2

b

$3+$

x

c

xyz

$$xyz||cab$$

$T = 10$

$$T = 2$$

O_{lm}

$\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y)$

a

E_{el}

H_{mix}

$$H_E + H_{int}$$

$$B_2^0$$

$E^1, \ldots, E^6$

$T = 20$

$\hat{I}_a, \hat{I}_b, \hat{I}_c \ldots$

$T =$

$$H = 0$$

4

9

3

m

$$\frac{1}{2}$$

$$m \neq 0$$

$m = 0$

$$\langle J || \theta_l || J \rangle$$

$$\langle L||\theta_l||L\rangle$$

L

d

λ_{lm}

$$\lambda_{lm} \equiv B_l^m/(\theta_l L_l^m) = A_{lm}\langle r^l\rangle/L_l^m$$

p_{lm}

$$\lambda_{l0} = \sqrt{\frac{4\pi}{2l+1}}|p_{l0}|$$

$$\lambda_{lm} = \sqrt{\frac{8\pi}{2l+1}}|p_{lm}|$$

$$B_m^l(\text{Newman}) \equiv (-1)^m L_l^m$$

$m > 0$

$$B_l^m$$

B_l^{-m}

$$B_4^4 = 5B_4^0$$

$$B_6^4 = -21B_6^0$$

$$xyz||abc$$

$$L_4^4 = 5/\sqrt{70}L_4^0$$

$$L_6^4 = -\sqrt{7/2} L_6^0$$

$$B_4^{3_{111}} = -20\sqrt{2}B_4^{0_{111}}$$

$$B_6^{3_{111}} = 35\sqrt{2}/4B_6^{0_{111}}$$

$$B_6^{6_{111}} = 77/8 B_6^{0_{111}}$$

$z||[111]$

$$L_4^{3_{111}} = -\sqrt{10/7}L_4^{0_{111}}$$

$$L_6^{3111} = \frac{1}{8}\sqrt{70/3}L_6^{0111}$$

$$L_6^{6111} = \frac{1}{8}\sqrt{77/3}L_6^{0111}$$

$$B_4^{0_{111}} = (-2/3)B_4^0$$

$$B_6^{0_{111}} = 16/9 B_6^0$$

5
6

0
6

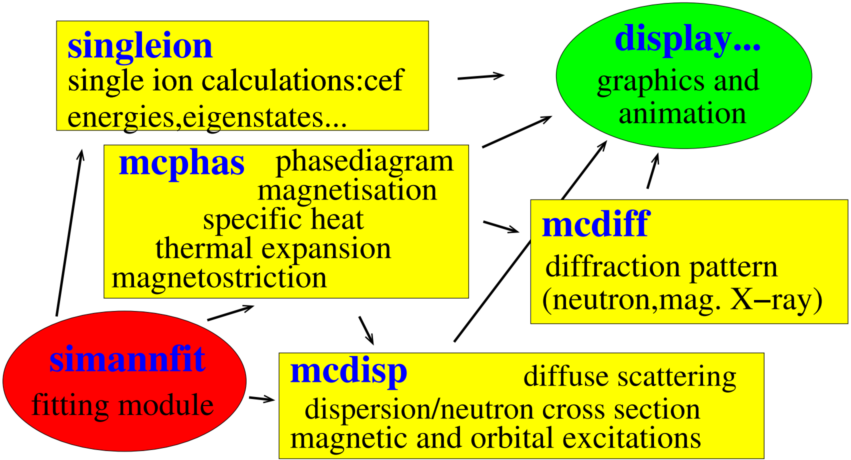
h

$$B_2^2$$

$\langle \mathbf{S} \rangle$

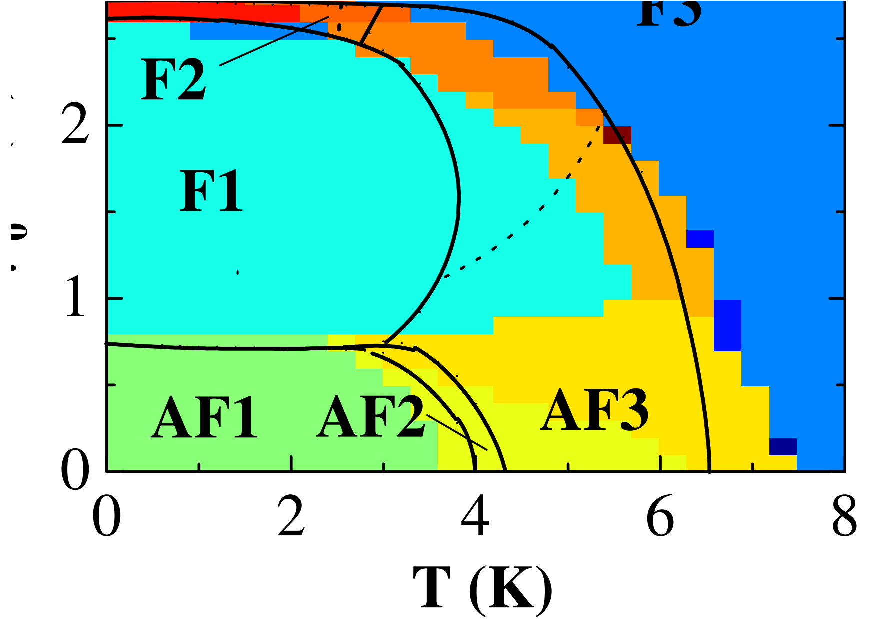
$\langle \mathbf{L} \rangle$

$$H = D_{x4}S_x^4 + D_{y4}S_y^4 + D_{z4}S_x^4$$


singleion
single ion calculations:cef
energies,eigenstates...
display...
graphics and
animation
mcphas
phasediagram
magnetisation
specific heat
thermal expansion
magnetostriction
mcdiff
diffraction pattern
(neutron,mag. X–ray)
simannfit
fitting module
mcdisp
diffuse scattering
dispersion/neutron cross section
magnetic and orbital excitations

T

H


F3
F2
F1
AF1
AF2
AF3
0
1
2
0
2
4
6
8
T (K)

6

20

$$\hat{\mathcal{H}} = \sum_{n=1}^{N} \hat{\mathcal{H}}(n) - \frac{1}{2} \sum_{n,n',\alpha,\beta} \mathcal{J}_{\alpha\beta}(\mathbf{R}_{n'} - \mathbf{R}_n) \hat{\mathcal{I}}_\alpha^n \hat{\mathcal{I}}_\beta^{n'}.$$

$$\hat{\mathcal{H}}(n)$$

n

$$\hat{\mathcal{I}}_{\alpha}^{n}$$

$\alpha = 1, 2, ..., m$

$$[\hat{\mathcal{I}}_{\alpha}^{n}, \hat{\mathcal{I}}_{\alpha}^{n'}] = 0$$

$$[\hat{\mathcal{H}}(n), \hat{\mathcal{I}}_{\alpha}^{n'}] = 0$$

$$[\hat{\mathcal{H}}(n), \hat{\mathcal{H}}(n')] = 0$$

$$n \neq n'$$

$\alpha = 1, 2, 3$

$$\hat{\mathcal{I}}_1 \leftrightarrow \hat{S}_x, \hat{\mathcal{I}}_2 \leftrightarrow \hat{S}_y, \hat{\mathcal{I}}_3 \leftrightarrow \hat{S}_z$$

$$\mathcal{J}_{\alpha\beta}(\mathbf{R}_n - \mathbf{R}_{n'})$$

α

$$\hat{\mathcal{I}}_{\alpha}^{n}$$

u^n

$$n = (1, x), (1, y), (1, z), (2, x), (2, y), (2, z), ...$$

$\mathcal{H}$

$$\mathrm{H}= \sum_{n,lm} B_l^m O_{lm}(\mathbf{J}^n) - \frac{1}{2} \sum_{nn'} \mathcal{J}(nn')\mathbf{J}^n\mathbf{J}^{n'} - \sum_n g_{Jn}\mu_B\mathbf{J}^n\mathbf{H}$$

$$O_l^m$$

$$\mathrm{H}_{JJ} = -\frac{1}{2}\sum_{nn'}\sum_{ll'}\sum_{mm'}\mathcal{K}_{ll'}^{mm'}(nn')O_{lm}(\mathbf{J}^n)O_{l'm'}(\mathbf{J}^{n'})$$

$\mathcal{J}(ij)$

$$\mathcal{K}_{ll'}^{mm'}(ij)$$

ϵ

$\mathcal{H}$

$=$

$$\sum_n \left\{ \sum_{i_n=1}^{\nu_n} \left[\frac{p_{i_n}^2}{2m_e} - \frac{Z_n e^2}{4\pi\epsilon_0 |\mathbf{r}_{i_n} - \mathbf{R}_n|} + \zeta_n \mathbf{l}^{i_n} \cdot \mathbf{s}^{i_n} + \sum_{lm} L_l^m(n) T_{lm}^n \right] + \sum_{i_n > j_n = 1}^{\nu_n} \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_{i_n} - \mathbf{r}_{j_n}|} \right\}$$

$$-\sum_n \mu_B(2\mathbf{S}^n + \mathbf{L}^n)\mathbf{H}$$

$$-\frac{1}{2}\sum_{nn'}\left[(\hat{\mathbf{L}}^n,\hat{\mathbf{S}}^n)\ \overset{=}{\mathcal{J}}\ (nn')\left(\begin{array}{c}\hat{\mathbf{L}}^{n'}\\ \hat{\mathbf{S}}^{n'}\end{array}\right)+\sum_{kk'}\sum_{qq'}\mathcal{K}^{qq'}_{kk'}(nn')\hat{T}^n_{kq}T^{n'}_{k'q'}\right]$$

ν_n

Z_n

$\mathbf{R}_n$

p

m_e

e

r

1

S

$\mathbf{S}_n$

$\mathbf{L}_n$

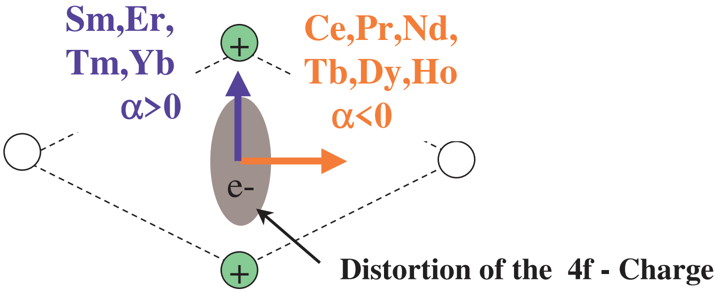
$$L_l^m$$

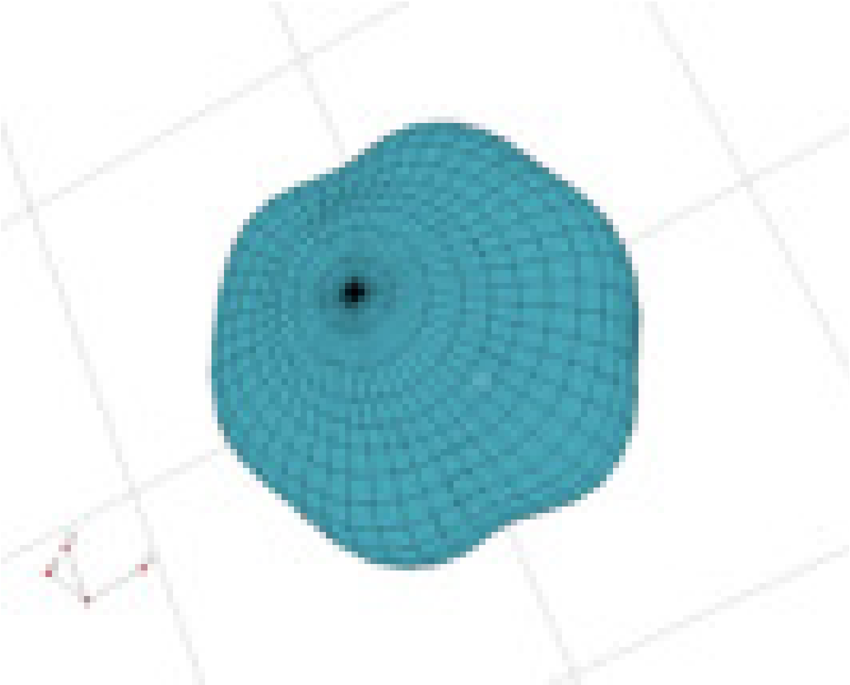
$$T_{lm}^{n}$$

$$T_{l0} = \sqrt{4\pi/(2l+1)} \sum_i Y_{l0}(\Omega_{i_n})$$

$$T_{l,\pm|m|} = \sqrt{4\pi/(2l+1)} \sum_i \sqrt{\pm 1}[Y_{l,-|m|}(\Omega_{i_n}) \pm (-1)^m Y_{l,|m|}(\Omega_{i_n})]$$

Crystal Field Effects and Magnetic Anisotropy





$$|JLSm_J\rangle$$

$$\mathrm{H}=\sum_{n,lm} B_{lm} O_{lm}(\mathbf{J}^n)-\sum_n g_{Jn}\mu_B \mathbf{J}^n \mathbf{H}$$

$$\sum_s D_x^2 (J_x^s)^2 + D_y^2 (J_y^s)^2 + D_z^2 (J_z^s)^2$$

$$\sigma(i \to k) = \left(\frac{\hbar \gamma e^2}{2mc^2} \right)^2 \frac{e^{-E_i/k_B T}}{\sum_j e^{-E_j/k_B T}} \frac{2}{3} \sum_{\alpha=x,y,z} |g_J \langle i | \hat{J}_\alpha - \langle \hat{J}_\alpha \rangle | k \rangle|^2$$

$$\gamma = g_n/2\hbar$$

$$g_n = -3.82608552$$

$$e^2/mc^2 = 2.81794$$

$$\frac{\hbar\gamma e^2}{mc^2} = r_0 = -5.3908$$

$\mathcal{Q}$

k'/k

$$exp(-W(Q))$$

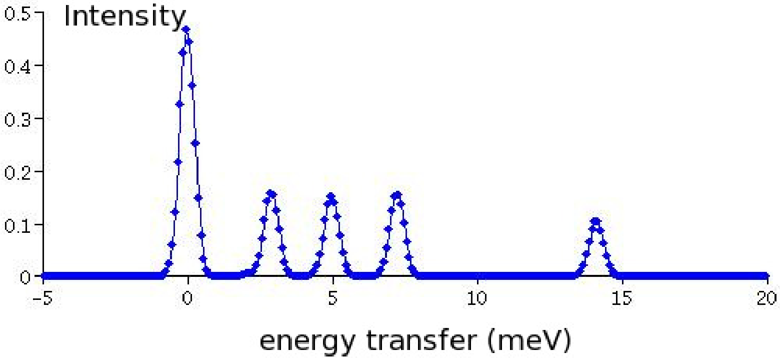
$$\frac{d^2\sigma}{d\Omega dE'}$$

$$N\frac{k'}{k}\left(\frac{\hbar\gamma e^2}{2mc^2}\right)^2 e^{-2W(Q)}|F(Q)|^2\times$$

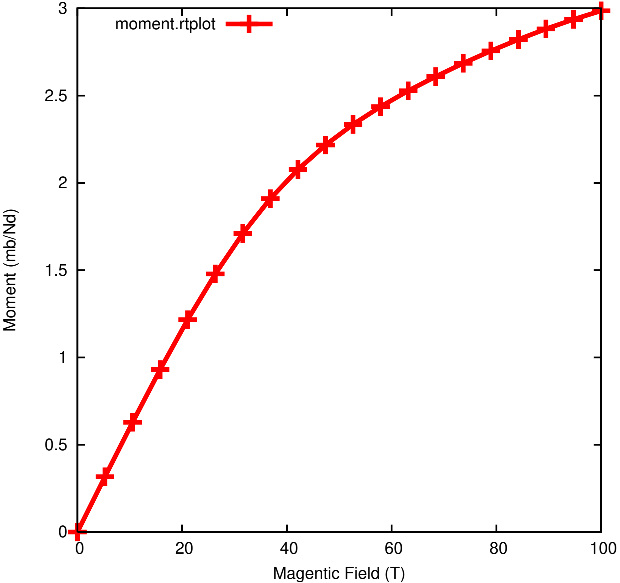
×

$$\sum_{i,f=1,2,\ldots,2J+1} \frac{e^{-E_i/k_BT}}{\sum_j e^{-E_j/k_BT}} \frac{2}{3} \sum_{\alpha=x,y,z} |g_J \langle i|\hat{J}_\alpha - \langle \hat{J}_\alpha \rangle |f\rangle|^2 \delta(E_f - E_i - \hbar\omega)$$

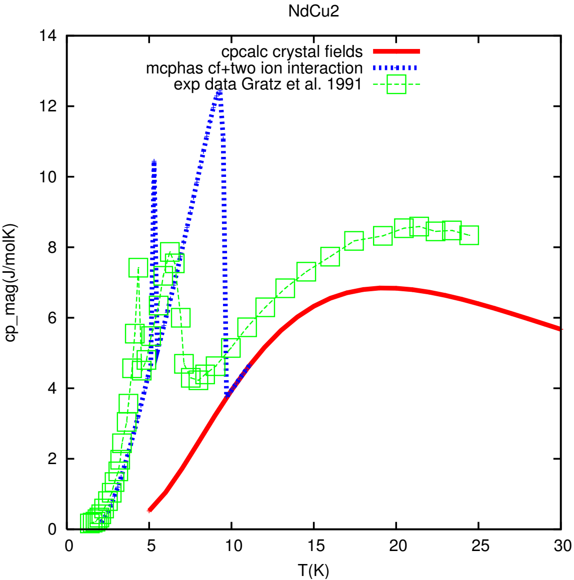
>


Intensity
0.5
0.4
0.3
0.2
0.1
0
-5
0
5
10
15
20
energy transfer (meV)

>>



moment.rtplot
Moment (mb/Nd)
Magentic Field (T)
0
0.5
1
1.5
2
2.5
3
0
20
40
60
80
100


NdCu2
cpcalc crystal fields
mcphas cf+two ion interaction
exp data Gratz et al. 1991
cp_mag(J/molK)
T(K)
0
2
4
6
8
10
12
14
0
5
10
15
20
25
30

S

f

$$\rho_{s-f}(T) = \frac{3\pi N m}{\hbar e^2 E_F} G^2 (g_J - 1)^2 \sum_{m_s, m'_s, i, i'} \langle m'_s, i' | \mathbf{s} \cdot \mathbf{J} | m_s, i \rangle^2 p_i f_{ii'}$$

G

p_i

$$e^{-\beta E_i}/Z$$

$f_{ii'}$

$$2/(1 + e^{-\beta(E_i - E_{i'})})$$

$$|i\rangle$$

$$\mathbf{s} \cdot J$$

$$\rho_0 = (3\pi N m/\hbar e^2 E_F) G^2 (g_J - 1)^2$$

$$\rho_0 = 0.2$$

Ω

$$2J+1$$

$$\rho_0 J(J+1)$$

$$\mathbf{H}^s$$

$$\langle \hat{\mathbf{J}} \rangle$$

$$\langle \hat{\mathbf{J}} \rangle = \sum_{i=1}^{2J+1} p_i \langle i | \hat{\mathbf{J}} | i \rangle$$

p_i

$$\frac{\exp(-E_i/kT)}{z}$$

$\mathcal{Z}$

$$\sum_{i=1}^{2J+1} \exp(-E_i/kT)$$

Z

E_i

$$\langle \mathbf{J}_i \rangle$$

$$u = \sum_{i=1}^{2J+1} p_i E_i$$

abc

$$\vec{a} || x$$

$$\vec{b} || y$$

$\vec{c}||z$

$\vec{a} || y$

$$\vec{b}||z$$

$\vec{c} \| x$

$y||\vec{b}$

$$z || (\vec{a} \times \vec{b})$$

y

$$Ha, Hb, Hc$$

$\mathbf{a}, \mathbf{b}, \mathbf{c}$

$Hb||\mathbf{b}$

$$Hc || (\mathbf{a} \times \mathbf{b})$$

Ha

Hb

Hc

N_b

$$\hat{\mathcal{H}} = \sum_{s=1}^{N_b} \hat{H}^{MF}(s) + E_{corr}$$

$$\hat{H}^{MF}(s) = \hat{H}(s) - \sum_{\alpha=1}^{\text{nofcomponents}} H_{\alpha}^{s} \hat{I}_{\alpha}^{s}$$

$$\text{nofcomponents} = 3$$

$$\hat{I}_\alpha = \hat{J}_\alpha$$

$$\mathbf{M} = g_J \mu_B \langle \hat{\mathbf{J}} \rangle$$

$$\hat{H}^{MF}_{\mathrm{so1ion}}(s) = \underbrace{B_l^m \hat{O}_{lm}(\hat{\mathbf{J}}^s) - g_{Js}\mu_B \hat{\mathbf{J}}^s \cdot \mathbf{H}}_{\hat{H}(s)} - \hat{\mathbf{I}}^s \cdot \mathbf{H}^s$$

$\mathbf{H}^s$

H

$$E_{corr} = \frac{1}{2} \sum_{s=1}^{N_b} \sum_{\alpha=1}^{\text{nofcomponents}} \langle \hat{I}_{\alpha}^{s} \rangle H_{\alpha}^{s}$$

$$\mathrm{H}^{s}_{\alpha} = \sum_{\mathbf{G}'} \sum_{s'=1}^{N_b} \sum_{\beta=1}^{\mathrm{nofcomponents}} \mathcal{J}_{\alpha\beta}(\mathbf{r}_s - (\mathbf{G}' + \mathbf{r}_{s'})) \langle \hat{I}^{s'}_{\beta} \rangle$$

$$\langle \hat{\mathbf{I}}^s \rangle$$

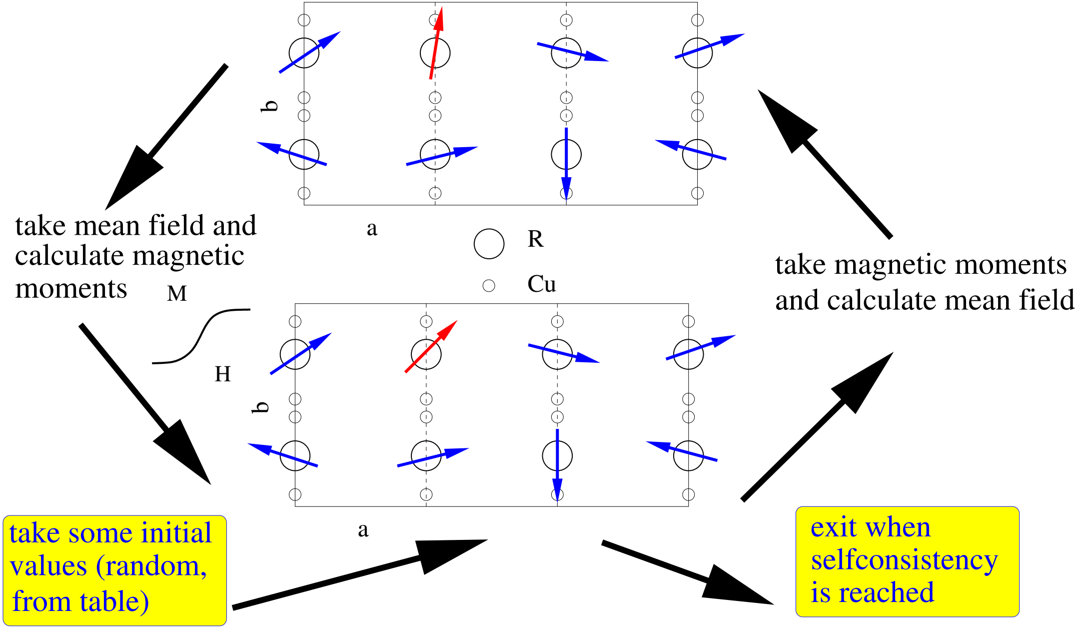
f

$$-kT\frac{1}{N_b}\sum_{s}\ln(z_s)+\frac{E_{corr}}{N_B}$$

z_s

$$\sum_i \exp(-\epsilon_i^s/kT)\ldots \text{partition sum of the site } s$$

$\epsilon_i^s \ldots$ eigenvalues of $\hat{H}^{MF}(s)$


take mean field and calculate magnetic moments
M
H
b
a
R
Cu
take magnetic moments and calculate mean field
b
a
take some initial values (random, from table)
exit when selfconsistency is reached

g_J

d_a

d_b

d_c

st

$\vec{a}$

$\vec{b}$

$\vec{c}$

$\vec{r}_1$

$\vec{r}_2$

$\vec{r}_3$

$$d_a\vec{a} + d_b\vec{b} + d_c\vec{c} = d_1\vec{r}_1 + d_2\vec{r}_2 + d_3\vec{r}_3$$

