Screened Exchange Interactions Applied to Spin and Orbital Magnetism

Spin-orbit interaction

Screening of Coulomb interactions

LDA and Exchange integrals

Examples
1.Fe, Co and Ni
2. CeFe2
3.US
4.UFe2

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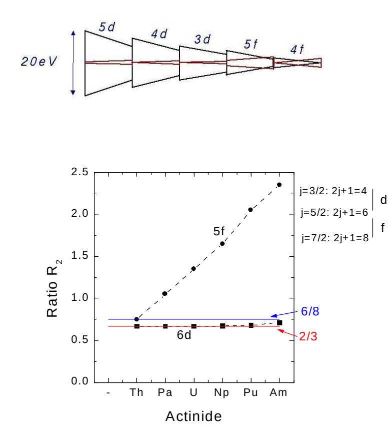
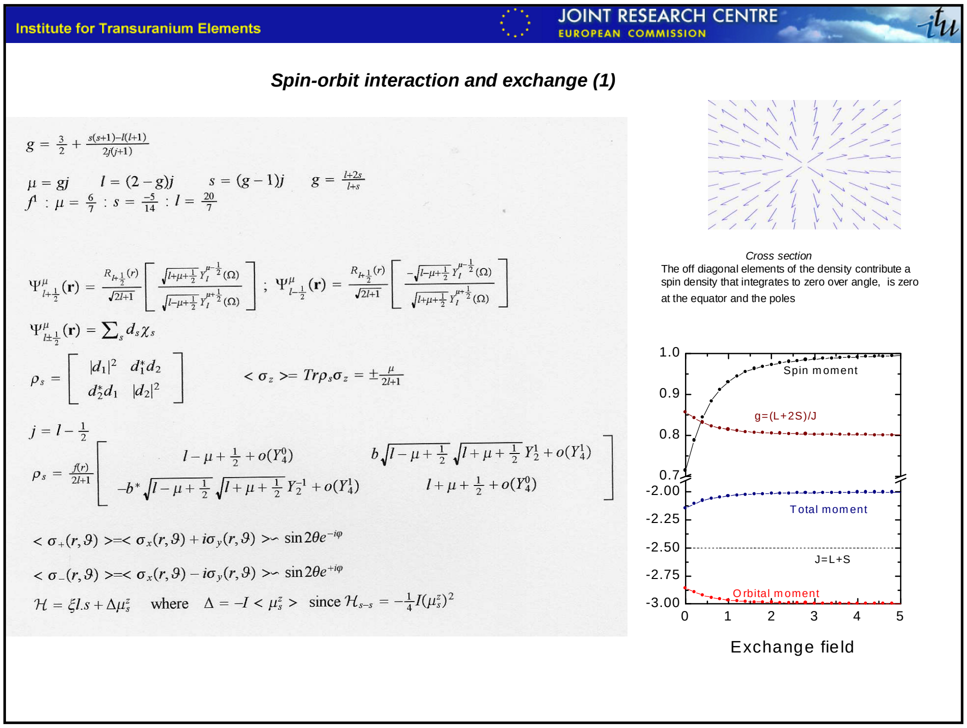
Bandwidth and spin-orbit interaction

