,\Delta\bar{n}^{\sigma(f)}_q\right\} g^{dd(o)}_k(\omega)$$

$$+ 2\pi\, g^{dd(o)}_{k+q}(\omega) V_{df}(k+q)\,\frac{1}{\omega - E^{(f)}_{K+q\,\sigma}}\left\{h_o\sigma + U_f\,\Delta\bar{n}^{\sigma(f)}_q + I_{df}\,\Delta\bar{n}^{\sigma(d)}_q\right\}\frac{1}{\omega - E^{(f)}_{k\sigma}} V_{fd}(k) g^{dd(o)}_k(\omega) \qquad (12\text{-b})$$

The physical meaning of (12-b) is quite clear. The first term describes intra d-band propagation where an electron of wave vector k scatters to k+q due to the external magnetic field or due to the fluctuations of wave vector q associated to the d electrons (through U_d) and f electrons (through I_{df}). The second term describes d-f mixing effects; a d electron of wave vector k is admixed into the f-band, propagates within it through $1/(\omega - E^{(f)}_{k\sigma})$ and is scattered to k+q. The sources of scattering are those associated to the f-band (h_o, $U_f\ \Delta n^{(f)}_q$ and $I_{df}\,\Delta n^{(d)}_q$). After scattering it propagates within f through $1/(\omega - E^{(f)}_{k+q\sigma})$ and it is admixed back to the d-band through $V_{df}(k+q)$. Quite similarly (or using the symmetry of d and f) one gets (in alternative form):

$$g^{ff(1)}_{k+q,k}(\omega) = \frac{1}{2\pi}\,\bar{g}^{dd}_{k+q}(\omega)(\omega - E^{(d)}_{k+q\sigma})\left\{h_o\sigma + U_f\,\Delta\bar{n}^{\sigma(f)}_q + I_{df}\,\Delta\bar{n}^{\sigma(d)}_q\right\}(\omega - E^{(d)}_{k\sigma})\,\bar{g}^{dd}_k(\omega)$$

$$+ \frac{1}{2\pi}\, V_{fd}(k+q) V_{df}(k)\left\{h_o\sigma + U_d\,\Delta\bar{n}^{\sigma(d)}_q + I_{df}\,\Delta\bar{n}^{\sigma(f)}_q\right\}\bar{g}^{dd}_{k+q}(\omega)\,\bar{g}^{dd}_k(\omega)$$

since $\bar{g}^{dd}_k = \bar{g}^{ff}_k$ (12-c)

Now we introduce the following notation:

$$\chi_d^\sigma(k,q) = \frac{1}{2\pi} F_\omega\left[\bar{g}^{dd}_{k+q}(\omega)(\omega-E^{(f)}_{k+q\sigma})(\omega-E^{(f)}_{k\sigma})\bar{g}^{dd}_{k}(\omega)\right]$$

$$\chi_f^\sigma(k,q) = \frac{1}{2\pi} F_\omega\left[\bar{g}^{dd}_{k+q}(\omega)(\omega-E^{(d)}_{k+q\sigma})(\omega-E^{(d)}_{k\sigma})\bar{g}^{dd}_{k}(\omega)\right] \qquad (13)$$

$$\chi^\sigma_{mix}(k,q) = \frac{1}{2\pi} F_\omega\left[\bar{g}^{dd}_{k+q}(\omega)\ \bar{g}^{dd}_{k}(\omega)\right]$$

where F_ω is defined as usually by $-2\pi i \int_{-\infty}^{+\infty} d\omega\ f(\omega)\left[G(\omega+i\delta)-G(\omega-i\delta)\right]$. Using these definitions and equations (12) one has:

$$\langle d^+_{k\sigma}\ d_{k+q\sigma}\rangle^{(1)} = \left\{h_o\sigma + U_d\ \Delta n_q^{-\sigma(d)} + I_{df}\ \Delta n_q^{-\sigma(f)}\right\}\chi_d^\sigma(k,q)$$
$$+\left\{h_o\sigma + U_f\ \Delta\bar{n}_q^{\sigma(f)} + I_{df}\ \Delta\bar{n}_q^{\sigma(d)}\right\}V_{df}(k+q)V_{fd}(k)\chi^\sigma_{mix}(k,q) \qquad (14\text{-a})$$

$$\langle f^+_{k\sigma}\ f_{k+q\sigma}\rangle^{(1)} = \left\{h_o\sigma + U_f\ \Delta\bar{n}_q^{\sigma(f)} + I_{df}\ \Delta\bar{n}_q^{\sigma(d)}\right\}\chi_f^\sigma(k,q)$$
$$+\left\{h_o\sigma + U_d\ \Delta\bar{n}_q^{\sigma(d)} + I_{df}\ \Delta\bar{n}_q^{\sigma(f)}\right\}V_{fd}(k+q)V_{df}(k)\chi^\sigma_{mix}(k,q) \qquad (14\text{-b})$$