$\overline{\overline{\mathcal{J}}}$

$$Ja, Jb, Jc, Jaa, Jbb, Jcc, Jab...$$

$\vec{a}, \vec{b}, \vec{c}$

$$Jb||\vec{b}$$

$$Jc||(\vec{a}\times\vec{b})$$

Ja

Jb

Jc

$$-d_a$$

$$-d_b$$

$$-d_c$$

$\|$

$\mathbf{r}_i$

$3n$

$n =$

$< J >$

$$mb||\vec{b}$$

$$mc || (\vec{a} \times \vec{b})$$

ma

mb

mc

u

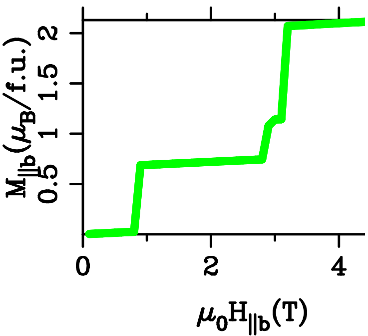
$$\mathrm{sta} = \sum_{\mathrm{datapointsi}} (m_i^{calc} - m_i^{meas})^2 / (\Delta m_i^{meas})^2$$

$$\Delta m_i^{meas}$$

$$m_i^{meas}$$

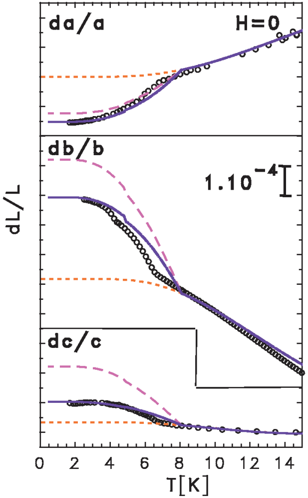
$H - T$

$$T - H$$



$M_{\|b}(\mu_B/\mathrm{f.u.})$
0.5
1
1.5
2
0
2
4
$\mu_0 H_{\|b}(\mathrm{T})$

$NdCu_2$



Kristallfeld

$$H = H_{cf}(\varepsilon = 0) + \varepsilon \frac{\partial H_{cf}}{\partial \varepsilon}$$

$$+ H_{ex}(\varepsilon = 0)$$

Austausch - Striktion

$$+ \varepsilon \frac{\partial H_{ex}}{\partial \varepsilon}$$

M. Rotter et al. J. Appl. Phys, 91 (2002) 8885

$\vec{a}^{*}, \vec{b}^{*}, \vec{c}^{*}$

$$\langle \hat{I}_{\alpha} \rangle$$

$$\alpha = 1, \ldots, \mathrm{nofcomponents}$$

$$\hat{I}_1 = \hat{J}_x, \hat{I}_2 = \hat{J}_y, \hat{I}_3 = \hat{J}_z, \hat{I}_4 = \hat{O}_2^{-2}, \hat{I}_5 = \hat{O}_2^{-1}, \ldots$$

$$H_{xc}(i)$$

$$u = f + Ts = f - T\partial f/\partial T = \frac{1}{N_b}\sum_{s,i} \epsilon_i^s \frac{e^{-\epsilon_i^s/kT}}{z^s} + \frac{E_{corr}}{N_b}$$

$$c_V = \partial u / \partial T$$

ma, mb, mc

$$H b \| \vec{b}$$

$$Hc||(\vec{a} \times \vec{b})$$

k

$$\frac{1}{N_b} \sum_{s=1}^{N_b} < \hat{\mathbf{I}}^s > \otimes < \hat{\mathbf{I}}^{s+k} >$$

$$< \hat{I}_\alpha >$$

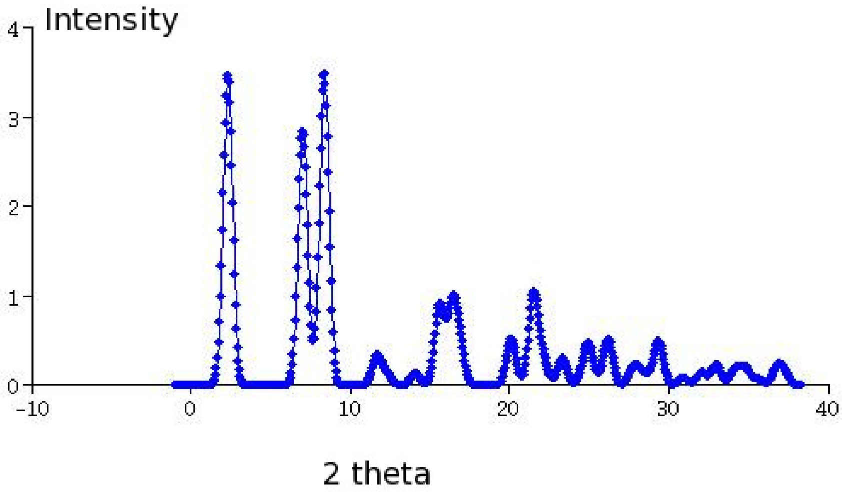
h, k, l

a, b, c

α, β, γ

Θ

2Θ



Intensity
4
3
2
1
0
−10
0
10
20
30
40
2 theta

$$R_{\mathrm{p}} = 100\frac{\sum_{hkl}|I_{calc}(hkl)-I_{exp}(hkl)|}{\sum_{hkl}|I_{\mathrm{exp}}(hkl)|}$$

$$\chi^2 = \sum_{hkl} \frac{(I_{calc}(hkl) - I_{exp}(hkl))^2}{n(\Delta I_{\text{experror}}(hkl))^2}$$

$$f_{nE1}^{RXMS} =$$

$$= \begin{pmatrix} \sigma \to \sigma & \pi \to \sigma \\ \sigma \to \pi & \pi \to \pi \end{pmatrix} = F^{(0)} \begin{pmatrix} 1 & 0 \\ 0 & \cos 2\Theta \end{pmatrix} - iF^{(1)}$$

$$\times \begin{pmatrix} 0 & z_1 \cos\Theta + z_3 \sin\Theta \\ z_3 \sin\Theta - z_1 \cos\Theta & -z_2 \sin 2\Theta \end{pmatrix} + F^{(2)}$$

$$\times \begin{pmatrix} z_2^2 & -z_2(z_1 \sin\Theta - z_3 \cos\Theta) \\ +z_2(z_1 \sin\Theta + z_3 \cos\Theta) & -\cos^2\Theta(z_1^2 \tan^2\Theta + z_3^2) \end{pmatrix}$$

z_1, z_2

z_3

$$[\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3]$$

k

$\mathbf{k}'$

$$\mathbf{u}_1$$

$\mathbf{u}_3$

$$\mathbf{Q} = \mathbf{k} - \mathbf{k}'$$

$$F^{(1)}$$

$$F^{(2)}$$

z_i

μ_x, μ_y

μ_z

z_1

$$\mu_x \sin\alpha_1 \cos(\Psi + \delta_1) + \mu_y \sin\alpha_2 \cos(\Psi + \delta_2)$$

$$+\mu_z \sin\alpha_3 \cos(\Psi + \delta_3),$$

z_2

$$\mu_x \sin\alpha_1 \sin(\Psi + \delta_1) + \mu_y \sin\alpha_2 \sin(\Psi + \delta_2)$$

$$+\mu_z \sin\alpha_3 \sin(\Psi + \delta_3)$$

z_3

$$\mu_x \cos\alpha_1 + \mu_y \cos\alpha_2 + \mu_z \cos\alpha_3$$

$$\alpha_i = \angle(\hat{\mathbf{x}}_i \cdot \mathbf{u}_3)_{\Psi=0}$$

$$\delta_i = \angle(\mathbf{x}_i^{\perp} \cdot \mathbf{u}_1)_{\Psi=0}$$

$$\hat{\mathbf{x}}_{1,2,3} = \hat{\mathbf{x}}, \hat{\mathbf{y}}, \hat{\mathbf{z}}$$

$$\mathbf{x}_i^{\perp}$$

$\hat{\mathbf{x}}_i$

Q

$$\Psi = 0$$

X

$$\mathbf{Q}||\mathbf{x}$$

y

$$\hat{\mathcal{H}} = B_l^m \hat{O}_{lm}(\hat{\mathbf{J}}) - g_J \mu_B \hat{\mathbf{J}} \cdot \mathbf{H} - \hat{\mathbf{J}} \cdot \mathbf{H}^s$$

$$\frac{d^2\sigma}{d\Omega dE'}$$

N

k'

$$\gamma = \frac{g_n}{2\hbar}$$

$e^2/m_e c^2 = 2.82$

$$\hbar\omega = E - E' = \frac{(\hbar\mathbf{k})^2}{2m_n} - \frac{(\hbar\mathbf{k}')^2}{2m_n}$$

S

S_{nuc}

$$S_{\mathrm{nuc}}^{\mathrm{el}} + S_{\mathrm{nuc}}^{\mathrm{inel}}$$

S_{mag}

$$S_{\mathrm{mag}}^{\mathrm{el}} + S_{\mathrm{mag}}^{\mathrm{inel}}$$

$$S_{\mathrm{nuc}}^{\mathrm{el}} = S_{\mathrm{nuc}}^{\mathrm{el,inc}} + S_{\mathrm{nuc}}^{\mathrm{el,coh}}$$

$$S_{\mathrm{nuc}}^{\mathrm{el,coh}}$$

$$\delta(\hbar\omega)\left(\frac{(2\pi)^3}{v_0}\sum_{\tau}\delta(\mathbf{Q}-\tau)\right)\frac{1}{N_B}\left(\sum_{dd'}\overline{b}_d^*\overline{b}_{d'}e^{-i\mathbf{Q}(\mathbf{B}_d-\mathbf{B}_{d'})}e^{-W_d-W_{d'}}\right)$$

$$\delta(\hbar\omega)\left(\frac{(2\pi)^3}{v_0}\sum_{\tau}\delta(\mathbf{Q}-\tau)\right)\frac{1}{N_B}|NSF|^2$$

N_B

τ

$$d = 1, \ldots, N_B$$

v_0

$\bar{b}_d$

$\mathbf{B}_d$

W_d

$$W_d = \langle (\mathbf{Q}.\mathbf{u}_d)^2 \rangle / 2 = \langle u_{\text{iso}}^2 \rangle Q^2 / 2 = B_{\text{iso}} Q^2 / 16\pi^2 = B_{\text{iso}} sin^2\Theta / \lambda^2$$

$$\sum_{\alpha\beta}(\delta_{\alpha\beta} - \hat{\mathbf{Q}}_\alpha \hat{\mathbf{Q}}_\beta) S^{\mathrm{el},\alpha\beta}_{\mathrm{mag}}$$

$$\delta(\hbar\omega)\left(\frac{(2\pi)^3}{v_0}\sum_{\tau}\delta(\mathbf{Q}-\tau)\right)\frac{1}{N_B}\left(\sum_{dd',\alpha\beta}(\delta_{\alpha\beta}-\hat{\mathbf{Q}}_\alpha\hat{\mathbf{Q}}_\beta)\frac{1}{2\mu_B}F_d(Q)M_{d\alpha}\right.$$

$$\left. \frac{1}{2\mu_B} F_{d'}(Q) M_{d'\beta} e^{-i\mathbf{Q}(\mathbf{B}_d - \mathbf{B}_{d'})} e^{-W_d - W_{d'}} \right)$$

$$\delta(\hbar\omega)\left(\frac{(2\pi)^3}{v_0}\sum_{\tau}\delta(\mathbf{Q}-\tau)\right)\frac{1}{N_B}|\mathrm{M\vec{S}F}|^2$$

$F_d(Q)M_{d\alpha}$

$$g_J \neq 0$$

$$F_d(Q) M_{d\alpha} = g_J \mu_B \langle J_{d\alpha} \rangle_{T,H} \left[\langle j_0(Q) \rangle + \frac{2-g_J}{g_J} \langle j_2(Q) \rangle \right]$$

$$g_J = 0$$

$$\langle Ma \rangle, \langle Mb \rangle, \langle Mc \rangle$$

$$F_d(Q) M_{d\alpha} = \langle M_{d\alpha} \rangle_{T,H} \left[\langle j_0(Q) \rangle \right]$$

$$\langle Sa \rangle, \langle La \rangle, \langle Sb \rangle, \langle Lb \rangle, \langle Sc \rangle, \langle Lc \rangle$$

$$F_d(Q)M_{d\alpha} = \mu_B \langle 2S_{d\alpha}\rangle_{T,H} \langle j_0(Q)\rangle + \mu_B \langle L_{d\alpha}\rangle_{T,H} \left[\langle j_0(Q)\rangle + \langle j_2(Q)\rangle\right]$$

$$F_d(Q)$$

$$\langle S_{d\alpha} \rangle_{T,H}$$

$$\langle L_{d\alpha} \rangle_{T,H}$$

$$\langle J_{d\alpha} \rangle_{T,H}$$

$$\mathbf{Q} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^*$$

$$\sin(\Theta) = \lambda \frac{|\mathbf{Q}|}{4\pi}$$

$$I_{hkl}^{nuc} = |\frac{\mathrm{NSF}}{N_B}|^2 \exp(-\frac{\mathrm{OTF} \times Q^2}{8\pi^2}) \times \mathrm{LF}$$

$$I_{hkl}^{mag} = \frac{3.65}{4\pi} \left| \frac{\mathrm{M}\vec{\mathrm{S}}\mathrm{F}}{N_B} \right|^2 \exp\left(-\frac{\mathrm{OTF} \times Q^2}{8\pi^2}\right) \times \mathrm{LF}$$

OTF

$$...\mathrm{OverallTemperatureFactor}(B_{\mathrm{iso}}), \mathrm{OTF}.Q^2/(8\pi^2) = \langle(\mathbf{Q}.\mathbf{u})^2\rangle = \langle u^2\rangle Q^2$$

LF

...Lorentzfactor

$\sin^{-2}(2\Theta)$...powderflatsample

$\sin^{-1}(2\Theta)\,\sin^{-1}(\Theta)$...powdercylindricalsample

$\sin^{-1}(2\Theta)$...singlecrystalsample

d^3...TOFpowdercylindricalsamplelogscaleddpattern

d^4...TOFpowdercylindricalsamplelinearscaleddpattern

NSF

…nuclearstructurefactor

$$\sum_d \bar{b}_d e^{i\mathbf{Q}\mathbf{B}_d} e^{-W_d}$$

$\vec{\text{MSF}}$

...magneticstructurefactor

$$\sum_{d} \frac{1}{2\mu_B} F_d(Q) \vec{M}_d^{\perp} e^{i\mathbf{Q}\mathbf{B}_d} e^{-W_d}$$

$$\langle j_4(Q) \rangle$$

$$\langle j_6(Q) \rangle$$

$$\langle j_0(Q) \rangle$$

$$\langle j_2(Q) \rangle$$

$$Z(K)$$

$$\langle M_{d\alpha} \rangle_{T,H}$$

$$|MSF|^2$$

$$|\mathrm{M}\vec{\mathrm{S}}\mathrm{F}|^2$$

$$\left(\sum_{dd',\alpha\beta}(\delta_{\alpha\beta}-\hat{\mathbf{Q}}_\alpha\hat{\mathbf{Q}}_\beta)\langle\hat{\mathcal{Q}}_\alpha^{d\dagger}\rangle_{T,H}\langle\hat{\mathcal{Q}}_\beta^{d'}\rangle_{T,H}e^{-i\mathbf{Q}(\mathbf{B}_d-\mathbf{B}_{d'})}e^{-W_d-W_{d'}}\right)$$

$$\langle \cdots \rangle_{T,H}$$

$$\hat{\mathcal{Q}}_{\alpha}$$

$$\hat{\mathcal{Q}} = \frac{1}{2\mu_B}\hat{M}(\mathbf{Q})$$

$$|SLJM\rangle$$

$$M = -J, -J+1, \ldots J$$

i

$$\langle SLJM|\hat{\mathcal{Q}}_x|SLJM'\rangle$$

$$\frac{1}{2}\sum_{K',Q'} f(K')P(K',Q')\times$$

$$\times[Y_{K'-1,Q'+1}(\hat{\mathbf{Q}})\sqrt{(K'-Q')(K'-Q'-1)} - Y_{K'-1,Q'-1}(\hat{\mathbf{Q}})\sqrt{(K'+Q')(K'+Q'-1)}]$$

$$\langle SLJM|\hat{\mathcal{Q}}_y|SLJM'\rangle$$

$$\frac{-i}{2} \sum_{K',Q'} f(K')P(K',Q') \times$$

$$\times[Y_{K'-1,Q'+1}(\hat{\mathbf{Q}})\sqrt{(K'-Q')(K'-Q'-1)}+Y_{K'-1,Q'-1}(\hat{\mathbf{Q}})\sqrt{(K'+Q')(K'+Q'-1)}]$$

$$\langle SLJM|\hat{\mathcal{Q}}_z|SLJM'\rangle$$

$$\sum_{K',Q'} f(K')P(K',Q')[Y_{K'-1,Q'}(\hat{\mathbf{Q}})\sqrt{(K'-Q')(K'+Q')}]$$

$Z(K')$

$$c_{K'-1}\langle j_{K'-1}(Q)\rangle + c_{K'+1}\langle j_{K'+1}(Q)\rangle$$

$f(K')$

$$\sqrt{4\pi}Z(K')/K'$$

$$P(K', Q')$$

$$(-1)^{J-M'} \begin{pmatrix} K' & J & J \\ -Q' & M' & -M \end{pmatrix} \begin{pmatrix} K' & J & J \\ 0 & J & -J \end{pmatrix}^{-1}$$

$c_{K'}$

$$Y_{lm}(\hat{\mathbf{Q}})$$

$$P(K', Q')$$

$3j$

ω

$$\hat{I}_1 = \hat{J}_x, \hat{I}_2 = \hat{J}_y, \hat{I}_3 = \hat{J}_z$$

$$\hat{I}_1 = \hat{S}_x, \hat{I}_2 = \hat{L}_x, \hat{I}_3 = \hat{S}_y, \hat{I}_4 = \hat{L}_y, \hat{I}_5 = \hat{S}_z, \hat{I}_6 = \hat{L}_z$$

$$\hat{\mathbf{S}}, \hat{\mathbf{L}}, \hat{\mathbf{J}}$$

$y||b$

$$z||(a \times b)$$

$$\mathcal{J}(\mathbf{Q})$$

H

q

sta

$$\sum_i |weight(i)| * [Eexp(i) - nearestEcalc(i)]^{[2*sign(weight(i))]}$$

sta_int

$$\sum_i |weight(i)| * [Eexp(i) - nearestEcalc_{\text{withInt>Iexp(i)>0.1mb/srf.u.}}]^{[2*sign(weight(i))]}$$

sta_without_antipeaks

$$\sum_{i,weight(i)>0} weight(i) * [Eexp(i) - nearestEcalc(i)]^2$$

sta_int_without_antipeaks

$$\sum_{i,weight(i)>0} weight(i) * [Eexp(i) - nearestEcalc_{\text{withInt>Iexp(i)>0.1mb/srf.u.}}]^2$$

sta_without_weights

$$\sum_i [Eexp(i) - nearestEcalc(i)]^{[2*sign(weight(i))]}$$

sta_int_without_weights

$$\sum_{i}[Eexp(i) - nearestEcalc_{\mathrm{withInt>Iexp(i)>0.1mb/srf.u.}}]^{[2*sign(weight(i))]}$$

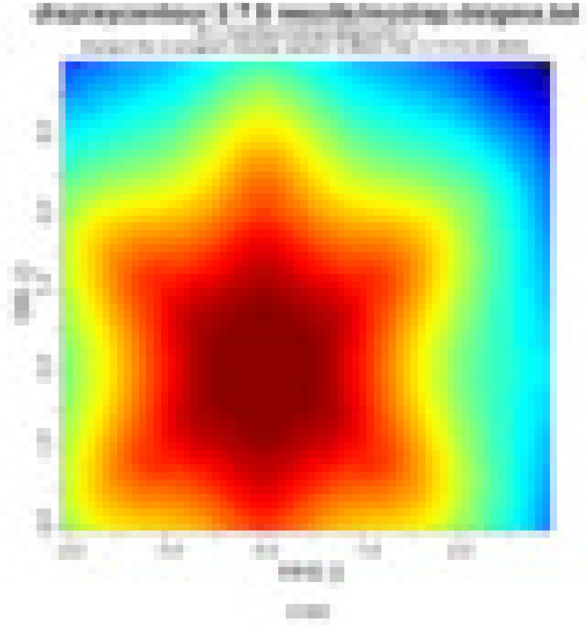
sta_without_antipeaks_weights

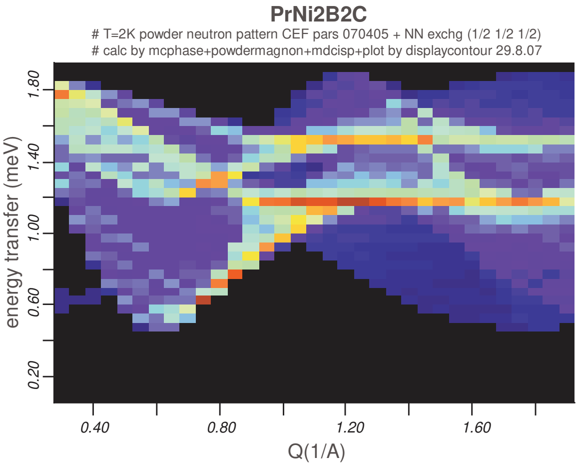
$$\sum_{i, weight(i) > 0} [Eexp(i) - nearestEcalc(i)]^2$$

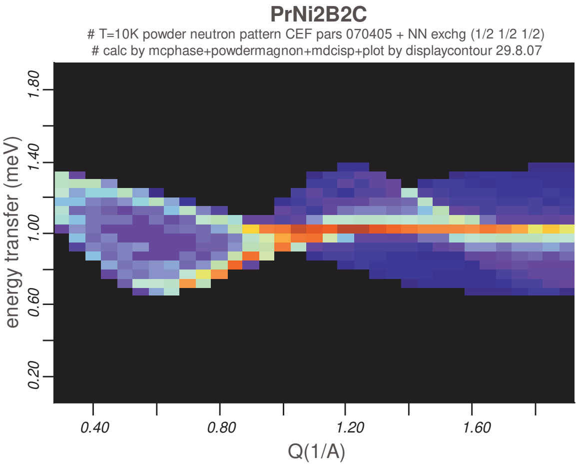
sta_int_without_antipeaks_weights

$$\sum_{i,weight(i)>0} [Eexp(i) - nearestEcalc_{\text{withInt>Iexp(i)>0.1mb/srf.u.}}]^2$$

γ




PrNi2B2C
T=2K powder neutron pattern CEF pars 070405 + NN exchg (1/2 1/2 1/2)
calc by mcphase+powdermagnon+mdcisp+plot by displaycontour 29.8.07
energy transfer (meV)
1.80
1.40
1.00
0.60
0.20
0.40
0.80
1.20
1.60
Q(1/A)


PrNi2B2C
T=10K powder neutron pattern CEF pars 070405 + NN exchg (1/2 1/2 1/2)
calc by mcphase+powdermagnon+mdcisp+plot by displaycontour 29.8.07
energy transfer (meV)
1.80
1.40
1.00
0.60
0.20
0.40
0.80
1.20
1.60
Q(1/A)

ϕ

$$\delta\phi = \delta\Theta * \pi / (4 * sin(\Theta))$$

$$k_f$$

k_i

$\hat{\mathcal{O}}_\alpha$

R

$$R^{\epsilon_i \epsilon_o}_{\omega,j}$$

$$R_{\omega,j}^{\epsilon_i \epsilon_o} = \epsilon_o^{\star} \cdot \mathbf{R} \cdot \epsilon_i$$

ϵ

Ŝ

$$R^{\epsilon_i \epsilon_o}_{\omega,j}$$

$$\epsilon_o^{\star} \cdot \mathbf{R} \cdot \epsilon_i$$

$$\sigma^{(0)}\epsilon_i \cdot \epsilon_o^\star + \frac{\sigma^{(1)}}{s}\epsilon_o^\star \times \epsilon_i \hat{\mathbf{S}}_j$$

$$\frac{\sigma^{(2)}}{s(2s-1)}\left(\epsilon_i\cdot\hat{\mathbf{S}}_j\epsilon_o^\star\cdot\hat{\mathbf{S}}_j+\epsilon_o^\star\cdot\hat{\mathbf{S}}_j\epsilon_i\cdot\hat{\mathbf{S}}_j-\frac{2}{3}\epsilon_i\cdot\epsilon_o^\star\hat{\mathbf{S}}_j^2\right)$$

σ

$\hat{\mathbf{J}}$

π

u2

$$\alpha_i = \angle(\mathbf{a}_i \cdot \mathbf{u}_3)_{\Psi=0}$$

$$\delta_i = \angle(\mathbf{a}_i^{\perp} \cdot \mathbf{u}_1)_{\Psi=0}$$

$$\mathbf{a}_{1,2,3} = \mathbf{a}, \mathbf{b}, \mathbf{c}$$

$$\mathbf{a}_i^{\perp}$$

$\mathbf{a}_i$

$$\mathbf{a}_1 = \mathbf{a}$$

$$\mathrm{H}_{JJ} = -\frac{1}{2}\sum_{nn'}\sum_{ll'}\sum_{mm'}\mathcal{K}_{ll'}^{mm'}(nn')\hat{O}_{lm}(\mathbf{J}^n)\hat{O}_{l'm'}(\mathbf{J}^{n'}) = -\frac{1}{2}\sum_{nn'}\sum_{\substack{\alpha=(lm)\\ \alpha'=(l'm')}} J_{\alpha\alpha'}(nn')\hat{I}_{\alpha}^{n}\hat{I}_{\alpha'}^{n'}$$

$J_{\alpha\alpha}$

$$\hat{I}_1 \cdot \hat{I}_1$$

$$\hat{I}_2 \cdot \hat{I}_2$$

$$\hat{I}_3 \cdot \hat{I}_3$$

$$\hat{I}_4 \cdot \hat{I}_4$$

Î

$$\hat{I}_1, \hat{I}_2, \hat{I}_3, \hat{I}_4, \ldots \equiv \hat{I}_a, \hat{I}_b, \hat{I}_c, \hat{I}_d, \ldots$$

$$\hat{I}_1, \hat{I}_2, \hat{I}_3, \hat{I}_4, \ldots =$$

$\hat{O}_{11}$

$$\hat{O}^s_{11}$$

$$\hat{O}_{10}$$

$$\hat{O}^{s}_{22}$$

$$\hat{O}^s_{21}$$

$$\hat{O}_{20}$$

$$\hat{O}_{21}$$

$$\hat{O}_{22}$$

$$\hat{O}^{s}_{33}$$

$$\hat{O}_{66}$$

$$\hat{J}_x^2$$

$$\hat{J}_y^2$$

$$\hat{J}_z^2$$

$$\hat{J}_x^4$$

$$\hat{J}_y^4$$

$$\hat{J}_z^4$$

$$< \hat{J}_a >$$

$$< \hat{J}_b >$$

$$< \hat{J}_c >$$

$$< \hat{I}_a >$$

$$< \hat{I}_b >$$

$$< \hat{I}_c >$$

$$< \hat{I}_d >$$

$$< \hat{I}_e >$$

$$< \hat{O}^s_{22} >$$

$$< \hat{O}_{21}^{s} >$$

$$< \hat{O}_{20} >$$

$$< \hat{O}_{21} >$$

$$< \hat{O}_{22} >$$

$$< \hat{O}^s_{33} >$$

$$\hat{I}_\alpha$$

$$(5\hat{O}_{44}(\hat{\mathbf{J}}^n) + \hat{O}_{40}(\hat{\mathbf{J}}^n)) \cdot (5\hat{O}_{44}(\hat{\mathbf{J}}^{n'}) + \hat{O}_{40}(\hat{\mathbf{J}}^{n'}))$$

$$\hat{O}_{00} = 1$$

$$O_{00}(\mathrm{so1ion}) = 0$$

$$\hat{O}_{11} = \frac{1}{2}[\hat{J}_+ + \hat{J}_-] = \hat{J}_x$$

$$\hat{I}_a$$

$$\hat{I}_c$$

$$\hat{O}_{11}(s) = \frac{-i}{2}[\hat{J}_+ - \hat{J}_-] = \hat{J}_y$$

$$\hat{I}_b$$

$$\hat{O}_{10} = \hat{J}_z$$

$$\hat{O}_{22}(s) = \frac{-i}{2}[\hat{J}_+^2 - \hat{J}_-^2] = \hat{J}_x\hat{J}_y + \hat{J}_y\hat{J}_x$$

$$= 2\hat{P}_{xy}$$

$\hat{I}_d$

$$\hat{O}_{21}(s) = \frac{-i}{4}[(\hat{J}_+ - \hat{J}_-)\hat{J}_z + \hat{J}_z(\hat{J}_+ - \hat{J}_-)] = \frac{1}{2}[\hat{J}_y\hat{J}_z + \hat{J}_z\hat{J}_y]$$

$$= \hat{P}_{yz}$$

$\hat{I}_e$

$$\hat{O}_{20} = [3\hat{J}_z^2 - J(J+1)]$$

$$O_2^0(s) = 0$$

$$\hat{I}_f$$

$$\hat{O}_{21} = \frac{1}{4}[(\hat{J}_+ + \hat{J}_-)\hat{J}_z + \hat{J}_z(\hat{J}_+ + \hat{J}_-)] = \frac{1}{2}[\hat{J}_x\hat{J}_z + \hat{J}_z\hat{J}_x]$$

$$= \hat{P}_{xz}$$

$$\hat{I}_g$$

$$\hat{O}_{22} = \frac{1}{2}[\hat{J}_+^2 + \hat{J}_-^2] = [\hat{J}_x^2 - \hat{J}_y^2]$$