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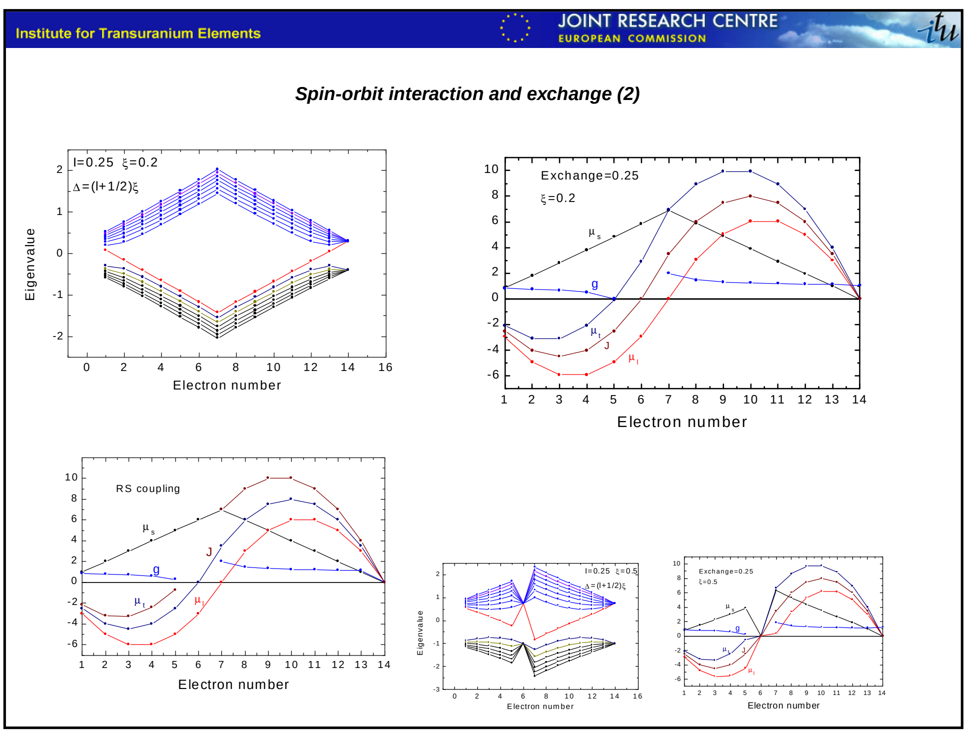
Spin-orbit interaction and exchange (1)
$g = \frac{3}{2} + \frac{s(s+1)-l(l+1)}{2j(j+1)}$
$\mu = gj \quad l = (2-g)j \quad s = (g-1)j \quad g = \frac{l+2s}{l+s}$
$f^1 : \mu = \frac{6}{7} : s = \frac{-5}{14} : l = \frac{20}{7}$
$\rho_s = \begin{bmatrix} |d_1|^2 & d_1^* d_2 \\ d_2^* d_1 & |d_2|^2 \end{bmatrix} \quad < \sigma_z >= Tr\rho_s\sigma_z = \pm\frac{\mu}{2l+1}$
$j = l - \frac{1}{2}$
$\mathcal{H} = \xi l.s + \Delta\mu_s^z$ where $\Delta = -I < \mu_s^z >$ since $\mathcal{H}_{s-s} = -\frac{1}{4}I(\mu_s^z)^2$
Cross section
The off diagonal elements of the density contribute a spin density that integrates to zero over angle, is zero at the equator and the poles
Spin moment
g=(L+2S)/J
Total moment
J=L+S
Orbital moment
Exchange field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Spin-orbit interaction and exchange (2)
I=0.25 ξ=0.2
Δ=(I+1/2)ξ
Eigenvalue
Electron number
Exchange=0.25
ξ=0.2
Electron number
RS coupling
Electron number
I=0.25 ξ=0.5
Exchange=0.25
ξ=0.5

Thomas Fermi screening

When the positive charge background cancels the uniform electron density, ρ_0, and an impurity, Z, is placed at r=0,

$$\nabla^2 V(r) = 8\pi[\delta(r) - \delta\rho(r)]$$

where $\delta\rho(r)$ is the screening density. This equation can be solved if one can find another relationship between V(r) and $\delta\rho(r)$.

(a) Here the total density is used to calculate κ.

$E_F = [3\pi^2\rho_0]^{\frac{2}{3}} = T_0$ is the Fermi energy of the uniform electron since V is zero. With the impurity

$$T(r) + V(r) = E_F$$

$$T(r) = [3\pi^2\rho(r)]^{\frac{2}{3}} = T_0[1 + \tfrac{2}{3}\delta\rho(r) + ...]$$

$$T_0[1 + \tfrac{2}{3}\delta\rho(r) + ...] + V(r) = T_0 \; ; \; \delta\rho(r) = -\frac{3\rho_0}{2T_0}V(r)$$

$$\nabla^2 V(r) = 8\pi\delta(r) + \kappa^2 V(r) \; ; \; \kappa^2 = 8\pi\frac{3\rho_0}{2T_0} = 4(\tfrac{3}{\pi}\rho_0)^{\frac{1}{3}};$$

$$V(r) = -\frac{2Z}{r}e^{-\kappa r}$$

(b) Here the density of states is used to calculate κ

$$\delta\rho(r) = -V(r)\frac{\partial\rho_0(E)}{\partial E}|_{E=E_F} = -V(r)D(E_F)$$

