

# **V. 3 Magnetische Anregungen**

- I. magnetische Wechselwirkung**
- II. Bestimmung der magnetischen Struktur**
- III. Magnetische Anregungen**
- IV. Polarisationsanalyse**

## V.3.1 Theorie - Zeitabhängigkeiten

Einfluss der Polarisation :

$$\left( \frac{d^2\sigma}{d\Omega dE'} \right)_{\sigma\lambda \rightarrow \sigma'\lambda'} = \frac{k'}{k} \left( \frac{m}{2\pi\hbar^2} \right)^2 |\langle \mathbf{k}'\sigma'\lambda' | V_m | \mathbf{k}\sigma\lambda \rangle|^2 \delta(E_\lambda - E_{\lambda'} + \hbar\omega).$$

Hierbei ist  $V_m$  Produkt von Dipolmoment Neutron und Feld

$$\boldsymbol{\sigma} \cdot \mathbf{B} = \sigma_x B_x + \sigma_y B_y + \sigma_z B_z$$

Wählt man z als Quantisierungsrichtung entsprechend den Zuständen u,v → nur quadratische Terme  $\sigma_x^2 \dots$  für unpol. Neutronen !

$$\begin{aligned} \frac{d^2\sigma}{d\Omega dE'} &= (\gamma r_0)^2 \frac{k'}{k} \sum_{\lambda\lambda'} p_\lambda \sum_{\alpha} \langle \lambda | Q_{\perp\alpha}^+ | \lambda' \rangle \langle \lambda' | Q_{\perp\alpha} | \lambda \rangle \delta(E_\lambda - E_{\lambda'} + \hbar\omega) \\ &= (\gamma r_0)^2 \frac{k'}{k} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \\ &\quad \times \sum_{\lambda\lambda'} p_\lambda \langle \lambda | Q_\alpha^+ | \lambda' \rangle \langle \lambda' | Q_\beta | \lambda \rangle \delta(E_\lambda - E_{\lambda'} + \hbar\omega). \end{aligned}$$

# Magnetisierung :

a) Spin-Teil :

$$\mathbf{Q}_{\perp S} = \sum_i \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}_i) \{ \hat{\boldsymbol{\kappa}} \times (\mathbf{s}_i \times \hat{\boldsymbol{\kappa}}) \}.$$

$$\mathbf{Q}_{\perp S} = \hat{\boldsymbol{\kappa}} \times (\mathbf{Q}_S \times \hat{\boldsymbol{\kappa}}).$$

$$\mathbf{Q}_S = \sum_i \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}_i) \mathbf{s}_i.$$

$\mathbf{Q}_S$  ist Fourier-Transformierte der  
Spin-Dichte

$$\boldsymbol{\rho}_S(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) \mathbf{s}_i$$

$$\mathbf{Q}_S = \int \boldsymbol{\rho}_S(\mathbf{r}) \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}) d\mathbf{r}.$$

## Magnetisierung :

$$\mathbf{M}_S(\mathbf{r}) = -2\mu_B \rho_S(\mathbf{r}).$$

$$\mathbf{Q}_S = -\frac{1}{2\mu_B} \mathbf{M}_S(\boldsymbol{\kappa}),$$

$$\mathbf{M}_S(\boldsymbol{\kappa}) = \int \mathbf{M}_S(\mathbf{r}) \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}) d\mathbf{r}.$$

Spin-Anteil der  
Magnetisierung

## b) Orbital-Komponente :

$$\mathbf{Q}_{\perp L} = \frac{i}{\hbar \kappa} \sum_i \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}_i) (\mathbf{p}_i \times \hat{\boldsymbol{\kappa}}) = -\frac{1}{2\mu_B} \hat{\boldsymbol{\kappa}} \times \{\mathbf{M}_L(\boldsymbol{\kappa}) \times \boldsymbol{\kappa}\}$$

where

$$\mathbf{M}_L(\boldsymbol{\kappa}) = \int \mathbf{M}_L(\mathbf{r}) \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}) d\mathbf{r}.$$

$$\mathbf{Q}_{\perp L} = \hat{\boldsymbol{\kappa}} \times (\mathbf{Q}_L \times \hat{\boldsymbol{\kappa}}),$$

$$\mathbf{Q}_L = -\frac{1}{2\mu_B} \mathbf{M}_L(\boldsymbol{\kappa}).$$

Orbitale Magnetisierung

# Übergang zu zeitabhängigen Operatoren

$$\begin{aligned} \frac{d^2\sigma}{d\Omega dE'} &= (\gamma r_0)^2 \frac{k'}{k} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \sum_{l'd'} \sum_{ld} F_{d'}^*(\boldsymbol{\kappa}) F_d(\boldsymbol{\kappa}) \\ &\quad \times \sum_{\lambda\lambda'} p_\lambda \langle \lambda | \exp(-i\boldsymbol{\kappa} \cdot \mathbf{R}_{l'd'}) S_{l'd'}^\alpha | \lambda' \rangle \\ &\quad \times \langle \lambda' | \exp(i\boldsymbol{\kappa} \cdot \mathbf{R}_{ld}) S_{ld}^\beta | \lambda \rangle \delta(E_\lambda - E_{\lambda'} + \hbar\omega). \end{aligned}$$

Summe über die Komponenten bei Atom **ld** !

Nun zeitabhängige Operatoren :

$$\begin{aligned} \delta(E_\lambda - E_{\lambda'} + \hbar\omega) &= \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \exp\{i(E_{\lambda'} - E_\lambda)t/\hbar\} \exp(-i\omega t) dt, \\ \exp(iHt/\hbar)|\lambda\rangle &= \exp(iE_\lambda t/\hbar)|\lambda\rangle. \end{aligned}$$

$$\begin{aligned}
& \sum_{\lambda\lambda'} p_{\lambda}(\lambda | \exp(-i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d'}) S_{T_d'}^{\alpha} | \lambda') \\
& \quad \times \langle \lambda' | \exp(i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d}) S_{T_d}^{\beta} | \lambda \rangle \delta(E_{\lambda} - E_{\lambda'} + \hbar\omega) \\
& = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \sum_{\lambda\lambda'} p_{\lambda}(\lambda | \exp(-i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d'}) S_{T_d'}^{\alpha} | \lambda') \\
& \quad \times \langle \lambda' | \exp(iHt/\hbar) \exp(i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d}) \exp(-iHt/\hbar) \\
& \quad \times \exp(iHt/\hbar) S_{T_d}^{\beta} \exp(-iHt/\hbar) | \lambda \rangle \exp(-i\omega t) dt \\
& = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} \langle \exp\{-i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d'}(0)\} S_{T_d'}^{\alpha}(0) \\
& \quad \times \exp\{i\boldsymbol{\kappa} \cdot \mathbf{R}_{T_d}(t)\} S_{T_d}^{\beta}(t) \rangle \exp(-i\omega t) dt, \\
& \quad \mathbf{S}_{T_d}^{\beta}(t) = \exp(iHt/\hbar) S_{T_d}^{\beta} \exp(-iHt/\hbar).
\end{aligned}$$

- Annahme : Bewegung der Kerne ist von den Spins entkoppelt =>

Faktorisierung :

$$\begin{aligned} & \langle \exp\{i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(0)\} S_{I'd'}^\alpha(0) \exp\{i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(t)\} S_{I'd'}^\beta(t) \rangle \\ & = \langle \exp\{-i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(0)\} \exp\{i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(t)\} \rangle \langle S_{I'd'}^\alpha(0) S_{I'd'}^\beta(t) \rangle. \end{aligned}$$

Damit folgt der magnetische Streuquerschnitt (lokalisierte Spins):

$$\begin{aligned} \frac{d^2\sigma}{d\Omega dE'} &= \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \sum_{I'd',I'd} \frac{1}{4} g_{d'} g_d F_{d'}^*(\boldsymbol{\kappa}) F_d(\boldsymbol{\kappa}) \\ & \quad \times \int_{-\infty}^{\infty} \langle \exp\{-i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(0)\} \exp\{i\boldsymbol{\kappa} \cdot \mathbf{R}_{I'd'}(t)\} \rangle \\ & \quad \times \langle S_{I'd'}^\alpha(0) S_{I'd}^\beta(t) \rangle \exp(-i\omega t) dt. \end{aligned}$$

- Im Falle eines Bravais-Gitters :

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} N \left\{ \frac{1}{2} g F(\boldsymbol{\kappa}) \right\}^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \sum_l \exp(i\boldsymbol{\kappa} \cdot \mathbf{l})$$

$$\times \int_{-\infty}^{\infty} \langle \exp\{-i\boldsymbol{\kappa} \cdot \mathbf{u}_0(0)\} \exp\{i\boldsymbol{\kappa} \cdot \mathbf{u}_l(t)\} \rangle$$

$$\times \langle S_0^\alpha(0) S_l^\beta(t) \rangle \exp(-i\omega t) dt, \quad ($$


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-Korrelationsfunktion :

nun muss man statische und zeitabhängige Terme auftrennen  
und dann Cross-Terme berücksichtigen

- a) Statische magnetische Streuung :  
statisch nuklear mal statisch magnetisch
- b) magneto-vibrationelle Streuung :  
magnetische elastisch plus nuklear inelastisch  
→ Phononenbeitrag aufgrund der magnetischen Wechselwirkung
- c) Inelastische magnetische Streuung  
keine Änderung in dem Phononensystem
- d) Streuung, die in beiden Bereichen inelastische ist  
→ inelastisch nuklear-magnetische Interferenz

## Verallgemeinerung : Magnetisierungskomponenten

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{(\gamma r_0)^2}{2\pi\hbar} \frac{k'}{k} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \int \langle Q_\alpha(-\boldsymbol{\kappa}, 0) Q_\beta(\boldsymbol{\kappa}, t) \rangle \exp(-i\omega t) dt,$$

$$Q_\beta(\boldsymbol{\kappa}, t) = \exp(iHt/\hbar) Q_\beta(\boldsymbol{\kappa}) \exp(-iHt/\hbar).$$

## Fourier-Koeffizienten der Magnetisierung

$$\left(\frac{d\sigma}{d\Omega}\right)_{el} = (\gamma r_0)^2 \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) \langle Q_\alpha(-\boldsymbol{\kappa}) \rangle \langle Q_\beta(\boldsymbol{\kappa}) \rangle.$$

# Streu-Querschnitt eines Paramagneten :

- keine Korrelationen : keine t-Abhängigkeit

$$\frac{d\sigma}{d\Omega} = (\gamma r_0)^2 \left\{ \frac{1}{2} g F(\boldsymbol{\kappa}) \right\}^2 \exp(-2W) \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) N \sum_l \exp(i\boldsymbol{\kappa} \cdot \mathbf{l}) \langle S_0^\alpha S_l^\beta \rangle.$$

- keine räumlichen Korrelationen außer „auto“-Korrelationen :

$$\langle S_0^\alpha S_l^\beta \rangle = \langle S_0^\alpha \rangle \langle S_l^\beta \rangle = 0.$$

For  $l = 0$

$$\langle S_0^\alpha S_l^\beta \rangle = \delta_{\alpha\beta} \langle (S_0^\alpha)^2 \rangle = \frac{1}{3} \delta_{\alpha\beta} \langle S^2 \rangle$$
$$= \frac{1}{3} \delta_{\alpha\beta} S(S+1).$$

$$\sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\kappa}_\alpha \hat{\kappa}_\beta) = \sum_\alpha (1 - \hat{\kappa}_\alpha^2) = 2.$$

- gesamte paramagnetische  
Streuung :

$$\frac{d\sigma}{d\Omega} = \frac{2}{3} (\gamma r_0)^2 N \left\{ \frac{1}{2} g F(\boldsymbol{\kappa}) \right\}^2 \exp(-2W) S(S+1).$$

## V.3.2 Streuung an geordneten Systemen

### Spin-Wellen

jedes Atom hat Spin  $S$  der Länge  $\{S(S+1)\}^{1/2}$

jede Komponente hat  $m=-S, \dots, +S$

bei endlicher Temperatur ist geordnetes Moment nicht vollständig

Reduktion aufgrund von ebenen Wellen : **Spin-Wellen**

Quantisierung :  $\rightarrow$  Magnonen

**Lineare Spin-Wellen-Theorie** (vgl. harmonische Gitterdynamik) :

$$H = -\sum_{ll'} J(l-l') \mathbf{S}_l \cdot \mathbf{S}_{l'}$$

**Ferromagnetisch !**

Achtung : hier taucht jedes Paar zwei mal auf !!!

$$J(l-l') = J(l'-l)$$

## Erinnerung Quantenmechanik : Drehimpulsmomente

$S_x$ ,  $S_y$  und  $S_z$  sind die x,y,z-Komponenten eines Drehimpulses  
in Einheiten von  $\hbar$   
(gleichgültig ob Spin oder orbitales Moment)

$S^2 = S_x^2 + S_y^2 + S_z^2$     jeder der  $S_x$ ,  $S_y$  und  $S_z$  vertauschen mit  $S^2$   
aber nicht untereinander

$$[S^2, S_x] = [S^2, S_y] = [S^2, S_z] = 0$$

aber  $[S_x, S_y] = i S_z$  etc.

man definiert :  $S^+ = S_x + iS_y$     und     $S^- = S_x - iS_y$

Eigenfunktionen existieren zu  $S^2, S_z$

Eigenwerte :  $S^2 : S(S+1)$  für  $S=0, 1/2, 1, 3/2, \dots$

$S_z : -S, -S+1, \dots, +S$

$S^+ |S, m\rangle = \{(S-m)(S+m+1)\}^{1/2} |S, m+1\rangle$     also  $S^+ |S, S\rangle = 0$

$S^- |S, m\rangle = \{(S+m)(S-m-1)\}^{1/2} |S, m-1\rangle$     also  $S^- |S, -S\rangle = 0$

# Holstein-Primakoff Transformation (1940) :

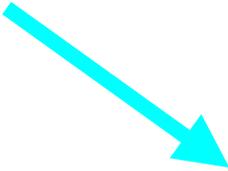
Einführung von Vernichter- und Erzeuger-Operatoren :

$$n = S - M.$$

Verschiebung der Komponente

$$S^+|n\rangle = (2Sn)^{1/2} \left(1 - \frac{n-1}{2S}\right)^{1/2} |n-1\rangle,$$

$$S^-|n\rangle = \{2S(n+1)\}^{1/2} \left(1 - \frac{n}{2S}\right)^{1/2} |n+1\rangle.$$


$$\begin{aligned} a|n\rangle &= n^{1/2}|n-1\rangle, & a^+|n\rangle &= (n+1)^{1/2}|n+1\rangle. \\ aa^+|n\rangle &= (n+1)|n\rangle, & a^+a|n\rangle &= n|n\rangle, \\ & & [a, a^+] &= 1. \end{aligned}$$

Lineare Näherung

$$S_l^+ = (2S)^{1/2} a_l, \quad S_l^- = (2S)^{1/2} a_l^+.$$

## Holstein-Primakoff Transformation (1940) :

Dann drückt man die S-Terme in den Erzeuger/Vernichtern aus  
Fourier-Koeffizienten :

$$a_l = N^{-1/2} \sum_{\mathbf{q}} \exp(i\mathbf{q} \cdot \mathbf{l}) b_{\mathbf{q}},$$
$$a_l^+ = N^{-1/2} \sum_{\mathbf{q}} \exp(-i\mathbf{q} \cdot \mathbf{l}) b_{\mathbf{q}}^+,$$

$$b_{\mathbf{q}} = N^{-1/2} \sum_l \exp(-i\mathbf{q} \cdot \mathbf{l}) a_l,$$
$$b_{\mathbf{q}}^+ = N^{-1/2} \sum_l \exp(i\mathbf{q} \cdot \mathbf{l}) a_l^+.$$

## Holstein Primakoff Transformation (1940) :

Komplikationen entstehen durch die x- und y-Terme :

$$S_l \cdot S_{l'} = \frac{1}{2} (S_l^+ S_{l'}^- + S_{l'}^+ S_l^-) + S_l^z S_{l'}^z.$$

keine  $l=l'$ -Terme       $S_l$  und  $S_{l'}$  kommutieren

$$H = -\sum_{ll'} J(l-l')(S_l^+ S_{l'}^- + S_l^z S_{l'}^z).$$

$$H = -NS^2 \mathcal{J}(0) + 2S\mathcal{J}(0) \sum_l a_l^\dagger a_l - 2S \sum_{ll'} J(l-l') a_l a_{l'}^\dagger,$$

$$\mathcal{J}(\mathbf{q}) = \sum_{\boldsymbol{\rho}} J(\boldsymbol{\rho}) \exp(i\mathbf{q} \cdot \boldsymbol{\rho}),$$

$$\boldsymbol{\rho} = l - l'.$$

ähnlich wie bei Phononen : Fourier-Transformierte der J's

$$\sum_l a_l^\dagger a_l = \frac{1}{N} \sum_{\mathbf{q}\mathbf{q}'} \sum_l \exp\{i(\mathbf{q}' - \mathbf{q}) \cdot l\} b_{\mathbf{q}}^\dagger b_{\mathbf{q}'} = \sum_{\mathbf{q}} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}.$$