$\hat{I}_h$

ζ

η

$$\hat{P}_{zx}$$

$$\hat{P}_{xy}$$

$$\hat{P}_{yz}$$

$$\hat{O}_2^2$$

$$(\hat{I}_h)$$

$$8 \times 8$$

$$< O_l^m >$$

$$< \hat{J}_d >$$

$$< \hat{J}_e >$$

$$< J_a >$$

$< J_b >$

$$< J_c >$$

$$< O_{22}(s) >$$

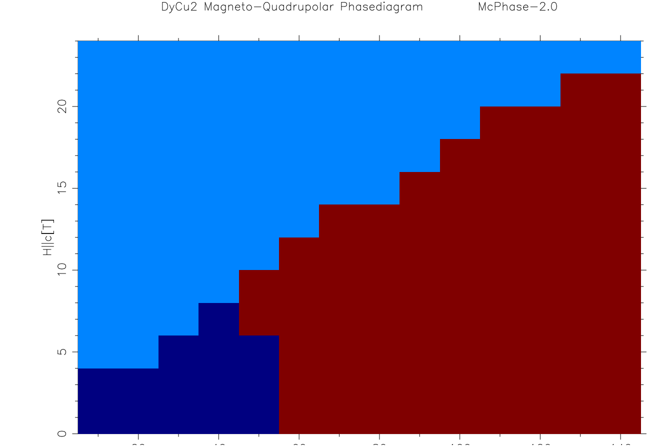
$$< O_{21}(s) >$$

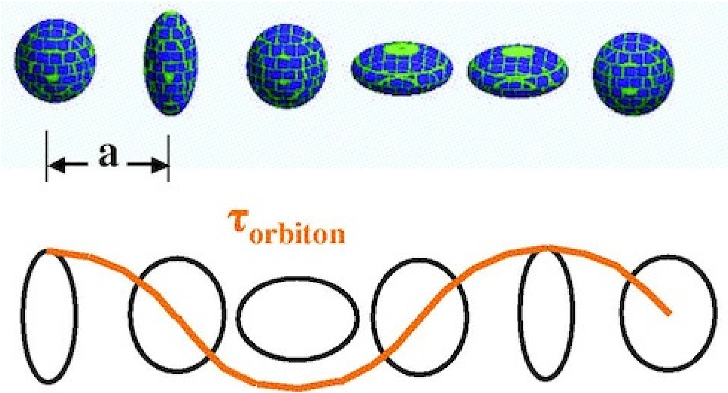
$$< O_{20} >$$

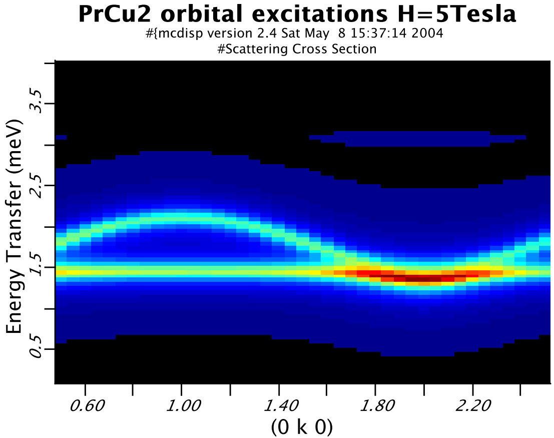
$< O_{21} >$

$$< O_{22} >$$

$$< O_{33}(s) >$$


DyCu2 Magneto-Quadrupolar Phasediagram McPhase-2.0
H||c[T]
0
5
10
15
20


a
$\tau_{orbiton}$


PrCu2 orbital excitations H=5Tesla
#{mcdisp version 2.4 Sat May 8 15:37:14 2004
#Scattering Cross Section
Energy Transfer (meV)
0.5
1.5
2.5
3.5
0.60
1.00
1.40
1.80
2.20
(0 k 0)

$$\hat{H}_E(i) = \frac{a_0^2 \hat{\mathbf{w}}_i^2}{2m_i} - \frac{1}{2}\hat{\mathbf{u}}_i^T \overline{K}(ii)\hat{\mathbf{u}}_i$$

$\hat{\mathbf{u}}$

$$\hat{\mathbf{u}}_i = \hat{\mathbf{P}}_i / a_0 = \Delta \hat{\mathbf{r}}_i / a_0$$

$$a_0 = 0.5219$$

m_i

$$\hat{\mathbf{w}}_i = d\hat{\mathbf{u}}_i/dt = \mathbf{p}_i/a_0$$

$\hat{\mathbf{u}}_i$

$\overline{K}(ii)$

$$\hat{H}_{phon} = \sum_{i} \hat{H}_E(i) - \frac{1}{2} \sum_{i \neq i'} \hat{\mathbf{u}}_i^T \overline{K}(ii') \hat{\mathbf{u}}_{i'}$$

$$K_{\alpha\beta}(ii') = -A_{\alpha\beta}(ii')$$

$$A_{\alpha\beta}$$

$$\hat{H}_E = \frac{a_0^2 \hat{\mathbf{w}}^2}{2m} - \frac{1}{2}\hat{\mathbf{u}}^T \overline{K} \hat{\mathbf{u}} - \mathbf{F}^T \hat{\mathbf{u}}$$

F

$$\mathbf{H}_{xc}$$

$$\overline{K}(nn')$$

$$\mathcal{J}(nn')$$

$$\overline{S}$$

$$\overline{K} = \overline{S}^T \overline{\Omega S}$$

$$\hat{\mathbf{u}}' = \overline{S}\hat{\mathbf{u}} + \overline{\Omega}^{-1}\overline{S}\mathbf{F}$$

$$\hat{H}_E = \frac{a_0^2 \hat{\mathbf{w}}'^2}{2m} - \frac{1}{2}\hat{\mathbf{u}}'^T \overline{\Omega} \hat{\mathbf{u}}' - \frac{1}{2}\mathbf{F}^T \mathbf{u}_0$$

$$\mathbf{u}_0 = -\overline{S}^T \overline{\Omega}^{-1} \overline{S} \mathbf{F}$$

$\overline{\Omega}$

$$\Omega_{11} = -ma_0^2(\Delta_1/\hbar)^2$$

$$\Omega_{22} = -ma_0^2(\Delta_2/\hbar)^2$$

$$\Omega_{33} = -ma_0^2(\Delta_3/\hbar)^2$$

Δ_1

$$\overline{\chi}^0$$

$$\sum_{\nu\mu} \frac{\langle\nu|\hat{\mathbf{u}}|\mu\rangle\langle\mu|\hat{\mathbf{u}}^T|\nu\rangle}{\Delta_1 - \hbar\omega}(p_\nu - p_\mu)$$

$$\sum_{\nu\mu} \frac{\langle\nu|\overline{S}^T \hat{\mathbf{u}}'|\mu\rangle\langle\mu|\hat{\mathbf{u}}'^T \overline{S}|\nu\rangle}{\Delta_1 - \hbar\omega}(p_\nu - p_\mu)$$

$$\mathbf{u}'$$

u_1'

$$\chi^0_{\alpha\beta}$$

$$S_{\alpha 1}^{T} \sum_{\nu\mu} \frac{\langle \nu | \hat{u}_1' | \mu \rangle \langle \mu | \hat{u}_1' | \nu \rangle}{\Delta_1 - \hbar\omega} (p_\nu - p_\mu) S_{1\beta}$$

$$S^T_{\alpha 1} S_{1\beta} \frac{\hbar^2}{2ma_0^2 \Delta_1} \left(\frac{1}{\Delta_1 - \hbar\omega} + \frac{1}{\Delta_1 + \hbar\omega} \right)$$

$$\hat{u}'_1$$

$$\hat{u}_1' = a_0^{-1}\hbar/\sqrt{2m\Delta_1}(\hat{a} + \hat{a}^\dagger)$$

$$\hat{a}^\dagger|\nu\rangle = \sqrt{\nu+1}|\nu+1\rangle$$

$$\hat{a}|\nu\rangle = \sqrt{\nu}|\nu - 1\rangle$$

$$\sum_{\nu=0}^{\infty}(p_\nu - p_{\nu+1})(\nu+1) = 1$$

$$p_\nu = exp(-\nu\Delta_1/kT)(1 - exp(-\Delta_1/kT))$$

$$\sum_{n=1,2,3} S_{\alpha n}^{T} S_{n\beta} \frac{\hbar^2}{2ma_0^2\Delta_n} \left(\frac{1}{\Delta_n - \hbar\omega} + \frac{1}{\Delta_n + \hbar\omega} \right)$$

u_{max}

$\langle \mathbf{u} \rangle$

$$u \leftarrow u_{max} * tanh(u/u_{max})$$

u

u_x, u_y, u_z

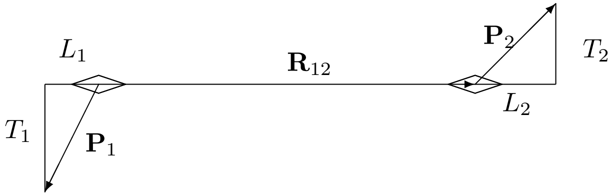
$$\mathbf{y}||\mathbf{b}$$

$$\mathbf{z} || \mathbf{a} \times \mathbf{b}$$

Z

$$\overline{K}(ii')$$

i'



$$E = \frac{c_L}{2}(L_1 + L_2)^2 + \frac{c_T}{2}(T_1 + T_2)^2$$

$$\mathbf{p}_i = a_0 \mathbf{w}_i$$

$$\hat{\mathbf{U}}_i$$

c_L

c_T

$$\hat{H}_{\text{phon}}$$

$$\sum_i \frac{a_0^2 \hat{\mathbf{w}}_i^2}{2m_i} + \frac{1}{2} \sum_{ij} \frac{c_L(ij) - c_T(ij)}{2|\mathbf{R}_{ij}|^2} (\hat{\mathbf{U}}_j.\mathbf{R}_{ij} - \hat{\mathbf{U}}_i.\mathbf{R}_{ij})^2$$

$$+\frac{c_T(ij)}{2}(\hat{\mathbf{U}}_j - \hat{\mathbf{U}}_i)^2$$

i, j

$1/2$

$$\mathbf{R}_{ij} = \mathbf{R}_j - \mathbf{R}_i$$

$$\bar{\epsilon}\mathbf{R}_i$$

$\bar{\omega}\mathbf{R}_i$

$$\hat{\mathbf{P}}_i$$

$$\hat{\mathbf{U}}_i = \bar{\epsilon}\mathbf{R}_i + \bar{\omega}\mathbf{R}_i + \hat{\mathbf{P}}_i = \bar{a}\mathbf{R}_i + \hat{\mathbf{P}}_i$$

$$(\hat{\mathbf{U}}_j.\mathbf{R}_{ij} - \hat{\mathbf{U}}_i.\mathbf{R}_{ij})^2$$

$$(\mathbf{R}_{ij}^T \bar{a} \mathbf{R}_{ij} + \mathbf{R}_{ij}^T \mathbf{P}_{ij})^2$$

$$(\mathbf{R}_{ij}^T \bar{a} \mathbf{R}_{ij})^2 + 2\mathbf{R}_{ij}^T \bar{a} \mathbf{R}_{ij} \mathbf{R}_{ij}^T \hat{\mathbf{P}}_{ij}$$

$$+(\mathbf{R}_{ij}^T \hat{\mathbf{P}}_{ij})^2$$

$$(\hat{\mathbf{U}}_j - \hat{\mathbf{U}}_i)^2$$

$$\mathbf{R}_{ij}^T \bar{a}^T \bar{a} \mathbf{R}_{ij}$$

$$2\mathbf{R}_{ij}^T \bar{a}^T \hat{\mathbf{P}}_{ij} + \hat{\mathbf{P}}_{ij}^T \hat{\mathbf{P}}_{ij}$$

$\bar{a}$

$\hat{\mathbf{P}}$

H_{E}

$$H_{\text{int}}$$

$$E_{el} + \hat{H}_{mix} + \hat{H}_{\mathrm{E}} + \hat{H}_{\mathrm{int}}$$

$$E_{el}$$

$$\frac{1}{2}\sum_{ij}\frac{c_L(ij)-c_T(ij)}{2|\mathbf{R}_{ij}|^2}(\mathbf{R}_{ij}^T\bar{a}\mathbf{R}_{ij})^2$$

$$+\frac{c_T(ij)}{2}\mathbf{R}_{ij}^T\bar{a}^T\bar{a}\mathbf{R}_{ij}$$

$$\frac{1}{2}\sum_{ij,\alpha\beta\gamma\delta}\frac{c_L(ij)-c_T(ij)}{2|\mathbf{R}_{ij}|^2}R_{ij}^{\alpha}R_{ij}^{\beta}R_{ij}^{\gamma}R_{ij}^{\delta}a_{\alpha\beta}a_{\gamma\delta}$$

$$+\frac{c_T(ij)}{2}R^{\alpha}_{ij}R^{\delta}_{ij}a_{\alpha\beta}\delta_{\beta\gamma}a_{\gamma\delta}$$

$a_{\alpha\beta}$

$$\frac{\partial E_{el}}{\partial a_{\alpha\beta}}$$

$$\frac{1}{2}\sum_{ij,\gamma\delta}\frac{c_L(ij)-c_T(ij)}{|\mathbf{R}_{ij}|^2}R_{ij}^{\alpha}R_{ij}^{\beta}R_{ij}^{\gamma}R_{ij}^{\delta}a_{\gamma\delta}$$

$$+\frac{c_T(ij)}{2}R^{\alpha}_{ij}R^{\delta}_{ij}\delta_{\beta\gamma}a_{\gamma\delta}+$$

$$\frac{c_T(ij)}{2} R_{ij}^{\gamma} R_{ij}^{\beta} a_{\gamma\delta} \delta_{\delta\alpha}$$

$$c^{\alpha\beta\gamma\delta}$$

$$\frac{\partial^2 E_{el}}{\partial a_{\alpha\beta} \partial a_{\gamma\delta}}$$

$$\frac{1}{2}\sum_{ij}\frac{c_L(ij)-c_T(ij)}{|\mathbf{R}_{ij}|^2}R_{ij}^{\alpha}R_{ij}^{\beta}R_{ij}^{\gamma}R_{ij}^{\delta}$$

$$+\frac{c_T(ij)}{2}R_{ij}^{\alpha}R_{ij}^{\delta}\delta_{\beta\gamma}+$$

$$\frac{c_T(ij)}{2} R_{ij}^{\gamma} R_{ij}^{\beta} \delta_{\delta\alpha}$$

$\overline{\epsilon}$

$$\epsilon_{\alpha\beta} = \epsilon_{\beta\alpha}$$

$$\omega_{\alpha\beta} = -\omega_{\beta\alpha}$$

$$\bar{a} = \bar{\epsilon} + \bar{\omega}$$

$$\frac{1}{2}\sum_{\alpha\beta\gamma\delta} c^{\alpha\beta\gamma\delta}\epsilon_{\alpha\beta}\epsilon_{\gamma\delta}$$

$\bar{\omega}$

$$R^\alpha R^\delta \omega_\sigma \epsilon_{\sigma\alpha\beta}\delta_{\beta\gamma}\omega_\eta \epsilon_{\eta\gamma\delta} = R^\alpha R^\delta \omega_\sigma \omega_\eta \epsilon_{\sigma\alpha\beta}\epsilon_{\eta\beta\delta} = R^\alpha R^\delta \omega_\sigma \omega_\eta (\delta_{\sigma\delta}\delta_{\alpha\eta} - \delta_{\sigma\eta}\delta_{\alpha\delta}) = (\mathbf{R}.\omega)^2 - R^2\omega^2 \neq 0$$

$$+\frac{c_T(ij)}{4}(R_{ij}^{\alpha}R_{ij}^{\delta}\delta_{\beta\gamma}+$$

$$R^{\gamma}_{ij} R^{\beta}_{ij} \delta_{\delta\alpha}$$

$$+R_{ij}^{\beta}R_{ij}^{\delta}\delta_{\alpha\gamma}+R_{ij}^{\gamma}R_{ij}^{\alpha}\delta_{\delta\beta})$$

$$\frac{\partial E_{el}}{\partial \epsilon_{\alpha\beta}}$$

$$\sum_{\gamma\delta=1,2,3} c^{\alpha\beta\gamma\delta}\epsilon_{\gamma\delta}$$

ϵ_1

ϵ_{11}

ϵ_2

ϵ_{22}

ϵ_3

ϵ_{33}

ϵ_4

$$2\epsilon_{23} = 2\epsilon_{32}$$

ϵ_5

$$2\epsilon_{31} = 2\epsilon_{13}$$

ϵ_6

$$2\epsilon_{12} = 2\epsilon_{21}$$

c^{11}

c^{1111}

c^{44}

c^{2323}

$$c^{\alpha\beta}$$

$\beta = 1, ..., 6$

$$\alpha \leq \beta$$

$$c^{\alpha\beta} = c^{\beta\alpha}$$

$$c^{\alpha\beta\gamma\delta} = c^{\beta\alpha\gamma\delta} = c^{\alpha\beta\delta\gamma}$$

$$\frac{1}{2} \sum_{\alpha\gamma=1,..,6} c^{\alpha\gamma} \epsilon_\alpha \epsilon_\gamma$$

$$\hat{H}_{mix}$$

$$\frac{1}{2}\sum_{ij}\frac{c_L(ij)-c_T(ij)}{|\mathbf{R}_{ij}|^2}\mathbf{R}_{ij}^T\bar{a}\mathbf{R}_{ij}\mathbf{R}_{ij}^T\hat{\mathbf{P}}_{ij}$$

$$+c_T(ij)\mathbf{R}_{ij}^T\bar{a}^T\mathbf{P}_{ij}$$

$$\frac{1}{2}\sum_{ij} 2\frac{c_L(ij) - c_T(ij)}{|\mathbf{R}_{ij}|^2}\mathbf{R}_{ij}^T \bar{a} \mathbf{R}_{ij} \mathbf{R}_{ij}^T \hat{\mathbf{P}}_i$$

$$+2c_T(ij)\mathbf{R}_{ij}^T\bar{a}^T\hat{\mathbf{P}}_i$$

$$\sum_{ij,\alpha\beta} \frac{c_L(ij) - c_T(ij)}{|\mathbf{R}_{ij}|^2} R_{ij}^{\alpha} a_{\alpha\beta} R_{ij}^{\beta} R_{ij}^{\gamma} \hat{P}_i^{\gamma}$$

$$+c_T(ij)R^{\beta}_{ij}a_{\alpha\beta}\delta_{\alpha\gamma}\hat{P}^{\gamma}_{i}$$

$$- \sum_{\substack{i,\alpha=1,..,6 \\ \gamma=1,2,3}} G^{\alpha\gamma}_{mix}(i)\epsilon_\alpha \hat{P}^\gamma_i / a_0 + \sum_{ij,\alpha\beta} c_T(ij) R^\beta_{ij} \omega_{\alpha\beta} \hat{P}^\alpha_i$$

$$\hat{H}_{mix}$$

$$\langle \hat{\mathbf{P}}_i \rangle$$

$$G_{mix}^{\alpha\gamma}(i)$$

$$\alpha = (\alpha\beta)$$

$$G_{mix}^{(\alpha\beta)\gamma}(i)$$

$$-a_0 \sum_j \frac{c_L(ij) - c_T(ij)}{|\mathbf{R}_{ij}|^2} R_{ij}^{\alpha} R_{ij}^{\beta} R_{ij}^{\gamma} -$$

$$-a_0 \frac{1}{2} \sum_j c_T(ij)(R_{ij}^{\beta} \delta_{\alpha\gamma} + R_{ij}^{\alpha} \delta_{\beta\gamma})$$

$$(\mathbf{R}_{ij}^T \hat{\mathbf{P}}_{ij})^2$$

$$\sum_{\alpha,\beta=1,2,3} R^{\alpha}_{ij} R^{\beta}_{ij} (\hat{P}^{\alpha}_{j} - \hat{P}^{\alpha}_{i})(\hat{P}^{\beta}_{j} - \hat{P}^{\beta}_{i})$$

$$\hat{\mathbf{P}}_{ij}^T \hat{\mathbf{P}}_{ij}$$

$$\sum_{\alpha=1,2,3} (\hat{P}_j^\alpha - \hat{P}_i^\alpha)^2$$

$$\sum_{\alpha=1,2,3} (\hat{P}_j^\alpha)^2 + (\hat{P}_i^\alpha)^2 - 2\hat{P}_i^\alpha \hat{P}_j^\alpha$$

$$\hat{H}_{\mathrm{E}}$$

$$\sum_i \hat{H}_{\mathrm{E}}(i)$$

$$\hat{H}_{\mathrm{E}}(i)$$

$\equiv$

$$\frac{a_0^2 \hat{\mathbf{w}}_i^2}{2m_i} - \frac{1}{2} \sum_{\alpha} K_{\alpha\beta}(ii) \hat{P}_i^{\alpha} \hat{P}_i^{\beta} a_0^{-2}$$

$$K_{\alpha\beta}(ii)$$

$$-a_0^2 \sum_j \frac{R_{ij}^{\alpha} R_{ij}^{\beta}}{|\mathbf{R}_{ij}|^2} [c_L(ij) - c_T(ij)] +$$

$$+\delta_{\alpha\beta}c_T(ij)$$

$$\hat{H}_{\text{int}}$$

$$-\frac{1}{2}\sum_{i\neq j,\alpha\beta} K_{\alpha\beta}(ij)\hat{P}_i^{\alpha}\hat{P}_j^{\beta}a_0^{-2}$$

$$K_{\alpha\beta}(ij)$$

$$a_0^2 \frac{R_{ij}^{\alpha} R_{ij}^{\beta}}{|\mathbf{R}_{ij}|^2} [c_L(ij) - c_T(ij)] + a_0^2 \delta_{\alpha\beta} c_T(ij)$$

$$B_{\gamma}(i) = B_{l}^{m}$$

lm

$$\mathrm{B}_{\gamma}(i) = B_l^m = -|e|\theta_l^i \langle r^l \rangle \gamma_{lm}(i) p_{lm}$$

$$\gamma_{lm}(i)$$

R_{ji}, Ω_{ji}

q_j

$$\gamma_{lm}(i) = \sum_j \frac{q_j}{2l+1} \frac{Z_{lm}(\Omega_{ji})}{\epsilon_0 R_{ji}^{l+1}}$$

$i = 1, ..., N_{\text{nuclei}}$

j

$$j = N_{\text{nuclei}} + 1, ...N_{\text{nuclei}} + N_{\text{magneticions}}$$

$i < j$

$$\hat{H}_{\text{tot}}$$

$$\hat{H}_{\text{phon}} + \sum_{i,\gamma} B_\gamma(i, \hat{\mathbf{U}}_1, ..., \hat{\mathbf{U}}_N) O_\gamma(\hat{\mathbf{J}}_i) - \sum_i g_{J_i} \mu_B \hat{\mathbf{J}}_i \mathbf{H}$$

$$\hat{H}_{\text{phon}} + \sum_{i,\gamma} B_\gamma(i, 0, \ldots, 0) O_\gamma(\hat{\mathbf{J}}_i) + \hat{H}_{\text{cfph}}$$

$\hat{H}_{\mathrm{cfph}}$

$$\sum_{i<j,\gamma} \nabla_{\hat{\mathbf{U}}_i} B_\gamma(j) \hat{\mathbf{U}}_i O_\gamma(\hat{\mathbf{J}}_j)$$

$$\sum_{i<j,\gamma} \nabla_{\hat{\mathbf{U}}_i} B_\gamma(j)(\bar{a}\mathbf{R}_i + \hat{\mathbf{P}}_i) O_\gamma(\hat{\mathbf{J}}_j)$$

$$\sum_{i<j,\alpha\beta=1,2,3,\gamma=1,\ldots} R_i^{\beta} \frac{\partial B_{\gamma}(j)}{\partial \hat{U}_i^{\alpha}} \epsilon_{\alpha\beta} O_{\gamma}(\hat{\mathbf{J}}_j)$$

$$+\sum_{i<j,\gamma}\nabla_{\hat{\mathbf{U}}_j}B_\gamma(j)\hat{\mathbf{P}}_iO_\gamma(\hat{\mathbf{J}}_j)$$

$$- \sum_{j,\alpha=1,..,6,\gamma=1,...} G^{\alpha\gamma}_{\mathrm{cfph}}(j)\epsilon_\alpha O_\gamma(\hat{\mathbf{J}}_j)$$

$$-\sum_{i<j,\alpha=1,2,3,\gamma=1,\ldots}\Gamma^{\alpha\gamma}(ij)\hat{P}_i^{\alpha}a_0^{-1}O_\gamma(\hat{\mathbf{J}}_j)$$

$$\mathrm{G}_{\mathrm{cfph}}^{(\alpha\beta)\gamma}(j) = -\frac{1}{2}\sum_i \left(R_i^{\beta}\frac{\partial B_\gamma(j)}{\partial \hat{U}_i^{\alpha}} + R_i^{\alpha}\frac{\partial B_\gamma(j)}{\partial \hat{U}_i^{\beta}}\right)$$

$$\Gamma^{\alpha\gamma}(ij) = -a_0 \frac{\partial B_\gamma(j)}{\partial \hat{U}_i^\alpha}$$

$$\hat{\mathbf{u}} = \hat{\mathbf{P}}/a_0$$

$$\sum_{i,\gamma} B_\gamma(i,0,\ldots,0) O_\gamma(\hat{\mathbf{J}}_i) - \sum_i g_{J_i} \mu_B \hat{\mathbf{J}}_i \mathbf{H} +$$

+

$$\sum_i \hat{H}_{\mathrm{E}}(i) + \frac{1}{2} \sum_{\alpha\gamma=1-6} c^{\alpha\gamma} \epsilon_\alpha \epsilon_\gamma -$$

—

$$\frac{1}{2}\sum_{i\neq j,\alpha\beta} K_{\alpha\beta}(ij)\hat{u}_i^\alpha \hat{u}_j^\beta - \sum_{i<j,\alpha=1-6,\gamma} \Gamma^{\alpha\gamma}(ij)\hat{u}_i^\alpha O_\gamma(\hat{\mathbf{J}}_j)$$

$$\sum_{i,\alpha=1-6,\gamma=1,2,3} G^{\alpha\gamma}_{mix}(i)\epsilon_\alpha \hat{u}^\gamma_i -$$

$$\sum_{i,\alpha=1-6,\gamma=1,\ldots} G^{\alpha\gamma}_{\mathrm{cfph}}(i)\epsilon_\alpha O_\gamma(\hat{\mathbf{J}}_i)$$

$$\langle \hat{O}_l^m(i) \rangle$$

$$\langle \hat{\mathbf{u}}_i \rangle$$

0

$$\sum_{ij} \frac{c_L(ij) - c_T(ij)}{|\mathbf{R}_{ij}|^2} (\mathbf{R}_{ij}^T \bar{\epsilon} \mathbf{R}_{ij}) R_{ij}^{\alpha} R_{ij}^{\beta}$$

$$+\frac{c_T(ij)}{2}(R_{ij}^{\alpha}(\bar{\epsilon}\mathbf{R}_{ij})^{\beta}+R_{ij}^{\beta}(\bar{\epsilon}R_{ij})^{\alpha})$$

$$+2\sum_{ij}\frac{c_L(ij)-c_T(ij)}{|\mathbf{R}_{ij}|^2}R_{ij}^{\alpha}R_{ij}^{\beta}\mathbf{R}_{ij}^{T}\langle\mathbf{P}_i\rangle$$

$$+2c_T(ij)\mathbf{R}_{ij}^{\beta}\langle\hat{P}_i^{\alpha}\rangle+\sum_{ij,\gamma}\frac{\partial B_\gamma(i)}{\partial\hat{U}_j^{\alpha}}R_j^{\beta}\langle O_\gamma(\hat{\mathbf{J}}_i)\rangle$$