Introducing the definitions:

$$\chi_d^\sigma(q) = \sum_k \chi_d^\sigma(k,q)$$

$$\chi_f^\sigma(q) = \sum_k \chi_f^\sigma(k,q)$$

and the mixing contributions

$$\chi_d^{\sigma\ mix}(q) = \sum_k V_{df}(k+q)\ V_{fd}(k)\ \chi^\sigma_{mix}(k,q)$$

$$\chi_f^{\sigma mix}(q) = \sum_k V_{fd}(k+q)\chi^\sigma_{mix}(k,q)\ V_{df}(k)$$

one has:

$$\Delta n_q^{\sigma(d)} = h_o\sigma \left\{\chi_d^{\sigma}(q) + \chi_d^{\sigma\ mix}(q)\right\} + \Delta\bar{n}_q^{\sigma(d)}\left\{ U_d\ \chi_d^{\sigma}(q) + I_{df}\ \chi_d^{\sigma\ mix}(q)\right\}$$
$$+ \Delta\bar{n}_q^{\sigma(f)}\left\{I_{df}\ \chi_d^{\sigma}(q) + U_f\ \chi_d^{\sigma\ mix}(q)\right\} \qquad (15\text{-a})$$

Quite similarly:

$$\Delta n_q^{\sigma(f)} = h_o\sigma \left\{\chi_f^{\sigma}(q) + \chi_f^{\sigma\ mix}(q)\right\} + \Delta n_q^{-\sigma(f)}\left\{U_f\ \chi_f^{\sigma}(q) + I_{df}\ \chi_f^{\sigma\ mix}(q)\right\}$$
$$+ \Delta n_q^{-\sigma(d)}\left\{I_{df}\ \chi_f^{\sigma}(q) + U_d\ \chi_f^{\sigma\ mix}(q)\right\} \qquad (15\text{-b})$$

Now we introduce effective values of Coulomb interactions, namely:

$$U_d^{eff}(q) = U_d\left\{1 + \frac{I_{df}}{U_d}\ \frac{\chi_d^{\sigma\ mix}(q)}{\chi_d^{\sigma}(q)}\right\}$$

$$U_f^{eff}(q) = U_f\left\{1 + \frac{I_{df}}{U_f}\ \frac{\chi_f^{\sigma\ mix}(q)}{\chi_f^{\sigma}(q)}\right\}$$

$$I_{df}^{(d)}(q) = I_{df}\left\{1 + \frac{U_f}{I_{df}}\ \frac{\chi_d^{\sigma\ mix}(q)}{\chi_d^{\sigma}(q)}\right\} \qquad (16)$$

and finally:

$$I_{df}^{(f)}(q) = I_{df}\left\{1 + \frac{U_d}{I_{df}}\ \frac{\chi_f^{\sigma\ mix}(q)}{\chi_f^{\sigma}(q)}\right\}$$

Then equations (15) can be written as:

$$\Delta n_q^{\sigma(d)} = h_o\sigma\left\{\chi_d^\sigma(q) + \chi_d^{\sigma\ mix}(q)\right\} + \Delta\bar{n}_q^{\sigma(d)}\ U_d^{eff}(q)\ \chi_d^\sigma(q) + \Delta\bar{n}_q^{\sigma(f)} I_{df}^{(d)}(q)\chi_d^\sigma(q)$$

$$\Delta n_q^{\sigma(f)} = h_o\sigma\left\{\chi_f^\sigma(q) + \chi_f^{\sigma\ mix}(q)\right\} + \Delta\bar{n}_q^{\sigma(f)} U_f^{eff}(q)\chi_f^\sigma(q) + \Delta\bar{n}_q^{\sigma(d)}\ I_{df}^{(f)}(q)\ \chi_f^\sigma(q) \qquad (17)$$