# Zeitabhängige Form der Erzeuger/Vernichter-Operatoren

$$a_l(t) = N^{-1/2} \sum_{\mathbf{q}} \exp\{i(\mathbf{q} \cdot \mathbf{l} - \omega_{\mathbf{q}}t)\} b_{\mathbf{q}},$$

$$a_l^+(t) = N^{-1/2} \sum_{\mathbf{q}} \exp\{-i(\mathbf{q} \cdot \mathbf{l} - \omega_{\mathbf{q}}t)\} b_{\mathbf{q}}^+.$$

- Spin-Wellen : Hamilton-Operator in Magnonen-Termen

$$H = H^0 + \sum_{\mathbf{q}} \hbar \omega_{\mathbf{q}} b_{\mathbf{q}}^+ b_{\mathbf{q}},$$

$$H^0 = -S^2 N \mathcal{J}(0) = -S^2 N \sum_{\boldsymbol{\rho}} J(\boldsymbol{\rho}),$$

$$\hbar \omega_{\mathbf{q}} = 2S \{ \mathcal{J}(0) - \mathcal{J}(\mathbf{q}) \}.$$

$$\hbar\omega_{\mathbf{q}} = 2S\{\mathcal{F}(0) - \mathcal{F}(\mathbf{q})\}.$$

Einfachstes Beispiel :  
Nur  $\mathbf{r}$  nächste Nachbarn koppeln mit  $\mathbf{J}$

$$\mathcal{F}(0) = rJ,$$

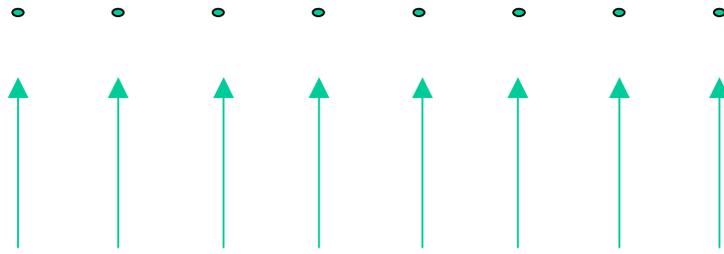
$$\mathcal{F}(\mathbf{q}) = rJ\gamma_{\mathbf{q}},$$

$$\gamma_{\mathbf{q}} = \frac{1}{r} \sum_{\boldsymbol{\rho}} \exp(i\mathbf{q} \cdot \boldsymbol{\rho}).$$

- einfach kubisch (Konstante  $a$ )  $\hbar\omega_{\mathbf{q}} = Dq^2$  mit  $D = 2JSa^2$
- höchste Energie „entspricht“ Flippen eines Spins !

# Beispiel: ferromagnetische Spinwellen

$T = 0$ : Ausrichtung der Spins entlang der Quantisierungsachse (bzw. Nullpunktsbewegung)



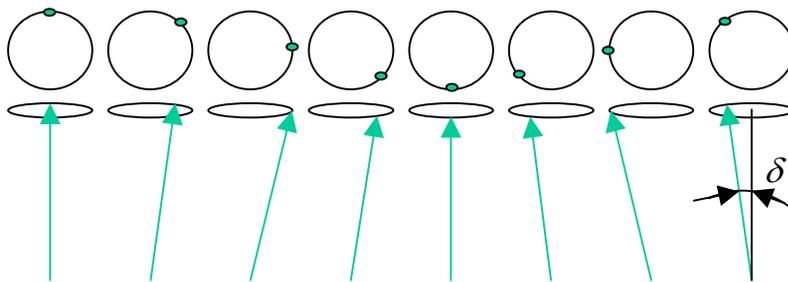
$N$  Ionen in linearer Kette

Richtungsquantelung:

**Gesamtspin** in einer Richtung  $N/2, N/2-1, \dots, -N/2$

$$U_{\min} = -N2JS^2$$

$T > 0$ : Abweichungen der Spins von der Quantisierungsachse, propagierende Spinwelle



diskrete Werte für Winkel  $\delta$ :  $SN \cos \delta = SN - n$

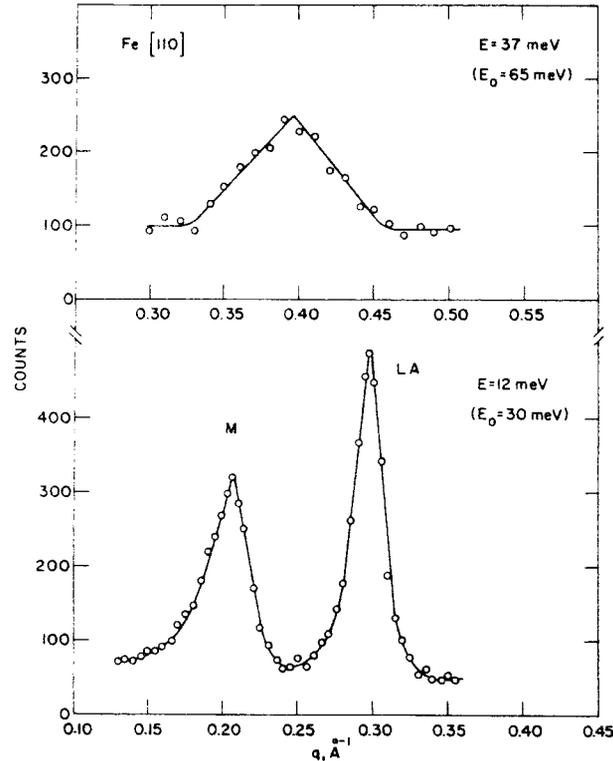
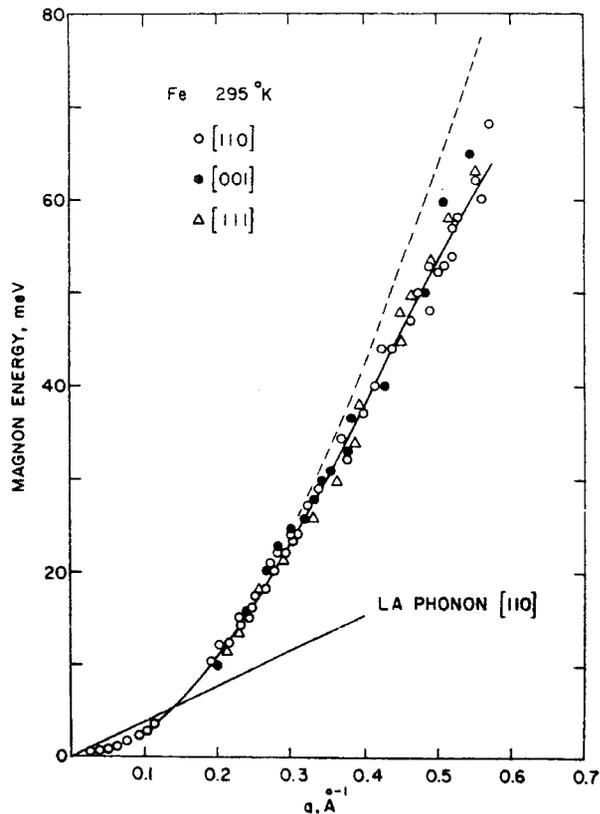
$n = 1, 2, \dots$

$$\frac{\delta^2}{2} = \frac{n}{SN}$$

# Klassisches Beispiel Fe

## magnon dispersion in Fe

Shirane et al. (1968)

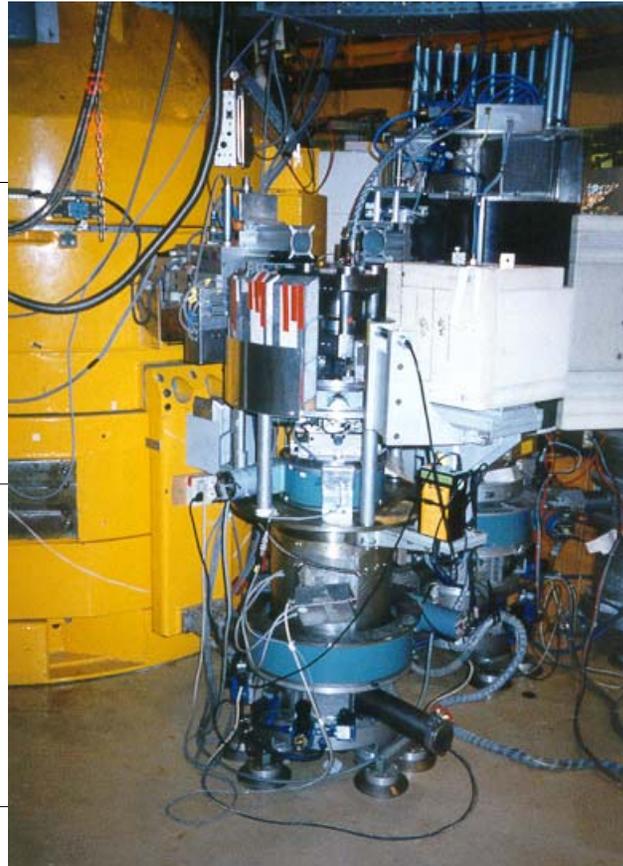
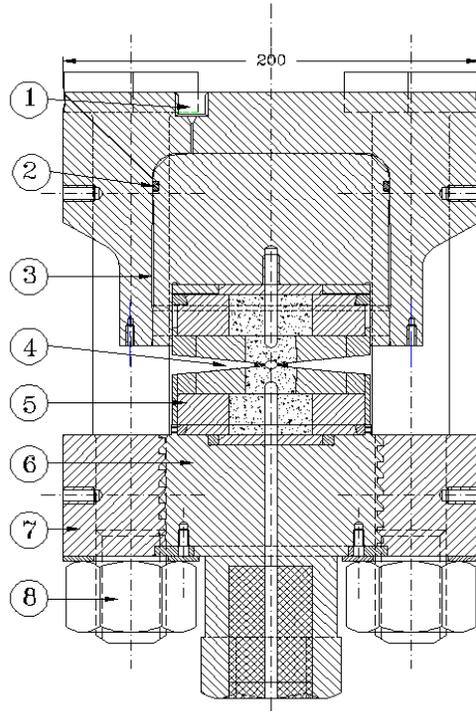


$$\omega = D \cdot q^2$$

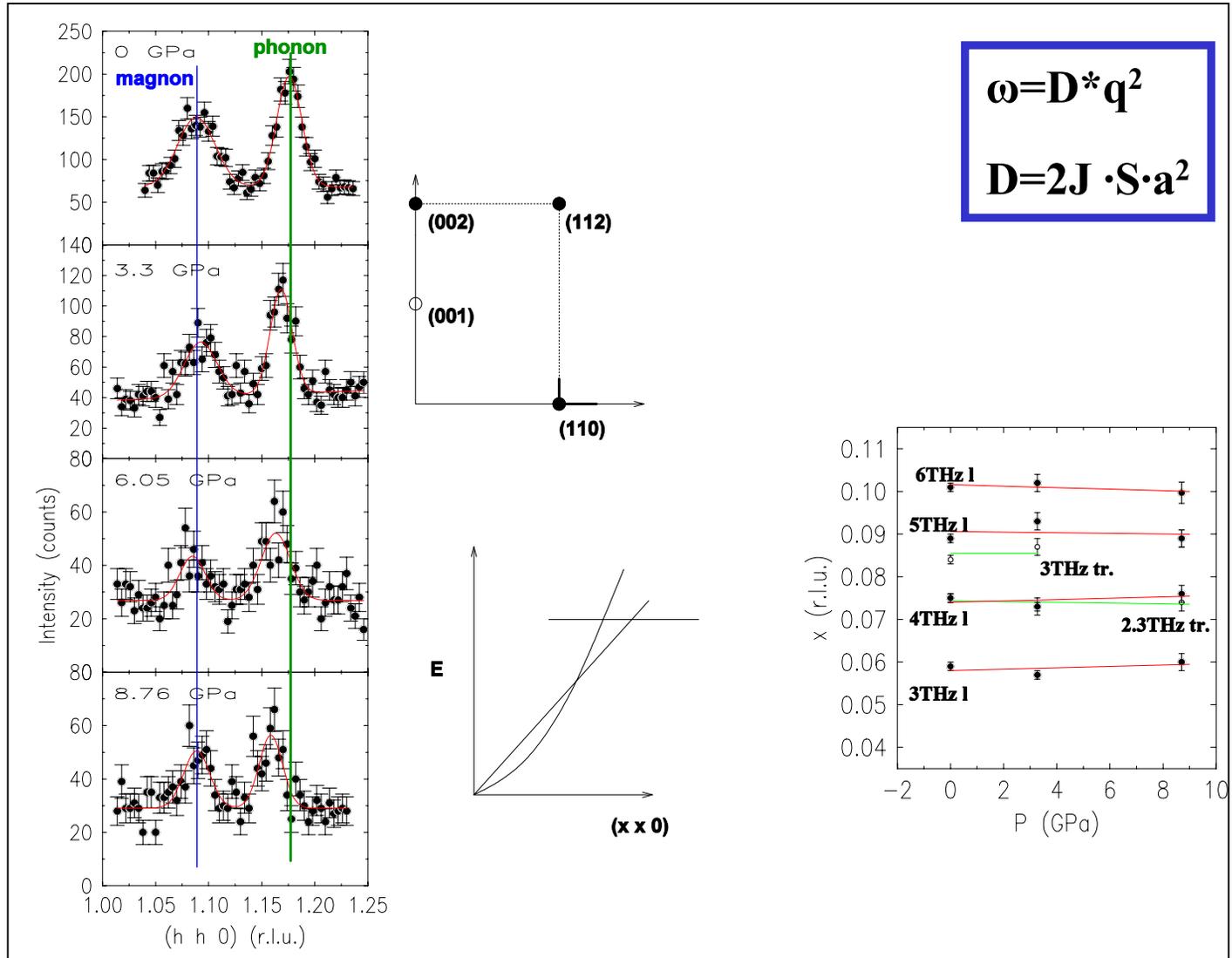
$$D = 2J \cdot S \cdot a^2$$

# Inelastic neutron scattering at high pressure ?

“Paris-Edinburgh” high pressure cell  
capacity 250 tn, mass: ~ 50 kg



# Magnons at high pressure



## Ein-Magnonen-Streuquerschnitt :

Analog zu dem Vorgehen bei Phononen kann man die Matrixelemente über die Spinwellen berechnen :

$$S_i^+(t) = \left(\frac{2S}{N}\right)^{1/2} \sum_{\mathbf{q}} \exp\{i(\mathbf{q} \cdot \mathbf{l} - \omega_{\mathbf{q}}t)\} b_{\mathbf{q}},$$

$$S_i^-(t) = \left(\frac{2S}{N}\right)^{1/2} \sum_{\mathbf{q}} \exp\{-i(\mathbf{q} \cdot \mathbf{l} - \omega_{\mathbf{q}}t)\} b_{\mathbf{q}}^+,$$

$$S_i^z(t) = S - \frac{1}{N} \sum_{\mathbf{q}\mathbf{q}'} \exp[i\{(\mathbf{q}' - \mathbf{q}) \cdot \mathbf{l} - (\omega_{\mathbf{q}'} - \omega_{\mathbf{q}})t\}] b_{\mathbf{q}}^+ b_{\mathbf{q}'}.$$

## Ein-Magnonen-Streuquerschnitt :

Analog zu dem Vorgehen bei Phononen kann man die Matrixelemente über die Spinwellen berechnen :

$$\begin{aligned} \frac{d^2\sigma}{d\Omega dE'} &= (\gamma r_0)^2 \frac{k'}{k} \frac{1}{2\pi\hbar} \frac{1}{2} S(1 + \hat{\kappa}_z^2) \left\{ \frac{1}{2} gF(\boldsymbol{\kappa}) \right\}^2 \exp(-2W) \sum_l \exp(i\boldsymbol{\kappa} \cdot \mathbf{l}) \\ &\times \int_{-\infty}^{\infty} \sum_q [\exp\{-i(\mathbf{q} \cdot \mathbf{l} - \omega_q t)\} \langle n_q + 1 \rangle \\ &+ \exp\{i(\mathbf{q} \cdot \mathbf{l} - \omega_q t)\} \langle n_q \rangle] \exp(-i\omega t) dt \\ &= (\gamma r_0)^2 \frac{k'}{k} \frac{(2\pi)^3}{v_0} \frac{1}{2} S(1 + \hat{\kappa}_z^2) \left\{ \frac{1}{2} gF(\boldsymbol{\kappa}) \right\}^2 \exp(-2W) \\ &\times \sum_{\tau, q} \{ \delta(\boldsymbol{\kappa} - \mathbf{q} - \boldsymbol{\tau}) \delta(\hbar\omega_q - \hbar\omega) \langle n_q + 1 \rangle \\ &+ \delta(\boldsymbol{\kappa} + \mathbf{q} - \boldsymbol{\tau}) \delta(\hbar\omega_q + \hbar\omega) \langle n_q \rangle \}. \end{aligned}$$

S-Faktor

Polarisations-Faktor

Bose-Faktor

The thermal average of  $n_q$  is

$$\langle n_q \rangle = \{ \exp(\hbar\omega_q \beta) - 1 \}^{-1}.$$

- nur transversale Terme geben inelastische Streuung (Achtung Domänen)!