$\alpha, \beta = 1, 2, 3$

$\epsilon_{\alpha\beta}$

$\alpha = 1, ..., 6$

$$\sum_{\beta=1,..6} c^{\alpha\beta} \epsilon_\beta$$

$$\sum_{i,\delta=1,2,3} G_{mix}^{\alpha\delta}(i)\langle\hat{u}_i^{\delta}\rangle$$

$$\sum_{i,\gamma=1,\ldots} G^{\alpha\gamma}_{\mathrm{cfph}}(i)\langle O_{\gamma}(\hat{\mathbf{J}}_i)\rangle$$

$$\hat{H} = \hat{H}_{\text{tot}} - \frac{1}{2} \sum_{ij,\alpha\beta} \mathcal{J}_{\alpha\beta}((1+\bar{a})(\mathbf{R}_j - \mathbf{R}_i))\hat{\mathcal{I}}^i_\alpha \hat{\mathcal{I}}^j_\beta$$

$$\mathcal{J}_{\alpha\beta}(\mathbf{R}_{ij})$$

$\mathcal{J}_{\alpha\beta}(\mathbf{R} = (1 + \bar{a})\mathbf{R}_{ij})$

$$\mathcal{J}_{\alpha\beta}(\mathbf{R}_{ij}) + \frac{\partial \mathcal{J}_{\alpha\beta}}{\partial R^{\alpha'}} \frac{\partial (\bar{a}\mathbf{R}_{ij})^{\alpha'}}{\partial \epsilon_{\beta'}} \epsilon_{\beta'} + \ldots$$

$$\mathcal{J}_{\alpha\beta}(\mathbf{R}_{ij}) + \sum_{\alpha'\gamma=1,2,3,\beta'=1,..,6} \frac{\partial \mathcal{J}_{\alpha\beta}}{\partial R^{\alpha'}} \frac{\partial \epsilon_{\alpha'\gamma} \mathbf{R}^{\gamma}_{ij}}{\partial \epsilon_{\beta'}} \epsilon_{\beta'}$$

$$\hat{H} = \hat{H}_{\rm tot} - \frac{1}{2}\sum_{ij,\alpha\beta}\mathcal{J}_{\alpha\beta}(\mathbf{R}_{ij})\hat{\mathcal{I}}^i_\alpha\hat{\mathcal{I}}^j_\beta - \frac{1}{2}\sum_{\substack{ij,\alpha\beta\alpha'\gamma=1,2,3\\ \beta'=1,..,6}}\frac{\partial\mathcal{J}_{\alpha\beta}}{\partial R^{\alpha'}}\frac{\partial\epsilon_{\alpha'\gamma}\mathbf{R}^\gamma_{ij}}{\partial\epsilon_{\beta'}}\epsilon_{\beta'}\hat{\mathcal{I}}^i_\alpha\hat{\mathcal{I}}^j_\beta$$

$$\sum_{\beta=1,..,6} c^{\alpha\beta}\epsilon_{\beta}$$

$$\sum_{i,\delta=1,2,3} G_{mix}^{\alpha\delta}(i)\langle u_i^{\delta}\rangle$$

$$\frac{1}{2}\sum_{ii',\delta,\delta'\alpha',\gamma=1,..,3}\frac{\partial\mathcal{J}_{\delta\delta'}(\mathbf{R}_{ii'})}{\partial R^{\alpha'}}\frac{\partial\epsilon_{\alpha'\gamma}R^{\gamma}_{ii'}}{\partial\epsilon_{\alpha}}\langle\hat{\mathcal{I}}^{i}_{\delta}\hat{\mathcal{I}}^{i'}_{\delta'}\rangle$$

$$\langle \hat{u}_j^{\alpha} \rangle$$

$$\langle O_{\gamma}(\hat{\mathbf{J}}_i)\rangle$$

$$G_{mix}$$

G_{cfph}

Γ_{cfph}

C_{Tm}

C_{Ni}

$$C_C$$

$$B_2^0 = 0.22$$

$$B_2^2 = -0.33$$

$$B_2^0$$

$$\mathrm{Ni}_{20}C_{Ni} + \mathrm{C}_{20}C_{C} + \mathrm{Tm}_{20}C_{Tm}$$

$$B_2^2$$

$$\mathrm{Ni}_{22} C_{Ni} + \mathrm{C}_{22} C_{C} + \mathrm{Tm}_{22} C_{Tm}$$

$$C_{Ni} + 2\mathrm{C}_C + C_{Tm}$$

Ni_{lm}

C_{lm}

Tm_{lm}

$1|e|$

C_{20}

C_{22}

$$r_{max} = 20$$

$$\langle r^l \rangle$$

$$\mathrm{Ni}_{20}C_{Ni} + \mathrm{C}_{20}C_{C} + \mathrm{Tm}_{20}C_{Tm} + \sum_{i=1}^{6} E_{20}^{i} C_{E^{i}}$$

$$\mathrm{Ni}_{22}C_{Ni} + \mathrm{C}_{22}C_C + \mathrm{Tm}_{22}C_{Tm} + \sum_{i=1}^{6} E_{22}^{i} C_{E^i}$$

$$C_{Ni} + 2\mathrm{C}_C + C_{Tm} + C_{E^1} + 2C_{E^2} + 2C_{E^3} + 4C_{E^4} + 2C_{E^5} + 2C_{E^6}$$

C_{E^i}

$$|e|$$

E^1

E^2

$$E^3$$

$$E^4$$

E^5

$$E^6$$

$$B_4^0$$

$$B_4^2$$

B_4^4

$$B_6^0$$

$$B_6^2$$

B_6^4

$$B_6^6$$

x, y, z

$$\langle I \rangle$$

$$\Delta L/L$$

$$\frac{\Delta L}{L} = \sum_{\alpha\beta} \epsilon_{\alpha\beta} \hat{L}_\alpha \hat{L}_\beta$$

$\hat{\mathbf{L}}$

$$C_{Tm} = 0.8|e|$$

$$C_{Cu} = -0.4|e|$$

$$\hat{J}_a, \hat{J}_b, \hat{J}_c, \hat{O}_{2-2}, \hat{O}_{2-1}, \hat{O}_{20}, \hat{O}_{21}, \hat{O}_{22}, \hat{O}_{3-3} \ldots \hat{O}_{66}, \hat{J}_a^2, \hat{J}_b^2, \hat{J}_c^2, \hat{J}_a^4, \hat{J}_b^4, \hat{J}_c^4$$

$$\hat{J}_a, \hat{J}_b, \hat{J}_c, \hat{O}_{2-2}, \hat{O}_{2-1}, \hat{O}_{20}, \hat{O}_{21}, \hat{O}_{22}, \hat{O}_{3-3} ... \hat{O}_{66}$$

$\hat{J}_a, \hat{J}_b, \hat{J}_c$

$\hat{u}_a, \hat{u}_b, \hat{u}_c$

$\hat{S}_a, \hat{S}_b, \hat{S}_c, \hat{L}_a, \hat{L}_b, \hat{L}_c, \hat{T}_2^{-2}, \hat{T}_2^{-1}, \hat{T}_2^{0}, \hat{T}_2^{1}, \hat{T}_2^{2}, \hat{T}_3^{-3} ... \hat{T}_6^{6}$

$$\hat{J}_a, \hat{J}_b, \hat{J}_c, \hat{O}_{2-2}, \hat{O}_{2-1}, \hat{O}_{20}, \hat{O}_{21}, \hat{O}_{22}, \hat{O}_{4-4} ..., \hat{O}_{44}, \hat{O}_{6-6} ... \hat{O}_{66}$$

J

$$\hat{I}_1$$

$$\hat{J}_x$$

$$\hat{I}_1 \equiv 5\hat{O}_4^4 + O_4^0$$

$$I_n$$

$$M(\mathbf{Q})$$

$Z(K')$

$$10^{-14}$$

$$\langle \hat{\mathbf{I}} \rangle$$

$$\langle -|\hat{\mathbf{I}}|+\rangle \sqrt{(p_- - p_+)}$$

$$\langle \hat{\mathrm{M}} \rangle$$

$$\langle -|\hat{\mathbf{M}}|+\rangle \sqrt{(p_- - p_+)}$$

$$\langle \hat{\mathbf{L}} \rangle$$

$$\langle -|\hat{\mathbf{L}}|+\rangle \sqrt{(p_- - p_+)}$$

$$\langle \hat{\mathrm{S}} \rangle$$

$$\langle -|\hat{\mathbf{S}}|+\rangle \sqrt{(p_- - p_+)}$$

$$\langle \hat{\mathbf{M}}(\mathbf{Q}) \rangle$$

$$\langle -|\hat{\mathbf{M}}(\mathbf{Q})|+\rangle \sqrt{(p_- - p_+)}$$

$$\hat{\mathbf{R}}$$

$$\langle \hat{\mathbf{P}} \rangle$$

$$\langle -|\hat{\mathbf{P}}|+\rangle \sqrt{(p_{-} - p_{+})}$$

$$-|e|Z_l^m(\Omega)R^2(r)$$

$$\langle \sum_i Z_l^m(\Omega_i) \rangle$$

$\langle -| \sum_i Z_l^m(\Omega_i) |+\rangle \sqrt{(p_- - p_+)}$

$$Z_l^m(\Omega) R^2(r)$$

$$Z_l^m(\Omega)F(r)$$

$H_2||\vec{b}$

$$H_3 || (\vec{a} \times \vec{b})$$

H_1

H_2

H_3

Î

$$\mathbf{H}_{ext}$$

$\langle \hat{I}_a \rangle, \langle \hat{I}_b \rangle, \langle \hat{I}_c \rangle etc$

I

$$\hat{H} = \hat{H}_0 - \hat{\mathbf{M}}\mathbf{H}_{ext} - \hat{I}_a \mathrm{Hxc}(1) - \hat{I}_b \mathrm{Hxc}(2) - \hat{I}_c \mathrm{Hxc}(3) - \hat{I}_d \mathrm{Hxc}(4) ...$$

$$Z = \sum_i e^{-\epsilon_i/kT}$$

$$U = \sum_i p_i = \sum_i \epsilon_i e^{-\epsilon_i/kT}/Z$$

$$T < 0$$

$$n = (-T)$$

$$p_n = 1$$

*

$$M^s_{\alpha\beta}$$

$$|-\rangle \rightarrow |+\rangle$$

M

$u1$

$$\mathbf{u}^s_{\alpha 1} = \sqrt{(p_- - p_+)}\langle -|I^s_\alpha - \langle I^s_\alpha\rangle_{\mathbf{H},T}|+\rangle$$

$$\mathcal{U}^{s}_{\alpha 1}$$

$$\mathbf{u}^{s}_{\alpha 1}$$

$$\mathbf{u}_{\alpha 1}^{s} = \sqrt{(p_{-} - p_{+})}\langle -|\hat{I}_{\alpha}^{s} - \langle \hat{I}_{\alpha}^{s} \rangle_{\mathbf{H},T}|+\rangle$$

$$\Delta(tn) = 0$$

$$(p_- - p_+)$$

(p_+/kT)

$$\Delta = -10^{-10}$$

m

μ_B

$m1$

$$\mathrm{m1}^s_\alpha = \sqrt{(p_- - p_+)}\langle -|\hat{m}^s_\alpha - \langle \hat{m}^s_\alpha \rangle_{\mathbf{H},T}|+\rangle$$

$$\mathbf{m}1^s_\alpha = \sqrt{(p_- - p_+)}\langle -|\hat{m}^s_\alpha - \langle \hat{m}^s_\alpha \rangle_{\mathbf{H},T}|+\rangle$$

$$\hat{\mathbf{m}} = 2\hat{\mathbf{S}} + \hat{\mathbf{L}}$$

L

$L1$

$$\mathrm{L1}^s_\alpha = \sqrt{(p_- - p_+)}\langle -|\hat{L}^s_\alpha - \langle \hat{L}^s_\alpha \rangle_{\mathbf{H},T}|+\rangle$$

S

$S1$

$$\mathrm{S1}^s_\alpha = \sqrt{(p_- - p_+)}\langle -|\hat{S}^s_\alpha - \langle \hat{S}^s_\alpha \rangle_{\mathbf{H},T}|+\rangle$$

$\hat{\mathcal{Q}}$

$\mathbf{M}(\mathbf{r})$

$$\mathrm{Q}\ \times(\hat{\mathcal{Q}} \times \mathbf{Q}) = \frac{-1}{2\mu_B}\mathbf{Q} \times (\hat{\mathbf{M}}(\mathbf{Q}) \times \mathbf{Q}) = \frac{-1}{2\mu_B}\int d\mathbf{r}e^{i\mathbf{Q}\mathbf{r}}\left[\mathbf{Q} \times (\hat{\mathbf{M}}(\mathbf{r}) \times \mathbf{Q})\right]$$

$$\hat{\mathbf{M}}(\mathbf{r}) = \hat{\mathbf{M}}_S(\mathbf{r}) + \hat{\mathbf{M}}_L(\mathbf{r})$$

$$\nabla \times \hat{\mathbf{M}}_L(\mathbf{r}) = \hat{\mathbf{j}}(\mathbf{r})$$

$$\hat{\mathbf{M}}(\mathbf{r})$$

$$\mathbf{Q} \times \mathbf{Q} \times \mathbf{Q} = 0$$

$$\langle \hat{\mathcal{Q}}_{\alpha}^{d\dagger} \rangle_{T,H}$$

$$\mathbf{m}^s_{\alpha 1}(\mathbf{Q}) = \sqrt{(p_- - p_+)}\langle -|\hat{\mathbf{M}}^\dagger_\alpha(\mathbf{Q}) - \langle\hat{\mathbf{M}}^\dagger_\alpha(\mathbf{Q})\rangle|+\rangle/\mu_B$$

$$\hat{\mathcal{Q}}_\alpha = \frac{\hat{\mathbf{M}}_\alpha(\mathbf{Q})}{-2\mu_B}$$

$$\mathbf{m}^s_{\alpha 1}(\mathbf{Q}) = \sqrt{(p_- - p_+)}\langle -|\hat{\mathbf{M}}^\dagger_\alpha(\mathbf{Q}) - \langle \hat{\mathbf{M}}^\dagger_\alpha(\mathbf{Q})\rangle|+\rangle/\mu_B$$

$\alpha = 1, ..3$

$$\mathbf{m}^{s}_{\alpha 1}(\mathbf{Q})$$

$$\mathbf{rixs}^{s}_{\alpha 1}(\mathbf{Q}) = \sqrt{(p_{-} - p_{+})}\langle - | \hat{\mathbf{R}}^{\dagger}_{\alpha}(\mathbf{Q}) - \langle \hat{\mathbf{R}}^{\dagger}_{\alpha}(\mathbf{Q}) \rangle | + \rangle$$

$$\hat{R}_{\alpha}$$

$$\alpha = xx, xy, xz, yx, yy, yz, zx, zy, zz$$

$$\mathbf{rixs}^{s}_{\alpha 1}(\mathbf{Q}) = \sqrt{(p_{-} - p_{+})}\langle - | \hat{\mathbf{R}}^{\dagger}_{\alpha}(\mathbf{Q}) - \langle \hat{\mathbf{R}}^{\dagger}_{\alpha}(\mathbf{Q}) \rangle | + \rangle$$

$\alpha = 1, ..9$

$$\mathbf{rixs}^{s}_{\alpha 1}(\mathbf{Q})$$

P_α

$$\langle -|\hat{P}_\alpha|+\rangle = S_{i\alpha}\frac{\hbar}{\sqrt{2m\Delta_i}}$$

$$\mathrm{P1}^s_\alpha = \sqrt{(p_- - p_+)}\langle -|\hat{P}^s_\alpha - \langle \hat{P}^s_\alpha \rangle_{\mathbf{H},T}|+\rangle$$

$$\langle -|\hat{P}_\alpha|+\rangle = S_{tn,\alpha}\frac{\hbar}{\sqrt{2m\Delta_{tn}}}$$

$$\mathbf{P1}^{s}_{\alpha} = \sqrt{(p_{-} - p_{+})}\langle -|\hat{P}^{s}_{\alpha} - \langle \hat{P}^{s}_{\alpha}\rangle_{\mathbf{H},T}|+\rangle$$

$$-|e|Z_l^m R^2(r)$$

$$\sum_i \hat{Z}_{lm}(\Omega_i)$$

$cd1$

$$\mathrm{cd1}^{s}_{\alpha=lm} = \sqrt{(p_- - p_+)}\langle -|\sum_i \hat{Z}^s_{lm}(\Omega_i) - \langle \sum_i \hat{Z}^s_{lm}(\Omega_i)\rangle_{\mathbf{H},T}|+\rangle$$

$$Z_l^m R^2(r)$$

$$M^{S}_{x,y,z} = \sum_{l,m} a^{x,y,z}_{S,lm} Z^{m}_{l} R^{2}(r)$$

$$a_{S,lm}^{x,y,z}$$

$aSlm1$

$$\mathrm{aS1}^{s}_{\alpha=lm} = \sqrt{(p_- - p_+)}\langle -|a^{x,y,z}_{S,lm} - \langle a^{x,y,z}_{S,lm}\rangle_{\mathbf{H},T}|+\rangle$$

$Z_l^m F(r)$

$$M_{x,y,z}^{L} = \sum_{l,m} a_{L,lm}^{x,y,z} Z_l^m F(r)$$

$$a_{L,lm}^{x,y,z}$$

$F(r)$

$R(r)$

$$F(r) = \frac{1}{r} \int_r^\infty R^2(\xi) d\xi$$

$$\mathrm{aL1}^{s}_{\alpha=lm} = \sqrt{(p_- - p_+)}\langle -|a^{x,y,z}_{L,lm} - \langle a^{x,y,z}_{L,lm}\rangle_{\mathbf{H},T}|+\rangle$$

l^{ν}

7

LS

$$\hat{T}_{kq}$$

$$\mathbf{M} = \mu_B(2 < \mathbf{S} > + < \mathbf{L} >)$$

F^k

nl^{ν}

$4f^1$

jj

$$\mathcal{H}_{\text{Coulomb}} \gg \mathcal{H}_{\text{SO}} \gg \mathcal{H}_{\text{CEF}}$$

L, S, J

J_z

m_J

$$\mathcal{H}_{\mathrm{SO}} \gg \mathcal{H}_{\mathrm{Coulomb}}$$

$$\mathcal{H}_{\text{Coulomb}} \gg \mathcal{H}_{\text{CEF}} \gg \mathcal{H}_{\text{SO}}$$

$$\mathcal{H}_{\text{Coulomb}}$$

$\mathcal{H}_{\mathrm{CEF}}$

$\mathcal{H}_{\mathrm{SO}}$

^{2S+1}L

$\mathcal{H}_{\mathrm{CF}}$

$$m_l = -l, ..., l$$

$$|m_l = 0, 2\rangle$$

E_g

$$|m_l = -2, -1, 1\rangle$$

T_{2g}

$$\mathcal{H}_{\text{Coulomb}} \sim \mathcal{H}_{\text{SO}} \sim \mathcal{H}_{\text{CEF}}$$

$nl^{\nu-1}$

ν^{th}

$$|\Omega\rangle$$

$$\sum_{\bar{\Omega},\omega} \langle \bar{\Omega}; \omega | \Omega \rangle |\omega\rangle$$

$$|\omega\rangle$$

$(\nu - 1)^{\text{th}}$

$$|\bar{\Omega}\rangle$$

$$\langle \bar{\Omega}; \omega | \Omega \rangle$$

$$\langle \Omega | V | \Omega' \rangle$$

$\mathcal{V}$

$$\langle \omega | v | \omega' \rangle$$

$$\langle \Omega | V | \Omega' \rangle = \nu \sum_{\bar{\Omega}, \omega, \omega'} \langle \Omega | \bar{\Omega}; \omega \rangle \langle \omega | v | \omega' \rangle \langle \bar{\Omega}; \omega' | \Omega' \rangle$$

$\hat{e}_0$

$\hat{e}_1$

$\hat{e}_2$

$\hat{e}_3$

$$\mathcal{H} = \mathcal{H}_{\text{coulomb}} + \mathcal{H}_{\text{spinorbit}} + \mathcal{H}_{\text{crystalfield}} + \mathcal{H}_{\text{zeman}}$$

$$\mathcal{H}_{\text{coulomb}} = \sum_{i>j=1}^{\nu} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_i - \mathbf{r}_j|} = \sum_k F^k \sum_{ij} \mathbf{T}_i^{(k)} \cdot \mathbf{T}_j^{(k)} = \sum_k F^k \hat{f}_k$$

$$|\mathbf{r}_i - \mathbf{r}_j|$$

$$Y_{kq}$$

$\mathbf{T}_i^{(k)}$

i^{th}

$$\hat{f}_k$$

$2l$

$\hat{e}_k$

$\times G_2$

$$\mathcal{H}_{\text{spinorbit}} = \zeta \sum_i (\mathbf{s}_i . \mathbf{l}_i)$$

$$\mathbf{R}_j$$

$$\mathrm{H}_{\text{crystalfield}} = \frac{1}{4\pi\epsilon_0} \sum_{i=1}^{\nu} \sum_j \frac{-|e|q_j}{|\mathbf{R}_j - \mathbf{r}_i|}$$

$$Z_{kq}(\Omega)$$

$$\mathcal{H}_{\text{crystalfield}} = -|e| \sum_{i=1}^{\nu} \sum_{j} q_j \sum_{k=0}^{\infty} \frac{r_i^k}{\epsilon_0 R_j^{k+1}} \sum_{q=-k}^{k} \frac{1}{2k+1} Z_{kq}(\Omega_i) Z_{kq}(\Omega_j)$$

$$\gamma_{kq} = \sum_j \frac{q_j}{2k+1} \frac{1}{\epsilon_0 R_j^{k+1}} Z_{kq}(\Omega_j)$$

$$\mathcal{H}_{\text{crystalfield}} = -|e| \sum_{i=1}^{\nu} \sum_{k=0}^{\infty} \sum_{q=-k}^{k} r_i^k \gamma_{kq} Z_{kq}(\Omega_i)$$

z_{kq}

$$z_{kq} = \sqrt{\frac{8\pi}{2k+1}} Z_{kq} \ldots q \neq 0$$

$$z_{k0} = \sqrt{\frac{4\pi}{2k+1}} Z_{k0} \ldots q = 0$$

$$L_{kq} = -|e|\langle r^k\rangle\gamma_{kq}\sqrt{\frac{2k+1}{8\pi}}\ldots q \neq 0$$

$$L_{k0} = -|e|\langle r^k \rangle \gamma_{kq} \sqrt{\frac{2k+1}{4\pi}} \ldots q = 0$$

$$\mathcal{H}_{\text{crystalfield}} = \sum_{k=0}^{\inf} \sum_{q=-k}^{k} L_{kq} \sum_{i=1}^{\nu} z_{kq}(\Omega_i)$$

$$\sum_i z_{kq}(\Omega_i)$$

$$\hat{T}_{kq}$$

$$|J, m_J\rangle$$

$$\Omega \equiv (\theta, \phi)$$

$$\hat{C}_{kq}$$

$$\hat{T}_{k0} = \hat{C}_{k0}, \qquad \hat{T}_{k,\pm|q|} = \sqrt{\pm 1}\left[\hat{C}_{k,-|q|} \pm (-1)^{|q|}\hat{C}_{k,|q|}\right]$$

$$\frac{d^2\sigma}{d\Omega dE'} = N\frac{k'}{k}\left(\frac{\hbar\gamma e^2}{m_e c^2}\right)^2 \sum_{\alpha\beta=x,y,z}(\delta_{\alpha\beta}-\hat{\mathbf{Q}}_\alpha\hat{\mathbf{Q}}_\beta)S^{\alpha\beta}_{\mathrm{mag}}(\mathbf{Q},\omega)+N\frac{k'}{k}S_{\mathrm{nuc}}(\mathbf{Q},\omega)$$

$$\langle l|\hat{c}_k|l\rangle = (-1)^l(2l+1)\begin{pmatrix} l & k & l \\ 0 & 0 & 0 \end{pmatrix}$$

$$L_x L_y L_z S_x S_y S_z$$

$\mathcal{H}_{\text{zeman}}$

$$\langle \theta J m_J | (L, S)_{x,y} | \theta' J' m'_J \rangle$$

$$\frac{(-1)^{J-m_J}}{\sqrt{\pm 2}}\left[\begin{pmatrix} J & 1 & J' \\ -m_J & 1 & m'_J \end{pmatrix} \pm \begin{pmatrix} J & -1 & J' \\ -m_J & 1 & m'_J \end{pmatrix}\right]$$

$$\times \langle \theta J || (L, S) ||| \theta' J' \rangle$$

$$\langle \theta J m_J | (L, S)_z | \theta' J' m'_J \rangle$$

$$(-1)^{J-m_J}\begin{pmatrix} J & 1 & J' \\ -m_J & 0 & m'_J \end{pmatrix}\langle\theta J||(L,S)||\theta' J'\rangle$$

$$\langle \theta J || (L,S) || \theta' J' \rangle = \delta_{\theta,\theta'} (-1)^{S+L+(J,J')} \sqrt{(2J+1)(2J'+1)}$$

$$\times\sqrt{(L,S)((L,S)+1)(2(L,S)+1)}\left\{\begin{array}{ccc} J' & 1 & J \\ (L,S) & (S,L) & (L,S)' \end{array}\right\}$$

$$\mathcal{H}_{\text{zeman}} = -\mu_B(2\mathbf{S}^n + \mathbf{L}^n)\mathbf{H}$$

$$\langle l^{\nu} v S L J M | \hat{\mathcal{Q}}_q | l^{\nu} v' S' L' J' M' \rangle$$

$$\sqrt{4\pi} \sum_{K',Q,Q'} \left[Y^{Q}_{K'-1}(\hat{\mathbf{Q}}) \left(\frac{2K'+1}{K'+1} \right)\right.$$

$$\times\{A(K'-1,K')+B(K'-1,K')(K'-1QK'Q'|1q)\}$$

$$+Y_{K'}^{Q}(\hat{\mathbf{Q}})B(K',K')(K'QK'Q'|1q)\Big]\,(K'Q'J'M'|JM)$$

$$q = -1, 0, 1$$

$$\hat{\mathcal{Q}}_x$$

$$+\frac{1}{\sqrt{2}}(\hat{\mathcal{Q}}_{+1}+\hat{\mathcal{Q}}_{-1})$$

$$\hat{Q}_y$$

$$-\frac{i}{\sqrt{2}}(\hat{\mathcal{Q}}_{+1}-\hat{\mathcal{Q}}_{-1})$$

$$\hat{\mathcal{Q}}_z$$

$\hat{\mathcal{Q}}_0$

$$A(K, K')$$

$$B(K, K')$$

#!