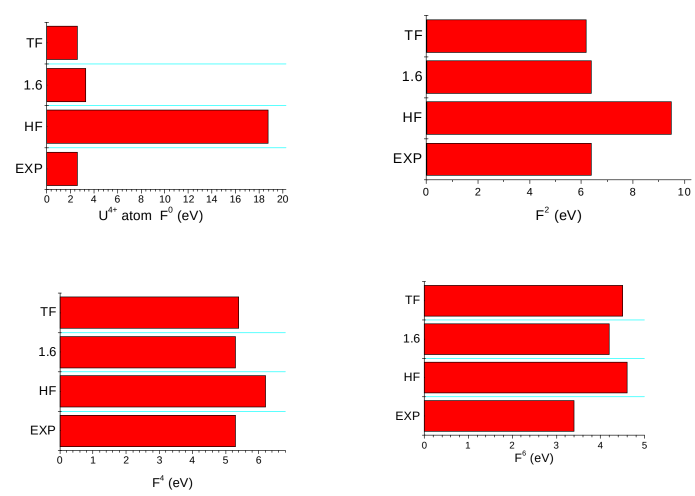
$$D(E_F) = \frac{3\rho_0}{2T_0} \qquad \kappa^2 = 8\pi D(E_F)$$

For the free electron gas, $D(E_F) = \frac{1}{2\pi}(\frac{3}{\pi}\rho_0)^{\frac{1}{3}}$,

$\kappa^2 = 4(\frac{3}{\pi}\rho_0)^{\frac{1}{3}}$. $D_{cell}(E_F) = N(E_F)/V_{cell}$

$D(E_F, r) = \frac{1}{4\pi}\sum N_l(E_F)\phi_l(r)^2 \int r^2\phi_l(r)^2 dr = 1.$

Uranium ion



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Screening of exchange interactions in atoms

$$E_{SP}^{LSDA} = -\frac{1}{4}\sum_{ll'} J_{ll'} m_l m_{l'}.$$

$$E_{SP}^{HFA} = -\frac{1}{4}\sum_{l,l'} V_{ll'} m_l m_{l'}.$$

The exchange integral matrices are

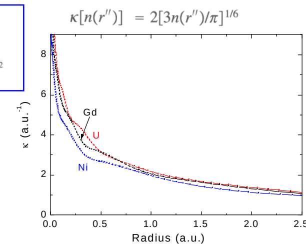
$$J_{ll'} = \frac{2}{3}\int r^2\phi_l^2(r)\phi_{l'}^2(r)A[n(r)]/n(r)dr$$

$$V_{ll'} = \sum_k \begin{pmatrix} l & l' & k \\ 0 & 0 & 0 \end{pmatrix}^2 G^k(ll'll')\ ;$$

$$l+l'+k \ even;\ \begin{pmatrix} ll'0 \\ 000 \end{pmatrix} = 0 \ for\ l \neq l';\ \begin{pmatrix} ll0 \\ 000 \end{pmatrix} = (2l+1)^{-1/2}$$

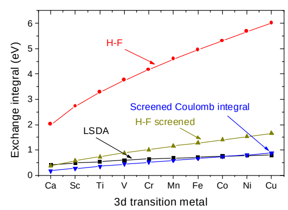
$$V(\mathbf{r},\mathbf{r}') = \frac{e^{-\kappa|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$$

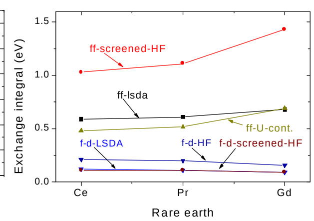
$$\kappa[n(r'')] = 2[3n(r'')/\pi]^{1/6}$$

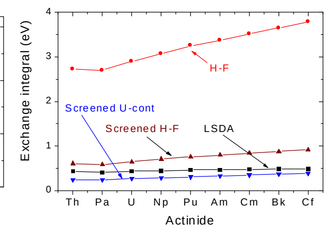


$$V(\mathbf{r},\mathbf{r}') = -\kappa\sum_l (2l+1)j_l(i\kappa r_<)h_l^{(1)}(i\kappa r_>)P_l(cos\theta)$$

$$G^k(ll'll') = -\int\int r^2r'^2 j_k(i\kappa r_<)h_k^{(1)}(i\kappa r_>)R_l(r)R_{l'}(r')R_l(r')R_{l'}(r)\,dr\,dr'$$