Now consider the paramagnetic phase; all spins dependence in the susceptibility disappears and as far the external field is concerned one has [4]:

$$\Delta\bar{n}_q^{\sigma(\alpha)} = -\Delta n_q^{\sigma(\alpha)}, \quad \alpha = d,f$$

Introducing $\tilde{\chi}_{(\alpha)}(q) = \chi_{(\alpha)}(q) + \chi_{(\alpha)}^{\ mix}(q)$, $\alpha = d,f$ one has from (17)

$$\Delta n_q^{\sigma(d)}\left\{1+U_{eff}^{(d)}(q)\ \chi_d(q)\right\} = h_o\sigma\ \tilde{\chi}_d(q) - \Delta n_q^{\sigma\ (f)}\ I_{df}^{(d)}(q)\ \chi_d(q)$$

$$\Delta n_q^{\sigma(f)}\left\{1 + U_{eff}^{(f)}(q)\ \chi_f(q)\right\} = h_o\sigma\ \tilde{\chi}_f(q) - \Delta n_q^{\sigma(d)}\ I_{df}^{(f)}(q)\ \chi_f(q) \qquad (18)$$

From equations (18) one finally gets:

$$\Delta n_q^{\sigma(d)} = h_o\sigma\ \frac{\tilde{\chi}_d + U_{eff}^{(f)}\ \tilde{\chi}_d\ \chi_f - I_{df}^{(d)}(q)\ \chi_d(q)\ \tilde{\chi}_f(q)}{(1+U_{eff}^{(d)}(q)\chi_d(q))(1+U_{eff}^{(f)}(q)\chi_f(q)) - I_{df}^{(d)}(q)I_{df}^{(f)}(q)\chi_d(q)\chi_f(q)} \qquad (19)$$

and a quite similar expression for $\Delta n_q^{\sigma(f)}$ (interchanging d with f) but with the same denominator as (19).

From expression (19) one sees that the role of V_{df} hybridization is two fold:

i) Firstly it introduces effective Coulomb interactions $U_{eff}^{(d)}(q)$, $U_{eff}^{(f)}(q)$ and $I_{df}^{(\alpha)}(q)$, $\alpha = d,f$ which reduce to their "bare" values when V_{df} tends to zero.

ii) Secondly the susceptibilities χ_d and χ_f are d-f renormalized susceptibilities, with predominantly d and f character respectively.

It should be emphasized that although the Coulomb interactions are q-independent, due to the existence of mixing and of the I_{df} coupling the effective interactions become q dependent.

Now it is interesting to consider some limiting cases. Consider firstly the case where mixing is zero; equation (19) reduces to:

$$\Delta n_q^{\sigma(d)}(V_{df}=0) = h_o\,\sigma\,\frac{\chi_d^{(o)}(q)(1+U_f\,\chi_f^{(o)}(q))-I_{df}\,\chi_d^{(o)}(q)\,\chi_f^{(o)}(q)}{(1+U_d\,\chi_d^{(o)}(q))(1+U_f\,\chi_f^{(o)}(q))-I_{df}^2\,\chi_d^{(o)}(q)\,\chi_f^{(o)}(q)}$$

which in the absence of interband Coulomb repulsion reduces to the usual result:

$$\Delta n_q^{\sigma(d)}(V_{df}=I_{df}=0) = h_o\sigma\,\frac{\chi_d^{(o)}(q)}{1+U_d\,\chi_d^{(o)}(q)}$$

Another interesting case corresponds to $I_{df}=0$ but non vanishing hybridization; one gets:

$$\Delta n_q^{\sigma(d)}(I_{df}=0)=h_o\,\sigma\,\frac{\tilde{\chi}_d(1+U_f\,\chi_f(q))-U_f\,\chi_d^{mix}(q)\,\tilde{\chi}_f(q)}{(1+U_d\,\chi_d(q))(1+U_f\,\chi_f(q))-U_d\,U_f\,\chi_d^{mix}(q)\,\chi_f^{mix}(q)}$$

where two band effects are present due to the coupled effect of mixing and U_f.