$\vec{Q}, \omega$

$$g = j_{ex}N(0)$$

$$p(n)$$

$\beta E(n)$

$$P(\mu)$$

$K_{n,m}$

$\Omega_{\nu\mu}$

$$\Phi_{\mu,\nu}(\omega)$$

$$\chi^{\alpha,\beta}(\omega) = \beta \sum_{\mu\nu} (J^{\alpha})_{\mu})^{*} \left[P_{\mu}\delta_{\mu\nu} - \omega\Phi_{\mu\nu}(\omega) \right] J^{\beta}_{\nu}$$

$$Im\chi^{\alpha\beta}(\omega)/(1-\exp(-\beta\omega))$$

$$S(\vec{Q},\omega) = \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \tilde{Q}^{\alpha}\tilde{Q}^{\beta}\right) Im\chi^{\alpha\beta}/(1 - \exp(-\beta\omega))$$

$$\chi^{\alpha\beta}(\omega)$$

$Npoint$

$emin$

$emax$

$Im\chi^{\alpha\alpha}(\omega)/\tanh\beta\omega/2$

$$\sum_{\alpha} \frac{1}{\pi} \int d\omega \frac{Im\chi^{\alpha\alpha}}{\tanh(\beta\omega/2)} = J(J+1)$$

$$S(\vec{Q},\omega) = \sum_{\alpha,\beta} (\delta_{\alpha,\beta} - \tilde{Q}_\alpha \tilde{Q}_\beta) \frac{\chi''_{\alpha\beta}(\omega)}{1 - \exp(-\beta\omega)}$$

$$\vec{Q}$$

$$(r_0 g_J F(\vec{Q})/2)^2 \frac{1}{\pi} S^{\alpha\beta}(\vec{Q},\omega), \quad S^{\alpha\beta}(\vec{Q},\omega) = \frac{Im\chi^{\alpha,\beta}(\omega)}{1 - exp(-\beta\omega)}$$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k} S(\vec{Q}, \omega)$$

$$S(\vec{Q},\omega) = (\frac{r_0}{2} gF(Q))^2 \frac{1}{\pi} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) \frac{Im\chi^{\alpha,\beta}(\omega)}{1 - exp(-\beta\omega)}$$

$$\vec{k}$$

$$E = k^2/2m$$

$$\vec{k}' = \vec{k} - \vec{Q}$$

$$E' = k'^2/2m$$

$$\omega = E - E'$$

$$\vec{k}'$$

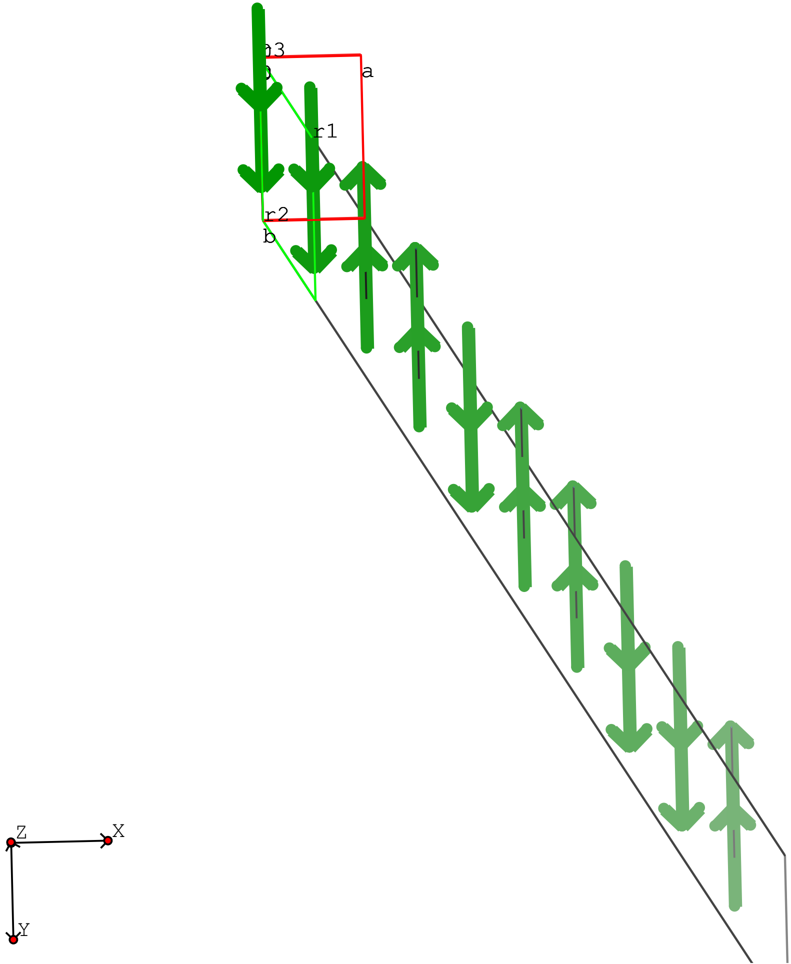
$$E'$$

E

$$E' = k^2/2m$$

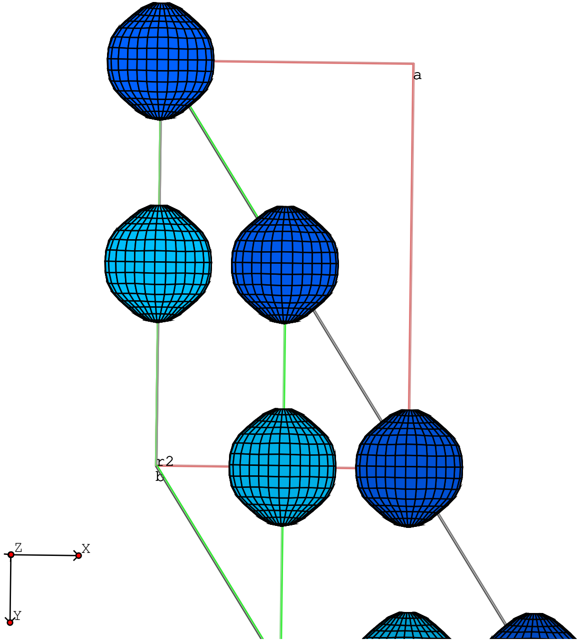
$\longrightarrow$

<

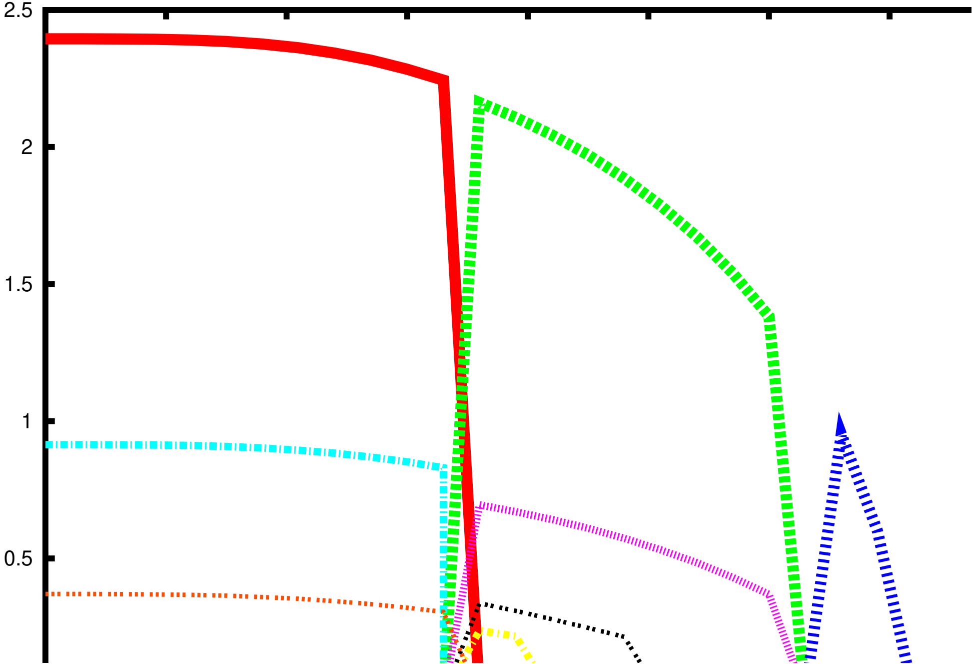


a3
a
r1
r2
b
Z
X
Y

$$\langle Mx\rangle\langle My\rangle\langle Mz\rangle$$

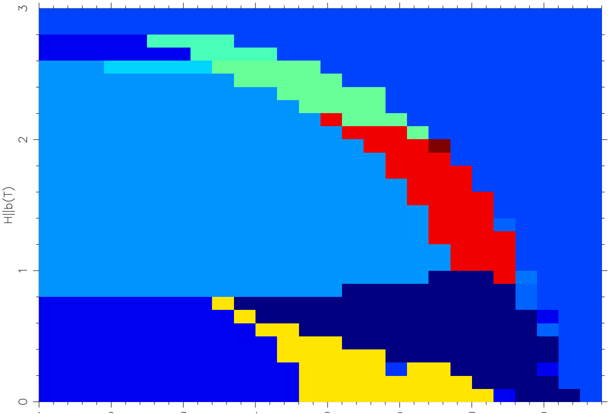

a
r2
b
Z
X
Y

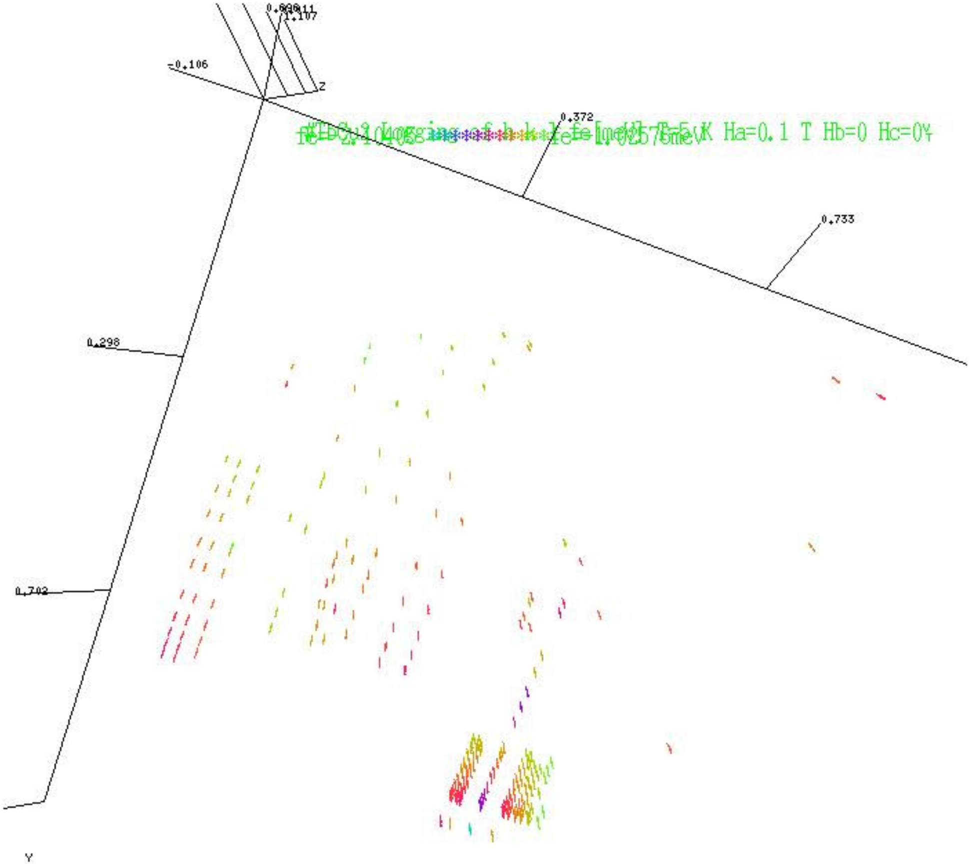
$\langle \mathbf{I} \rangle$


2.5
2
1.5
1
0.5

HT

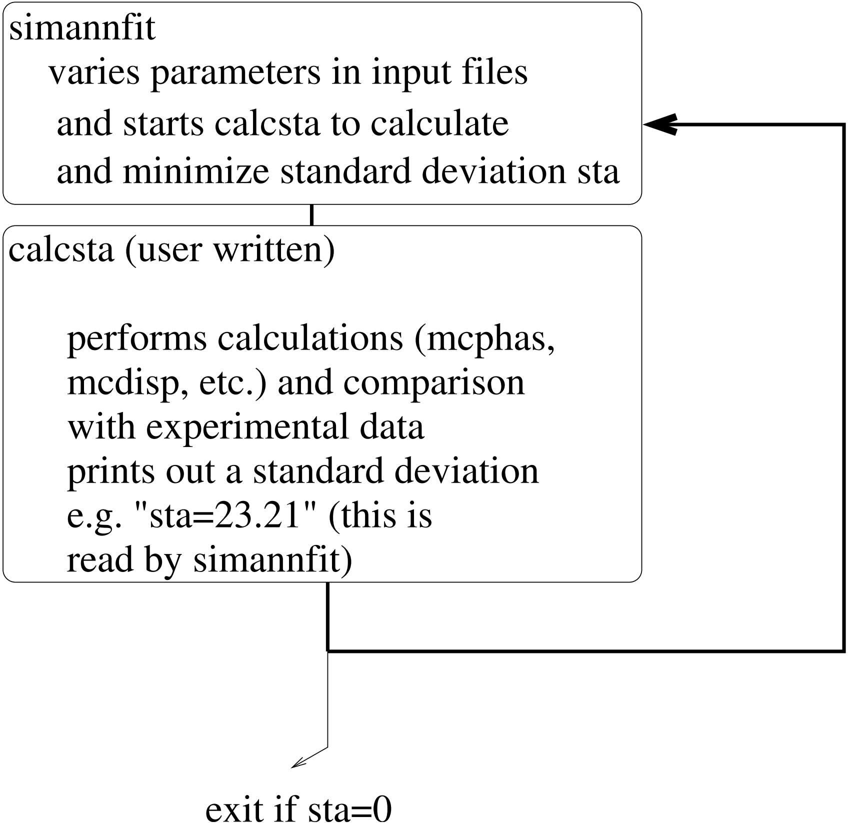
NdCu2 calculated magnetic phasediagram

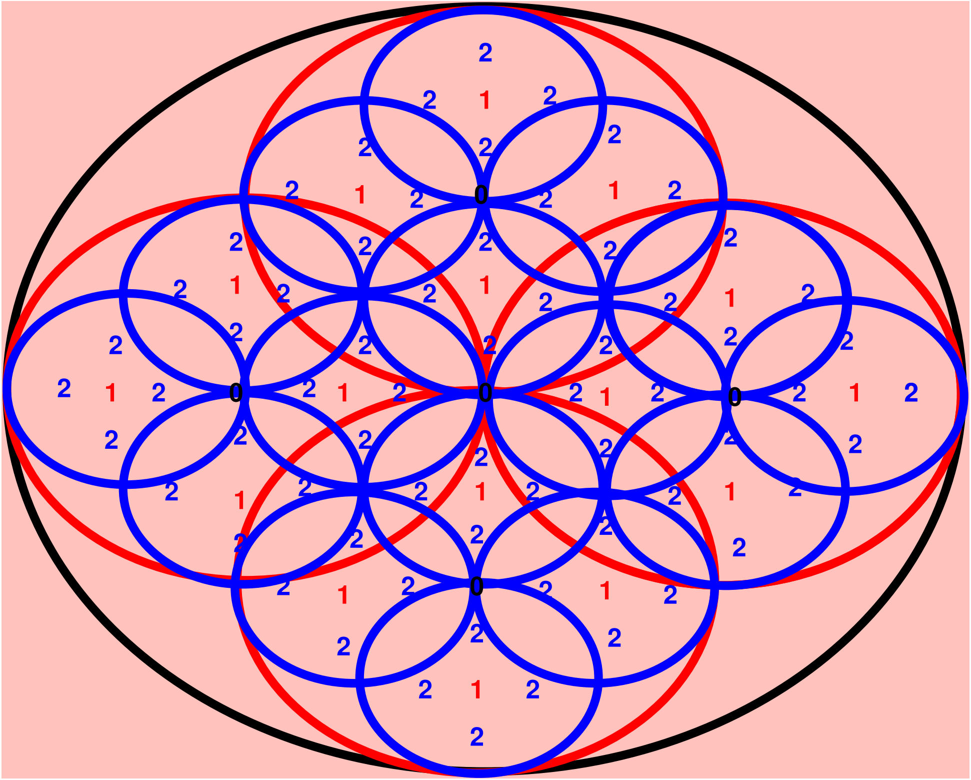




-0.106
0.372
0.733
0.298
0.702
Z
Y
T=5 K Ha=0.1 T Hb=0 Hc=0

$$exp([sta(par') - sta(par)]/T) < \mathrm{a random number out of } [0, 1]$$


simannfit
varies parameters in input files
and starts calcsta to calculate
and minimize standard deviation sta
calcsta (user written)
performs calculations (mcphas,
mcdisp, etc.) and comparison
with experimental data
prints out a standard deviation
e.g. "sta=23.21" (this is
read by simannfit)
exit if sta=0



0
1
2

δ_i^2

$$s^2 = 1/N \sum_i \delta_i^2$$

$$\mathrm{err}^2$$

$$\delta_i^2 =$$

2

$= s^2 = 1/N \sum_i \delta_i^2$

$$\chi^2 = 1/N \sum_i \delta_i^2/\mathrm{err}^2$$

$$F_{ij} = \partial\delta_i/\mathrm{err}_i\partial\mathrm{par}_j$$

$$\text{cov} = \chi^2 (F^T F)^{-1}$$

j

$parn$

$$d = \sum_i^N (par_i - parn_i)^2 / stepwidth_i^2$$

$d > N$

sta

$$sta <= sta$$

> 11

$sta < 0.2$

<

〉

B_2^m

$$B_4^m$$

$$B_6^m$$

$$\epsilon = S * T * D(\Theta_D / T)$$

$$D(z) = \frac{3}{z^3} \int_0^z \frac{x^3 dx}{e^x - 1}$$

$$f(E) = b + l(E - EF) + [d + k(E - EF)]/(\exp((E - EF)/kT) + 1)$$

$$f(E)$$

$$J_{\alpha\beta}(\vec{R}) = \frac{\mu_0}{4\pi}(g_J\mu_B)^2 \frac{3R_\alpha R_\beta - \delta_{\alpha\beta}R^2}{R^5}$$

$$J(R) = Acos(2k_f R)/(2k_f R)^3$$

$$J(R) = Acos(2\kappa)/(2\kappa)^3$$

$$\kappa^2 = k_a^2 R_a^2 + k_b^2 R_b^2 + k_c^2 R_c^2$$

$$J(R) = A(sin(2k_fR) - 2k_fRcos(2k_fR))/(2k_fR)^4$$

$$J(R) = A(sin(2\kappa) - 2\kappa cos(2\kappa))/(2\kappa)^4$$

$$\kappa^2 = k_a^2 R_a^2 + k_b^2 R_b^2 + k_c^2 R_c^2$$

$$J(R) = A[-(R/D)^2 + (R/D)^4] exp[-\alpha(R/D)^2]$$

D

$$J(R) = A[-\rho^2 + \rho^4]exp[-\alpha\rho^2]$$

$$\rho^2 = R_a^2/D_a^2 + R_b^2/D_b^2 + R_c^2/D_c^2$$

H

$$\sum_{ij} \frac{c_L(ij) - c_T(ij)}{2|R_{ij}|^2}(\mathbf{P}_i.\mathbf{R}_{ij} - \mathbf{P}_j.\mathbf{R}_{ij})^2 + \frac{c_T(ij)}{2}(\mathbf{P}_i - \mathbf{P}_j)^2$$

$$C_L(ij) = 25\exp(-0.1 * r_{ij}^2/\mathring{A}^2)$$

$$\partial B_{lm}/\partial u$$

$$\mathbf{J}_i$$

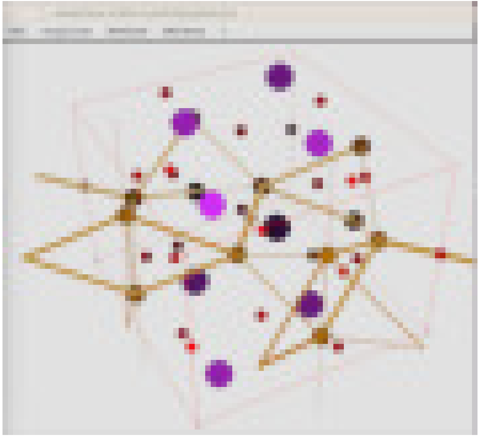
$\mathbf{J}_j$

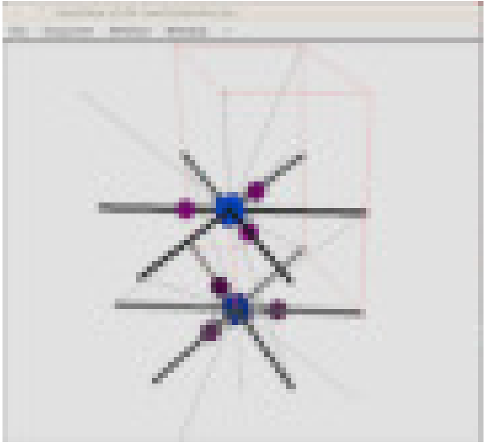
$$\mathcal{J}\mathbf{J}_i.\mathbf{J}_j$$

$$\mathbf{J}_i.\begin{pmatrix} \mathcal{J} & 0 & 0 \\ 0 & \mathcal{J} & 0 \\ 0 & 0 & \mathcal{J} \end{pmatrix}.\mathbf{J}_j$$

$$\mathcal{D}(\mathbf{J}_i \times \mathbf{J}_j)$$

$$\mathbf{J}_i . \left(\begin{array}{ccc} 0 & \mathcal{D}_z & -\mathcal{D}_y \\ -\mathcal{D}_z & 0 & \mathcal{D}_x \\ \mathcal{D}_y & -\mathcal{D}_x & 0 \end{array} \right) . \mathbf{J}_j$$





$0.2|e|$

$$0.1|e|$$

$$0.3|e|$$

$$dB_l^m/du$$

dL_l^m/du

$u =$

$(\mathring{A})/a_0$

< 1

$J(Q)$

$$< Ia >, < Ib >$$

$< I >$

$$2^4 = 8$$

$$\chi^2 = \frac{1}{n}\sum_{i=1}^{n}\frac{(\mathrm{col2}_i - \mathrm{col1}_i)^2}{\mathrm{col3_i}^2}$$

x_i, y_i

$c(x)$

$$f(x) = \sum_i y_i c(x - x_i)$$

$$f(x)$$

x_i, y_i, z_i

$$c(x, y)$$

$$f(x, y) = \sum_i z_i c(x - x_i, y - y_i)$$

$$\sigma = \mathrm{fwhm}/\sqrt{8 * log(2)}$$

$$\mathrm{gauss}(x) = \frac{\mathrm{area} exp(-(x - \mathrm{position})^2/2\sigma^2)}{\sqrt{2 * \pi}\sigma}$$

$$\int f(x)dx$$

$$\mu_1 = \int x f(x) dx$$

$$\mu_n = \int (x - \mu_1)^n f(x) dx$$

$$\mathrm{lorentz}(x) = \frac{1.0}{\pi \mathrm{fwhm}(1.0 + (x - \mathrm{position})^2 / fwhm^2)}$$

const

x'

$$\cos(\alpha) * x + \sin(\alpha) * y$$

y'

$$-\sin(\alpha) * x + \cos(\alpha) * y$$

R_p

$$R_p = 100 * \frac{\sum_{i=1}^{N} |(x(i) - y(i)|}{\sum_{i=1}^{N} |x(i)|}$$

$$\mathrm{fwhm} = \sqrt{u \tan^2(\theta) + v \tan(\theta) + w}$$

$$\text{gauss}(x) = \frac{exp(-x^2/2\sigma^2)}{\sqrt{2*\pi}\sigma}$$

$$\text{gauss}(x, y) = \frac{exp(-u_1^2/2\sigma_1^2)}{\sqrt{2*\pi}\sigma_1} \frac{exp(-u_2^2/2\sigma_2^2)}{\sqrt{2*\pi}\sigma_2}$$

$$u_1 = xcos(\theta) - ysin(\theta)$$

$$u_2 = ycos(\theta) + xsin(\theta)$$

θ

$$\mathrm{lorentz}(x) = \frac{1.0}{\pi \mathrm{fwhm}(1.0 + x^2/fwhm^2)}$$

|土 >

$$< \pm|\hat{\mathbf{J}}_a|\mp >= A$$

$$A^{\star} = A$$

A... saturation moment in a direction

$$< \pm|\hat{\mathbf{J}}_b|\pm >= \pm B$$

$$B^{\star} = B$$

B... saturation moment in b direction

$$< \pm|\hat{\mathbf{J}}_c|\mp >= C$$

$$C^{\star} = -C$$

C... saturation moment in c direction

$$H = H_{cf} - g_J \mu_b \mathbf{HJ}$$

$$\hat{H} = g_J \mu_B \begin{pmatrix} BH_b & -AH_a - CH_c \\ -AH_a + CH_c & -BH_b \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \beta^\star & -\alpha \end{pmatrix}$$

$\lambda_{\pm}$

$$\Delta = \lambda_+ - \lambda_-$$

$$\lambda_{\pm} = \pm\sqrt{\alpha^2 + \beta^\star \beta}$$

$$|\lambda_\pm >= \frac{-\beta|+> + (\alpha - \lambda_\pm)|->}{\sqrt{|\alpha - \lambda_\pm|^2 + \beta^\star \beta}}$$

$$Z = \exp(-\Delta/2kT) + \exp(\Delta/2kT)$$

$$< \hat{\mathbf{M}} >= \sum_{\pm} < \lambda_{\pm} | g_J \hat{\mathbf{J}} | \lambda_{\pm} > \frac{\exp(-\lambda_{\pm}/kT)}{Z}$$

$$< \lambda_{\pm} | \hat{J}_a | \lambda_{\pm} >= \frac{-2A\Re[\beta^{\star}(\alpha - \lambda_{\pm})]}{|\alpha - \lambda_{\pm}|^2 + \beta^{\star}\beta}$$

$$< \lambda_{\pm}|\hat{J}_b|\lambda_{\pm} >= \frac{-B\beta^{\star}\beta + B|\alpha - \lambda_{\pm}|^2}{|\alpha - \lambda_{\pm}|^2 + \beta^{\star}\beta}$$

$$< \lambda_{\pm}|\hat{J}_c|\lambda_{\pm} >= \frac{2\Re(\beta C)(\alpha - \lambda_{\pm})}{|\alpha - \lambda_{\pm}|^2 + \beta^{\star}\beta}$$

U

$$U = \sum_{\pm} \lambda_{\pm} \frac{\exp(-\lambda_{\pm}/kT)}{Z}$$

$$M_{\alpha\beta} = < \lambda_- | \hat{J}_\alpha | \lambda_+ >< \lambda_+ | \hat{J}_\beta | \lambda_- > \tanh(\Delta/2kT)$$

$$< \lambda_- | \hat{J}_a | \lambda_+ >= \frac{-2A(\alpha \Re(\beta) + i\lambda_+ \Im(\beta))}{\sqrt{(|\alpha - \lambda_+|^2 + \beta^\star \beta)(|\alpha - \lambda_-|^2 + \beta^\star \beta)}}$$

$$< \lambda_- | \hat{J}_b | \lambda_+ >= \frac{-2B\beta^\star \beta}{\sqrt{(|\alpha - \lambda_+|^2 + \beta^\star \beta)(|\alpha - \lambda_-|^2 + \beta^\star \beta)}}$$

$$< \lambda_- | \hat{J}_c | \lambda_+ >= \frac{2|C|(-\alpha \Im(\beta) + i\lambda_+ \Re(\beta))}{\sqrt{(|\alpha - \lambda_+|^2 + \beta^\star \beta)(|\alpha - \lambda_-|^2 + \beta^\star \beta)}}$$

$$<>_T$$

J

$$\mathbf{M} = g_J \mu_B < \mathbf{J} >_T$$

$2+$

$$\mathbf{M} = g_J \mu_B < \hat{\mathbf{J}} >_T$$

$$< \hat{\mathbf{J}} >= \frac{\mathbf{H}}{|\mathbf{H}|} B_J(x = g_J \mu_B |\mathbf{H}|/kT)$$

$$B_J(x) = \frac{\sum_{m=-J}^{J} m x^m}{\sum_{m=-J}^{J} x^m} = \frac{J(x^{J+2} - x^{-J}) + (J+1)x(x^{-J} - x^J)}{(1-x)(x^{-J} - x^{J+1})}$$

Z

$$Z = \sum_{m=-J}^{J} x^m = \frac{x^{J+1} - x^{-J}}{x-1}$$

$$\Delta = g_J \mu_B H$$

$$M_{\alpha\beta} = \frac{-b_\alpha b_\beta R_J}{Z}$$

b

b_x

$$\frac{-H_y + iH_x \frac{H_z}{|\mathbf{H}|}}{2|\mathbf{H}| sin\Theta}$$

$$b_y$$

$$\frac{H_x + iH_y \frac{H_z}{|\mathbf{H}|}}{2|\mathbf{H}|sin\Theta}$$

b_z

$$\frac{H_x^2 + H_y^2}{2i|\mathbf{H}|^2 sin\Theta} = \frac{-isin\Theta}{2}$$

$$sin\Theta = \frac{\sqrt{H_x^2 + H_y^2}}{|\mathbf{H}|}$$

R_J

$$R_J = (x-1)\sum_{m=-J}^{J-1}(J+m+1)(J-m)x^m = \frac{2Jx^{-J} + (2J+2)x(x^J - x^{-J}) - 2Jx^{J+2}}{(1-x)^2}$$

$$J = 15/2$$

Δ

$$H = \begin{pmatrix} -\Delta/2 & 0 & 0 & 0 \\ 0 & -\Delta/2 & 0 & 0 \\ 0 & 0 & \Delta/2 & 0 \\ 0 & 0 & 0 & \Delta/2 \end{pmatrix} - g_J \mu_B (H_a J_a + H_b J_b + H_c J_b)$$

$$J_a = \begin{pmatrix} 0 & b & 0 & c \\ b & 0 & c & 0 \\ 0 & c & 0 & e \\ c & 0 & e & 0 \end{pmatrix}$$

$$J_b = \begin{pmatrix} 0 & -ib & 0 & ic \\ +ib & 0 & -ic & 0 \\ 0 & +ic & 0 & -ie \\ -ic & 0 & +ie & 0 \end{pmatrix}$$

$$J_c = \begin{pmatrix} +a & 0 & 0 & 0 \\ 0 & -a & 0 & 0 \\ 0 & 0 & -d & 0 \\ 0 & 0 & 0 & +d \end{pmatrix}$$