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Average exchange interaction for the electron gas

$$E_{int} = \frac{1}{2}\int \frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}[\rho(r_1)\rho(r_2) - \frac{1}{2}\rho^2(r_1,r_2)]dr_1dr_2$$

$$\rho(r_1,r_2) = \rho(R) = \frac{K_F^2}{\pi^2 R}J_1(K_F R)\ ; \quad R = |r_1 - r_2|$$

$$E_{ex}/N = -\frac{e^2K_F^4}{\pi^3\rho}\int^{k_F} J_1^2(x)xdx = -\frac{e^2K_F^4}{4\pi^3\rho}$$

Since $\rho = \frac{k_F^3}{3\pi^2}$; $\mu_x = \frac{d}{d\rho}(\rho E_{ex}/N) = -\frac{e^2}{\pi}(3\pi^2\rho)^{\frac{1}{3}}$

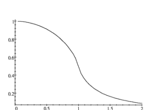
The Hartee-Fock equation

$$[-\nabla^2(1) + V_N(\mathbf{r}_1) + V_H(\mathbf{r}_1) + V_{EX}(r_1)]u_i(\mathbf{r}_1) = \varepsilon_i(\mathbf{r}_1)$$

$$V_{EX}(r_1) = -\frac{\sum_j n_j \int u_i^*(\mathbf{r}_1)u_j^*(\mathbf{r}_2)u_j(\mathbf{r}_1)u_i(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}d\mathbf{r}_2}{u_i^*(\mathbf{r}_1)u_i(\mathbf{r}_1)}$$

$$I_{ij} = \int u_i^*(\mathbf{r}_1)u_j^*(\mathbf{r}_2)u_j(\mathbf{r}_1)u_i(\mathbf{r}_2)\frac{e^2}{|\mathbf{r}_1-\mathbf{r}_2|}d\mathbf{r}_2 = \frac{4\pi}{V^2|k-k'|^2}$$

$$V_{EX}(r_1) = -V\sum_j n_j I_{ij} = -\frac{2e^2k_F}{\pi}F(\eta)\ ;\ \eta = \frac{k}{k_F}$$



$$F(\eta) = \frac{1}{2} + \frac{1-\eta^2}{4\eta}\ln\left|\frac{1+\eta}{1-\eta}\right|$$

$$< F(\eta) > = \frac{3}{4}\ ;\ F(1) = \frac{1}{2}$$

$$< V_{EX}(r_1) > = -\frac{3e^2k_F}{2\pi} = -\frac{3e^2}{2\pi}(3\pi^2\rho)^{\frac{1}{3}}$$

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Role of the Coulomb integral (1)

$$E_{\text{int}} = \frac{e^2}{2}\sum_{i,j}[<ij|\frac{1}{|r-r'|}|ij> - <ij|\frac{1}{|r-r'|}|ji>]n_i n_j$$

The spherical part of $\frac{1}{|r-r'|}$ *is* $\frac{1}{r_>}$

$$E_{\text{int}} = \frac{e^2}{2}F^0\sum_{i,j}[<ij|ij> - <ij|ji>]n_i n_j = \frac{e^2}{2}F^0\sum_{i,j}[n_i n_j - n_i^2\delta_{i,j}]$$

$$\frac{\partial E_{\text{int}}}{\partial n_i} = e^2F^0[n_l - n_i] \quad where \quad n_l = \sum_i n_i$$

$n_i = 1$

LDA+U (1) identifies LDA as the spherical average

$$E_{\text{int}}^{lda} = \frac{e^2}{2}F^0\overline{n}^2N_l(N_l-1) = \frac{e^2}{2}F^0n_l(n_l - \frac{n_l}{N_l}) \quad \text{where } \overline{n} = \frac{n_l}{N_l} \quad \text{and} \quad N_l = 2(2l+1)$$

$$E_1 = E_{lda} - \frac{e^2}{2}F^0\overline{n}^2N_l(N_l-1) + \frac{e^2}{2}F^0\sum_{i,j}[n_in_j - n_i^2\delta_{i,j}] = E_{lda} + \frac{e^2}{2}F^0\sum_{i,j}[n_i-\overline{n}][n_j-\overline{n}] - \frac{e^2}{2}F^0\sum_{i,j}[n_i-\overline{n}]^2$$

$$\frac{\partial E_1}{\partial n_i} = \varepsilon_{lda} + e^2F^0\left[\sum_j[n_j-\overline{n}] - [n_i-\overline{n}]\right]$$