# V.3.3 Einteilchensysteme: Kristallfeldanregungen - Theorie

**Kristall mit schwacher magnetischer Kopplung zwischen Ionen: Einteilchenproblem**

**z.B. seltene Erden mit niedriger Übergangstemperatur für magnetische Ordnung  
dominante Wechselwirkung wird von den umgebenden Ionen bereitgestellt:**

**einzelnes Ion in elektrostatischem Potential benachbarter Ionen (Kristallfeld)**

**Grundzustand des isolierten Ions: J Multiplett mit (2J+1)-facher Entartung**

**Entartung wird durch Symmetrie des Kristallfelds aufgehoben,**

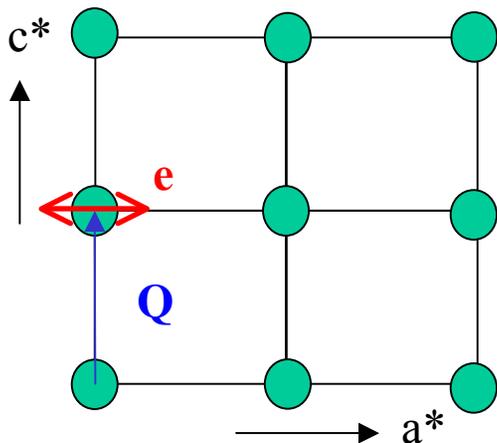
**Anzahl nicht-entarteter Kristallfeldniveaus wird durch Kristallsymmetrie bestimmt**

Magnetische Streufunktion

$$\frac{d^2\sigma}{d\Omega d\omega} = N \left( \frac{1}{2} g \gamma_0 \right)^2 \frac{k_f}{k_i} |F(\mathbf{Q})|^2 \exp(-2W(\mathbf{Q})) \sum_{\alpha} \left( 1 - \frac{Q_{\alpha}^2}{Q^2} \right) |\langle \Gamma_m | \hat{J}^{\alpha} | \Gamma_n \rangle|^2 \delta(\hbar\omega + E_n - E_m)$$

Kristallfeldzustände:  $|\Gamma_n\rangle = \sum_{M=-J}^{+J} A_n(M) |M\rangle$

Anregungsenergien sind unabhängig vom Streuvektor  $\mathbf{Q}$ , gestreute Intensität nicht!



$\mathbf{Q} \perp \mathbf{e}$ : transversale Übergänge

$\mathbf{Q} \parallel \mathbf{e}$ : longitudinale und transversale Übergänge mit halber Intensität

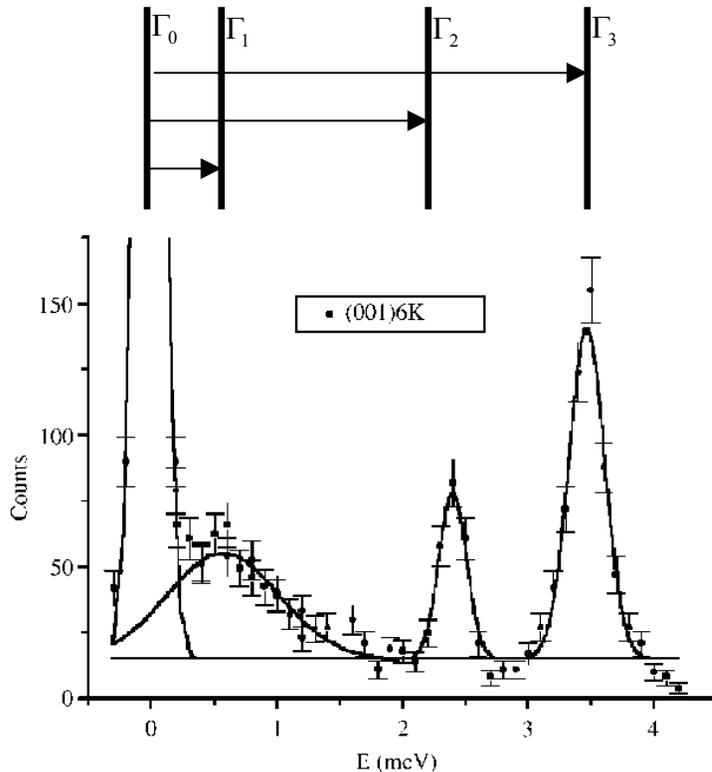
# Experimentelles Beispiel: Kristallfeldanregungen in einkristallinem PrNiSn

$\text{Pr}^{3+}$  :  $J = 4$ , maximal 9 Kristallfeldniveaus

frühere Messung mit HET (ISIS): 8 Anregungen im Energiebereich 2-28 meV

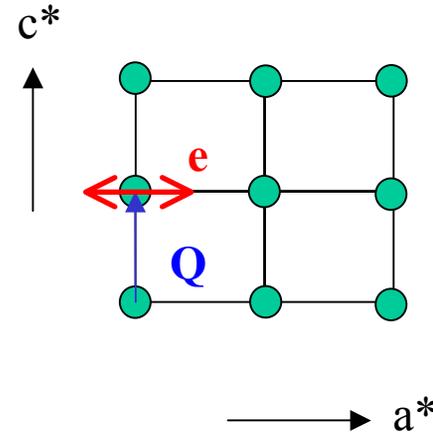
Vorhersage eines Energieniveaus bei 0.5 meV

Messung am kalten Dreiachsengerät V2 (FLEX), HMI: Anregungen im Energiebereich 0.4 - 4 meV



**Fig. 1.** Inelastic scattering from PrNiSn at  $Q = (001)$  at  $T = 6$  K, showing the 0.5, 2.4 and 3.5 meV modes. The lines are fits to gaussian functions. The counting time of 1E6 monitor counts corresponds to 7 min at 2 meV energy transfer

$$\frac{d^2\sigma}{d\Omega d\omega} \propto \left(1 - \frac{Q_\alpha^2}{Q^2}\right) |\langle \Gamma_m | \hat{J}^\alpha | \Gamma_n \rangle|^2$$

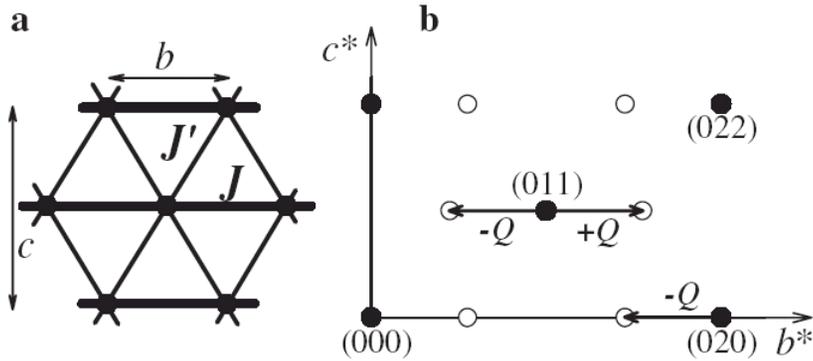


2.4 meV Mode wird nicht in  $[100]$  gefunden:  
polarisiert  $\parallel a^*$

0.5 meV Mode und 3.5 meV Mode werden mit  
gleicher Intensität entlang  $[100]$  und  $[001]$  gefunden :  
polarisiert  $\parallel b^*$

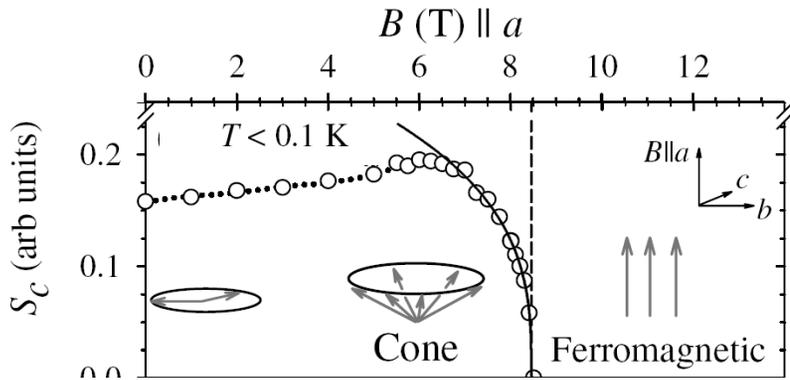
# V.3.4 Aktuelle Beispiele

## V.3.4.1 Spinwellendispersion in $\text{Cs}_2\text{CuCl}_4$

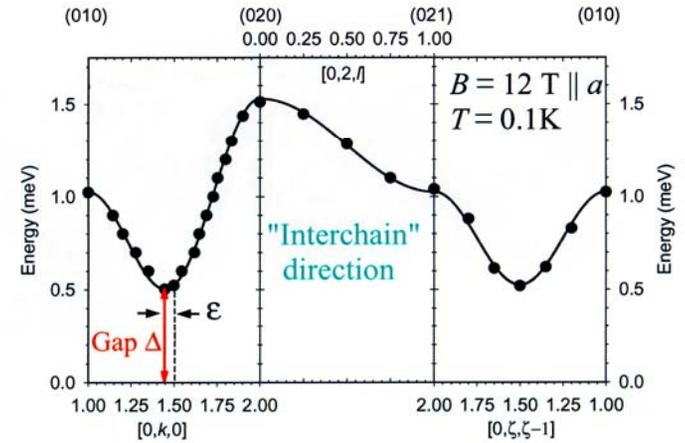


a: Magnetische Kopplungen in  $\text{Cs}_2\text{CuCl}_4$  Ebenen: Dreiecksgitter mit anisotroper Kopplung  $J' < J$

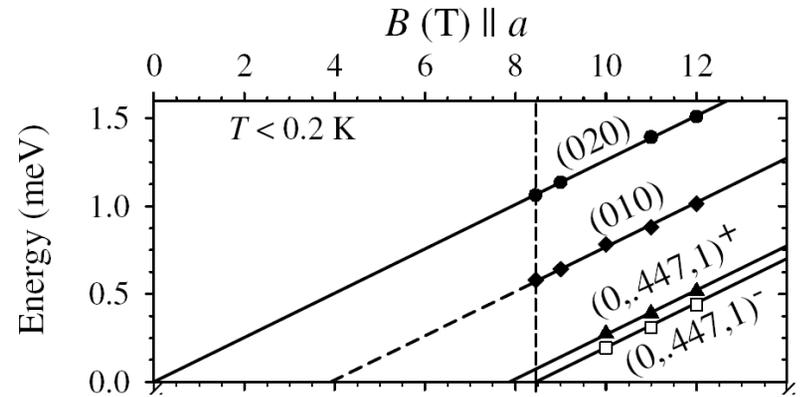
b: in der Konusphase auftretende magnetische Satellitenpeaks (offene Kreise) nukleare Peaks (gefüllte Kreise)



Skalierte Intensitäten der magnetischen Bragg-Peaks



Dispersionsrelation in der gesättigten Phase



Feldabhängigkeit der Anregungsenergien

## V.3.4.2. Mehrteilchensysteme (Cluster): Dimere - Theorie

Heisenberg Hamilton-Operator:  $H = -2J\hat{S}_1 \cdot \hat{S}_2$   $J$  : Austauschintegral

$$\frac{d^2\sigma}{d\Omega d\omega} = N(\gamma r_0)^2 \frac{k_f}{k_i} |F(\mathbf{Q})|^2 \exp(-2W(\mathbf{Q})) n_S$$
$$\times \sum_{\alpha} \left(1 - \frac{Q_{\alpha}^2}{Q^2}\right) \frac{2}{3} (1 - \cos(\mathbf{Q} \cdot \mathbf{R})) |\langle S' | \hat{T}_1 | S \rangle|^2 \delta(\hbar\omega + E_S - E_{S'})$$

charakteristischer Term

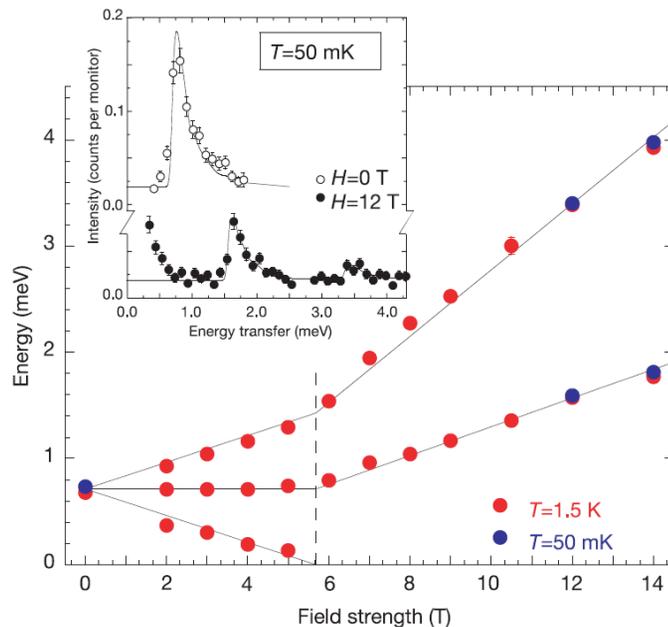
direkter Zusammenhang zwischen Kopplungsparameter  $J$  und meßbaren Energieniveaus

$$E_S = -J(S(S+1) - 2S_1(S_1+1))$$

# Experimentelles Beispiel: Tripletzustände in $\text{TlCuCl}_3$

$\text{TlCuCl}_3$  : paarweise Anordnung der magnetischen  $\text{Cu}^{2+}$  Ionen (Dimere) mit antiferromagnetischer Kopplung

Grundzustand: Singulett; Angeregte Zustände: Triplet-Zustände



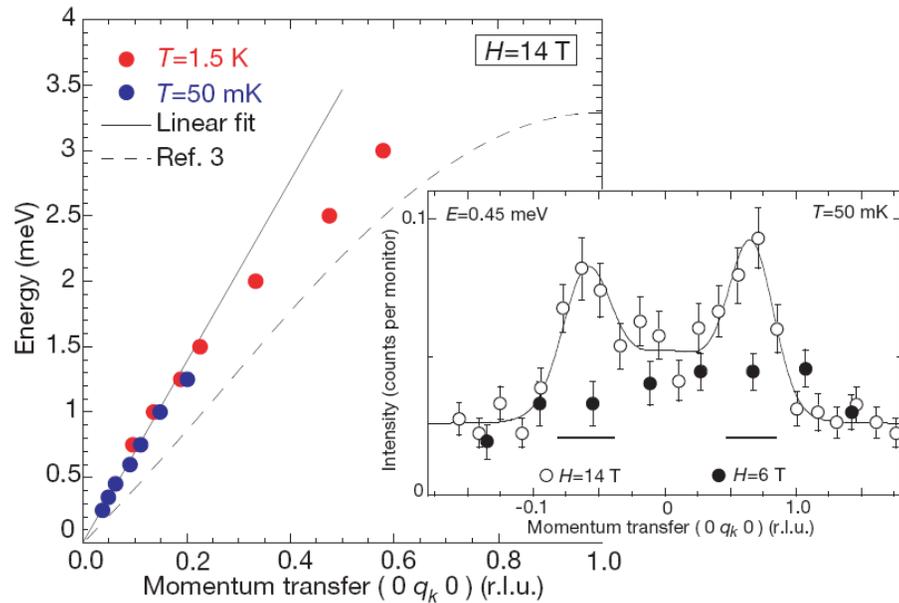
Äußeres Magnetfeld hebt die Entartung der angeregten Tripletzustände auf.