M

$\max(...)$

$$M_{001} = g_J \mu_B \max(|a|, |d|)$$

M_{100}

$$g_J \mu_B \lambda$$

$$2\lambda^2$$

$$e^2 + 2c^2 + b^2 + \sqrt{(e^2 + 2c^2 + b^2)^2 - 4(be - c^2)}$$

M_{110}

$$e^2 + 2c^2 + b^2 + \sqrt{(e^2 + 2c^2 + b^2)^2 - 4(be+c^2)}$$

$$J_a = \begin{pmatrix} 0 & b & 0 & c \\ b & 0 & -c & 0 \\ 0 & -c & 0 & e \\ c & 0 & e & 0 \end{pmatrix}$$

$$J_b = \begin{pmatrix} 0 & -ib & 0 & ic \\ +ib & 0 & +ic & 0 \\ 0 & -ic & 0 & -ie \\ -ic & 0 & +ie & 0 \end{pmatrix}$$

J_x

$$J_y$$

$$\mathcal{H}_{\text{cf}} = \sum_{l,m} A_{lm} \langle r^l \rangle \langle J || \theta_l || J \rangle \hat{O}_l^m(J)$$

$$A_{lm}\langle r^l\rangle$$

A_{lm}

$$B_l^m = A_{lm} \langle r^l \rangle \langle J || \theta_l || J \rangle$$

$$\theta_l = \langle J || \theta_l || J \rangle$$

$$l = 0, 2, 4, 6$$

$\nu, \alpha_J, \beta_J, \gamma_J$

$\hat{C}_{lm}$

$$C_{lm}(\theta, \phi) = \sqrt{4\pi/(2l+1)}Y_{lm}(\theta, \phi)$$

$$Y_{lm}(\theta, \phi)$$

$$\lambda_{l0} = p_{l0}\sqrt{4\pi/(2l+1)}$$

$$\lambda_{lm} = p_{lm}\sqrt{8\pi/(2l+1)}$$

$l \neq 0$

$$\mathcal{H}_{\mathrm{cf}} = \sum_{l,m} D_l^m \hat{C}_{lm}$$

$$\hat{T}_{lm}$$

$$\hat{T}_{l0} = \hat{C}_{l0}, \qquad \hat{T}_{l,\pm|m|} = \sqrt{\pm 1}\left[\hat{C}_{l,-|m|} \pm (-1)^{|m|}\hat{C}_{l,|m|}\right]$$

$$\mathcal{H}_{\mathrm{cf}} = \sum_{l,m} L_l^m \hat{T}_{lm}$$

$x||a, y||b, z||c$

$$A_l^m$$

$$\lambda_{lm} L_l^m / \langle r^l \rangle$$

$$\left\{\begin{array}{lr} \lambda_{lm} L_l^m \langle J||\theta_l||J\rangle & \text{for rare earth} \\ \lambda_{lm} L_l^m \langle L||\theta_l||L\rangle & \text{for trans metals} \end{array}\right.$$

B_m^l

$$V_l^m$$

$$\lambda_{lm} L_l^m$$

$$\lambda_{lm} L_l^m \langle J || \theta_l || J \rangle$$

B_0^l
$B_m^l(c)$
$B_m^l(s)$

$$\left\{\begin{array}{l} L_l^0 \\ L_l^m \\ -L_l^{-m} \end{array}\right.$$

$$B_m^l$$

$$\begin{cases} L_l^0 & m = 0 \\ (-1)^m (L_l^m - i L_l^{-m}) & m > 0 \\ L_l^{-m} + i L_l^m & m < 0 \end{cases}$$

B_{lm}

$Ak(), CAk()$

$$(-1)^m L_l^m$$

$$|m|$$

l

0

1

2

3

4

5

6

$$\sqrt{6}$$

$$\frac{1}{2}\sqrt{6}$$

$$\frac{1}{8}$$

$$\frac{1}{2}\sqrt{5}$$

$$\frac{1}{4}\sqrt{10}$$

$$\frac{1}{2}\sqrt{35}$$

$$\frac{1}{8}\sqrt{70}$$

$$\frac{1}{16}$$

$$\frac{1}{8}\sqrt{42}$$

$$\frac{1}{16}\sqrt{105}$$

$$\frac{1}{8}\sqrt{105}$$

$$\frac{3}{16}\sqrt{14}$$

$$\frac{3}{8}\sqrt{77}$$

$$\frac{1}{16}\sqrt{231}$$

$$B_m^l(\text{Newman}) \equiv (-1)^m L_l^m$$

Z_{n0}

Y_n^0

$$Z_{n\alpha} \equiv Z^c_{n,\alpha}$$

$$\frac{1}{\sqrt{2}}[Y_n^{-\alpha} + (-1)^\alpha Y_n^\alpha] \ldots \alpha > 0$$

$$Z_{n\alpha} \equiv Z^{s}_{n,|\alpha|}$$

$$\frac{i}{\sqrt{2}}[Y_n^\alpha - (-1)^\alpha Y_n^{-\alpha}] \ldots \alpha < 0$$

$$Z_{41}^{c}$$

$$Z_{43}^{c}$$

$$Z_{52}^{c}$$

$$Z_{00} = \frac{1}{\sqrt{4\pi}}$$

$$\begin{aligned}
Z_{11}^{s} &= \sqrt{\frac{3}{4\pi}}[y/r] \\
Z_{10} &= \sqrt{\frac{3}{4\pi}}[z/r] \\
Z_{11}^{c} &= \sqrt{\frac{3}{4\pi}}[x/r]
\end{aligned}$$

$$\begin{aligned}
Z_{22}^{s} &= \frac{1}{4}\sqrt{\frac{15}{\pi}}[2xy/r^2] \\
Z_{21}^{s} &= \frac{1}{2}\sqrt{\frac{15}{\pi}}[yz/r^2] \\
Z_{20} &= \frac{1}{4}\sqrt{\frac{5}{\pi}}[(3z^2-r^2)/r^2] \\
Z_{21}^{c} &= \frac{1}{2}\sqrt{\frac{15}{\pi}}[xz/r^2] \\
Z_{22}^{c} &= \frac{1}{4}\sqrt{\frac{15}{\pi}}[(x^2-y^2)/r^2]
\end{aligned}$$

$$\begin{aligned}
Z_{33}^{s} &= \sqrt{\frac{35}{32\pi}}[(3x^2y-y^3)/r^3] \\
Z_{32}^{s} &= \sqrt{\frac{105}{16\pi}}[2xyz/r^3] \\
Z_{31}^{s} &= \sqrt{\frac{21}{32\pi}}[y(5z^2-r^2)/r^3] \\
Z_{30} &= \sqrt{\frac{7}{16\pi}}[z(5z^2-3r^2)/r^3] \\
Z_{31}^{c} &= \sqrt{\frac{21}{32\pi}}[x(5z^2-r^2)/r^3] \\
Z_{32}^{c} &= \sqrt{\frac{105}{16\pi}}[(x^2-y^2)z/r^3] \\
Z_{33}^{c} &= \sqrt{\frac{35}{32\pi}}[(x^3-3xy^2)/r^3]
\end{aligned}$$

$$\begin{aligned}
Z_{44}^{s} &= \frac{3}{16}\sqrt{\frac{35}{\pi}}[4(x^3y-xy^3)/r^4] \\
Z_{43}^{s} &= \frac{3}{8}\sqrt{\frac{70}{\pi}}[(3x^2y-y^3)z/r^4] \\
Z_{42}^{s} &= \frac{3}{8}\sqrt{\frac{5}{\pi}}[2xy(7z^2-r^2)/r^4] \\
Z_{41}^{s} &= \frac{3}{4}\sqrt{\frac{5}{2\pi}}[yz(7z^2-3r^2)/r^4] \\
Z_{40} &= \frac{3}{16}\frac{1}{\sqrt{\pi}}[35z^4-30z^2r^2+3r^4)/r^4] \\
Z_{41}^{c} &= \frac{3}{4}\sqrt{\frac{5}{2\pi}}[xz(7z^2-3r^2)/r^4] \\
Z_{42}^{c} &= \frac{3}{8}\sqrt{\frac{5}{\pi}}[(x^2-y^2)(7z^2-r^2)/r^4] \\
Z_{43}^{c} &= \frac{3}{8}\sqrt{\frac{70}{\pi}}[(x^3-3xy^2)z/r^4] \\
Z_{44}^{c} &= \frac{3}{16}\sqrt{\frac{35}{\pi}}[(x^4-6x^2y^2+y^4)/r^4]
\end{aligned}$$

$$\begin{aligned}
Z_{55}^{s} &= \sqrt{\frac{693}{512\pi}}[(5x^4y-10x^2y^3+y^5)/r^5] \\
Z_{54}^{s} &= \sqrt{\frac{3465}{256\pi}}[4(x^3y-xy^3)z/r^5] \\
Z_{53}^{s} &= \sqrt{\frac{385}{512\pi}}[(3x^2y-y^3)(9z^2-r^2)/r^5] \\
Z_{52}^{s} &= \sqrt{\frac{1155}{64\pi}}[2xy(3z^3-zr^2)/r^5] \\
Z_{51}^{s} &= \sqrt{\frac{165}{256\pi}}[y(21z^4-14z^2r^2+r^4)/r^5] \\
Z_{50} &= \sqrt{\frac{11}{256\pi}}[(63z^5-70z^3r^2+15zr^4)/r^5] \\
Z_{51}^{c} &= \sqrt{\frac{165}{256\pi}}[x(21z^4-14z^2r^2+r^4)/r^5] \\
Z_{52}^{c} &= \sqrt{\frac{1155}{64\pi}}[(x^2-y^2)(3z^3-zr^2)/r^5] \\
Z_{53}^{c} &= \sqrt{\frac{385}{512\pi}}[(x^3-3xy^2)(9z^2-r^2)/r^5] \\
Z_{54}^{c} &= \sqrt{\frac{3465}{256\pi}}[(x^4-6x^2y^2+y^4)z/r^5] \\
Z_{55}^{c} &= \sqrt{\frac{693}{512\pi}}[(x^5-10x^3y^2+5xy^4)/r^5]
\end{aligned}$$

$$\begin{aligned}
Z_{66}^{s} &= \frac{231}{64}\sqrt{\frac{26}{231\pi}}[(6x^5y-20x^3y^3+6xy^5)/r^6] \\
Z_{65}^{s} &= \sqrt{\frac{9009}{512\pi}}[(5x^4y-10x^2y^3+y^5)z/r^6] \\
Z_{64}^{s} &= \frac{21}{32}\sqrt{\frac{13}{7\pi}}[4(x^3y-xy^3)(11z^2-r^2)/r^6] \\
Z_{63}^{s} &= \frac{1}{32}\sqrt{\frac{2730}{\pi}}[(3x^2y-y^3)(11z^3-3zr^2)/r^6] \\
Z_{62}^{s} &= \frac{1}{64}\sqrt{\frac{2730}{\pi}}[2xy(33z^4-18z^2r^2+r^4)/r^6] \\
Z_{61}^{s} &= \frac{1}{8}\sqrt{\frac{273}{4\pi}}[yz(33z^4-30z^2r^2+5r^4)/r^6] \\
Z_{60} &= \frac{1}{32}\sqrt{\frac{13}{\pi}}[(231z^6-315z^4r^2+105z^2r^4-5r^6)/r^6] \\
Z_{61}^{c} &= \frac{1}{8}\sqrt{\frac{273}{4\pi}}[xz(33z^4-30z^2r^2+5r^4)/r^6] \\
Z_{62}^{c} &= \frac{1}{64}\sqrt{\frac{2730}{\pi}}[(x^2-y^2)(33z^4-18z^2r^2+r^4)/r^6] \\
Z_{63}^{c} &= \frac{1}{32}\sqrt{\frac{2730}{\pi}}[(x^3-3xy^2)(11z^3-3zr^2)/r^6] \\
Z_{64}^{c} &= \frac{21}{32}\sqrt{\frac{13}{7\pi}}[(x^4-6x^2y^2+y^4)(11z^2-r^2)/r^6] \\
Z_{65}^{c} &= \sqrt{\frac{9009}{512\pi}}[(x^5-10x^3y^2+5xy^4)z/r^6] \\
Z_{66}^{c} &= \frac{231}{64}\sqrt{\frac{26}{231\pi}}[(x^6-15x^4y^2+15x^2y^4-y^6)/r^6]
\end{aligned}$$

$$I_\alpha$$

$X = J(J+1)$

$$
\begin{aligned}
O_{00} &= 1
\end{aligned}
$$

$$
\begin{aligned}
O_{11} &= \frac{1}{2}[J_+ + J_-] = J_x = I_1 \\
O_{11}^s &= \frac{-i}{2}[J_+ - J_-] = J_y = I_2 \\
O_{10} &= J_z = I_3
\end{aligned}
$$

$$
\begin{aligned}
O_{22}^s &= \frac{-i}{2}[J_+^2 - J_-^2] = J_xJ_y + J_yJ_x = 2P_{xy} = I_4 \\
O_{21}^s &= \frac{-i}{4}[J_z(J_+ - J_-) + (J_+ - J_-)J_z] = \frac{1}{2}[J_yJ_z + J_zJ_y] = P_{yz} = I_5 \\
O_{20} &= [3J_z^2 - X] = I_6 \\
O_{21} &= \frac{1}{4}[J_z(J_+ + J_-) + (J_+ + J_-)J_z] = \frac{1}{2}[J_xJ_z + J_zJ_x] = P_{xz} = I_7 \\
O_{22} &= \frac{1}{2}[J_+^2 + J_-^2] = J_x^2 - J_y^2 = I_8
\end{aligned}
$$

$$
\begin{aligned}
O_{33}^s &= \frac{-i}{2}[J_+^3 - J_-^3] = I_9 \\
O_{32}^s &= \frac{-i}{4}[(J_+^2 - J_-^2)J_z + J_z(J_+^2 - J_-^2)] = I_{10} \\
O_{31}^s &= \frac{-i}{4}[(J_+ - J_-)(5J_z^2 - X - 1/2) + (5J_z^2 - X - 1/2)(J_+ - J_-)] = I_{11} \\
O_{30} &= [5J_z^3 - (3X-1)J_z] = I_{12} \\
O_{31} &= \frac{1}{4}[(J_+ + J_-)(5J_z^2 - X - 1/2) + (5J_z^2 - X - 1/2)(J_+ + J_-)] = I_{13} \\
O_{32} &= \frac{1}{4}[(J_+^2 + J_-^2)J_z + J_z(J_+^2 + J_-^2)] = I_{14} \\
O_{33} &= \frac{1}{2}[J_+^3 + J_-^3] = I_{15}
\end{aligned}
$$

$$
\begin{aligned}
O_{44}^s &= \frac{-i}{2}[(J_+^4 - J_-^4] = I_{16} \\
O_{43}^s &= \frac{-i}{4}[(J_+^3 - J_-^3)J_z + J_z(J_+^3 - J_-^3)] = I_{17} \\
O_{42}^s &= \frac{-i}{4}[(J_+^2 - J_-^2)(7J_z^2 - X - 5) + (7J_z^2 - X - 5)(J_+^2 - J_-^2)] = I_{18} \\
O_{41}^s &= \frac{-i}{4}[(J_+ - J_-)(7J_z^3 - (3X+1)J_z) + (7J_z^3 - (3X+1)J_z)(J_+ - J_-)] = I_{19} \\
O_{40} &= [35J_z^4 - (30X-25)J_z^2 + 3X^2 - 6X] = I_{20} \\
O_{41} &= \frac{1}{4}[(J_+ + J_-)(7J_z^3 - (3X+1)J_z) + (7J_z^3 - (3X+1)J_z)(J_+ + J_-)] = I_{21} \\
O_{42} &= \frac{1}{4}[(J_+^2 + J_-^2)(7J_z^2 - X - 5) + (7J_z^2 - X - 5)(J_+^2 + J_-^2)] = I_{22} \\
O_{43} &= \frac{1}{4}[(J_+^3 + J_-^3)J_z + J_z(J_+^3 + J_-^3)] = I_{23} \\
O_{44} &= \frac{1}{2}[(J_+^4 + J_-^4] = I_{24}
\end{aligned}
$$

$$
\begin{aligned}
O_{55}^s &= \frac{-i}{2}[J_+^5 - J_-^5] = I_{25} \\
O_{54}^s &= \frac{-i}{4}[(J_+^4 - J_-^4)J_z + J_z(J_+^4 - J_-^4)] = I_{26} \\
O_{53}^s &= \frac{-i}{4}[(J_+^3 - J_-^3)(9J_z^2 - X - 33/2) + (9J_z^2 - X - 33/2)(J_+^3 - J_-^3)] = I_{27} \\
O_{52}^s &= \frac{-i}{4}[(J_+^2 - J_-^2)(3J_z^3 - (X+6)J_z) + (3J_z^3 - (X+6)J_z)(J_+^2 - J_-^2)] = I_{28} \\
O_{51}^s &= \frac{-i}{4}[(J_+ - J_-)\{21J_z^4 - 14J_z^2X + X^2 - X + 3/2\} + \{\ldots\}(J_+ - J_-)] = I_{29} \\
O_{50} &= [63J_z^5 - (70X - 105)J_z^3 + (15X^2 - 50X + 12)J_z] = I_{30} \\
O_{51} &= \frac{1}{4}[(J_+ + J_-)(21J_z^4 - 14J_z^2X + X^2 - X + 3/2) + (21J_z^4 - 14J_z^2X + X^2 - X + 3/2)(J \\
O_{52} &= \frac{1}{4}[(J_+^2 + J_-^2)(3J_z^3 - (X+6)J_z) + (3J_z^3 - (X+6)J_z)(J_+^2 + J_-^2)] = I_{32} \\
O_{53} &= \frac{1}{4}[(J_+^3 + J_-^3)(9J_z^2 - X - 33/2) + (9J_z^2 - X - 33/2)(J_+^3 + J_-^3)] = I_{33} \\
O_{54} &= \frac{1}{4}[(J_+^4 + J_-^4)J_z + J_z(J_+^4 + J_-^4)] = I_{34} \\
O_{55} &= \frac{1}{2}[J_+^5 + J_-^5] = I_{35}
\end{aligned}
$$

$$
\begin{aligned}
O_{66}^s &= \frac{-i}{2}[J_+^6 - J_-^6] = I_{36} \\
O_{65}^s &= \frac{-i}{4}[(J_+^5 - J_-^5)J_z + J_z(J_+^5 - J_-^5)] = I_{37} \\
O_{64}^s &= \frac{-i}{4}[(J_+^4 - J_-^4)(11J_z^2 - X - 38) + (11J_z^2 - X - 38)(J_+^4 - J_-^4)] = I_{38} \\
O_{63}^s &= \frac{-i}{4}[(J_+^3 - J_-^3)(11J_z^3 - (3X+59)J_z) + (11J_z^3 - (3X+59)J_z)(J_+^3 - J_-^3)] = I_{39} \\
O_{62}^s &= \frac{-i}{4}[(J_+^2 - J_-^2)\{33J_z^4 - (18X+123)J_z^2 + X^2 + 10X + 102\} + \{\ldots\}(J_+^2 - J_-^2)] = I_{40} \\
O_{61}^s &= \frac{-i}{4}[(J_+ - J_-)\{33J_z^5 - (30X-15)J_z^3 + (5X^2 - 10X + 12)J_z\} + \{\ldots\}(J_+ - J_-)] = I_4 \\
O_{60} &= [231J_z^6 - (315X - 735)J_z^4 + (105X^2 - 525X + 294)J_z^2 - 5X^3 + 40X^2 - 60X] = I_{42} \\
O_{61} &= \frac{1}{4}[(J_+ + J_-)\{33J_z^5 - (30X-15)J_z^3 + (5X^2 - 10X + 12)J_z\} + \{\ldots\}(J_+ + J_-)] = I_{43} \\
O_{62} &= \frac{1}{4}[(J_+^2 + J_-^2)\{33J_z^4 - (18X+123)J_z^2 + X^2 + 10X + 102\} + \{\ldots\}(J_+^2 + J_-^2)] = I_{44} \\
O_{63} &= \frac{1}{4}[(J_+^3 + J_-^3)(11J_z^3 - (3X+59)J_z) + (11J_z^3 - (3X+59)J_z)(J_+^3 + J_-^3)] = I_{45} \\
O_{64} &= \frac{1}{4}[(J_+^4 + J_-^4)(11J_z^2 - X - 38) + (11J_z^2 - X - 38)(J_+^4 + J_-^4)] = I_{46} \\
O_{65} &= \frac{1}{4}[(J_+^5 + J_-^5)J_z + J_z(J_+^5 + J_-^5)] = I_{47} \\
O_{66} &= \frac{1}{2}[J_+^6 + J_-^6] = I_{48}
\end{aligned}
$$

$abc||$

$B_2^0, B_4^0, B_4^4, B_6^0$

$$abc||yzx$$

Blm

$B20$

$$-\frac{1}{2}B_2^0$$

$B22$

$$+\frac{3}{2}B_2^0$$

$B40$

$$+\frac{3}{8}B_4^0 + \frac{1}{8}B_4^4$$

$B42$

$$-\frac{5}{2}B_4^0 + \frac{1}{2}B_4^4$$

$B44$

$$\frac{35}{8}B_4^0 + \frac{1}{8}B_4^4$$

$B60$

$$-\frac{5}{16}B_6^0 - \frac{1}{16}B_6^4$$

$B62$

$$+\frac{105}{32}B_6^0+\frac{5}{32}B_6^4$$

$B64$

$$-\frac{63}{16}B_6^0+\frac{13}{16}B_6^4$$

$B66$

$$\frac{231}{32}B_6^0 + \frac{11}{32}B_6^4$$

$$B_2^0, B_2^2, B_4^0, B_4^2, B_4^4, B_6^0, B_6^2, B_6^4$$

$$-\frac{1}{2}B_2^0 - \frac{1}{2}B_2^2$$

$$+\frac{3}{2}B_2^0 - \frac{1}{2}B_2^2$$

$$+\frac{3}{8}B_4^0+\frac{1}{8}B_4^2+\frac{1}{8}B_4^4$$

$$-\frac{5}{2}B_4^0-\frac{1}{2}B_4^2+\frac{1}{2}B_4^4$$

$$\frac{35}{8}B_4^0 - \frac{7}{8}B_4^2 + \frac{1}{8}B_4^4$$

$$-\frac{5}{16}B_6^0-\frac{1}{16}B_6^2-\frac{1}{16}B_6^4-\frac{1}{16}B_6^6$$

$$+\frac{105}{32}B_6^0+\frac{5}{32}B_6^4+...$$

$$-\frac{63}{16}B_6^0 + \frac{13}{16}B_6^4 + ...$$

$$\frac{231}{32}B_6^0 + \frac{11}{32}B_6^4 + ...$$

$B_2^0, B_2^{-1}, B_2^2, B_4^0, B_4^{-1}, B_4^2, B_4^{-3}, B_4^4, B_6^0, B_6^{-1}, B_6^2, B_6^{-3}, B_6^4$

$B21$

$$-2B_2^{-1}$$

$B4-3$

$$-\frac{7}{4}B_4^{-1} - \frac{3}{4}B_4^{-3}$$

$$B4 - 1$$

$$+\frac{3}{4}B_4^{-1} - \frac{1}{4}B_4^{-3}$$

$$-\frac{5}{16}B_6^0-\frac{1}{16}B_6^4+...$$

o

Φ

$$\overset{=}{\mathbf{S}}_2\ (\pi/2, \pi/2) = \begin{pmatrix} 0 & 0 & 0 & 1/2 & 0 \\ -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1/2 & 0 & -1/2 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 3/2 & 0 & -1/2 \end{pmatrix}$$

$$\overset{=}{\mathbf{S}}_4\ (\pi/2,\pi/2) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/8 & 0 \\ 1 & 0 & -7/2 & 0 & 0 & 7/8 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1/4 & 0 \\ 1 & 0 & 1/2 & 0 & 0 & -1/4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3/8 & 0 & 1/8 & 0 & 1/8 \\ 0 & -2/5 & 0 & -3/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5/2 & 0 & -1/2 & 0 & 1/2 \\ 0 & -3/4 & 0 & 7/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 35/8 & 0 & -7/8 & 0 & 1/8 \end{pmatrix}$$

$$\overset{=}{\mathbf{S}}_6\ (\pi/2, \pi/2) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -11/32 & 0 & 1/32 & 0 \\ -3/8 & 0 & 11/4 & 0 & -33/8 & 0 & 0 & 33/32 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -3/8 & 0 & 1/8 & 0 \\ -5/8 & 0 & 5/4 & 0 & 9/8 & 0 & 0 & -3/8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9/32 & 0 & 5/32 & 0 \\ -3/4 & 0 & -1/2 & 0 & -1/4 & 0 & 0 & 5/32 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -5/16 & 0 & -1/16 & 0 & -1/16 & 0 & -1/16 \\ 0 & 1/8 & 0 & 3/8 & 0 & 5/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 105/32 & 0 & 17/32 & 0 & 5/32 & 0 & -15/32 \\ 0 & 5/16 & 0 & 1/16 & 0 & -15/16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -63/16 & 0 & -3/16 & 0 & 13/16 & 0 & -3/16 \\ 0 & 5/16 & 0 & -33/16 & 0 & 33/16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 231/32 & 0 & -33/32 & 0 & 11/32 & 0 & -1/32 \end{pmatrix}$$

Θ_1

Φ_1

$$\Theta_2$$

Φ_2

$$\overset{=}{\mathbf{S}}^{-1}{}_{2}\ (\pi/2, \pi/2) = \begin{pmatrix} 0 & -1/2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1/2 & 0 & 1/2 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & 0 & -3/2 & 0 & -1/2 \end{pmatrix}$$

$$\stackrel{=}{\mathbf{S}}^{-1}{}_4\ (\pi/2, \pi/2) = \begin{pmatrix} 0 & 1/8 & 0 & 7/8 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -7/4 & 0 & -3/4 & 0 \\ 0 & -1/4 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3/4 & 0 & 1/4 & 0 \\ 0 & 0 & 0 & 0 & 3/8 & 0 & -1/8 & 0 & 1/8 \\ 1 & 0 & -1/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5/2 & 0 & -1/2 & 0 & -1/2 \\ -1 & 0 & -7/2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 35/8 & 0 & 7/8 & 0 & 1/8 \end{pmatrix}$$

$$\overset{=}{\mathbf{S}}^{-1}{}_{6}\ (\pi/2,\pi/2)=\begin{pmatrix}
0 & -1/32 & 0 & -11/32 & 0 & -33/32 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 33/16 & 0 & 33/16 & 0 & 5/16 & 0\\
0 & 1/8 & 0 & 3/8 & 0 & -3/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 15/16 & 0 & -1/16 & 0 & -5/16 & 0\\
0 & -5/32 & 0 & 9/32 & 0 & -5/32 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 5/8 & 0 & -3/8 & 0 & 1/8 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -5/16 & 0 & 1/16 & 0 & -1/16 & 0 & 1/16\\
3/4 & 0 & -1/2 & 0 & 1/4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -105/32 & 0 & 17/32 & 0 & -5/32 & 0 & -15/32\\
-5/8 & 0 & -5/4 & 0 & 9/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -63/16 & 0 & 3/16 & 0 & 13/16 & 0 & 3/16\\
3/8 & 0 & 11/4 & 0 & 33/8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -231/32 & 0 & -33/32 & 0 & -11/32 & 0 & -1/32
\end{pmatrix}$$