LDA+U (2) identifies LDA as $\frac{e^2}{2}F^0n_l(n_l-1)$

$$E_2 = E_{lda} - \frac{e^2}{2}F^0n_l(n_l-1) + \frac{e^2}{2}F^0\sum_{i,j}[n_in_j - n_i^2\delta_{i,j}] = E_{lda} + \frac{e^2}{2}F^0\sum_i[n_i - n_i^2]$$

$$\frac{\partial E_2}{\partial n_i} = \varepsilon_{lda} + \frac{e^2}{2}F^0[1-2n_i]$$

$n_i = 0$

$n_i = 1$

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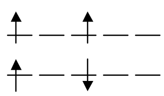
Role of the Coulomb integral (2)

Hydrogen — para — ferro

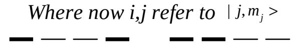
$$E_{\text{int}} = \frac{e^2}{2}F^0\frac{1}{2}*\frac{1}{2}*2 = \frac{e^2}{4}F^0 \qquad E_{\text{int}} = 0$$



Equal energies

e^2F^0

Relativistic case j=5/2, j=7/2 $E_{\text{int}} = \frac{e^2}{2}F^0[n_in_j - n_i^2\delta_{i,j}]$ *Where now i,j refer to* $|j,m_j>$



-3/2 -1/2 1/2 3/2 -3/2 -1/2 1/2 3/2

Equal energies

Polarization and time reversal

$$\rho = \overline{\rho} + \hat{\rho} \qquad R\rho = \overline{\rho} - \hat{\rho}$$

$$\overline{\rho} = (\rho + R\rho)/2 \qquad \hat{\rho} = (\rho - R\rho)/2$$

$$E[\rho] = \frac{e^2}{2}\int dr_1\int dr_2[\rho(r_1)\rho(r_2) - \rho(r_1,r_2)\rho(r_2,r_1)]$$

$$E[\rho] = \frac{e^2}{2}\int dr_1\int dr_2\frac{1}{|r_1-r_2|}[\overline{\rho}(r_1)\overline{\rho}(r_2) - \overline{\rho}(r_1,r_2)\overline{\rho}(r_2,r_1)] \quad \text{LDA}$$

$$-\frac{e^2}{2}\int dr_1\int dr_2\frac{1}{|r_1-r_2|}\hat{\rho}(r_1,r_2)\hat{\rho}(r_2,r_1) \quad \textbf{Polarization}$$

Screened exchange interactions applied to the calculation of spin and orbital moments

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Hubbard approximation

$$E_{ex} = -\frac{e^2}{2}\sum_{k,k'\le k_F}\sum_{\mu,\mu'}\iint dr dr' \Psi_k^{\mu *}(r)\Psi_{k'}^{\mu' *}(r')\frac{1}{|r-r'|}\Psi_k^{\mu}(r')\Psi_{k'}^{\mu'}(r) n_k^{\mu} n_{k'}^{\mu'}$$

Wannier Basis $\Psi_k^{\mu}(r) = \frac{1}{\sqrt{N}}\sum_j e^{ik.R_j} W_{\mu}(r-R_j)$ $\qquad W_{\mu}(r-R_j) = \sum_m c_{\mu,m} W_m(r-R_j)$

Select onsite interaction

$$E_{ex} = -\frac{e^2}{2}\sum_j \sum_{1234} g(1243)\rho_{14}\rho_{23} \qquad \textbf{where} \qquad \rho_{ij} = \sum_{k,\mu}\rho_k^{\mu} c^*_{\mu,i} c_{\mu,j}$$

$$g(1234) = \iint dr dr' W_1^*(r) W_2^*(r')\frac{1}{|r-r'|} W_3(r') W_4(r)$$

One centre expansion

$$E_{ex} = -\frac{e^2}{2}\sum_j \sum_{1234} g(1243)\rho_{14}\rho_{23}$$

$$g(1234) = \iint dr dr' \phi_1^*(r)\phi_2^*(r')\frac{1}{|r-r'|}\phi_3(r')\phi_4(r)$$

$$g(1234) = \delta_{\sigma_1,\sigma_4}\delta_{\sigma_2,\sigma_3}\delta_{m_1+m_2,m_3+m_4}\sum_k F^k c_k(l_1 m_1, l_4 m_4) c_k(l_3 m_3, l_2 m_2)$$