Bei kritischem Magnetfeld  $H_C = 6 \text{ T}$ :

Singulett und unterster Tripletzustand sind energetisch entartet und langreichweitige magnetische Ordnung wird beobachtet.

$H_C$ : Quantenkritischer Punkt (Bose-Einstein-Kondensation)

# Bose-Einstein Kondensation in $\text{TlCuCl}_3$



Dispersion der niedrigsten Triplet-Mode im feldinduzierten, geordneten Zustand eines Dimersystems in Übereinstimmung mit theoretischen Vorhersagen aus BEC Theorie.

# BENSC-Probenumgebung:

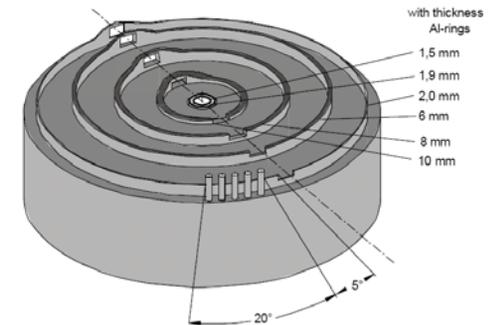
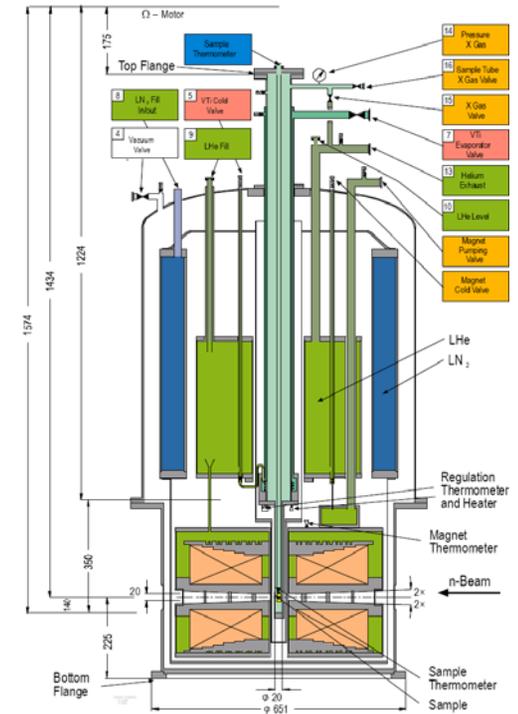


## Magnet Cryostats with Vertical Field

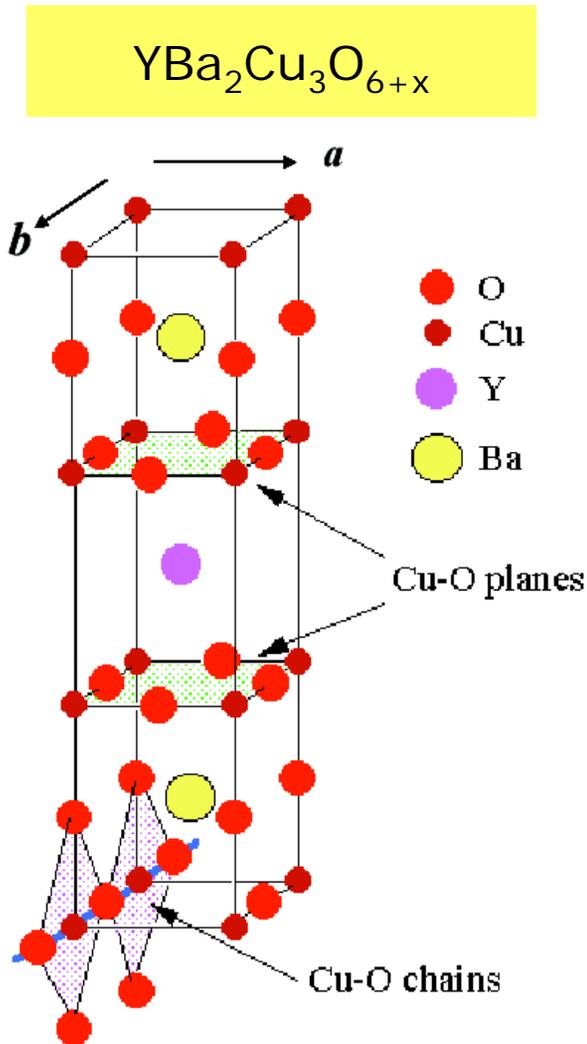
System Code	System Construct.	Temperature Range	Magnetic Field Max./Asy./Acc.	Sample Space Dia./Split/Angle	Thermometry Sensors
VM-1	OI	1.5K - 200K	12T /no/rings	<20mm/20mm/2°	Cernox®
	OI	1.5K - 100K	14,5T /no/rings	<20mm/20mm/2°	Cernox®
+ DY-booster	OI	1.5K - 80K	14,5+2,5T /no/rings	<20mm/20mm/2°	Cernox®
VM-1B	OI	1.5K - 200K	12T /no/rings	<20mm/20mm/2°	Cernox®
	OI	1.5K - 100K	15T /no/rings	<20mm/20mm/2°	Cernox®
+ DY-booster	OI	1.5K - 80K	15+2,5T /no/rings	<20mm/20mm/2°	Cernox®
VM-2	OI	1.5K - 300K	7T /yes/rings	<50mm/30mm/5°	Cernox®
VM-3	AS / OI	1.5K - 300K	5T /no/3x5°wedges	<50mm/30mm/0°	Cernox®
VM-4	AS / Thor	1.5K - 300K	5.5T /yes/3x55°wedges	<50mm/40mm/+35°	Cernox®

Kombination von  $^3\text{He}/^4\text{He}$  - Dilution Insert ("Dilution Stick") mit Vertikalmagnet VM-1/VM-1B:  
Temperaturen bis zu 50 mK bei  $B = 14.5 - 15 \text{ T}$

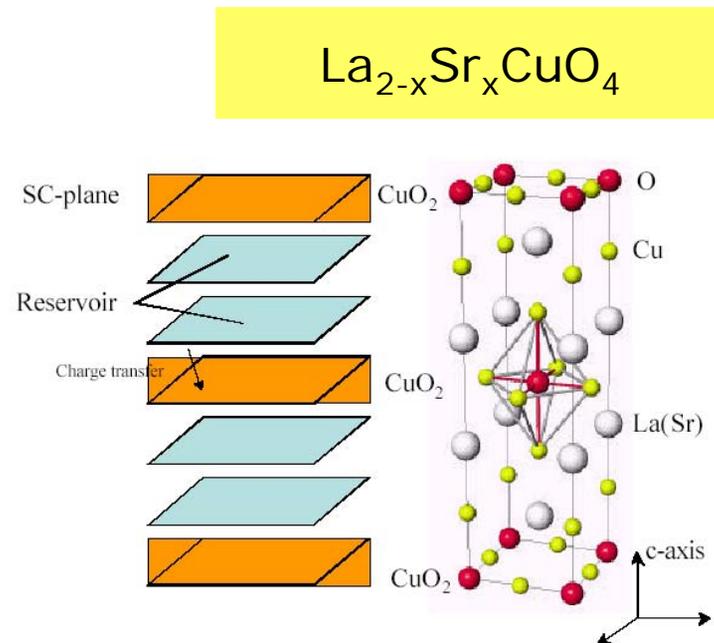
Kombination von Dy-Insert mit Vertikalmagnet VM-1/VM-1B:  
Temperaturen bis zu 1.5 K bei  $B = 17.0 - 17.5 \text{ T}$



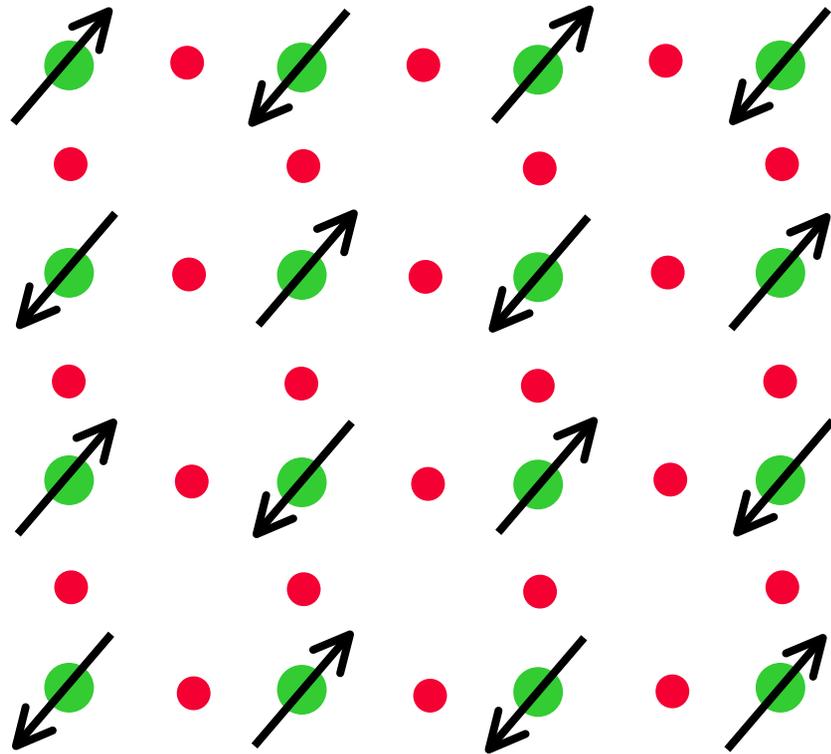
# V.3.4.3 Magnetismus der Kuprate



- Quasi-2D Materialien
- Gestapelte  $\text{CuO}_2$ -Ebenen
- Getrennt durch Ladungsreservoir (kontrollieren Ladungstransfer-Mechanismus)
- $\text{CuO}_2$  – Ebenen tragen anomale physik. Eigenschaften



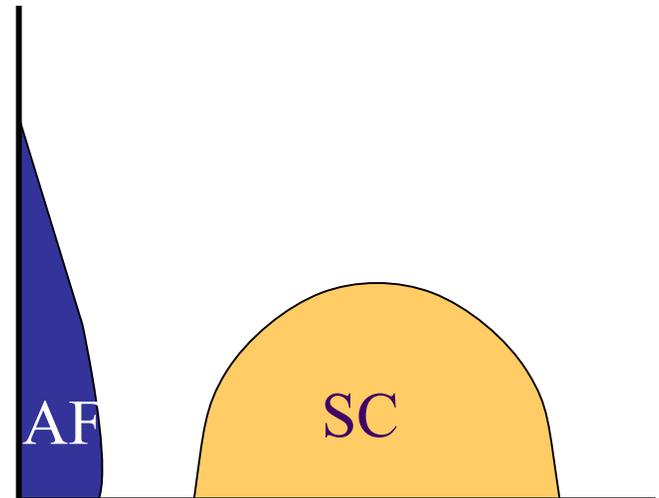
# Eine $\text{CuO}_2$ -Ebene



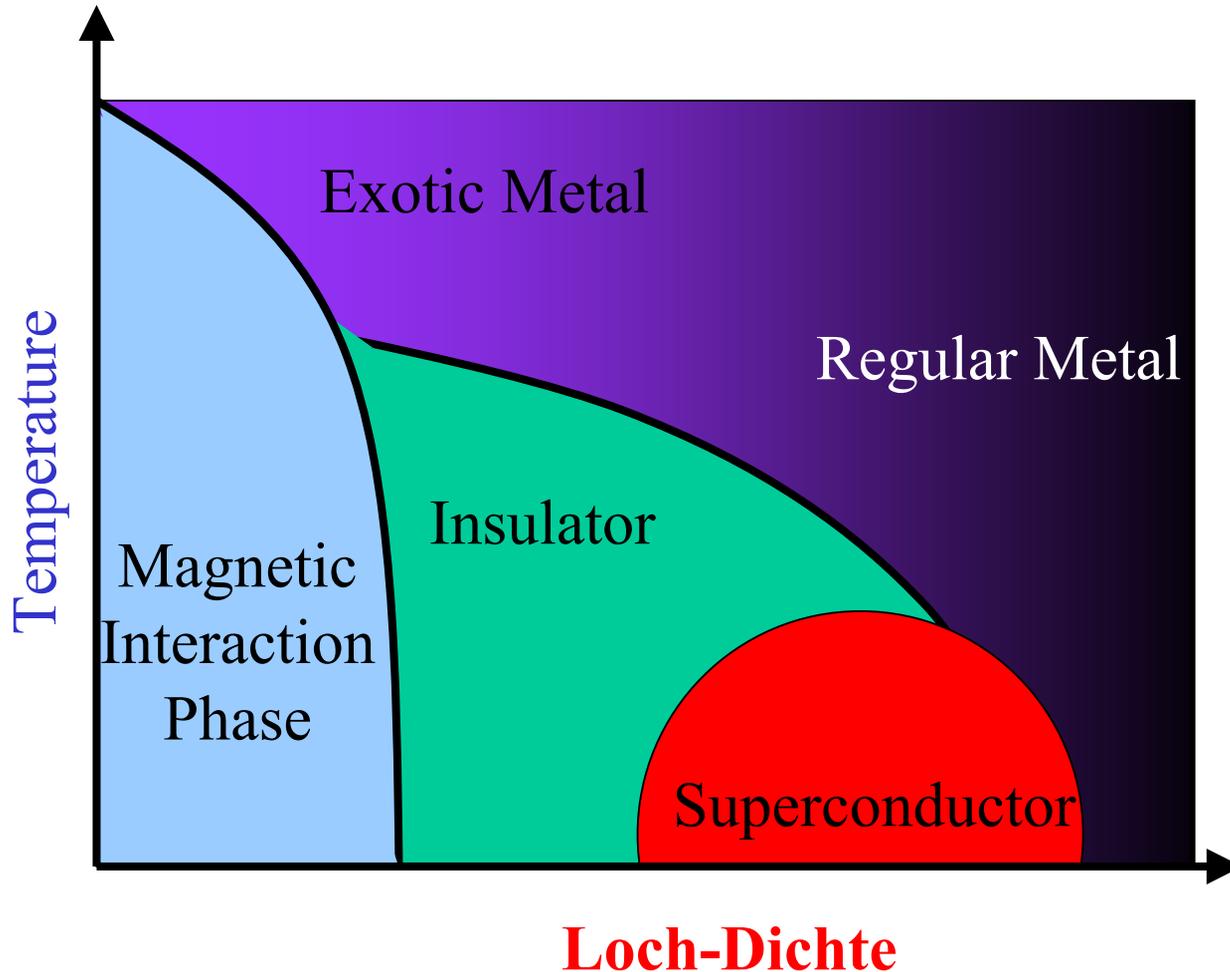
● Oxygen ● Cu

**Dotierung mit Löchern**

**Supraleitung bei  
spezieller Dotierung**



# Generelles Phasendiagramm?





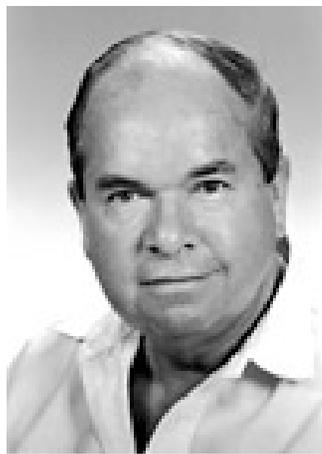
# Mechanism I ?