Next step is to explicitly calculate the involved susceptibilities as defined in equations (13). The explicit form of $\chi_d(k,q)$ is given by:

$$\chi_d(k,q) = \frac{1}{2\pi} F_\omega \left[\frac{\omega - E_{k+q}^{(f)}}{(\omega - E_{k+q}^{(1)})(\omega - E_{k+q}^{(2)})} \times \frac{\omega - E_k^{(f)}}{(\omega - E_k^{(1)})(\omega - E_k^{(2)})} \right] \tag{20-a}$$

where $E_k^{(1)}$ and $E_k^{(2)}$ are the roots of

$$(\omega - E_k^{(d)})(\omega - E_k^{(f)}) - |V_{df}(k)|^2 = 0 \tag{20-b}$$

Incidentally one notes that in the absence of d-f hybridization, equation (20-a) reduces to

$$\chi_d^{(o)}(k,q) = \frac{1}{2\pi} F_\omega \left[\frac{1}{\omega - E_{k+q}^{(d)}} \cdot \frac{1}{\omega - E_k^{(d)}} \right] = \frac{f(E_{k+q}^{(d)}) - f(E_k^{(d)})}{E_{k+q}^{(d)} - E_k^{(d)}}$$

which is the usual d-like susceptibility, the same occuring for $\chi_f^{(o)}(k,q)$. We expect then for (20-a) that the main contribution arises from d-like electron-hole pairs. Now the final form of the susceptibility $\chi_d(k,q)$ is obtained separating the bracketed terms in (20-a) in partial fractions; one gets:

$$\chi_d(k,q) = \sum_{\mu,\nu=1}^{2} (-1)^{\mu+\nu} \frac{(E_{k+q}^{(\mu)} - E_{k+q}^{(f)})(E_{k+q}^{(\mu)} - E_k^{(f)}) f(E_{k+q}^{(\mu)}) - (E_k^{(\nu)} - E_{k+q}^{(f)})(E_k^{(\nu)} - E_k^{(f)}) f(E_k^{(\nu)})}{(E_{k+q}^{(1)} - E_{k+q}^{(2)})(E_k^{(1)} - E_k^{(2)})(E_{k+q}^{(\mu)} - E_k^{(\nu)})} \tag{21}$$

A quite similar expression can be obtained for $\chi_f(k,q)$ just by replacing in (21) $E_k^{(f)}$ by $E_k^{(d)}$ where it appears. Finally the "susceptibility" $\chi_{mix}(k,q)$ is given by:

$$\chi_{mix}(k,q) = \sum_{\mu,\nu=1}^{2} (-1)^{\mu+\nu} \frac{f(E_{k+q}^{(\mu)}) - f(E_k^{(\nu)})}{(E_{k+q}^{(1)} - E_{k+q}^{(2)})(E_k^{(1)} - E_k^{(2)})(E_{k+q}^{(\mu)} - E_k^{(\nu)})} \tag{22}$$

It should be emphasized at this point that the complete determination of (21) and (22) involve the solution of a self-consistence problem, namely, given the Coulomb repulsions U_d, U_f and I_{df} and the total number of d and f electrons, to find out the value of the chemical potential, and the occupation numbers $\langle n_f \rangle$ and $\langle n_d \rangle$ in presence of the mixing V_{df}. We will return latter to this problem.

III. DISCUSSION OF THE FERROMAGNETIC INSTABILITIES

The general criterion for magnetic instabilities is provided by the poles of (19), or equivalently the roots of:

$$(1+U^{(d)}_{eff}\,\chi_d(q)(1+U^{(f)}_{eff}\,\chi_f(q)) - I^{(d)}_{df}(q)\,I^{(f)}_{df}(q)\,\chi_d(q)\,\chi_f(q) = 0 \quad (23)$$

where q can be zero (ferromagnetic instability), π/a (antiferromagnetic instability) etc.

Here we consider in a certain detail the case of a ferromagnetic instability, namely $q = 0$. The criterion for ferromagnetism is then:

$$(1 + U^{(d)}_{eff}(0)\,\chi_d(0)(1 + U^{(f)}_{eff}(0)\,\chi_f(0)) - I^{(d)}_{df}(0)\,I^{(f)}_{df}(0)\,\chi_d(0)\,\chi_f(0) \leq 0 \quad (24)$$

the equality providing the border line of the ferromagnetic instability. Now we intend to cast equation (23) in a form that can be compared to Stoner's criterion for ferromagnetism. Suppose one wants to emphasize the f-electrons; equation (23) can be written in a quite suggestive way:

$$(1 + U^{(d)}_{eff}(q)\,\chi_d(q))(1 + U^{(f)}_{eff}(q)\,\chi_f(q)) - I^{(d)}_{df}(q)\,I^{(f)}_{df}\,\chi_d(q)\,\chi_f(q) = 1 + J^{(f)}_{eff}(q)\,\chi_f(q) \quad (25\text{-a})$$

where the effective "exchange interaction" among f electrons, $J^{(f)}_{eff}(q)$ is defined as:

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

$$+ I_{df} \frac{\chi_f^{mix}(q) + \chi_d^{mix}(q)}{\chi_f(q)} \qquad (25\text{-b})$$

and the criterion for magnetic instabilities of wave vector q reads:

$$1 + J^{(f)}_{eff}(q)\, \chi_f(q) \leq 0 \qquad (25\text{-c})$$

Now we specialize equations (25) to the case of a ferromagnetic instability· then one needs explicit expressions for $J^{(f)}_{eff}(0)$ and $\chi_f(0)$. According to (25) this amonts in calculating $\chi_d(0)$, $\chi_f(0)$ and $\chi_{(i)}^{mix}(0)$. It is important to emphasize that in the limiting process ($q \to 0$) one must consider separately the terms in (21) and (22) with $\mu \neq \nu$ and $\mu = \nu$. In (21) the terms with $\mu = \nu$ give:

$$\lim_{q\to 0} (-1)^{2\mu} \frac{(E^{(\mu)}_k - E^{(f)}_{k+q})(E^{(\mu)}_k - E^{(f)}_k)\left[f(E^{(\mu)}_{k+q}) - f(E^{(\mu)}_k)\right]}{(E^{(1)}_{k+q} - E^{(2)}_{k+q})(E^{(1)}_k - E^{(2)}_k)(E^{(\mu)}_{k+q} - E^{(\mu)}_k)}$$

$$\lim_{q\to 0} (-1)^{2\mu} \frac{(E^{(\mu)}_{k+q} - E^{(f)}_{k+q})(E^{(\mu)}_{k+q} - E^{(f)}_k) - (E^{(\mu)}_k - E^{(f)}_{k+q})(E^{(\mu)}_k - E^{(f)}_k)}{(E^{(1)}_{k+q} - E^{(2)}_{k+q})(E^{(1)}_k - E^{(2)}_k)(E^{\mu}_{k+q} - E^{(\mu)}_k)} f(E^{(\mu)}_{k+q})$$

Now the first term of (26) can be trivially calculated to give:

$$(-1)^{2\mu}\left(\frac{E_k^{(\mu)} - E_k^{(f)}}{E_k^{(1)} - E_k^{(2)}}\right)^2 f'(E_k^{(\mu)}), \quad \text{where } f'(\varepsilon) = \frac{df}{d\varepsilon} \tag{27-a}$$

The numerator of the second term in (26) can be written as:

$$(E_{k+q}^{(\mu)} + E_k^{(\mu)} - E_{k+q}^{(f)} - E_k^{(f)})(E_{k+q}^{(\mu)} - E_k^{(\mu)})$$

giving then to the second term of (26)

$$(-1)^{2\mu}\, 2\, \frac{E_k^{(\mu)} - E_k^{(f)}}{(E_k^{(1)} - E_k^{(2)})^2}\, f(E_k^{(\mu)}) \tag{27-b}$$

Then the total contribution of the $\mu = \nu$ term in (21) is:

$$(-1)^{2\mu}\left\{\left(\frac{E_k^{(\mu)} - E_k^{(f)}}{E_k^{(1)} - E_k^{(2)}}\right)^2 f'(E_k^{(\mu)}) + 2\,\frac{E_k^{(\mu)} - E_k^{(f)}}{(E_k^{(1)} - E_k^{(2)})^2}\, f(E_k^{(\mu)})\right\} \tag{28-a}$$

The $\mu \neq \nu$ terms in (21) give:

$$(-1)^{\mu+\nu}\,\frac{(E_k^{(\mu)} - E_k^{(f)})^2 f(E_k^{(\mu)}) - (E_k^{(\nu)} - E_k^{(f)})^2\, f(E_k^{\nu})}{(E_k^{(1)} - E_k^{(2)})^2\,(E_k^{(\mu)} - E_k^{(\nu)})} \tag{28-b}$$