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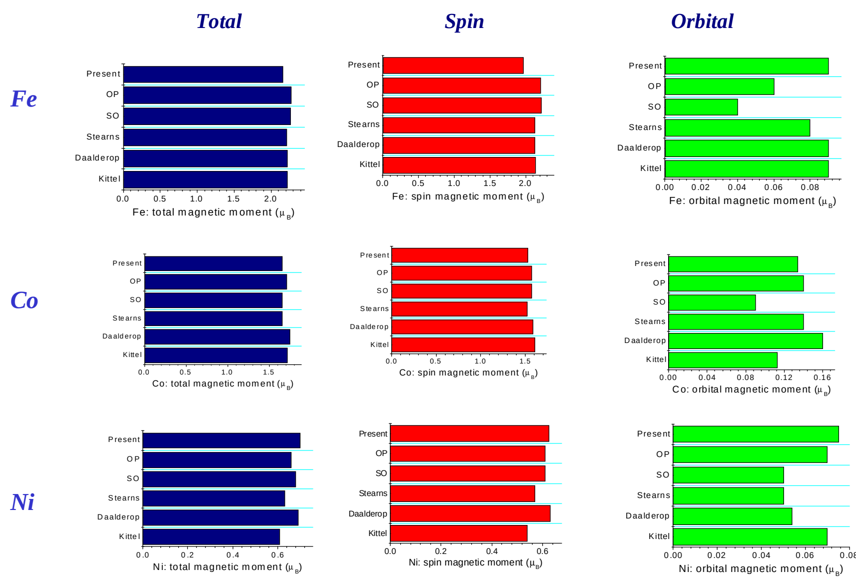
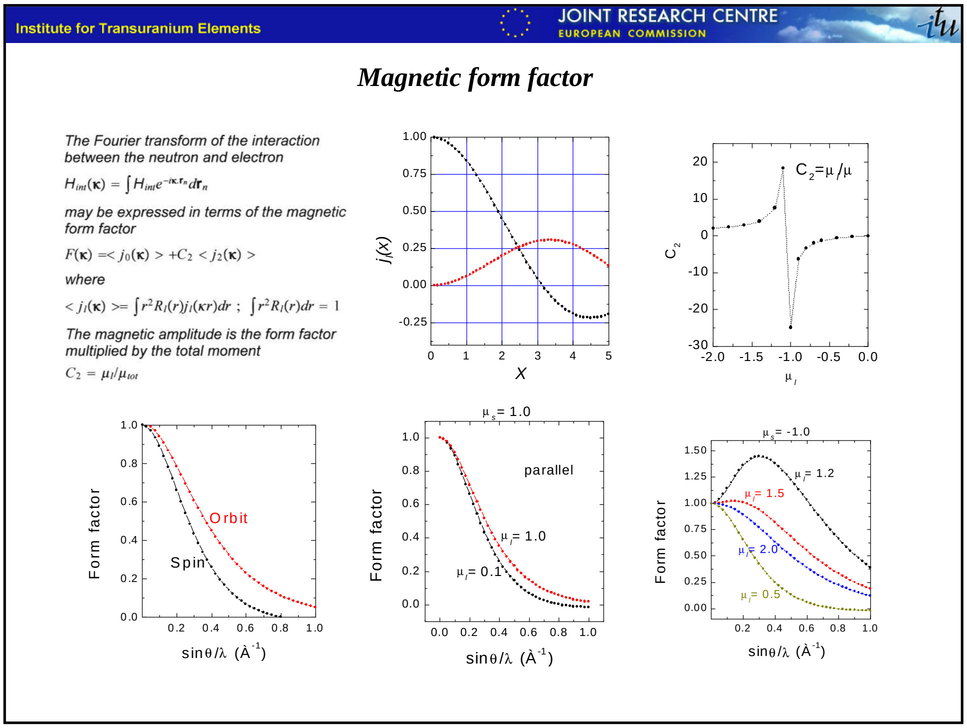
Fe, Co and Ni Magnetic Moments