Superconductivity in High  $T_c$  Cuprates: The Cause is No Longer A Mystery

Philip W. Anderson  
*Joseph Henry Laboratories of Physics*  
*Princeton University, Princeton, NJ 08544*

(2001)

**I discuss various direct calculations of the properties of the one-band Hubbard model on a square lattice and conclude that these properties sufficiently resemble those of the cuprate superconductors that no more complicated interactions are necessary to cause high  $T_c$  superconductivity. In particular, I discuss phonon effects and conclude that these may be effective in reducing  $T_c$  and the gap in electron-doped materials.**



# Mechanism II ?

## Theory of High-T<sub>c</sub> Superconducting Cuprates Based on Experimental Evidence

A.A. Abrikosov

*Materials Science Division, Argonne National Laboratory  
9700 South Cass Avenue, Argonne, Illinois 60439, USA  
(January 8, 2004)*

**A model of superconductivity in layered high-temperature superconducting cuprates is proposed, based on the extended saddle point singularities in the electron spectrum, weak screening of the Coulomb interaction and **phonon-mediated interaction between electrons** plus a small short -range repulsion of Hund's, or spin-fluctuation, origin. This permits to explain the large values of T<sub>c</sub> ....**



**TOSANOUMI**  
(Sumo Wrestler)

Height of Tosanoumi 186cm  
Weight of Tosanoumi 142kg  
Weight of disk 60kg  
Total weight 202kg

As of February '90

浮いた  
土佐ノ海

Es geht auch  
ohne  
Theo-rie/retiker

# Lineare Spin-Wellen-Theorie : Antiferromagneten

$$\begin{aligned}\mathcal{H} = & \sum_{\mathbf{m},\mathbf{r}} J(\mathbf{r}) \hat{\mathbf{S}}_{\mathbf{m}} \cdot \hat{\mathbf{S}}_{\mathbf{m}+\mathbf{r}} + \sum_{\mathbf{n},\mathbf{r}} J(\mathbf{r}) \hat{\mathbf{S}}_{\mathbf{n}} \cdot \hat{\mathbf{S}}_{\mathbf{n}+\mathbf{r}} + \\ & + \sum_{\mathbf{m},\mathbf{R}} J_1(\mathbf{R}) \hat{\mathbf{S}}_{\mathbf{m}} \cdot \hat{\mathbf{S}}_{\mathbf{m}+\mathbf{R}} + \sum_{\mathbf{n},\mathbf{R}} J_2(\mathbf{R}) \hat{\mathbf{S}}_{\mathbf{n}} \cdot \hat{\mathbf{S}}_{\mathbf{n}+\mathbf{R}} - \\ & - g_1 \mu_B (H + H_{A,1}) \sum_{\mathbf{m}} \hat{S}_{\mathbf{m}}^z - g_2 \mu_B (H - H_{A,2}) \sum_{\mathbf{n}} \hat{S}_{\mathbf{n}}^z,\end{aligned}$$

Grundsätzlicher Unterschied :

Gitter *bipartit* (zwei Untergitter)

↔ Summen über  $\mathbf{m}$  und  $\mathbf{n}$  und Verbindungsvektoren  $\mathbf{r}$

Kopplungen innerhalb eines Gitters :  $\mathbf{R}$

hier zusätzlich : **Anisotropieterme** und **externes Feld**

Bemerkung : jedes Paar zwischen den beiden Gittern tritt doppelt auf

# Lineare Spin-Wellen-Theorie : Antiferromagneten

For an antiferromagnet  $g_1 = g_2 = g$ ,  $H_{A,1} = H_{A,2} = H_A$ ,  $S_1 = S_2 = S$ , and  $\mathcal{J}_1 = \mathcal{J}_2 = \mathcal{J}'$ . This means that the functions  $a_1$ ,  $a_2$ ,  $b_1$ , and  $b_2$  satisfy  $a_1 = a_2 = g\mu_B H$  and

$$b_1 = b_2 = 2S\mathcal{J}(0) - 2S\{\mathcal{J}'(0) - \mathcal{J}'(\mathbf{q})\} + g\mu_B H_A = b, \text{ say,} \quad (9.238)$$

so 
$$\Omega(\mathbf{q}) \equiv [b^2 - \{2S\mathcal{J}(\mathbf{q})\}^2]^{\frac{1}{2}}$$

with 
$$\hbar\omega_{\mathbf{q},a} = (-1)^a g\mu_B H + \Omega(\mathbf{q}) \quad (a = 0, 1). \quad (9.239)$$

For small values of  $\mathbf{q}$  and cubic crystals

$$\mathcal{J}(\mathbf{q}) = \sum_{\mathbf{r}} \exp(-i\mathbf{q} \cdot \mathbf{r}) J(\mathbf{r}) \simeq \mathcal{J}(0) - \frac{1}{6}q^2 \sum_{\mathbf{r}} r^2 J(\mathbf{r})$$

and we define 
$$J^{(2)} = \sum_{\mathbf{r}} r^2 J(\mathbf{r}), \quad (9.240)$$

i.e. 
$$\mathcal{J}(0) - \mathcal{J}(\mathbf{q}) \simeq \frac{1}{6}q^2 J^{(2)}. \quad (9.241)$$

Similarly, 
$$\mathcal{J}'(0) - \mathcal{J}'(\mathbf{q}) \simeq \frac{1}{6}q^2 J'^{(2)}. \quad (9.242)$$

(In (9.22) we defined the moments  $\bar{l}^n$  through  $\bar{l}^n = \Sigma_1 l^{n+2} J(l) / \Sigma_1 l^2 J(l)$ . In the notation of (9.240) this would read  $J^{(n+2)} / J^{(2)}$ .)

Though (9.241) and (9.242) hold rigorously at small  $\mathbf{q}$  only for cubic crystals, it is often a good approximation to use them in other cases.

$$\begin{aligned} \hbar\omega_{\mathbf{q},a} = & [g\mu_B H_A \{4S\mathcal{J}(0) + g\mu_B H_A\} + \\ & + \frac{1}{3}q^2 S \{4S\mathcal{J}(0)(J^{(2)} - J'^{(2)}) - 2g\mu_B H_A J'^{(2)}\}]^{\frac{1}{2}} + (-1)^a g\mu_B H \end{aligned}$$

and this simplifies to

$$\hbar\omega_{\mathbf{q},a} = q \left\{ \frac{4S^2}{3} \mathcal{J}(0)(J^{(2)} - J'^{(2)}) \right\}^{\frac{1}{2}} + (-1)^a g\mu_B H$$

when  $H_A = 0$ .

für kleines  $q$  : lineare Dispersion

eine Art magnetischer Atome !  
unterscheide  $\mathbf{J}$  und  $\mathbf{J}'$  inter- und intra-Subgitter

# Antiferromagnet mit nächster Nachbarkopplung :

$$\hbar\omega_{\mathbf{q},a} = q \left\{ \frac{4S^2}{3} \mathcal{J}(0)(J^{(2)} - J'^{(2)}) \right\}^{\frac{1}{2}} + (-1)^a g\mu_B H$$

$$\hbar\omega_{\mathbf{q}} = 2rJS \left\{ (1 + h_A)^2 - \gamma_{\mathbf{q}}^2 \right\}^{\frac{1}{2}} = 2rJS \mathcal{E}_{\mathbf{q}},$$

$$\gamma_{\mathbf{q}} = \frac{1}{r} \sum_{\boldsymbol{\rho}} \exp(i\mathbf{q} \cdot \boldsymbol{\rho}).$$

- maximale Energie :  $2J \cdot S \cdot \text{Anzahl der Nachbarn } (r) !$

# Untergittermagnetisierung :

$$\begin{aligned}\langle \hat{S}_m^z \rangle &= S - \frac{1}{2S} \frac{1}{N^2} \sum_{\mathbf{q}} \langle \hat{S}_{\mathbf{q}}^- \hat{S}_{\mathbf{q}}^+ \rangle \\ &= S - \frac{1}{2N} \sum_{\mathbf{q}} \left\{ \left( \frac{1+h_A}{\mathcal{E}_{\mathbf{q}}} \right) \coth(\frac{1}{2} \hbar \omega_{\mathbf{q}} \beta) - 1 \right\}.\end{aligned}$$

$$\delta \langle \hat{S}^z \rangle_0 = \frac{1}{2N} \sum_{\mathbf{q}} \left( \frac{1+h_A}{\mathcal{E}_{\mathbf{q}}} \right) - 1.$$

-Untergittermagnetisierung  
nimmt mit Magnonen-  
Besetzung ab

$$\langle \hat{S}^z \rangle = S - \delta \langle \hat{S}^z \rangle_0 - \frac{1}{N} \sum_{\mathbf{q}} \left( \frac{1+h_A}{\mathcal{E}_{\mathbf{q}}} \right) \frac{1}{\exp(\hbar \omega_{\mathbf{q}} \beta) - 1}.$$

- Effekt bei T=0

- T<sup>2</sup> Abhängigkeit  
vgl. T<sup>1.5</sup> bei FM

For small  $q$  and  $h_A = 0$  (see eqn (9.17))

$$\mathcal{E}_{\mathbf{q}} = q(\rho^2/3)^{\frac{1}{2}} = Dq/2rJS,$$

which defines the parameter  $D$  for an antiferromagnet. Hence

$$\begin{aligned}\frac{1}{N} \sum_{\mathbf{q}} \frac{1}{(1-\gamma_{\mathbf{q}}^2)^{\frac{1}{2}}} \frac{1}{\exp(\hbar \omega_{\mathbf{q}} \beta) - 1} \\ \simeq \frac{1}{N} \frac{V}{(2\pi)^3} \int_0^{\infty} dq \, 4\pi q^2 \frac{\sqrt{3}}{\rho q} \frac{1}{\exp(\beta D q) - 1} = v_0 \frac{\sqrt{3}}{2\rho} \left( \frac{k_B T}{\pi D} \right)^2 \zeta(2),\end{aligned}$$

# Strukturfaktor :

$$\left(\frac{d^2\sigma}{d\Omega dE'}\right)^{(\pm)} = \left(\frac{\gamma e^2}{m_e c^2}\right)^2 \left\{\frac{1}{2}gF(\mathbf{x})\right\}^2 \frac{1}{4} \frac{k'}{k} (1 + \kappa_z^2) \exp\{-2W(\mathbf{x})\} \times \\ \times \frac{(2\pi)^3}{v_0} \sum_{a=0,1} \sum_{\mathbf{q}, \boldsymbol{\tau}} (n_{\mathbf{q},a} + \frac{1}{2} \pm \frac{1}{2}) \delta(\hbar\omega_{\mathbf{q},a} \mp \hbar\omega) \delta(\mathbf{x} \mp \mathbf{q} - \boldsymbol{\tau}) \times \\ \times \{u_{\mathbf{q}}^2 + v_{\mathbf{q}}^2 + 2u_{\mathbf{q}}v_{\mathbf{q}} \cos \boldsymbol{\rho} \cdot \boldsymbol{\tau}\}.$$

$$\left(\frac{1}{2SN}\right)u_{\mathbf{q}}^2 = (1 + h_A + \mathcal{E}_{\mathbf{q}})/2\mathcal{E}_{\mathbf{q}}, \\ \left(\frac{1}{2SN}\right)v_{\mathbf{q}}^2 = (1 + h_A - \mathcal{E}_{\mathbf{q}})/2\mathcal{E}_{\mathbf{q}}, \\ \left(\frac{1}{2SN}\right)u_{\mathbf{q}}v_{\mathbf{q}} = -\gamma_{\mathbf{q}}/2\mathcal{E}_{\mathbf{q}}.$$

If  $2\boldsymbol{\rho} = \mathbf{m}$ , where  $\mathbf{m}$  is some lattice vector of a sublattice, it follows by definition of the reciprocal lattice vectors  $\boldsymbol{\tau}$  that

$$\boldsymbol{\rho} \cdot \boldsymbol{\tau} = \frac{1}{2}\mathbf{m} \cdot \boldsymbol{\tau} = \pi \times \text{integer}. \quad (9.263)$$

Thus  $\cos \boldsymbol{\tau} \cdot \boldsymbol{\rho} = \pm 1$  (9.264)

according to whether the integer is even (+) or odd (-).

For instance, consider a b.c.c. lattice. In this case the sublattices are simple cubic lattices,  $\boldsymbol{\rho} = \frac{1}{2}a(1, 1, 1)$  and the reciprocal lattice vectors  $\boldsymbol{\tau}$  are given by

$$\boldsymbol{\tau} = \frac{2\pi}{a}(\tau_1, \tau_2, \tau_3),$$

where  $\tau_1, \tau_2, \tau_3$  are arbitrary integers. The reciprocal lattice vectors for a b.c.c. structure, however, are given by

$$\boldsymbol{\tau}_n = \frac{2\pi}{a}(\tau_1, \tau_2, \tau_3),$$

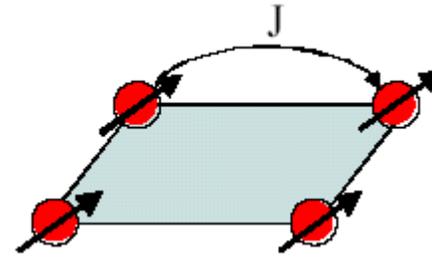
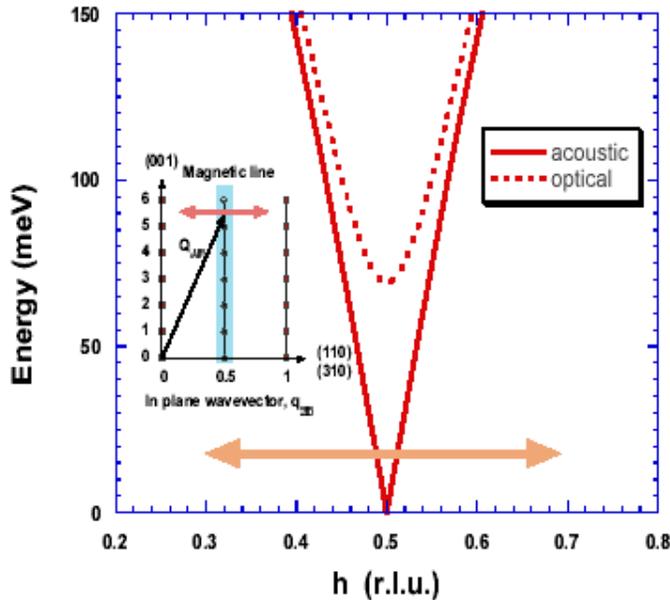
- Struktur-Faktor abhängig vom Streuvektor
- Messung an AF Bragg-Pkt.en
- 1/E Term !

# Vergleich AFM und FM :

FM :  $\hbar\omega_q = Dq^2$  mit  $D = 2JSa^2$  für kleine  $q$   
 $S(Q, \omega) = S * \text{Bose (+1 bei Erzeugung)} * \delta \text{ Funktionen (E,q)}$

AFM :  $\hbar\omega_q = \hbar cq$  mit  $c = rJSa/\hbar$  für kleine  $q$   
 $S(Q, \omega) = S * \frac{1}{E} * \text{Bose (+1 bei Erzeugung)} * \delta \text{ Funktionen (E,q)}$   
\* **Strukturfaktor !**  
 $\hbar\omega_0 = 2 * r * J * S$  maximale Energie

# Kuprate : Anregung im AF - Zustand



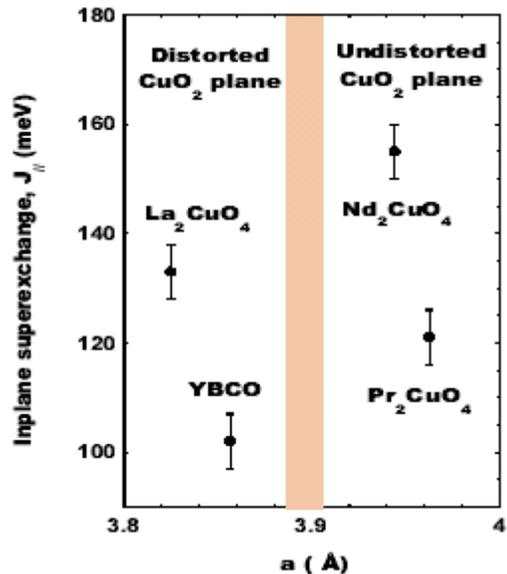
➤ Wichtiger Parameter :  
Cu–O–Cu Superaustausch-WW  $J$

➤ Spinwellen-Anregung:

startet linear gemäß  $\omega_q = cq$

aus  $c$  folgt  $J$ :  $c = \sqrt{2} \cdot 2 \cdot S \cdot Z_c \cdot a \cdot J$

YBCO<sub>6.1</sub> :  $J = 130$  meV



*Bourges et al., 1997*

High-Energy Spin Waves in  $\text{La}_2\text{CuO}_4$

S. M. Hayden,<sup>(1)</sup> G. Aeppli,<sup>(2)</sup> R. Osborn,<sup>(3)</sup> A. D. Taylor,<sup>(5)</sup> T. G. Perring,<sup>(4)</sup> S.-W. Cheong,<sup>(2)</sup> and Z. Fisk<sup>(5)</sup>

<sup>(1)</sup>H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom

<sup>(2)</sup>AT&T Bell Laboratories, Murray Hill, New Jersey 07974

<sup>(3)</sup>Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, United Kingdom

<sup>(4)</sup>Claarendon Laboratory, University of Oxford, Parks Road, Oxford, United Kingdom

<sup>(5)</sup>Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 30 July 1991)

Time-of-flight spectroscopy using neutrons produced by a spallation source is used to measure the one-magnon scattering throughout the Brillouin zone for  $\text{La}_2\text{CuO}_4$ . The zone-boundary magnons have an energy  $\hbar\omega_m = 0.312 \pm 0.005$  eV and are good eigenstates of the quantum Heisenberg Hamiltonian in that they possess lifetimes  $> 10/\omega$ . A multiplicative renormalization of the overall frequency scale of classical spin-wave theory accounts for the quantum effects in the one-magnon spectrum.