Finally the explicit expression for $\chi_d(0)$ is:

$$\chi_d(0) = \sum_k \left\{ \left(\frac{E_k^{(1)} - E_k^{(f)}}{E_k^{(1)} - E_k^{(2)}} \right)^2 f'(E_k^{(1)}) + \left(\frac{E_k^{(2)} - E_k^{(f)}}{E_k^{(1)} - E_k^{(2)}} \right)^2 f'(E_k^{(2)}) \right\}$$

$$+ 2 \sum_k \left\{ \frac{E_k^{(1)} - E_k^{(f)}}{(E_k^{(1)} - E_k^{(2)})^2} f(E_k^{(1)}) + - \frac{E_k^{(2)} - E_k^{(f)}}{(E_k^{(1)} - E_k^{(2)})^2} f(E_k^{(2)}) \right\}$$

$$- 2 \sum_k \left\{ \frac{(E_k^{(1)} - E_k^{(f)})^2 f(E_k^{(1)}) - (E_k^{(2)} - E_k^{(f)})^2 f(E_k^{(2)})}{(E_k^{(1)} - E_k^{(2)})^3} \right\} \qquad (29)$$

A quite similar expression can be obtained for $\chi_f(0)$ just by replacing $E_k^{(f)}$ in (29) by $E_k^{(d)}$. It remains to calculate $\chi_{mix}(k, 0)$ as given by (22); the $\mu = \nu$ terms give:

$$\lim_{q \to 0} (-1)^{2\mu} \frac{f(E_{k+q}^{(\mu)}) - f(E_k^{\mu})}{(E_k^{(1)} - E_k^{(2)})^2 (E_{k+q}^{(\mu)} - E_k^{(\mu)})} = \frac{1}{(E_k^{(1)} - E_k^{(2)})^2} f'(E_k^{(\mu)}) \qquad (30\text{-a})$$

the $\mu \neq \nu$ terms give:

$$(-1)^{\mu+\nu} \lim_{q \to 0} \frac{f(E_{k+q}^{(\mu)}) - f(E_k^{(\nu)})}{(E_k^{(1)} - E_k^{(2)})^2 (E_{k+q}^{(\mu)} - E_k^{(\nu)})} = (-1)^{\mu+\nu} \frac{f(E_k^{(\mu)}) - f(E_k^{(\nu)})}{(E_k^{(1)} - E_k^{(2)})(E_k^{(\mu)} - E_k^{(\nu)})} \qquad (30\text{-b})$$

Using the definitions of χ_d^{mix} and χ_f^{mix} one gets:

$$\chi_d^{mix}(0) = \chi_f^{mix}(0) = \sum_k |V_{df}(k)|^2 \left\{ \frac{1}{(E_k^{(1)} - E_k^{(2)})^2} \left[f'(E_k^{(1)}) + f'(E_k^{(2)}) \right] \right.$$

$$\left. - 2 \frac{f(E_k^{(1)}) - f(E_k^{(2)})}{(E_k^{(1)} - E_k^{(2)})^3} \right\} \qquad (31)$$

Equations (29) and (31) complete the determination of $\chi_f(0)$ and of $J_{eff}(0)$, and consequently the criterion of ferromagnetism. It remains only to determine the chemical potential which appears in $f(E_k^{(i)})$ and the Hartree-Fock renomalized energies, which in the paramagnetic phase are:

$$E_k^{(d)} = \varepsilon_k^{(d)} + U_d \langle n_d \rangle + I_{df} \langle n_f \rangle$$

$$E_k^{(f)} = \varepsilon_k^{(d)} + U_f \langle n_f \rangle + I_{df} \langle n_d \rangle \qquad (32)$$

At this point we adopt a simplifying approximation which consists in taking the Coulomb interactions approximately equal, namely

$$U_d \cong U_f \cong I_{df} \qquad (33)$$

In rare-earths, where the f level is quite localized, (33) is not a quite good, but we expect that in actinides this approximation may be reasonable. In any case, we use (33) only in order to simplify the mathematics of the self-consistency problem. The general case $U_d \neq U_f \neq I_{df}$ may be discussed in a similar but much more complicated way. Using (33) the effective "exchange" interaction is:

$$J_{eff}^{(f)}(0) = U_f \left\{ 1 + \frac{\chi_d(0)}{\chi_f(0)} + 2 \frac{\chi_d^{mix}(0)}{\chi_f(0)} \right\} \qquad (34)$$

and what one needs is $J_{eff}^{(f)}(0)$ as a function of the band structure $(\varepsilon_k^{(d)}, \varepsilon_k^{(f)})$, the mixing matrix elements $|V_{df}(k)|^2$ and the number of electrons. From (29), (31) and (20-b) one sees that it remains only to determine the energies (32), the chemical potential μ and to obtain formal expressions for the energies $E_k^{(i)}$, $i = 1, 2$.