$j_l(|\mathbf{Q}|r)$

$$\langle j_l(|\mathbf{Q}|)\rangle = \int_0^{\inf} R^2(r) j_l(|\mathbf{Q}|r) 4\pi r^2 dr$$

$$|Q|$$

$$F(|\mathbf{Q}|) = \langle j_0(|\mathbf{Q}|)\rangle + \frac{2-g}{g}\langle j_2(|\mathbf{Q}|)\rangle$$

$$\langle j_l(|\mathbf{Q}|)\rangle$$

$$\langle j_0(Q) \rangle$$

$$Aexp(-aQ^2) + Bexp(-bQ^2) + Cexp(-cQ^2) + D$$

$$\langle j_2(Q) \rangle$$

$$AQ^2exp(-aQ^2) + BQ^2exp(-bQ^2) + CQ^2exp(-cQ^2) + DQ^2$$

$$\langle j_4(Q) \rangle$$

$$\langle j_6(Q) \rangle$$

$$Aexp(-aQ^2) + Bexp(-bQ^2) + Cexp(-cQ^2) + Dexp(-dQ^2) + E$$

$$AQ^2exp(-aQ^2) + BQ^2exp(-bQ^2) + CQ^2exp(-cQ^2) + DQ^2exp(-dQ^2) + EQ^2$$

$$Z(K') = c_{K'-1}\langle j_{K'-1}(Q)\rangle + c_{K'+1}\langle j_{K'+1}(Q)\rangle$$

$c_{K'\pm 1}$

Gd^{3+}

$$L = 0$$

$l > 0$

Eu^{3+}

$$J = 0$$

$$\hat{\rho}(\mathbf{r}) = \sum_i -|e|\delta(\mathbf{r}_i - \mathbf{r})$$

$$\delta(\mathbf{r}_i - \mathbf{r}) = \frac{1}{r^2}\delta(r - r_i)\delta(\Omega - \Omega_i)$$

$$\delta(\Omega - \Omega_i) = \sum_{l,m} Y_l^{m\star}(\Omega_i) Y_l^m(\Omega) = \sum_{l,m} Z_l^m(\Omega_i) Z_l^m(\Omega)$$

$$\langle \hat{\rho}(\mathbf{r}) \rangle = -|e||R(r)|^2 \sum_{l,m} Z_l^m(\Omega) \langle \sum_i Z_l^m(\Omega_i) \rangle$$

$$\langle \sum_i Z_l^m(\Omega_i) \rangle = |p_{lm}| \theta_l \langle O_l^m(\mathbf{J}) \rangle_T$$

p_{nm}

$$Z_{lm}(\Omega)$$

θ_l

$4f$

$4f^{\nu}$

$$l = 0$$

β

$l =$

$$\langle \hat{\rho}(\mathbf{r}) \rangle = -|e||R_{4f}(r)|^2 \sum_{l=0,2,4,6} \sum_{m=-l,\ldots,l} |p_{lm}| \theta_l \langle O_l^m(\mathbf{J}) \rangle_T Z_{lm}(\Omega)$$

$$\hat{\mathcal{H}} = \sum_{n=1}^{N} \hat{\mathcal{H}}(n) - \frac{1}{2} \sum_{n,n',\alpha,\beta} \mathcal{J}_{\alpha\beta}(\mathbf{R}_{n'} - \mathbf{R}_n) \hat{\mathcal{I}}_\alpha^n \hat{\mathcal{I}}_\beta^{n'}.$$

$$\hat{\mathcal{I}}_1 \leftrightarrow \hat{S}_x, \hat{\mathcal{I}}_2 \leftrightarrow \hat{S}_y, \hat{\mathcal{I}}_3 \leftrightarrow \hat{S}_z$$

ℓ

$\mathbf{b}_s$

$$s = 1, 2, ..., N_b$$

$$H^s_\alpha = \sum_{\boldsymbol{\ell}' s' \beta} \mathcal{J}_{\alpha\beta}(\boldsymbol{\ell}' + \mathbf{b}_{s'} - \boldsymbol{\ell} - \mathbf{b}_s) \langle \hat{\mathcal{I}}^{s'}_\beta \rangle,$$

$$\langle \hat{\mathcal{I}}_{\beta}^{s'} \rangle$$

s'

$$\hat{\mathcal{H}}^{\mathrm{MF}}(s) = \hat{\mathcal{H}}(s) - \sum_{\alpha=1}^{m} H_{\alpha}^{s} \hat{\mathcal{I}}_{\alpha}^{s}$$

$$s' = 1, 2, ..., m$$

$$\chi_{BA}(\omega) = \lim_{\varepsilon \to 0^+} \left[\sum_{aa'}^{E_a \neq E_{a'}} \frac{\langle a|\hat{B}|a'\rangle\langle a'|\hat{A}|a\rangle}{E_{a'} - E_a - \hbar(\omega + i\varepsilon)}(n_a - n_{a'}) + \frac{i\varepsilon}{\omega + i\varepsilon}\chi'_{BA}(el) \right]$$

$$\chi'_{BA}(el) = \frac{1}{kT} \sum_{aa'}^{E_a = E_{a'}} \langle a|\hat{B} - \langle \hat{B} \rangle|a'\rangle\langle a'|\hat{A} - \langle \hat{A} \rangle|a\rangle \, n_a$$

$$n_a = \frac{\exp(-E_a/kT)}{\sum_{a'} \exp(-E_{a'}/kT)}; \qquad \langle \hat{A} \rangle = \sum_a \langle a|\hat{A}|a\rangle \, n_a$$

$$E_a$$

$$|a\rangle$$

n_a

$$\hat{A}$$

$\hat{B}$

$$\chi_{BA}(z = \omega + i\varepsilon)$$

$$\chi''_{BA}(\omega) \equiv \lim_{\varepsilon \to 0^+} \frac{1}{2i} \left[\chi_{BA}(z) - \chi_{AB}(-z^*) \right]$$

δ

$$\hbar\omega$$

$$E_{a'} - E_a$$

$$\chi''_{BA}(\omega)/\omega = \pi\chi'_{BA}(el)\delta(\omega)$$

$$E_{a'} - E_a - i\Upsilon_{a'a}$$

$$\Upsilon_{a'a} \geq 0$$

$$\chi''_{BA}(\omega) \simeq \sum_{aa'} \frac{\langle a|\hat{B}|a'\rangle\langle a'|\hat{A}|a\rangle\, \Upsilon_{a'a}}{(E_{a'} - E_a - \hbar\omega)^2 + \Upsilon_{a'a}^2}(n_a - n_{a'}) + \frac{\hbar\omega\, \Upsilon_0}{(\hbar\omega)^2 + \Upsilon_0^2}\chi'_{BA}(el)$$

$\mathcal{E}$

$$\varepsilon \to 0^+$$

$$\varepsilon = \Upsilon_{a'a}/\hbar$$

$$\varepsilon = \Upsilon_0/\hbar$$

$$\chi^{ss'}_{\alpha\beta}(\mathbf{Q},\omega) \equiv \chi_{BA}$$

$\hat{A}$

$$\frac{1}{\sqrt{N}} \exp(\mathrm{i}\mathbf{Q} \cdot \mathbf{b}_{s'}) \sum_{\boldsymbol{\ell}'} \exp(\mathrm{i}\mathbf{Q} \cdot \boldsymbol{\ell}') \hat{\mathcal{I}}_{\beta}^{(\boldsymbol{\ell}' s')}$$

$$\hat{B}$$

$$\frac{1}{\sqrt{N}} \exp(\mathrm{i}\mathbf{Q} \cdot \mathbf{b}_s) \sum_{\boldsymbol{\ell}} \exp(\mathrm{i}\mathbf{Q} \cdot \boldsymbol{\ell}) \hat{\mathcal{I}}_{\alpha}^{(\boldsymbol{\ell} s)},$$

$$\mathcal{J}_{\alpha\beta}^{ss'}(\mathbf{Q}) = \sum_{\boldsymbol{\ell}'} \mathcal{J}_{\alpha\beta}(\boldsymbol{\ell}' + \mathbf{b}_{s'} - \mathbf{b}_s) \exp\{\mathrm{i}\mathbf{Q} \cdot (\boldsymbol{\ell}' + \mathbf{b}_{s'} - \mathbf{b}_s)\}$$

$$\ell = 0$$

—

χ

$$\chi_{\alpha\beta}^{ss'}$$

$\overline{\chi}(\mathbf{Q}, \omega)$

$$\hat{\mathcal{I}}^n(t) - \langle \hat{\mathcal{I}}^n(t) \rangle$$

$$s = s' = 0$$

$$1 = \left[\overline{\chi}^0(\omega)^{-1} - \overline{\mathcal{J}}(\mathbf{Q})\right]\overline{\chi}(\mathbf{Q},\omega),$$

$$\overline{\chi}^{0}(\omega)$$

$$s = 1, 2, 3, 4, ..., N_B$$

$$\delta_{ss'} = \sum_{s''=1}^{N_B} \left[\delta_{ss''} [\overline{\chi}^s(\omega)]^{-1} - \overline{\mathcal{J}}^{ss''}(\mathbf{Q}) \right] \overline{\chi}^{s''s'}(\mathbf{Q}, \omega),$$

$$\delta_{ss'}\delta_{\alpha\beta} = \sum_{s''=1}^{N_B} \sum_{\delta=1}^{m} \left[\delta_{ss''} [\chi^s(\omega)]^{-1}_{\alpha\delta} - \mathcal{J}^{ss''}_{\alpha\delta}(\mathbf{Q}) \right] \chi^{s''s'}_{\delta\beta}(\mathbf{Q},\omega),$$

$$\chi^{s}_{\alpha\beta}(\omega)$$

$$\chi^{s}_{\alpha\beta}(\omega) = \sum_{jj'} \frac{\langle j|\hat{\mathcal{I}}_{\alpha} - \langle\hat{\mathcal{I}}_{\alpha}\rangle|j'\rangle\langle j'|\hat{\mathcal{I}}_{\beta} - \langle\hat{\mathcal{I}}_{\beta}\rangle|j\rangle}{\epsilon_{j'} - \epsilon_{j} - \hbar\omega}(p_j - p_{j'}).$$

ϵ_j

$\epsilon_{j'}$

$$|j\rangle$$

$$|j'\rangle$$

p_j

$$p_j = \frac{\exp(-\epsilon_j/kT)}{\sum_{j'} \exp(-\epsilon_{j'}/kT)}.$$

$$\omega + i\varepsilon$$

$\epsilon_{j'} + d$

$$\epsilon_{j'} = \epsilon_j$$

$$|d| \ll kT$$

$$p_j - p_{j'} = p_j\, d/kT$$

$$j = j'$$

$$d \to 0$$

$$\omega \to \omega + i\epsilon$$

$\chi_{\delta\beta}^{s''s'}(\mathbf{Q},\omega)$

Q

$$\hbar\omega \to \hbar\omega + i\Upsilon$$

$$3N_b \times 3N_b$$

(Q, ω)

$$\epsilon_- \to \epsilon_+$$

$$m \times m$$

$$\overline{\chi}^{s}$$

$$\chi^{s}_{\alpha\beta}$$

$\alpha, \beta = 1, \ldots, m$

$N_b \times N_b$

$$\chi_{\alpha\beta}^{ss'}(\mathbf{Q},\omega)$$

$\underline{\chi}(\mathbf{Q}, \omega)$

$$\overline{\chi}^s(\omega) = \frac{\overline{M}^s}{\Delta^s - \hbar\omega}$$

$$\Delta^s \equiv \epsilon^s_+ - \epsilon^s_-$$

$$M^s_{\alpha\beta} = \langle -|\hat{\mathcal{I}}^s_\alpha - \langle \hat{\mathcal{I}}^s_\alpha \rangle|+\rangle\langle +|\hat{\mathcal{I}}^s_\beta - \langle \hat{\mathcal{I}}^s_\beta \rangle|-\rangle(p_- - p_+)$$

$$\Delta^s = 0$$

$$\overline{M}^s$$

$$\gamma^s$$

Δ^s

$$\gamma^s = \mathrm{Tr}\{\overline{\mathrm{M}}^{\mathrm{s}}\}$$

$$\overline{\mathcal{U}}^{s}$$

$$\overline{\mathcal{U}}^{s\dagger}\overline{\mathcal{U}}^{s} = \overline{1}$$

$$\overline{\mathcal{U}}^{s}$$

$$\mathcal{U}_{\alpha 1}^{s} = \sqrt{(p_{-} - p_{+})/\gamma^{s}} \langle - | \hat{\mathcal{I}}_{\alpha}^{s} - \langle \hat{\mathcal{I}}_{\alpha}^{s} \rangle_{\mathbf{H},T} | + \rangle$$

$$\mathcal{J}^{ss'}_{\alpha\beta}(\mathbf{Q})$$

$$\overline{\mathcal{L}}^{ss'}(\mathbf{Q}) \equiv \overline{\mathcal{U}}^{s\dagger}\overline{\mathcal{J}}^{ss'}(\mathbf{Q})\overline{\mathcal{U}}^{s'}$$

$$A^{ss'}(\mathbf{Q}) = \Lambda^{ss'}\Delta^{s} - \sqrt{\gamma^{s}}\mathcal{L}^{ss'}(\mathbf{Q})\left(\sqrt{\gamma^{s'}}\right)^{*}$$

$$\underline{A}(\mathbf{Q})\mathbf{t} = \hbar\omega\underline{\mathbf{\Lambda}}\mathbf{t}$$

Λ

$$\Lambda^{ss'} = \delta_{ss'} \mathrm{sgn}(\Delta^s)$$

$$\underline{\mathcal{T}} = \left(\mathbf{t}^1, \mathbf{t}^2, \ldots, \mathbf{t}^r, \ldots\right)$$

$\hbar\omega^r$

$$\Omega^{rr'} = \delta_{rr'} \hbar \omega^r$$

$$\underline{A}(\mathbf{Q})$$

L

$\mathcal{T}$

$$\underline{\mathcal{T}}^{\dagger}\underline{A}\underline{\mathcal{T}} = \underline{1}$$

$$\chi_{\alpha\beta}^{ss'}(\mathbf{Q},\omega) = \left(\sqrt{\gamma^s}\right)^* \sum_r \mathcal{U}_{\alpha 1}^{s} \mathcal{T}^{sr}(\mathbf{Q}) \frac{\hbar\omega^r(\mathbf{Q})}{\hbar\omega^r(\mathbf{Q}) - \hbar\omega} \mathcal{T}^{rs'\dagger}(\mathbf{Q}) \mathcal{U}_{1\beta}^{s'\dagger} \sqrt{\gamma^{s'}}$$

$$\langle \hat{\mathcal{I}}_{\alpha}^{s} \rangle$$

$\alpha = 1, \ldots, m$

$$\mathbf{t}^r$$

$$\omega^r$$

$$\underline{\chi}(\mathbf{Q}, \omega)$$

$$\overline{X}(\mathbf{Q}, \omega)$$

$\alpha = 1, ..., m'$

$$n = (\boldsymbol{\ell} s)$$

$$\overline{\Sigma}(\mathbf{Q},\omega)$$

$\Sigma^{ss'}_{\alpha\beta}(\mathbf{Q},\omega)$

$$\int_{-\infty}^{+\infty} dt e^{i\omega t} e^{-i\mathbf{Q}\cdot(\mathbf{b}_s - \mathbf{b}_{s'})} \frac{1}{N_g} \sum_{\boldsymbol{\ell}\boldsymbol{\ell}'} e^{-i\mathbf{Q}\cdot(\boldsymbol{\ell}-\boldsymbol{\ell}')} \times$$

$$\times(\langle\hat{\mathcal{O}}_{\alpha}^{\boldsymbol{\ell}s\dagger}(t)\hat{\mathcal{O}}_{\beta}^{\boldsymbol{\ell}'s'}(0)\rangle_{T,H}-\langle\hat{\mathcal{O}}_{\alpha}^{\boldsymbol{\ell}s\dagger}\rangle_{T,H}\langle\hat{\mathcal{O}}_{\beta}^{\boldsymbol{\ell}'s'}\rangle_{T,H})$$

$$\hat{\mathcal{O}}^{\ell s}_{\alpha}$$

Σ

X

$$\underline{\Sigma}(\mathbf{Q}, \omega) = \frac{2\hbar}{1 - e^{-\hbar\omega/kT}} \left(\underline{X}\right)'' (\mathbf{Q}, \omega)$$

$$\left(X_{\alpha\beta}^{ss'}\right)''(\mathbf{Q},\omega) \equiv \frac{1}{2i}\left[X_{\alpha\beta}^{ss'}(\mathbf{Q},\omega) - \left(X_{\alpha\beta}^{ss'}(\mathbf{Q},\omega)\right)^*\right]$$

$$\overline{\chi}$$

$$\hat{\mathcal{I}}_{\alpha}$$

$$\overline{X}$$

$$\overline{X}(\mathbf{Q}, \omega)$$

$$\chi_{BA}(\omega)$$

$$\langle \hat{B}(t) \rangle$$

$\mathcal{O}_\alpha$

$$X_{\alpha\beta}^{ss'}(\mathbf{Q},\omega) \equiv \chi_{DC}(\omega)$$

$$\hat{C} = \frac{1}{\sqrt{N_g}} e^{i\mathbf{Q}\cdot\mathbf{b}_{s'}} \sum_{\boldsymbol{\ell}'} e^{i\mathbf{Q}\cdot\boldsymbol{\ell}'} \hat{\mathcal{O}}_{\beta}^{\mathbf{l}'s'}$$

$$\hat{D} = \frac{1}{\sqrt{N_g}} e^{i\mathbf{Q}\cdot\mathbf{b}_s} \sum_{\boldsymbol{\ell}} e^{i\mathbf{Q}\cdot\boldsymbol{\ell}} \hat{\mathcal{O}}_{\alpha}^{\mathbf{l}s}$$

$$|\alpha\rangle$$

$$\langle -|\hat{\mathcal{I}}^{s}_{\alpha}|+\rangle\langle +'|\hat{\mathcal{I}}^{s'}_{\beta}|-'\rangle$$

$$\langle -|\hat{\mathcal{O}}^{s}_{\alpha}|+\rangle\langle +'|\hat{\mathcal{O}}^{s'}_{\beta}|-'\rangle$$

$$X_{\alpha\beta}^{ss'}(\mathbf{Q}, \omega)$$

$$\mu^s_{\alpha\beta} = \langle -|\hat{\mathcal{I}}^s_\alpha - \langle \hat{\mathcal{I}}^s_\alpha \rangle|+\rangle\langle +|\hat{\mathcal{I}}^s_\beta - \langle \hat{\mathcal{I}}^s_\beta \rangle|-\rangle$$

$$\nu^{s}_{\alpha\beta} = \langle -|\mathcal{O}^{s\dagger}_{\alpha} - \langle \mathcal{O}^{s\dagger}_{\alpha}\rangle|+\rangle\langle +|\mathcal{O}^{s}_{\beta} - \langle \mathcal{O}^{s}_{\beta}\rangle|-\rangle$$

$$\overline{\mathcal{U}}^{s\dagger}\overline{\mathcal{U}}^{s} = \overline{1}$$

$$\overline{\mathcal{V}}^s$$

$$\overline{\mathcal{V}}^{s\dagger}\overline{\mathcal{V}}^{s}=\overline{1}$$

ϕ^s

$$\xi^s$$

$$\phi^s \equiv \gamma^s/(p_- - p_+) = \mathrm{Trace}\{\overline{\mu^s}\}$$

$$\xi^s \equiv \Gamma^s/(p_- - p_+) = \mathrm{Trace}\{\overline{\nu^{\mathrm{s}}}\}$$

$$X_{\alpha\beta}^{ss'} = (\sqrt{\Gamma^s})^* \sum_r \mathcal{V}_{\alpha 1}^s \mathcal{T}^{sr} \frac{\hbar\omega^r}{\hbar\omega^r - \hbar\omega} \mathcal{T}^{rs'\dagger} \mathcal{V}_{1\beta}^{s'\dagger} \sqrt{\Gamma^{s'}}$$

$$\hat{\mathcal{I}}^{s}_{\alpha}$$

$$\hbar\omega + i\hbar\varepsilon$$

$\varepsilon \to 0^+$

$$\lim_{\varepsilon \to 0^+} \frac{1}{\hbar\omega^r - \hbar\omega - i\hbar\varepsilon} = \mathcal{P}\frac{1}{\hbar\omega^r - \hbar\omega} + i\pi\delta(\hbar\omega^r - \hbar\omega)$$

$$\left(X^{ss'}_{\alpha\beta}\right)'' = \pi(\sqrt{\Gamma^s})^* \sum_r \mathcal{V}^s_{\alpha 1} \mathcal{T}^{sr} \hbar\omega^r \delta(\hbar\omega^r - \hbar\omega) \mathcal{T}^{rs'\dagger}(\mathbf{Q}) \mathcal{V}^{s'\dagger}_{1\beta} \sqrt{\Gamma^{s'}}$$

$$\Sigma$$

$$\Sigma_{\alpha\beta}^{ss'}(\mathbf{Q},\omega) = \frac{2\pi\hbar(\sqrt{\Gamma^s})^*\sqrt{\Gamma^{s'}}}{1-e^{-\hbar\omega/kT}} \sum_r \mathcal{V}_{\alpha 1}^{s} \mathcal{T}^{sr} \hbar\omega^r \delta(\hbar\omega^r - \hbar\omega) \mathcal{T}^{rs'\dagger} \mathcal{V}_{1\beta}^{s'\dagger}$$

$$\overline{\nu}^{s}$$

Γ^s

A

$$\underline{\mathcal{T}}^{\dagger}\underline{A}(\mathbf{Q})\underline{\mathcal{T}} = \underline{1}$$

$d \to 0$

$$\hat{\mathcal{H}}_{\text{perturb}} = \sum_{n',\beta} H_{\beta}^{n'} \hat{\mathcal{O}}_{\beta}^{n'}$$

$$H_\beta^{n'} = H_\beta^{s'} \exp(i\mathbf{Q} \cdot \mathbf{R}_{n'} - i\omega t), \qquad \mathbf{R}_{n'} \equiv \boldsymbol{\ell}' + \mathbf{b}_{s'}$$

$$\Delta\langle\hat{\mathcal{O}}_\alpha\rangle$$

$$\langle \hat{\mathcal{O}}_\alpha \rangle$$

$$\Delta\langle\hat{\mathcal{O}}_{\alpha}^{s}\rangle(\mathbf{Q},\omega)=\sum_{s'\beta}X_{\alpha\beta}^{ss'}(\mathbf{Q},\omega)H_{\beta}^{s'}$$

$$\Delta\langle\hat{\mathcal{O}}^n_\alpha\rangle = \Delta\langle\hat{\mathcal{O}}^s_\alpha\rangle(\mathbf{Q},\omega)\exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega t) = \exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega t)\sum_{s'\beta} X^{ss'}_{\alpha\beta}(\mathbf{Q},\omega)H^{s'}_\beta$$

$$H_{\beta}^{s'} = H\delta_{1s'}\delta_{1\beta}$$

$$\Delta\langle\hat{\mathcal{O}}_{\alpha}^{n}\rangle = \exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega t)X_{\alpha 1}^{s1}(\mathbf{Q},\omega)H$$

$$\omega = \omega^r$$

$$a_1$$

$$a_1 = H/(\hbar\omega - \hbar\omega^r)$$

$$\Delta\langle\hat{\mathcal{O}}^n_\alpha\rangle = a_1 \exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega^r t)\left(\sqrt{\Gamma^s}\right)^* \mathcal{V}^s_{\alpha 1}\mathcal{T}^{sr}(\mathbf{Q})\hbar\omega^r\mathcal{T}^{r1\dagger}(\mathbf{Q})\mathcal{V}^{1\dagger}_{11}\sqrt{\Gamma^1}$$

$$\mathcal{T}^{r1\dagger}(\mathbf{Q})$$

$$\mathcal{V}_{11}^{1\dagger}$$

r

$$s = 1$$

$$\langle \hat{\mathcal{O}}_1^1 \rangle$$

$$a = a_1 \mathcal{T}^{r1\dagger}(\mathbf{Q}) \mathcal{V}_{11}^{1\dagger} \sqrt{\hbar \omega^r \Gamma^1}$$

$$\Delta\langle\hat{\mathcal{O}}^n_\alpha\rangle = a\exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega^r t)\left(\sqrt{\hbar\omega^r\Gamma^s}\right)^* \mathcal{V}^s_{\alpha 1}\mathcal{T}^{sr}(\mathbf{Q}) \equiv a\exp(i\mathbf{Q}\cdot\mathbf{R}_n - i\omega^r t)e^s_\alpha$$

$$e_{\alpha}^{s}$$

$$\omega^r(\mathbf{Q})$$

t

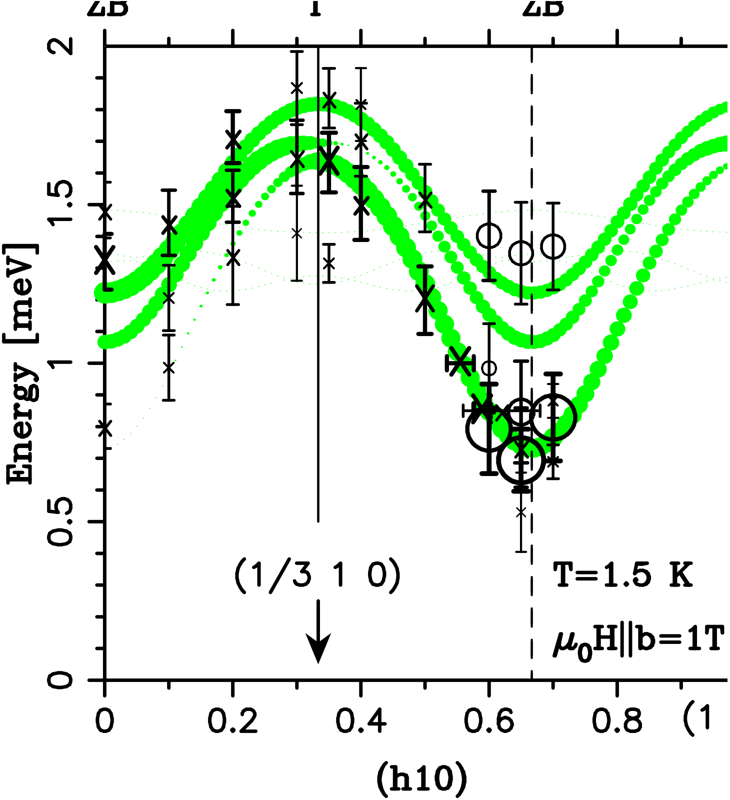
$$s = (ijklt)$$

$ijkl$

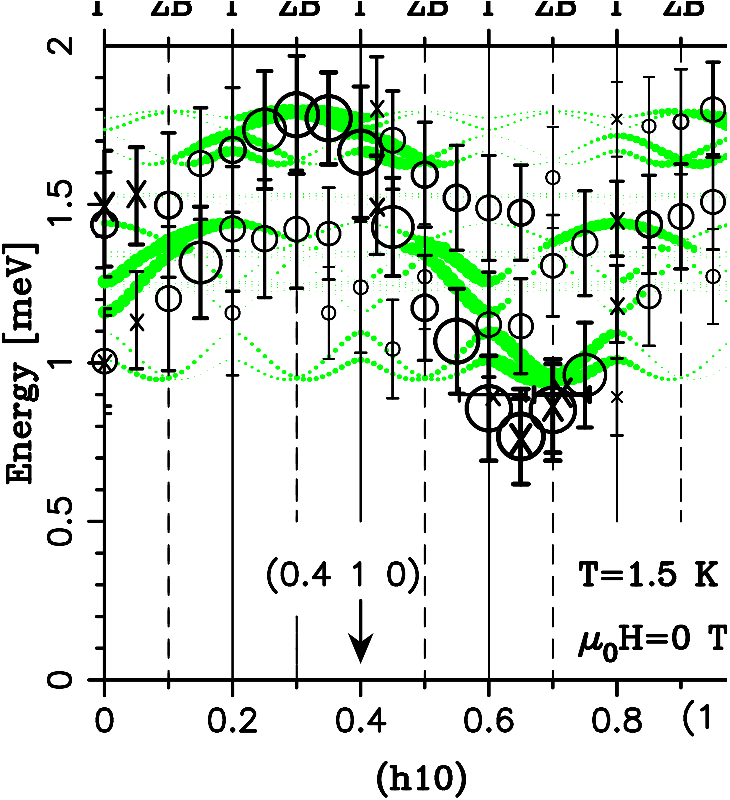
$$e^{s}_{r\alpha}$$

$\alpha = 1, ..., 28$

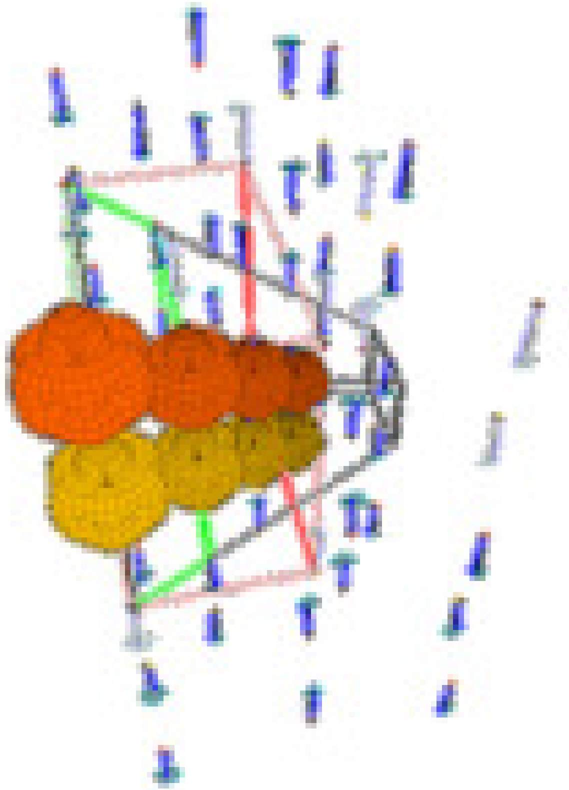
$$\Delta\langle\hat{\mathcal{O}}^n_{\alpha=(lm)}\rangle = \Delta\langle\sum_i Z^m_l(\Omega_i)\rangle_n = \Delta|p_{lm}|\theta_l\langle O^m_l(\mathbf{J}_n)\rangle$$