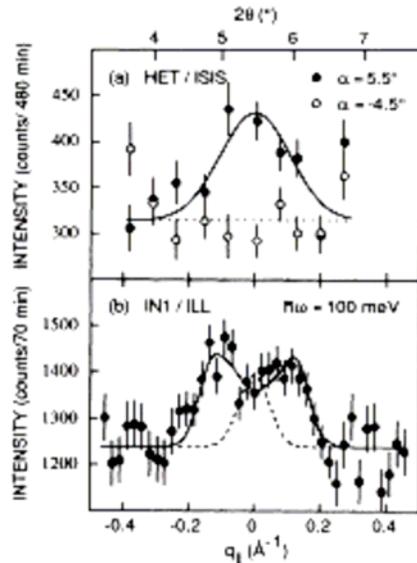


FIG. 2. (a) Measurements (spallation source) of the 2D magnetic scattering in  $\text{La}_2\text{CuO}_4$  for  $E_i = 307$  meV and  $\hbar\omega = 100$  meV. The energy resolution is 50 meV (FWHM) and the sample mass is 100 g. Solid points ( $\alpha = 5.5^\circ$ ) correspond to the condition that gives rise to a peak in the magnetic scattering for  $2\theta = 5.5^\circ$ . Open circles are with the crystal rotated ( $\alpha = -4.5^\circ$ ). (b) A transverse scan (reactor source) collected using the triple-axis spectrometer IN1 [11]; the dashed line shows the instrumental resolution. The energy resolution was 20 meV (FWHM) and the sample mass is 15 g.

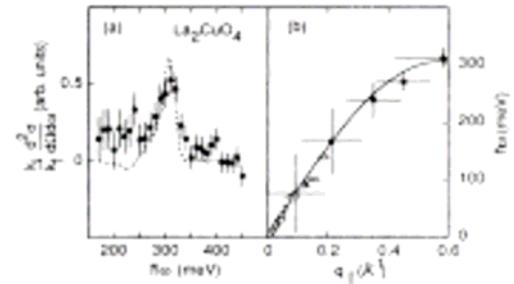


FIG. 3. (a) The difference between a combination of four detectors chosen to emphasize scattering near the magnetic zone boundary,  $Q = (1, k, 0.5)$ , and a background combination with the same  $2\theta$ . The dashed line is a resolution-corrected nearest-neighbor spin-wave model described in the text. (b) The dispersion relation deduced from the spectra in (a) and Fig. 4 (closed circles) and previous measurements [11,12] (open circles). Horizontal bars represent the range in wave vector parallel to  $(1,0,0)$  over which the detectors integrate. Energies are the fitted values at the centers of the detectors.

Conventional spin-wave theory of the Holstein-Primakoff type [17] for a 2D Heisenberg square lattice antiferromagnet with a Hamiltonian

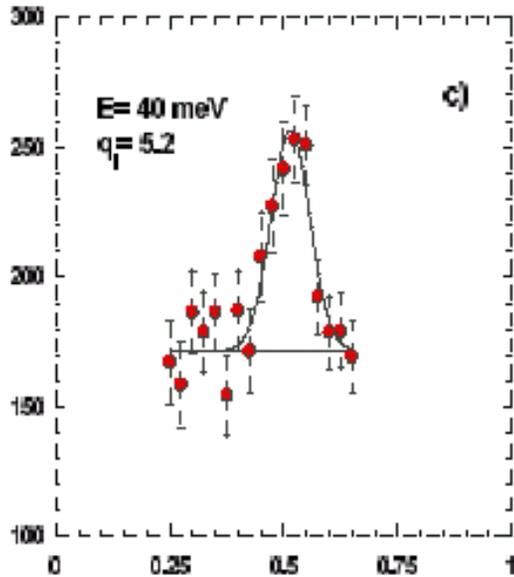
$$H = \sum_{ij} J S_i \cdot S_j, \tag{1}$$

where the sum is over nearest-neighbor spins ( $S = \frac{1}{2}$ ), yields a cross section (for magnon creation)

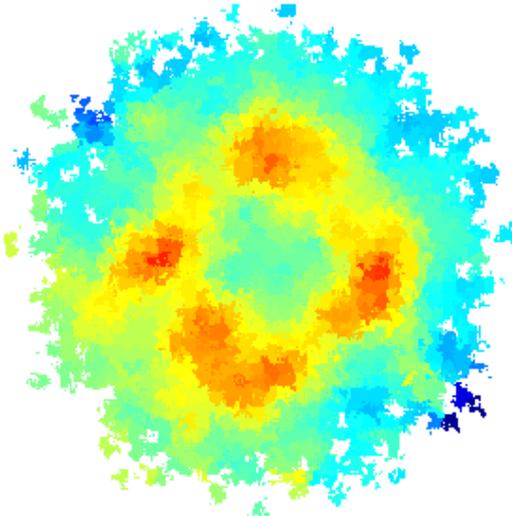
$$\hbar\omega_q = 2J[1 - \cos^2(h\pi) \cos^2(l\pi)]^{0.5}$$

Achtung : Unterschied ob Bindungen oder Plätze summiert werden (hier Bindungen)

# Kommensurabilität und Inkommensurabilität



*Bourges et al., 1999*



➤ **Kommensurabilität:**  
magn. Streuung beim AF-Impuls  $(\frac{1}{2}, \frac{1}{2})$

➤ **Inkommensurabilität:**  
Versetzung der Peaks (magn. Korrelation) um  $\delta$  in  $(100) + (010)$  Richtung von  $(\frac{1}{2}, \frac{1}{2})$  weg

**Magn. Anregungen** bei

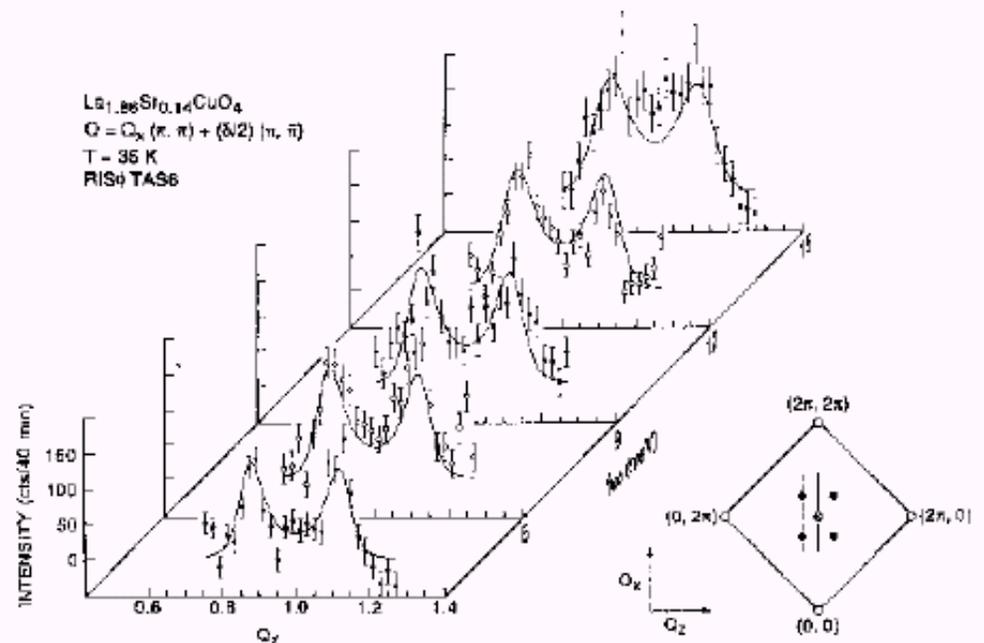
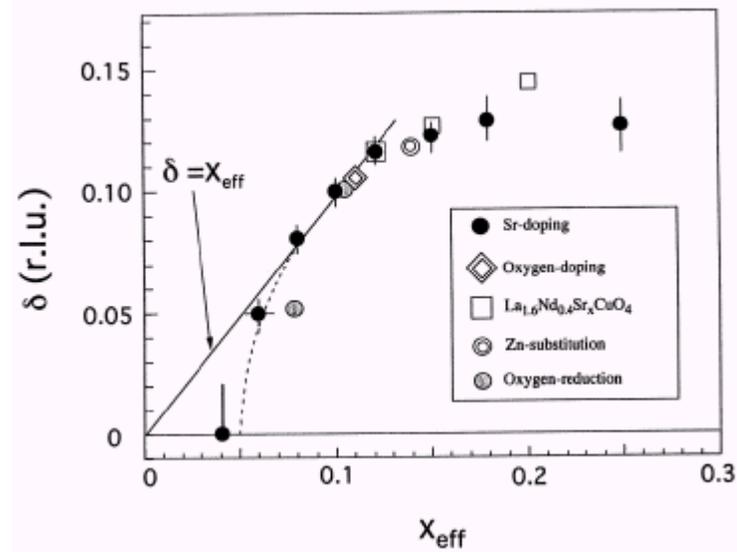
$$\mathbf{Q}_{\text{mag}} = (\pi/a \cdot (1 \pm \delta); \pi/a) \text{ und } (\pi/a; \pi/a \cdot (1 \pm \delta))$$

*Mook, Dai et al.*

# Kommensurabilität und Inkommensurabilität in YBCO und LSCO

## LSCO

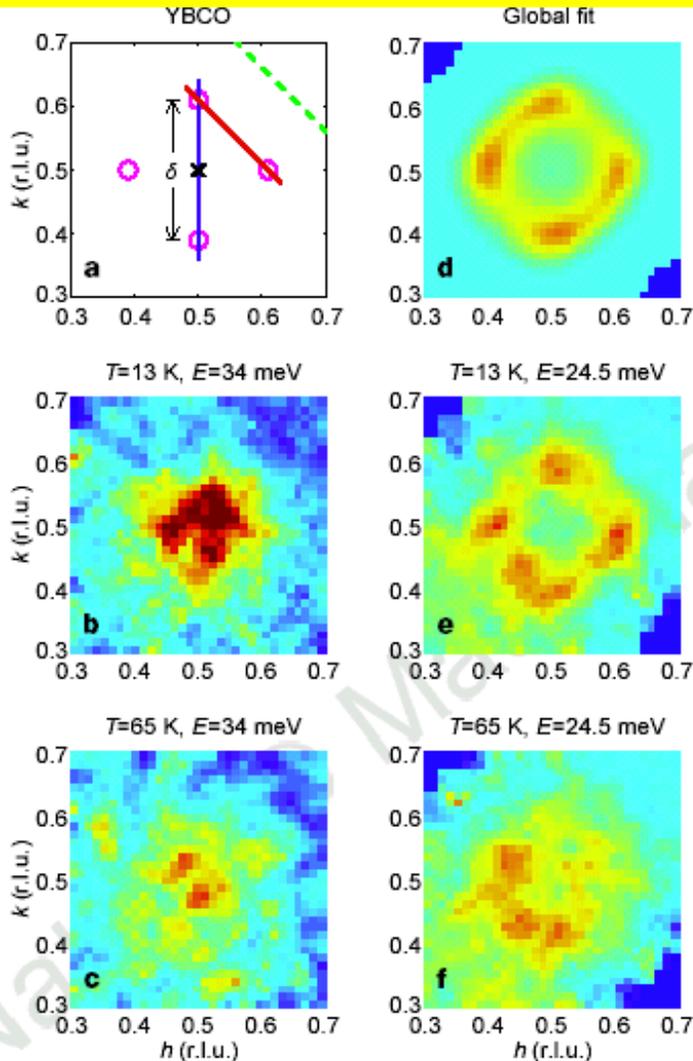
- Erhöhung der Energie führt zum Verschwinden der Inkommensurabilität
- Steigt linear mit der Dotierung an Sättigung bei  $x \geq 0,12$



*Yamada et al.,  
1998*

*Mason et al., 1992*

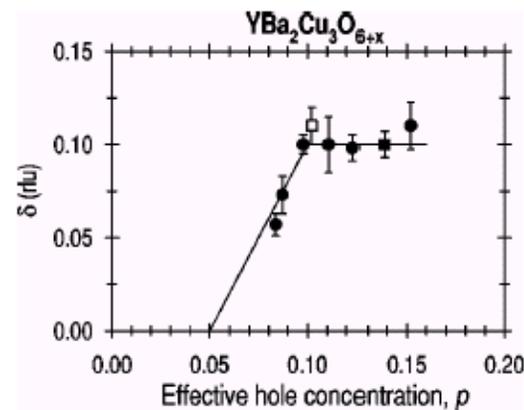
# Kommensurabilität und Inkommensurabilität in YBCO und LSCO



Mook et al. 1998

## YBCO

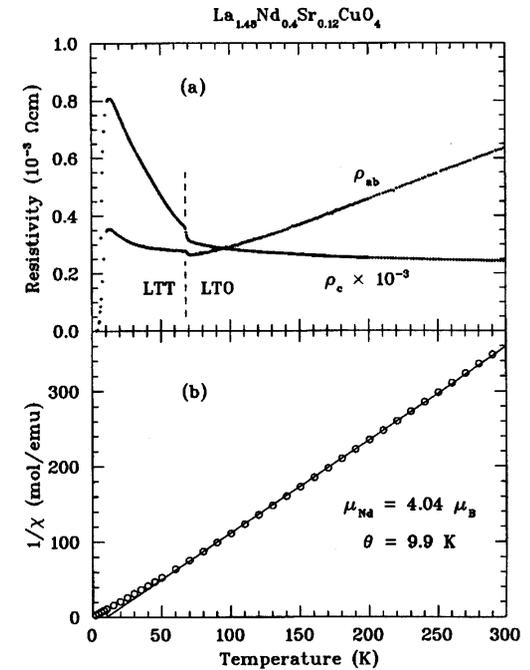
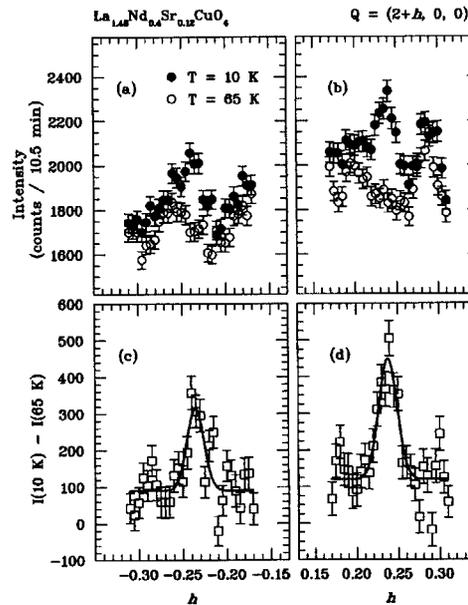
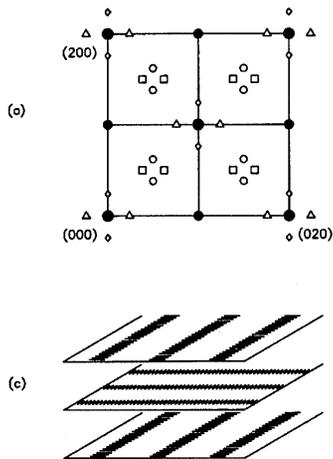
- Erst fand man um  $(\pi/a; \pi/a)$  zentrierte magn. Fluktuationen
- IK Peaks bei  $E \approx 25$  meV in  $\text{YBCO}_{6.6}$   
→ LSCO ähnliche IK bei Energien  $< 35-40$  meV
- Abnahme der IK mit steigender Temperatur und Energie
- Erhöhung der IK mit steigender Dotierung  
Sättigung bei  $\delta = 0,1$  für  $x \geq 0,6$



Arai et al., 1999  
Bourges et al., 2000

# Streifen-Phasen

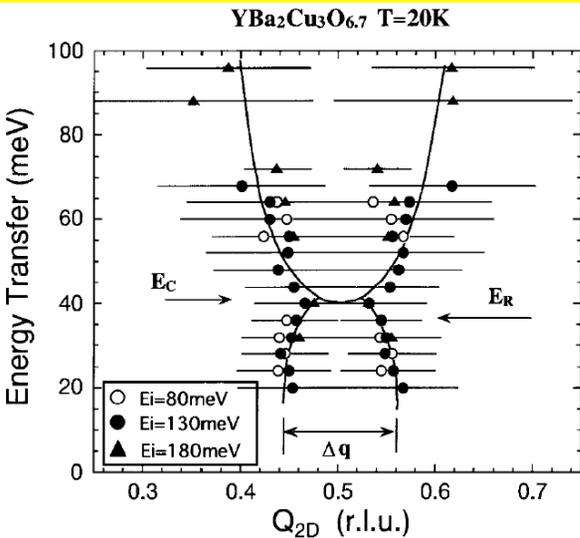
## Streifenordnung in $\text{La}_{1.48}\text{Nd}_{0.4}\text{Sr}_{0.12}\text{CuO}_4$ J. Tranquada et al., nature (1995).