Using approximation (33) and introducing n_o^d and n_o^f as the number of d and f electrons (of both spins) and $n = n_o^d + n_o^f$ one has:

$$E_k^{(d)} = \varepsilon_k^{(d)} + \frac{U_f}{2}(n_o^d + n_o^f) = \varepsilon_k^{(d)} + \frac{U_f}{2} n$$

$$E_k^{(f)} = \varepsilon_k^{(f)} + \frac{U_f}{2}(n_o^d + n_o^f) = \varepsilon_k^{(f)} + \frac{U_f}{2} n \qquad (35)$$

Incidentally one notes that from (35) that

$$E_k^{(d)} + E_k^{(f)} = \varepsilon_k^{(d)} + \varepsilon_k^{(f)} + U_f n \qquad (36\text{-a})$$

and

$$E_k^{(d)} - E_k^{(f)} = \varepsilon_k^{(d)} - \varepsilon_k^{(f)}$$

which imply that the solutions of (20-b) are of the form;

$$E_k^{(i)} = \frac{1}{2}\left\{\varepsilon_k^{(d)} + \varepsilon_k^{(f)} + U_f n \mp \Delta_k\right\} \quad i = 1, 2 \qquad (36\text{-b})$$

where

$$\Delta_k = \left\{(\varepsilon_k^{(d)} - \varepsilon_k^{(f)})^2 + 4|V_{df}(k)|^2\right\}^{1/2}$$

Now we determine the chemical potential μ; in order perform this one imposes:

$$\frac{n}{2} = \langle n_d \rangle + \langle n_f \rangle = \sum_k \left\{\langle n_k^d \rangle + \langle n_k^f \rangle\right\} \qquad (37)$$

The occupation numbers are directly obtained from the one electron

propagators $g_k^{dd(o)}(\omega)$ and $g_k^{ff(o)}(\omega)$, which in the Hartree-Fock approximation used are given by:

$$g_k^{dd(o)}(\omega) = \frac{1}{2\pi} \frac{\omega - E_k^{(f)}}{(\omega-E_k^{(d)})(\omega-E_k^{(f)})-|V_{df}(k)|^2} = \frac{1}{2\pi} \frac{\omega - E_k^{(f)}}{(\omega-E_k^{(1)})(\omega-E_k^{(2)})} \qquad (38\text{-a})$$

and

$$g_k^{ff(o)}(\omega) = \frac{1}{2\pi} \frac{\omega - E_k^{(d)}}{(\omega-E_k^{(d)})(\omega-E_k^{(f)})-|V_{df}(k)|^2} = \frac{1}{2\pi} \frac{(\omega-E_k^{(d)})}{(\omega-E_k^{(1)})(\omega-E_k^{(2)})} \qquad (38\text{-b})$$

The occupation numbers follow directly from (38) using

$$\langle n^{(i)} \rangle = \sum_k \langle n_k^{(i)} \rangle = -2\pi i \int_{-\infty}^{+\infty} f(\omega) \left[g_k^{ii}(\omega+i\delta) - g_k^{ii}(\omega-i\delta) \right] d\omega$$

$$i = d,f$$

Performing the calculation one gets:

$$\langle n_d \rangle = \sum_k \langle n_k^d \rangle = \sum_k \frac{(E_k^{(1)} - E_k^{(f)})\, f(E_k^{(1)}) - (E_k^{(2)} - E_k^{(f)})\, f(E_k^{(2)})}{E_k^{(1)} - E_k^{(2)}} \qquad (39)$$

$$\langle n_f \rangle = \sum_k \langle n_k^f \rangle = \sum_k \frac{(E_k^{(1)} - E_k^{(d)})\, f(E_k^{(1)}) - (E_k^{(2)} - E_k^{(d)}) f(E_k^{(2)})}{E_k^{(1)} - E_k^{(2)}}$$

where in order to explicitate the chemical potential we introduce $f_o(E_k^{(i)} - \mu)$, where $f_o(x) = (e^{\beta x} + 1)^{-1}$. Now the condition determining μ(37) can be written:

$$\frac{n}{2} = \sum_k \frac{(2\,E_k^{(1)} - E_k^{(d)} - E_k^{(f)})\, f_o(E_k^{(1)}-\mu) - (2\,E_k^{(2)} - E_k^{(d)} - E_k^{(f)})\, f_o(E_k^{(2)}-\mu)}{E_k^{(1)} - E_k^{(2)}} \qquad (40)$$