ZB
Γ
ZB
2
1.5
1
0.5
0
Energy [meV]
(1/3 1 0)
T=1.5 K
μ_0H||b=1T
0
0.2
0.4
0.6
0.8
(1
(h10)



Γ
ZB
Γ
ZB
Γ
ZB
Γ
ZB
Γ
ZB
Energy [meV]
2
1.5
1
0.5
0
(0.4 1 0)
T=1.5 K
μ_0H=0 T
0
0.2
0.4
0.6
0.8
(1
(h10)



$$\hat{\mathbf{M}}(\mathbf{Q})$$

$$\hat{\mathbf{M}}(\mathbf{Q}) = \hat{\mathbf{M}}_S(\mathbf{Q}) + \hat{\mathbf{M}}_L(\mathbf{Q})$$

$$\hat{\mathcal{Q}}_\alpha \equiv -\hat{M}_\alpha(\mathbf{Q})/(2\mu_B)$$

$\alpha = x, y, z$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}\left(\frac{m_n}{2\pi\hbar^2}\right)^2 \sum_{if,s_n} P_{s_n} P_i \left|\langle s_n|\langle i|H_{int}(\mathbf{Q})|f\rangle|s_n'\rangle\right|^2 \delta(\hbar\omega + E_i - E_f)$$

m_n

$$\left|s_n\right\rangle$$

$|s_n'\rangle$

$$P_{s_n}$$

$|s_n>$

$$|f\rangle$$

E_i

E_f

P_i

$$H_{int}(\mathbf{Q})$$

$$H_{int}(\mathbf{Q}) = \hat{\beta}(\mathbf{Q}) + \hat{\mathbf{s}}_n \cdot \hat{\boldsymbol{\alpha}}(\mathbf{Q})$$

$$\hat{\beta}$$

$\hat{\alpha}$

$$\hat{\beta}^{\dagger} \ldots \hat{\beta}$$

$$\hat{\alpha}^{\dagger} \ldots \hat{\alpha}$$

$$\alpha^{\dagger} \ldots \beta$$

$$N\frac{k'}{k}S_{\mathrm{nuc}}(\mathbf{Q},\omega)+N\frac{k'}{k}Tr\{S_{\mathrm{mag}\perp}(\mathbf{Q},\omega)\}$$

$$\hbar\omega = E - E'$$

S_{mag}

S_{nuc}

$$S_{\mathrm{nuc}}^{\mathrm{inel}}(\mathbf{Q}, \omega)$$

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt e^{i\omega t}\frac{1}{N}\sum_{nn'} b_n b_{n'} e^{-W_n(Q)-W_{n'}(Q)}$$

$$e^{-i\mathbf{Q}\cdot(\mathbf{R}_n-\mathbf{R}_{n'})}(\langle\mathbf{Q}\cdot\hat{\mathbf{u}}^n(t)\mathbf{Q}\cdot\hat{\mathbf{u}}^{n'}(0)\rangle_{T,H}$$

$\hat{\mathbf{u}}$

$$n = (\boldsymbol{\ell}, s)$$

$$\mathbf{Q} \cdot \hat{\mathbf{u}}$$

$$\mathcal{O} \leftrightarrow b_s e^{-W_s(Q)} \mathbf{Q} \cdot \hat{\mathbf{u}}^s$$

$$\sum_{ss'} \frac{\Sigma^{ss'}(\mathbf{Q},\omega)}{2\pi\hbar N_b}$$

$W_s(Q)$

$$\sum_{r,ss'} \frac{(\sqrt{\Gamma^{s}_{\mathrm{nuc}}(\mathbf{Q})})^{*}\sqrt{\Gamma^{s'}_{\mathrm{nuc}}(\mathbf{Q})}}{N_b(1-e^{-\hbar\omega^{r}(\mathbf{Q})/kT})}\times$$

$$\times\mathcal{V}^{s}_{\mathrm{nuc},\alpha 1}(\mathbf{Q})\mathcal{T}^{sr}(\mathbf{Q})\hbar\omega^{r}(\mathbf{Q})\delta(\hbar\omega^{r}(\mathbf{Q})-\hbar\omega)\mathcal{T}^{rs'\dagger}(\mathbf{Q})\mathcal{V}^{s'\dagger}_{\mathrm{nuc},1\beta}(\mathbf{Q})$$

$$I_{\mathrm{nuc}}$$

$$S^{\text{inel},\alpha\beta}_{\text{mag}\perp}(\mathbf{Q},\omega)$$

$$\left(\frac{\gamma r_0}{2\mu_B}\right)^2 \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dt e^{i\omega t} \frac{1}{N} \sum_{nn'} e^{-W_n(Q)-W_{n'}(Q)}$$

$$e^{-i\mathbf{Q}\cdot(\mathbf{R}_n-\mathbf{R}_{n'})}\left(\langle \hat{M}^{n\dagger}_{\perp\alpha}(t,\mathbf{Q})\hat{M}^{n'}_{\perp\beta}(0,\mathbf{Q})\rangle_{T,H}-\langle \hat{M}^{n\dagger}_{\perp\alpha}(\mathbf{Q})\rangle_{T,H}\langle \hat{M}^{n'}_{\perp\beta}(\mathbf{Q})\rangle_{T,H}\right)$$

$$4\pi(\gamma r_0)^2 = 4\pi\left(\frac{\hbar\gamma e^2}{mc^2}\right)^2 = 3.65$$

$$\hat{\mathbf{M}}_{\perp}(\mathbf{Q}) = \hat{\mathbf{M}}(\mathbf{Q}) - \mathbf{Q}(\hat{\mathbf{M}}_{\perp}(\mathbf{Q}) \cdot \mathbf{Q})/Q^2$$

$$\mathcal{O} \leftrightarrow \frac{\gamma r_0}{2\mu_B} e^{-W(Q)} \hat{\mathbf{M}}_\perp(\mathbf{Q})$$

$$S_{\mathrm{mag}\perp}^{\mathrm{inel},\alpha\beta}(\mathbf{Q},\omega) = \sum_{ss'} \frac{\Sigma_{\alpha\beta}^{ss'}(\mathbf{Q},\omega)}{2\pi\hbar N_b}$$

$$\sum_{r,ss'} \frac{(\sqrt{\Gamma^{s}_{\mathrm{mag}}(\mathbf{Q})})^{*}\sqrt{\Gamma^{s'}_{\mathrm{mag}}(\mathbf{Q})}}{N_b(1-e^{-\hbar\omega^{r}(\mathbf{Q})/kT})}\times$$

$$\times \mathcal{V}^{s}_{\mathrm{mag},\alpha 1}(\mathbf{Q}) \mathcal{T}^{sr}(\mathbf{Q}) \hbar\omega^{r}(\mathbf{Q}) \delta(\hbar\omega^{r}(\mathbf{Q}) - \hbar\omega) \mathcal{T}^{rs'\dagger}(\mathbf{Q}) \mathcal{V}^{s'\dagger}_{\mathrm{mag},1\beta}(\mathbf{Q})$$

$$S_{\mathrm{mag}}^{\mathrm{inel},\alpha\beta}(\mathbf{Q},\omega)$$

α, β

$$\mathbf{u} || \mathbf{Q} = \mathbf{k} - \mathbf{k}'$$

W

V

$$\hat{\mathbf{M}}_{\perp}(\mathbf{Q})$$

$$\mathcal{O} \leftrightarrow \hat{\mathbf{M}}_{\perp}(\mathbf{Q})$$

$1/Q$

$$\hat{M}^n_\alpha(\mathbf{Q}) \approx -\mu_B[F^n_S(Q)g_S\hat{S}^n_\alpha + F^n_L(Q)g_L\hat{L}^n_\alpha]$$

g

$$g_S \approx 2$$

$$g_L = 1$$

$$F_S(Q) = \langle j_0(Q) \rangle$$

$$F_L(Q) = \langle j_0(Q) \rangle + \langle j_2(Q) \rangle$$

$$\hat{S}^n_\alpha$$

$$\hat{L}_{\alpha}^{n}$$

$$\hat{M}^n_\alpha(\mathbf{Q}) \leftrightarrow -\mu_B\{F^n_S(Q)g_S\hat{S}^n_\alpha + F^n_L(Q)g_L\hat{L}^n_\alpha\}$$

$$\hat{M}^n_\alpha(\mathbf{Q}) \leftrightarrow -\mu_B F^n_S(Q) g_S \hat{S}^n_\alpha$$

$$\hat{M}_\alpha^n(\mathbf{Q}) \leftrightarrow -\mu_B g_J F^n(Q) \hat{J}_\alpha^n$$

$$\hat{M}_\alpha^n \approx -\mu_B g_J F^n(Q) \hat{J}_\alpha^n$$

$$F(Q) = \langle j_0(Q) \rangle + \frac{2-g_J}{g_J} \langle j_2(Q) \rangle$$

$$S_{\mathrm{mag}}^{\mathrm{inel},\alpha\beta}(\mathbf{Q},\omega)$$

$$e^{-i\mathbf{Q}\cdot(\mathbf{R}_n-\mathbf{R}_{n'})}(\langle\hat{M}_\alpha^{n\dagger}(t,\mathbf{Q})\hat{M}_\beta^{n'}(0,\mathbf{Q})\rangle_{T,H}-\langle\hat{M}_\alpha^{n\dagger}(\mathbf{Q})\rangle_{T,H}\langle\hat{M}_\beta^{n'}(\mathbf{Q})\rangle_{T,H})$$

$$\chi_{\alpha\beta}(t) = \frac{i}{\hbar}\Theta(t)\langle[J_{\alpha}^{\dagger}(t), J_{\beta}(0)]\rangle$$

$$\chi_{\alpha,\beta}(z) = \int_{-\infty}^{+\infty} dt e^{izt} \chi_{\alpha\beta}(t), \quad z = \omega + i\delta$$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\frac{r_0}{2}g_J F(Q))^2 \frac{1}{\pi}\sum_{\alpha\beta}(\delta_{\alpha\beta} - \tilde{Q}_\alpha \tilde{Q}_\beta)\frac{\chi"_{\alpha,\beta}(\omega)}{1-e^{-\beta\hbar\omega}}$$

$$\vec{Q} = \vec{k} - \vec{k}'$$

$$\tilde{Q} = \vec{Q}/|\vec{Q}|$$

$$r_0 = -0.54 \cdot 10^{-12}$$

$F(Q)$

$$\chi_{i,k}(t) = i\Theta(t)\langle[A_i^\dagger(t), A_k(0)]\rangle$$

$$A(t)$$

$$A(t) = \exp(iHt)A\exp(-iHt)$$

$$\mathcal{L}A = [H, A]$$

$$A(t) = \exp(i\mathcal{L}t)A$$

$$\chi_{i,k}$$

A_i, A_k

$$\chi_{i,k}(z) = i \int_0^\infty dt e^{izt} \langle [A_i^\dagger(t), A_k(0)] \rangle$$

$$\chi_{i,k}(t) = i\Theta(t)\langle[A_i^\dagger, A_k \exp^{-i\mathcal{L}t}\rangle$$

$$\chi_{i,k}(z) = -\langle [A_i^\dagger, \frac{1}{z - \mathcal{L}} A_k(0)] \rangle$$

$$\chi_{i,k}(0) = \int_0^\beta d\lambda \langle e^{\lambda H} A_i^\dagger e^{-\lambda H} A_k \rangle = \int_0^\beta d\lambda \langle (e^{\lambda \mathcal{L}} A_i^\dagger) A_k \rangle$$

$$(A_i|A_k) = \frac{1}{\beta}\int_0^\beta d\lambda \langle (e^{\lambda\mathcal{L}}A_i^\dagger)A_k\rangle = \frac{1}{\beta}\chi_{ik}(0)$$

$$(\mathcal{L}A_i|A_k) = (A_i|\mathcal{L}A_k) = \frac{1}{\beta}\langle[A_i^\dagger, A_k]\rangle$$

$$\chi_{i,k}(z) = -\beta(A_i|\frac{\mathcal{L}}{z-\mathcal{L}}A_k)$$

$$\chi_{ik}(z) = \chi_{ik}(0) - z\beta(A_i|\frac{1}{z-\mathcal{L}}A_k)$$

$$\Phi_{ik}(z) = (A_i|\frac{1}{z-\mathcal{L}}A_k)$$

$$H = H_{cf} + H_{el} + H_{el,cf}$$

$$H_{cf} = \sum_n E_n K_{nn}, \quad K_{nm} = |n\rangle\langle m|$$

$$|n\rangle$$

$$H_{el} = \sum_{k\alpha} \epsilon_k c_{k\alpha}^{\dagger} c_{k\alpha}$$

$$H_{el,cf} = -J_{ex}\vec{J}\cdot\vec{\sigma}, \quad \vec{\sigma} = \sum_{k\alpha Q\beta} \vec{\sigma}_{\alpha\beta} c^{\dagger}_{k\alpha} c_{k+Q\beta}, \quad \vec{J} = \sum_{n,m} \vec{J}_{n,m} K_{nm}.$$

E_n

$$A_\mu = K_\mu$$

$$\mu = [nm]$$

$$\mathcal{L}A_\mu = (E_n - E_m)A_\mu$$

$\chi_{\alpha\beta}$

A

A_i

$$\mathcal{P}A = \sum_{\nu\mu} A_\nu P^{-1}_{\nu\mu}(A_\mu|A) \quad P_{\nu\mu} = (A_\nu|A_\mu)$$

$$P^{-1}_{\nu\mu} = [P^{-1}]_{\nu\mu}$$

$\nu\mu$

P

$$\mathcal{F}(z) = \frac{1}{z - \mathcal{L}}, \quad (z - \mathcal{L})\mathcal{F}(z) = 1$$

$$(\mathcal{P}(z-\mathcal{P}\mathcal{L}\mathcal{P}-\mathcal{P}\mathcal{M}(z)\mathcal{P})\mathcal{P}\mathcal{F}(z)\mathcal{P}=\mathcal{P}$$

$$\mathcal{M}(z) = \mathcal{PLQ}\frac{1}{z - \mathcal{QLQ}}\mathcal{QLP}$$

$$\mathcal{Q} = 1 - \mathcal{P}$$

$$\Phi_{\nu\mu}(z) = (A_\nu | \frac{1}{z - \mathcal{L}} A_\mu)$$

$$\sum_{\lambda}\left(z\delta_{\nu\lambda}-\sum_{\kappa}\big[L_{\nu\kappa}+M_{\nu\kappa}(z)\big]P^{-1}_{\kappa\lambda}\right)\Phi_{\lambda\mu}(z)=P_{\nu\mu}$$

$$L_{\nu\mu} = (A_\nu|\mathcal{L}A_\mu)$$

$$M_{\nu\mu}(z) = (A_\nu|\mathcal{M}(z)A_\mu)$$

$$J^{\alpha} = \sum_{n_1,n_2} J^{\alpha}_{n_2,n_1} K_{n_2,n_1} = \sum_{\nu} J^{\alpha}_{\nu} A_{\nu}, \quad A_{\nu} = K_{n_1 n_2}$$

$$n_2 \leftarrow n_1$$

$$|n_2\rangle\langle n_1|$$

$$\mathcal{L}A_\nu = (E_{n_2} - E_{n_1})A_\nu$$

$$P_{\nu\mu} = (A_\nu | A_\mu) \simeq \delta_{\nu\mu} P_\nu, \quad P_\nu = (A_\nu | A_\nu) = \frac{p(n_1) - p(n_2)}{\beta(E_{n2} - E_{n_1})}$$

$$p(n) = \exp(-\beta E_n)/Z$$

$$L_{\nu\mu} = \delta_{\nu\mu}(A_\nu|A_\nu)(E_{n_2} - E_{n_1}) + O(J_{ex}^2)$$

$$\Phi_{\nu\mu}(z) = \left[\Omega^{-1}\right]_{\nu\mu}(z) P_\mu, \quad \Omega_{\nu\mu}(z) = (z - E_\nu)\delta_{\nu\mu} - M_{\nu\mu}(z)[P^{-1}]_\mu, \quad E_\nu = E_{n_2} - E_{n_1}$$

$\mathcal{QLA}_\nu$

$\mathcal{L}_{el,cf} A_\nu$

$$M_{\nu\mu}(z) = (\mathcal{L}_{el,cf} A_\nu | \frac{1}{z - \mathcal{L}_0} \mathcal{L}_{el,cf} A_\mu) = M_{n_2 n_1, m_2 m_1}(z)$$

$$M_{n_2n_1,m_2m_1}(z) = (\mathcal{L}_{el,cf}K_{n_2n_1}|\frac{1}{z-\mathcal{L}_0}\mathcal{L}_{el,cf}K_{m_2m_1})$$

$$\mathcal{L}_{el,cf} K_{n_2 n_1} = J_{ex} \sum_t \vec{\sigma} (\vec{J}_{n_1 t} K_{n_2 t} - \vec{J}_{t n_2} K_{t n_1})$$

$$\vec{\sigma} = \sum_{k\alpha, k+Q\beta} \vec{\sigma}_{\alpha\beta} c^{\dagger}_{k\alpha} c_{k+Q\beta}$$

$$(\sigma^i K_{nm}|\frac{1}{z-\mathcal{L}_0}\sigma^j K_{n'm'}) = \delta_{ij}\delta_{nn'}\delta_{mm'}G_{nm}(z)$$

$$G_{nm}(z) = (\sigma^i K_{nm} | \frac{1}{z - \mathcal{L}_0} \sigma^i K_{nm})$$

$$M_{n_2 n_1, m_2 m_1}(z) = J_{ex}^2 \sum_i \Big[$$

$$\delta_{n_2 m_2} \sum_t J^i_{m_1 t} J^i_{t n_1} G_{n_2 t} + \delta_{n_1 m_1} \sum_t J^i_{n_2 t} J^i_{t m_2} G_{t n_1}$$

$$-J^i_{m_1 n_1} J^i_{n_2 m_2} G_{n_2 m_1} - J^i_{n_2 m_2} J^i_{m_1 n_1} G_{m_2 n_1} \Big]$$

$G_{n,m}(z)$

$$\chi(z) = \chi(0) - \beta z \Phi(z)$$

$\sigma^i\sigma^i) = 2$

$$G_{nm}(z)$$

$$= \frac{2}{\beta\omega} \sum_{k,k+Q} \langle \Big[K_{mn} c^\dagger_{k+Q} c_k, (z - E_n + E_m - \epsilon_k + \epsilon_{k+Q})^{-1} K_{nm} c^\dagger_k c_{k+Q} \Big] \rangle$$

$$= \frac{2}{\beta\omega} \sum_{k,Q} (f_{k+Q}(1 - f_k)p_m - f_k(1 - f_{k+Q})p_n)(z - E_n + E_m - \epsilon_k + \epsilon_{k+Q})^{-1}$$

$$ImG_{nm}(\omega + i\delta) = -\frac{2\pi}{\beta\omega}\sum_{k,Q}\Big(f_{k+Q}(1-f_k)p_m - f_k(1-f_{k+Q})p_n\Big)\delta(\omega - E_n + E_m - \epsilon_k + \epsilon_{k+Q})$$

$$\rho = \omega - \omega_{nm}$$

$$\omega_{nm} = E_n - E_m$$

$$ImG_{nm}(\omega + i\delta) = -\frac{2\pi N^2(0)}{\beta\omega}\int d\epsilon (f(\epsilon)(1 - f(\epsilon + \rho)p_m - f(\epsilon + \rho)(1 - f(\epsilon))p_n)$$

$$\int d\epsilon f(\epsilon)(1 - f(\epsilon + \rho) =$$

$$\int d\epsilon \exp(\beta(\epsilon+\rho))/(1+\exp(\beta\epsilon))(1+\exp(\beta(\epsilon+\rho))$$

$=$

$(\omega - \omega_{nm}) \exp(\beta(\omega - \omega_{nm}))/(-1 + \exp(\beta(\omega - \omega_{nm})$

$$\int d\epsilon f(\epsilon + \rho)(1 - f(\epsilon) =$$

$$\int d\epsilon \exp(\beta(\epsilon)/(1+\exp(\beta\epsilon))(1+\exp(\beta(\epsilon+\rho))$$

$$(\omega - \omega_{nm})/(-1 + \exp(\beta(\omega - \omega_{nm}))$$

$$ImG_{nm} = -\frac{2\pi N^2(0)}{\beta\omega}(\omega - \omega_{nm})\frac{1-\exp(-\beta\omega)}{1-\exp[(\omega_{nm}-\omega)\beta]}p_m$$

$$F_{nm}(\omega) = \frac{1}{\beta\omega}(\omega - \omega_{nm})\frac{1 - \exp(-\beta\omega)}{1 - \exp[(\omega_{nm} - \omega)\beta]}p_m$$

$$F_{nm}(\omega) = \frac{\sqrt{p_n p_m}}{\beta} \frac{(\omega - \omega_{nm})}{\omega} \frac{\exp(\beta\omega)/2) - \exp(-\beta\omega)/2)}{\exp(\beta(\omega - \omega_{nm})/2) - \exp(-\beta(\omega - \omega_{nm})/2)}$$

$$g = J_{ex} N(0)$$

$$M_{n_2 n_1, m_2 m_1}(\omega) = -i2\pi g^2 \sum_i \Big[$$

$$\delta_{n_2 m_2} \sum_t J^i_{m_1 t} J^i_{t n_1} F_{n_2 t} + \delta_{n_1 m_1} \sum_t J^i_{n_2 t} J^i_{t m_2} F_{t n_1}$$

$$-J^i_{m_1 n_1} J^i_{n_2 m_2} F_{n_2 m_1} - J^i_{n_2 m_2} J^i_{m_1 n_1} F_{m_2 n_1} \Big]$$

$$M_{\nu\mu}(\omega) = M_{n_2 n_1, m_2 m_1}(\omega)$$

$$Im\chi^{\alpha\beta}(\omega + i\delta)/(1 - \exp(-\beta\omega)$$

$$\chi^{\alpha\beta}(z)$$

J^{α}

$$J^{\beta}$$

$$\Phi^{\alpha,\beta}$$

$$\chi^{\alpha\beta}(z) = \chi^{\alpha\beta}(0) - \beta z \Phi^{\alpha\beta}(z)$$

$$\chi^{\alpha\beta}(0)$$

$$\chi^{\alpha\beta}(0) = \sum_{\nu} (J_{\nu}^{\alpha})^{\dagger} \beta P_{\nu} J_{\nu}^{\beta}$$

$$\Phi^{\alpha\beta}(z) = \sum_{\mu\nu} (J_\nu^\alpha)^* \Phi_{\nu\mu}(z) J_\mu^\beta$$

n_1

n_2

$$\Phi_{\nu\mu}(z) = [\Omega^{-1}]_{\nu\mu} P_{\mu}$$

$$\Omega_{\nu\mu}(z) = (z - \omega_\nu)\delta_{\nu\mu} - M_{\nu\mu}(z)/P_\mu$$

$$\omega_\nu = E_{n_2} - E_{n_1}$$

$$\Phi_{\nu\mu}(z) = P_\nu [\bar{\Omega}^{-1}]_{\nu\mu} P_\mu$$

$$\bar{\Omega}_{\nu\mu}(z) = P_{\nu}(z - \omega_{\nu})\delta_{\nu\mu} - M_{\nu\mu}(z)$$

$$S(\vec{Q},\omega) = (\frac{r_0}{2} g_J F(\kappa))^2 \frac{1}{\pi} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) Im\Phi^{\alpha,\beta}(\omega) \frac{-\beta\omega}{1 - e^{-\beta\hbar\omega}}$$

$$(\hbar)\omega = E(k) - E(k')$$

$\hbar$

$$\beta = 11.6/T$$

$$S^{\alpha\beta}(\vec{Q},\omega)$$

$$S(\vec{Q},\omega) = \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta) S^{\alpha\beta}(\vec{Q},\omega)$$

$$S^{\alpha\beta}(\vec{Q},\omega) = Im\chi^{\alpha\beta}/(1-e^{-\beta\hbar\omega}) = Im\Phi^{\alpha,\beta}(\omega)\frac{-\beta\omega}{1-e^{-\beta\hbar\omega}}$$

$$\chi^{\alpha\beta}(\omega) = \chi^{\alpha\beta}(0) - \beta\omega\Phi^{\alpha\beta}(\omega) = \sum_{\mu\nu} \beta(J_\mu^\alpha)^*(P_{\mu\nu} - \omega\Phi_{\mu\nu}(\omega))J_\nu^\beta$$

$\beta P_{\mu\nu}$

D_2^h

$$-\frac{1}{2}\sum_{ij}\mathbf{J}_i^{alpha}\mathcal{J}_{\alpha\beta}(ij)\mathbf{J}_j^{\beta}$$

$$\mathcal{J}_{\alpha\beta}(ij)$$

$$\mathcal{J}_{\alpha\beta}(ij) = \mathcal{J}_{\beta\alpha}(ji)$$

士

$$\mathcal{J}_{\alpha\beta}(\pm 100)$$

$$\mathcal{J}_{\alpha\beta}(\pm 100) = \begin{pmatrix} \mathcal{J}_{aa}(\pm 100) & 0 & 0 \\ 0 & \mathcal{J}_{bb}(\pm 100) & 0 \\ 0 & 0 & \mathcal{J}_{cc}(\pm 100) \end{pmatrix}$$

$B_{iso}/2$

$\boldsymbol{\mu}$

10^{-12}

$$a_0^2$$

$$a0 = 0.5292$$

λ

$1-x$

x

$LaCoO_3$

2

$(Pu, Lu)Pd_3$

$$f^n$$

p^N

d^N

f^N

D_{3h}