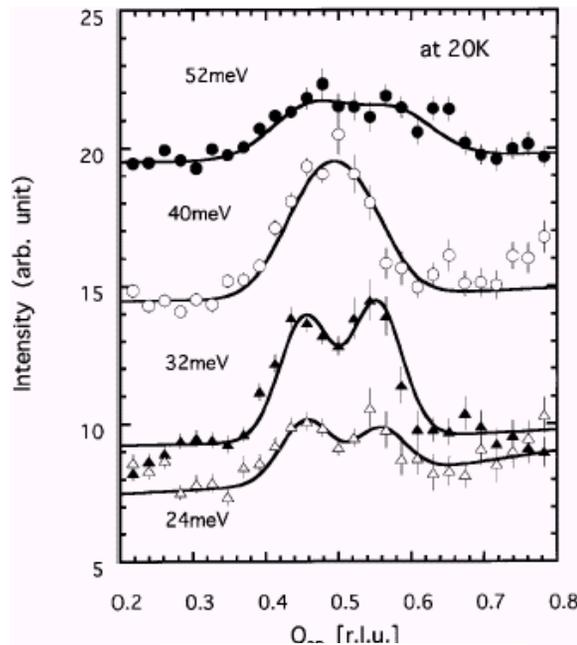
Widerstand :  
Halbleitende Charakteristik

Streifenordnung :  
Ladungen ordnen sich in Streifen  
→ AF-Ordnung dazwischen wiederhergestellt

# Kommensurabilität und Inkommensurabilität in YBCO und LSCO



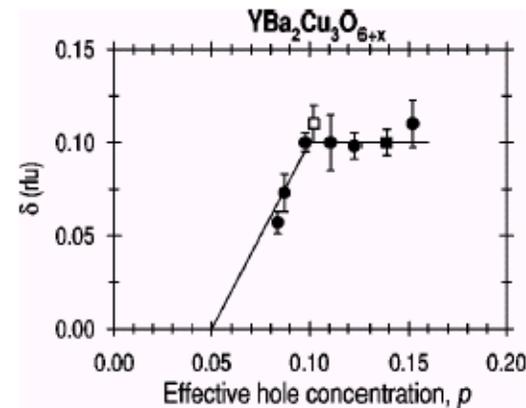
*Arai et al., 1999*



*Arai et al., 1998*

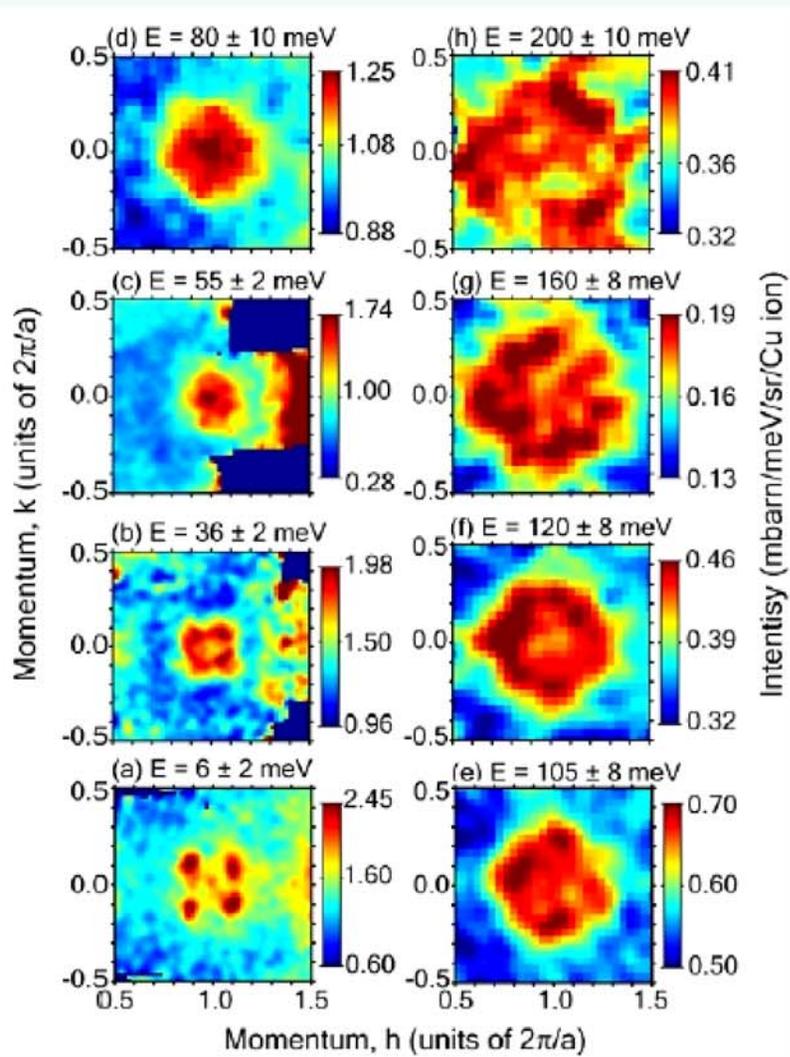
## YBCO

- Erst fand man um  $(\pi/a; \pi/a)$  zentrierte magn. Fluktuationen
- IK Peaks bei  $E \approx 25$  meV in  $\text{YBCO}_{6.6}$   
→ LSCO ähnliche IK bei Energien  $< 35-40$  meV
- Abnahme der IK mit steigender Temperatur und Energie
- Erhöhung der IK mit steigender Dotierung  
Sättigung bei  $\delta = 0,1$  für  $x \geq 0,6$

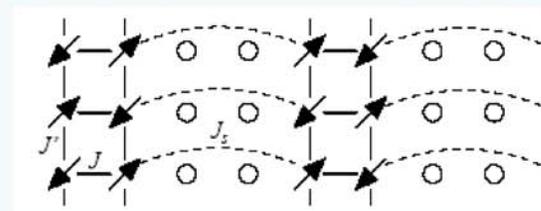
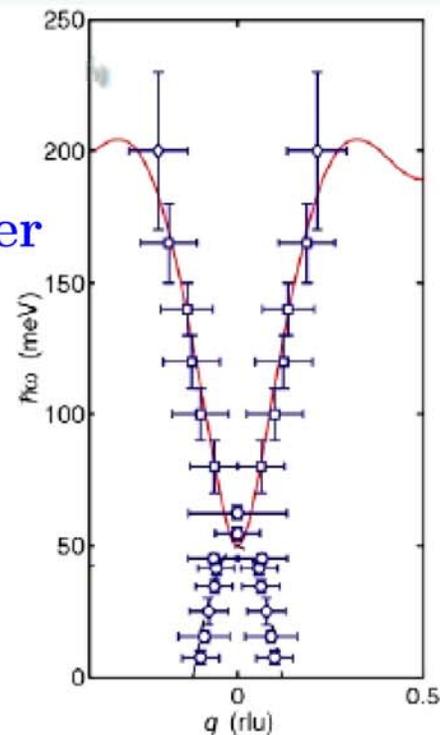


*Arai et al., 1999*  
*Bourges et al., 2000*

## Non-superconducting



Two-leg  
spin ladder



Bond-centered stripes

Vojta et al, Uhrig et al, Seibold et al

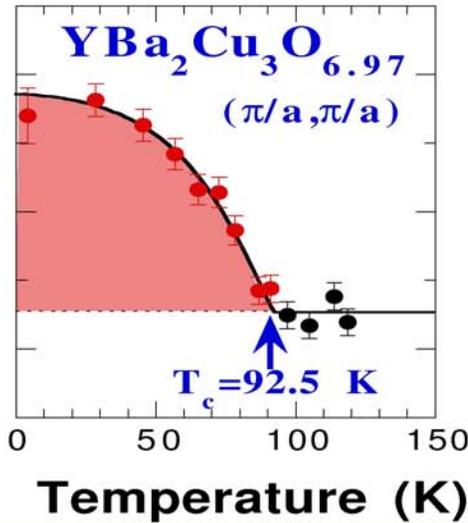
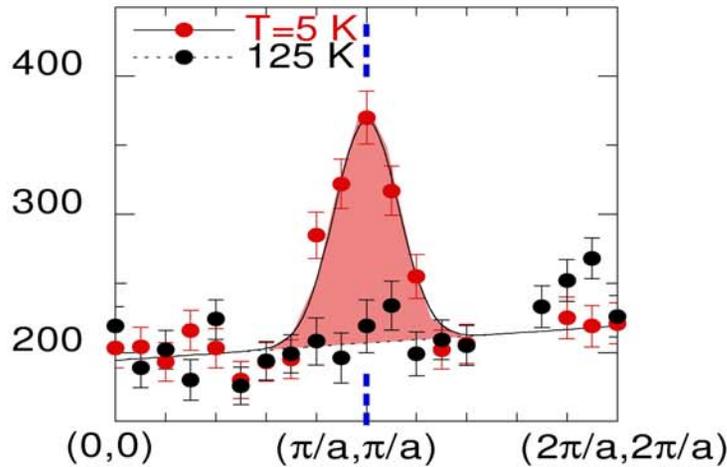
PRL 2004-2005



# Resonance peak (optimally doped): Q- and T dependences

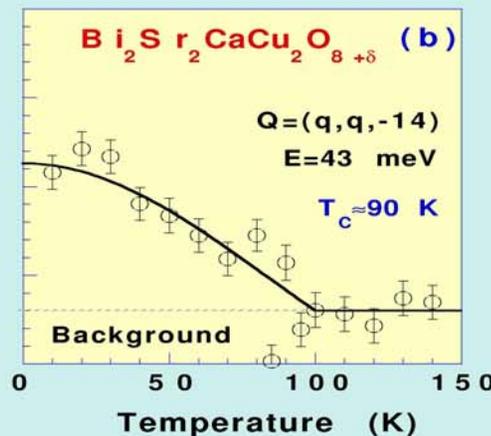
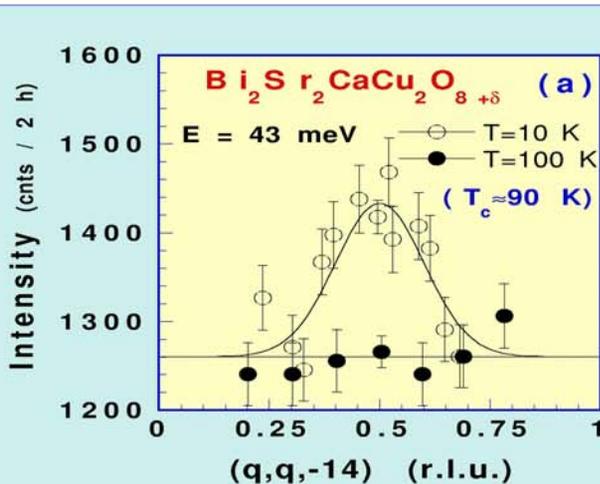
Discovered by J. Rossat-Mignod et al, *Physica C*, **185-189**, 86 (1991). 41 meV peak

Neutron Intensity (a. u.)



$$Q_{AF} = (1/2, 1/2) \equiv (\pi/a, \pi/a)$$

PRB, **53** 876 (1996)



Nature, **398** 588 (1999)

# RPA-approximation : itinerant magnetism

Pauli -paramagnetism  $\sim$  DOS(E-Fermi)  
Stoner interaction yields an enhancement of the  
susceptibility :  $\chi_{\text{mag}} = I N_{\text{up}} N_{\text{down}}$

Mazin and Singh : 1997, 1998, 1999

$$I = I_{\text{Ru}} v_{\text{Ru}}^2 + 2 I_{\text{O}} v_{\text{O}}^2$$

$v_{\text{Ru,O}}$  : contribution of Ru-d and O-p orbitals to the DOS

O can not contribute for antiferromagnetic fluctuations !

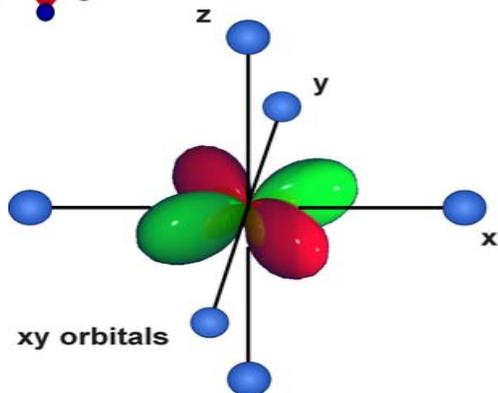
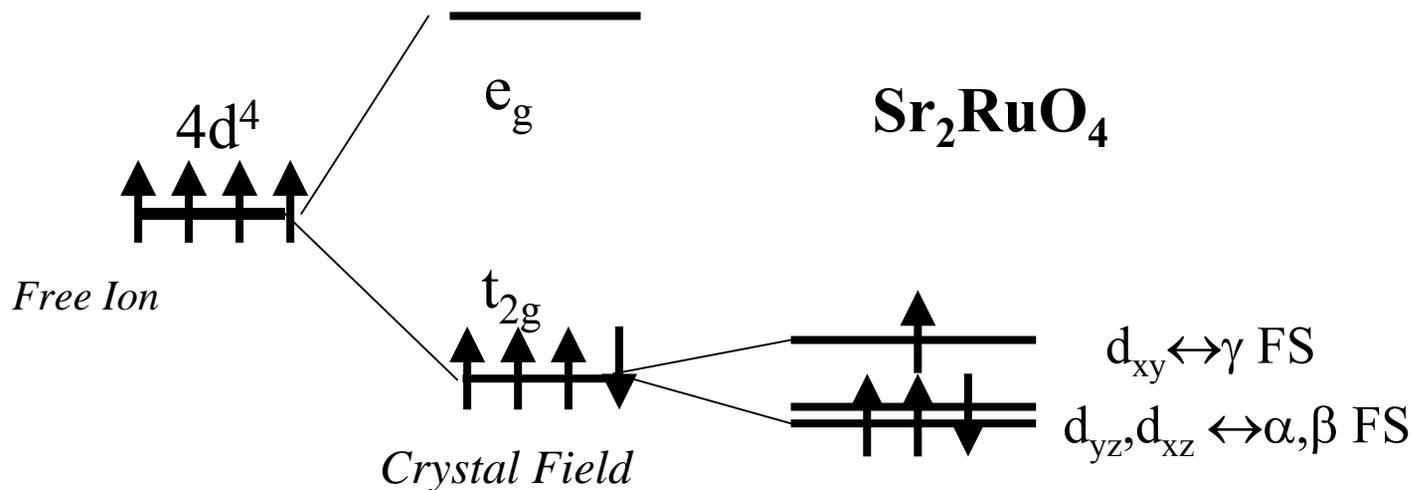
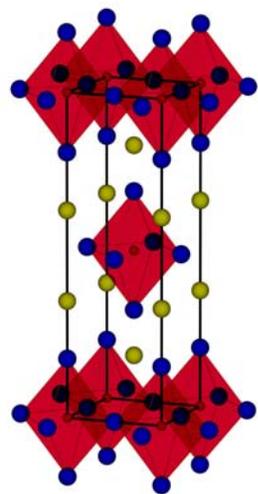
$$I(q) = 0.43 \text{eV} [1 + (0.08q^2)]^{-1}$$

$$\chi(q) = \frac{\chi_0(q)}{1 - I(q)\chi_0(q)}$$
$$\alpha = I(q)\chi_0(q)$$

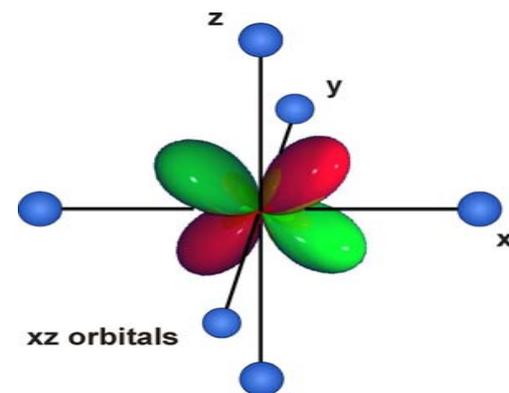
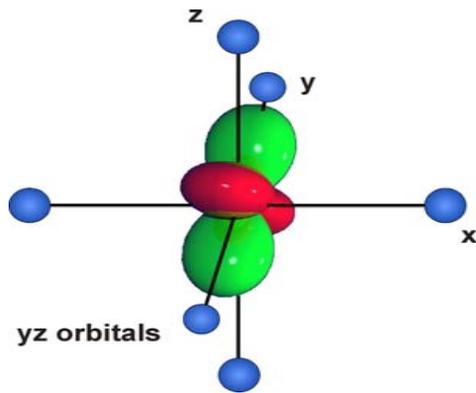
$\alpha > 1$  :  
divergency and magnetic order

# Electronic band structure

Ru<sup>4+</sup>: 4d<sup>4</sup>



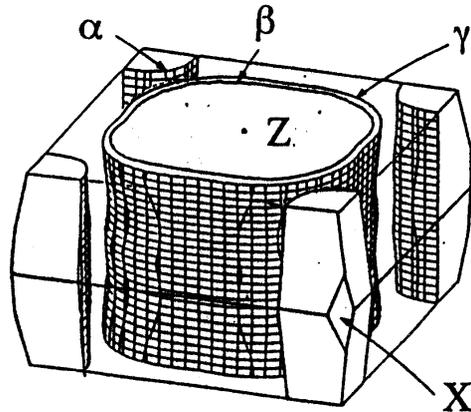
γ FS (2 dim.)