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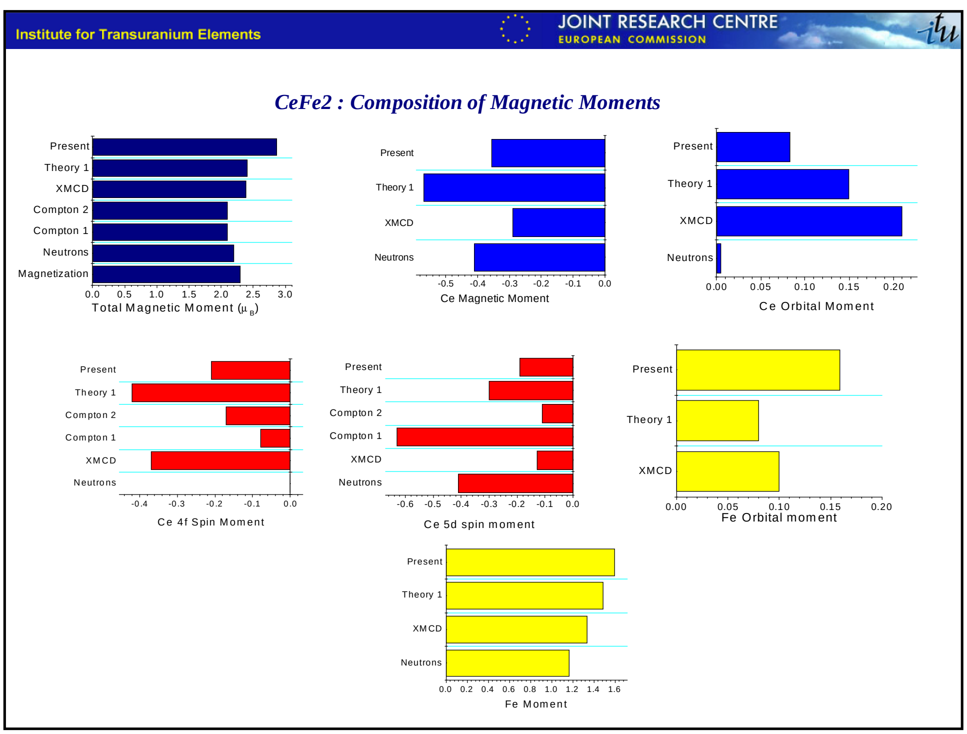
Magnetic form factor
The Fourier transform of the interaction between the neutron and electron
$H_{int}(\mathbf{\kappa}) = \int H_{int} e^{-i\mathbf{\kappa}\cdot\mathbf{r}_n} d\mathbf{r}_n$
may be expressed in terms of the magnetic form factor
$F(\mathbf{\kappa}) = \langle j_0(\mathbf{\kappa}) \rangle + C_2 \langle j_2(\mathbf{\kappa}) \rangle$
where
$\langle j_l(\mathbf{\kappa}) \rangle = \int r^2 R_l(r) j_l(\kappa r) dr \; ; \; \int r^2 R_l(r) dr = 1$
The magnetic amplitude is the form factor multiplied by the total moment
$C_2 = \mu_l / \mu_{tot}$
j(x)
X
$C_2 = \mu_l/\mu$
C_2
μ_l
Form factor
Orbit