Equation (40) can be further simplyfied introducing the results obtained from (36-b), namely:

$$E_k^{(1)} - E_k^{(2)} = -\Delta_k \qquad (41\text{-a})$$

$$E_k^{(1)} - E_k^{(d)} = \frac{\varepsilon_k^{(f)} - \varepsilon_k^{(d)} - \Delta_k}{2}$$

$$E_k^{(2)} - E_k^{(d)} = \frac{\varepsilon_k^{(f)} - \varepsilon_k^{(d)} + \Delta_k}{2} \qquad (41\text{-b})$$

and finally

$$E_k^{(1)} - E_k^{(f)} = \frac{\varepsilon_k^{(d)} - \varepsilon_k^{(f)} - \Delta_k}{2} \qquad (41\text{-c})$$

$$E_k^{(2)} - E_k^{(f)} = \frac{\varepsilon_k^{(d)} - \varepsilon_k^{(f)} + \Delta_k}{2}$$

Introducing equations (41) into (40) one has:

$$\frac{n}{2} = \sum_k \frac{-\Delta_k\, f_o(E_k^{(1)}-\mu) - \Delta_k\, f_o(E_k^{(2)}-\mu)}{-\Delta_k} = \sum_k \left\{ f_o(E_k^{(1)}-\mu) + f_o(E_k^{(2)}-\mu) \right\} \qquad (42)$$

Now we cast equation (42) in a more illustrative way; we rewrite the roots of equation (20-b) as

$$E_k^{(1)} = \frac{\varepsilon_k^{(d)} + \varepsilon_k^{(f)} - \Delta_k}{2} + \frac{U_f}{2} n = \varepsilon_k^{(1)} + \frac{1}{2} U_f n \qquad (43)$$

$$E_k^{(2)} = \frac{\varepsilon_k^{(d)} + \varepsilon_k^{(f)} + \Delta_k}{2} + \frac{U_f}{2} n = \varepsilon_k^{(2)} + \frac{1}{2} U_f n$$

Where $\varepsilon_k^{(1)}$ and $\varepsilon_k^{(2)}$ involve only the band structure details namely $\varepsilon_k^{(d)}$, $\varepsilon_k^{(f)}$ and $|V_{df}(k)|^2$. Then (43) shows explicitly the n-dependence of the energy. The condition determining μ is finally:

$$\frac{n}{2} = \sum_k \left\{ f_o(\varepsilon_k^{(1)} + \frac{1}{2} U_f\, n - \mu) + f_o(\varepsilon_k^{(2)} + \frac{1}{2} U_f n - \mu) \right\} \qquad (44)$$

CONCLUSION AND DISCUSSIONS

In the above calculations the criterion for magnetic instabilities in actinides was obtained within the Hartree-Fock picture. This criterion turns out to be of the same form of Stoner criterion for the one-band problem, but with effective, q dependent "exchange" interaction. It should be emphasized that although Coulomb interactions are described by q-independent parameters, the q-dependence arise from the ratio of the d and f-like susceptibilities and the "mixing" susceptibility. The d-f mixing strength appears in this picture as having two different roles; firstly it contributes in modifying the value of the f-like susceptibility $\chi_f(q)$. A rough idea of this effect (at least for $q = 0$) has been provided by a previous work where the electronic density of states is calculated in the three-band model [6]. One sees that a quite strong effect can be obtained when d-f hybridication is turned on; the density of states of f-like electrons may be considerably changed. Secondly the "effective exchange interaction" may be changed by this effect by changing the d and f susceptibilities and through the $|V_{df}|^2$ coefficient appearing in the definition of $J_{eff}(q)$. Then one expects that if Stoner criterion is satisfied for a non-hybridized band, when mixing is turned on both $J_{eff}(q)$ and $\chi_f(q)$ change, implying in a deviation from the

condition of magnetic instability. All these effects however require a quite detailed numerical investigation and this is the subject of our future work. In the last part of this work, the case of ferromagnetic instability was examined in more detail, and the results are ready for numerical computation. Such a computation involves several steps, namely, the determination of the chemical potential as a function of the number of electrons, the calculation of the involved susceptibilities, and finally the computation of the effective exchange.

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