Spin
$\sin\theta/\lambda$ (Å^{-1})
$\mu_s = 1.0$
parallel
$\mu_l = 1.0$
$\mu_l = 0.1$
$\mu_s = -1.0$
$\mu_l = 1.2$
$\mu_l = 1.5$
$\mu_l = 2.0$
$\mu_l = 0.5$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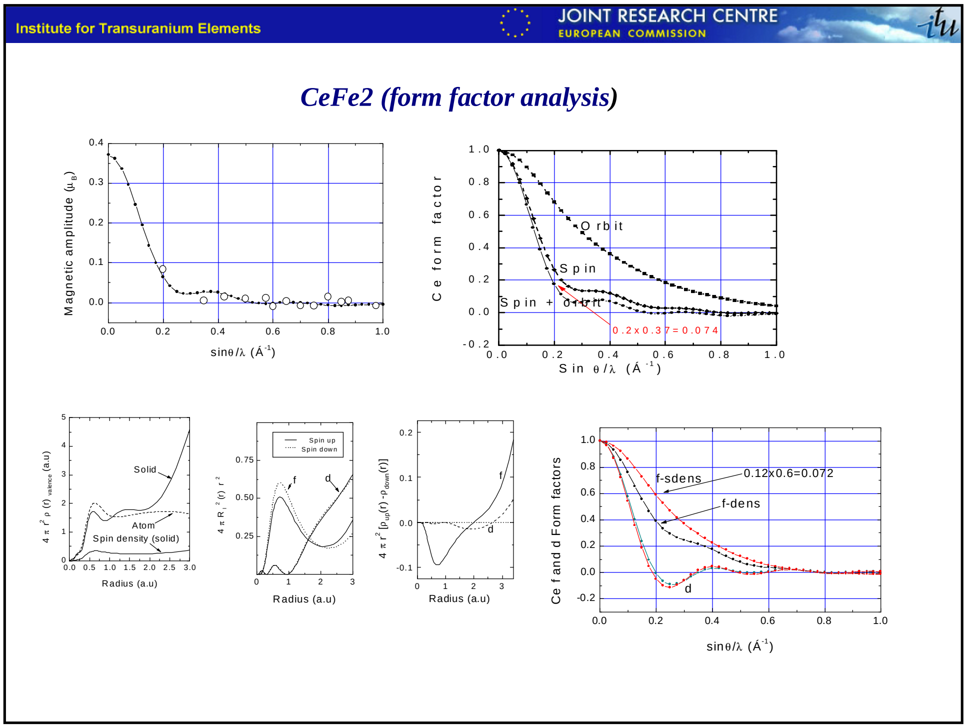
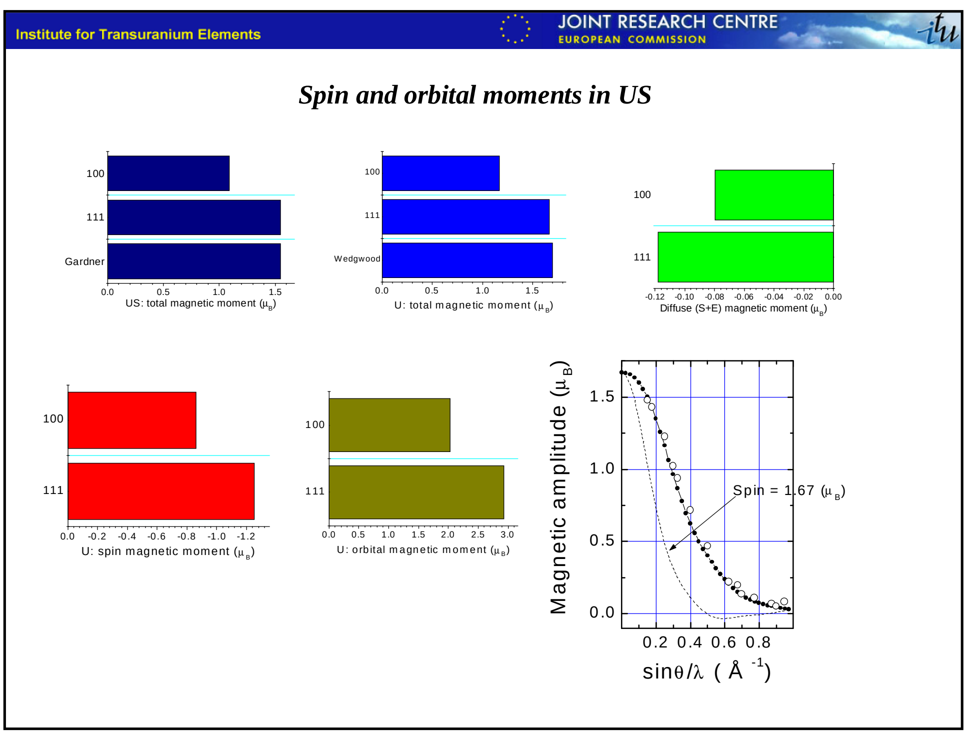
CeFe2 : Composition of Magnetic Moments
Present
Theory 1
XMCD
Compton 2
Compton 1
Neutrons
Magnetization
Total Magnetic Moment (μ_B)
Ce Magnetic Moment
Ce Orbital Moment
Ce 4f Spin moment
Ce 5d spin moment
Fe Orbital moment
Fe Moment

Screened exchange interactions applied to the calculation of spin and orbital moments





Screened exchange interactions applied to the calculation of spin and orbital moments