α and β FS (1 dim.)

# Fermi-surface

dHvA A. Mackenzie et al. PRL (1996)

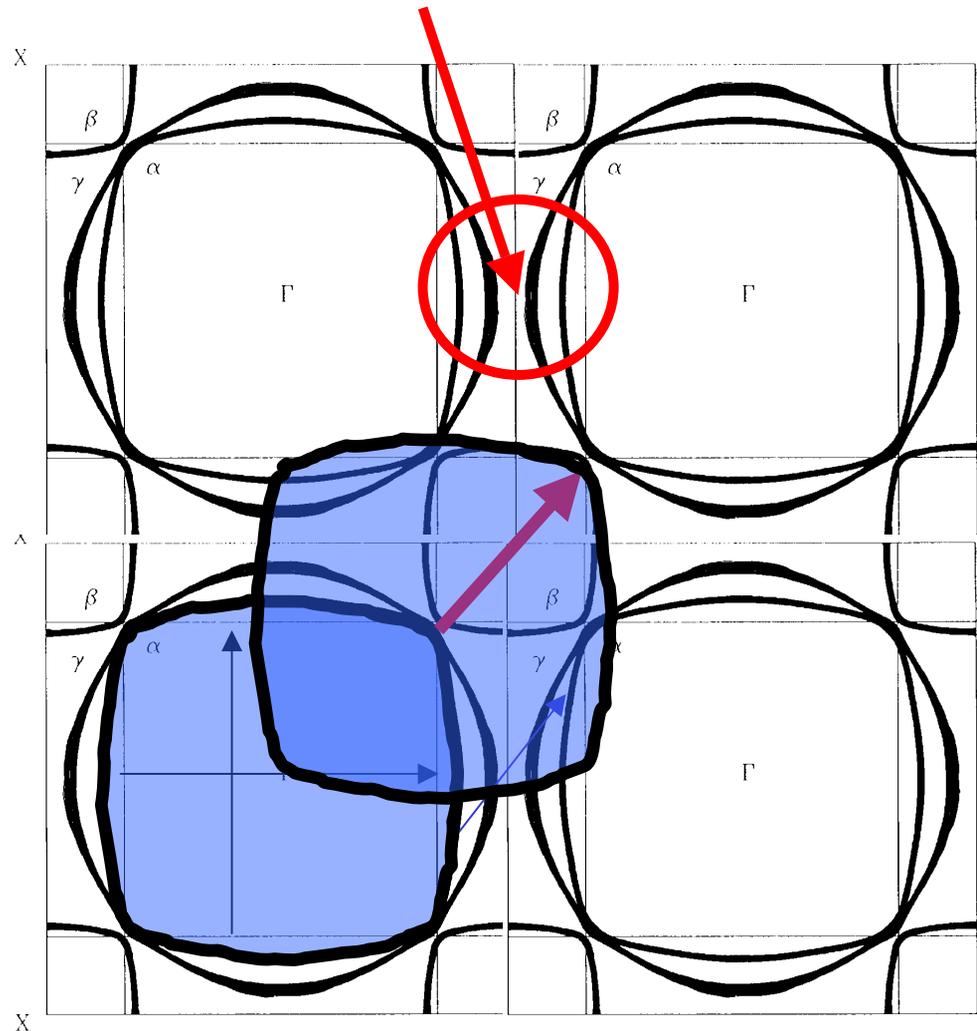


van Hove singularity

FS	e/h	character	DOS
$\alpha$	h	$d_{xz}, d_{yz}$	13%
$\beta$	e	$d_{xz}, d_{yz}$	30%
$\gamma$	e	$d_{xy}$	57%

$$\chi_0(q) = \sum_{k_{ij}} \frac{M_{k_i;(k+q)_j} [f(\epsilon_{k_i}) - f(\epsilon_{(k+q)_j})]}{\epsilon_{(k+q)_j} - \epsilon_{k_i}}$$

**M = 1 intraband = 0 interband**



# Fermi-surface nesting

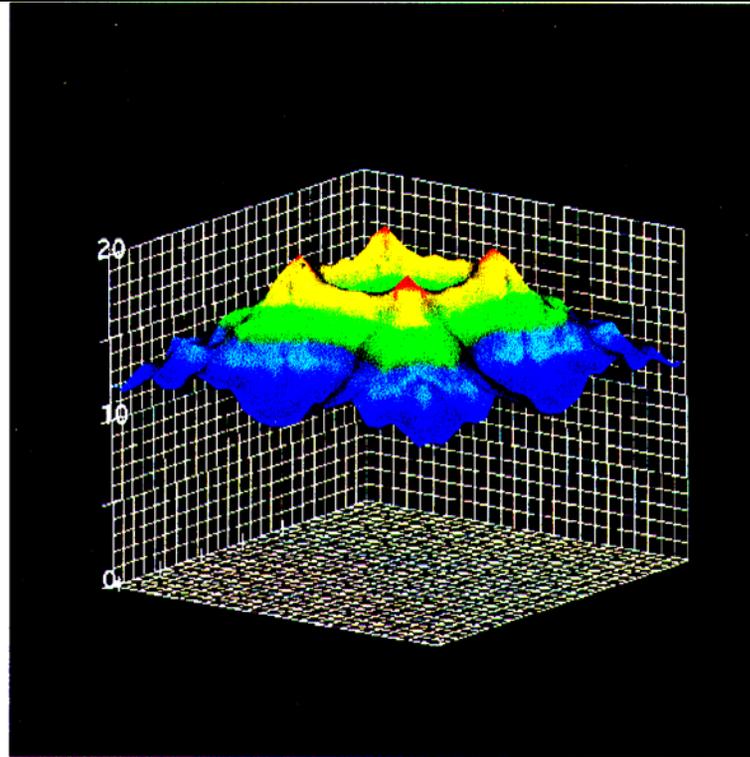


FIG. 1. Calculated bare susceptibility for  $\text{Sr}_2\text{RuO}_4$

Mazin and Singh ,  
PRL (1999)

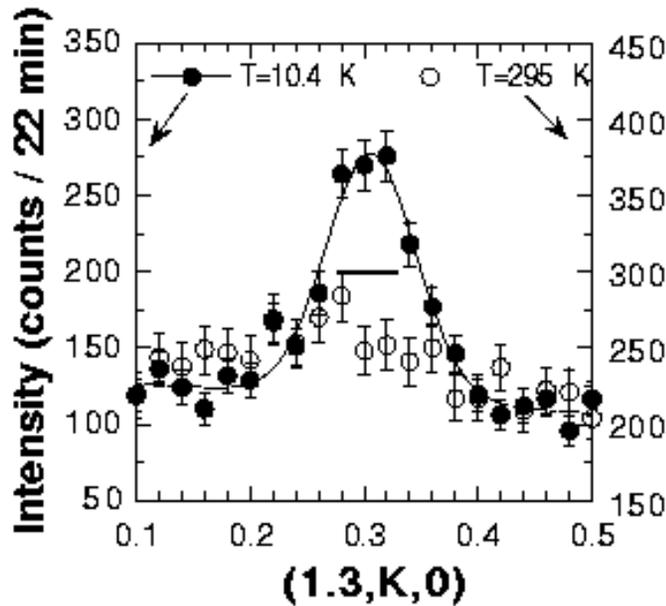
$$\chi_0(q) = \sum_{k_{ij}} \frac{M_{k_i;(k+q)_j} [f(\varepsilon_{k_i}) - f(\varepsilon_{(k+q)_j})]}{\varepsilon_{(k+q)_j} - \varepsilon_{k_i}}$$

**M = 1 intraband = 0 interband**

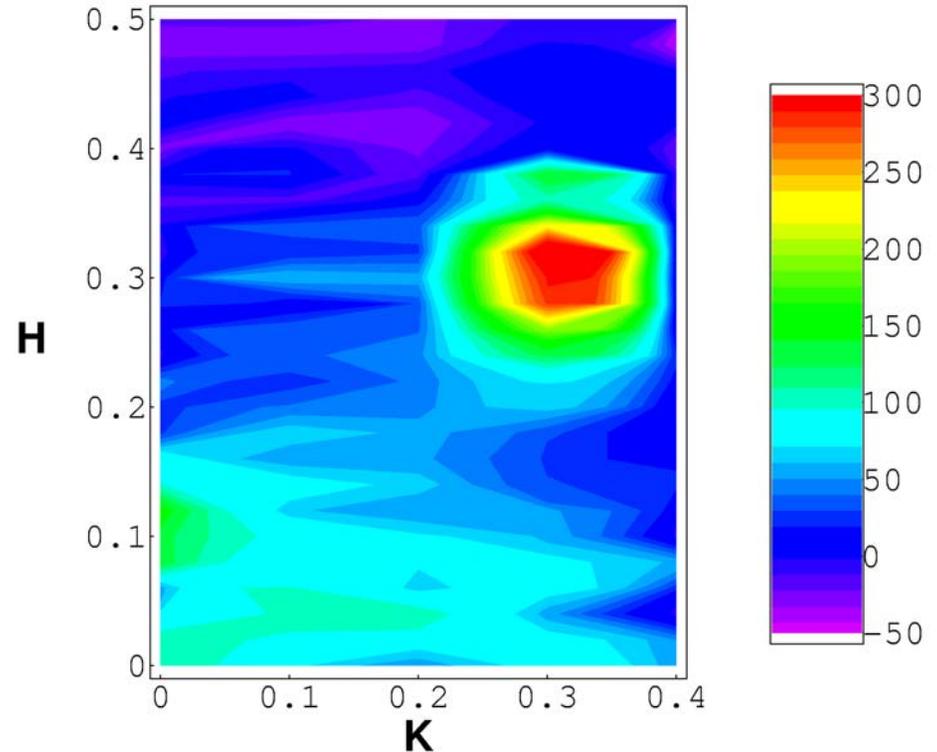
-  $d_{xz}$  and  $d_{yz}$  Fermi surface-sheets are flat  
 $\implies$  large susceptibility at  $(0.3 q_y)$  and  $(q_x 0.3)$   
**AND Peak at (0.3 0.3)**

# Inelastic neutron scattering

$$\frac{d^2\sigma}{d\Omega d\omega} = r_0^2 \cdot \frac{2F^2(Q)}{\pi(g\mu_B)^2} \cdot \frac{\chi''(Q, \omega)}{1 - \exp(-\frac{\hbar\omega}{kt})}$$



Sidis et al., PRL 1999



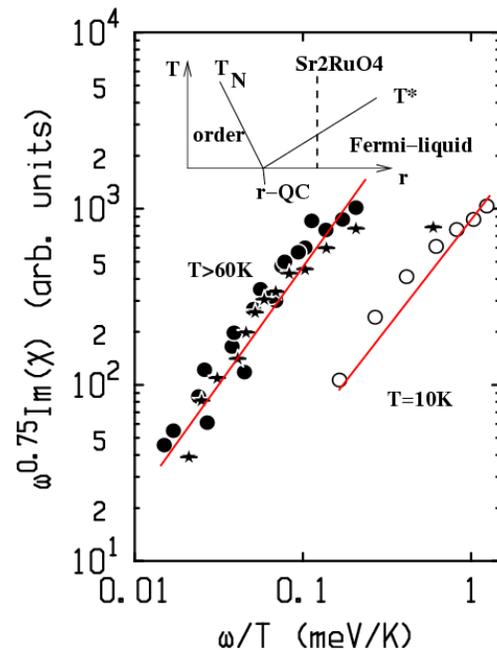
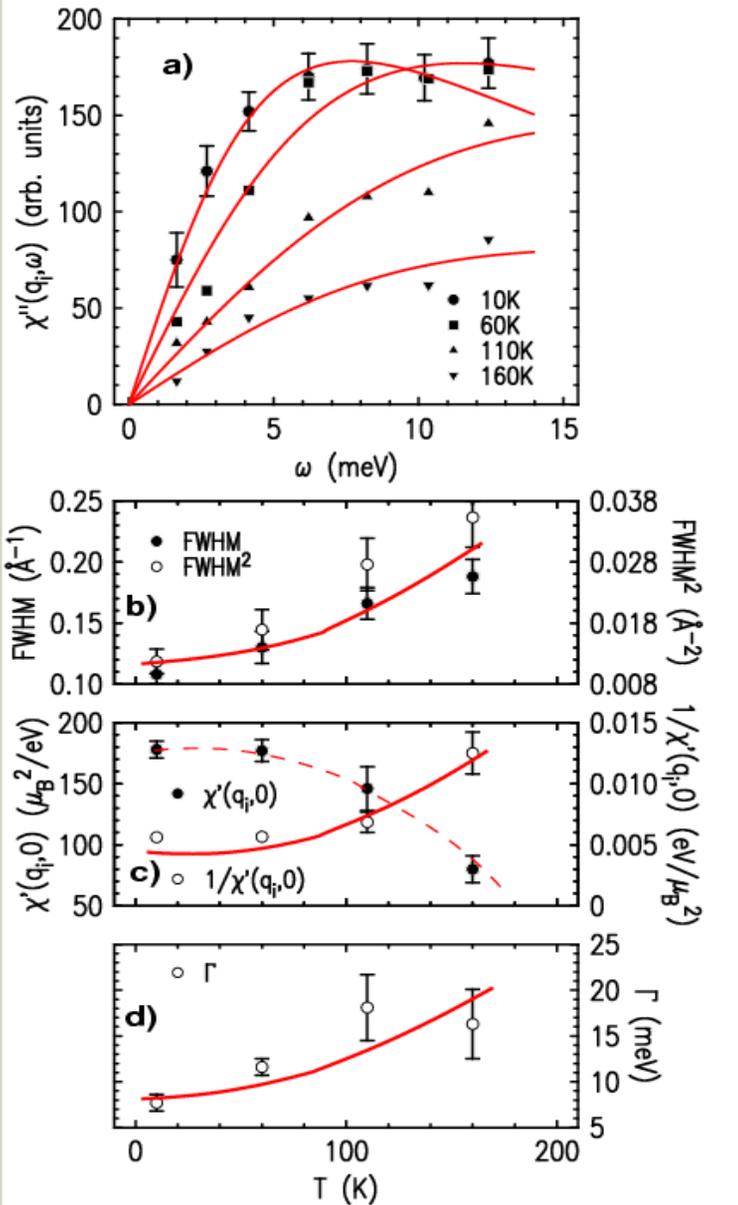
Braden et al., PRB66, 064522 2002; PRL92, 097402, 2004.

- Scans at constant energy,  $E=6.2\text{meV}$ , along  $Q=(1.3 \text{ y } 0)$  show a clear peak
- incommensurate fluctuations due to nesting in one-dimensional bands

# Energy-Temperature-dependency

$$\chi''(q_i, \omega) = \chi'(q_i, 0) \cdot \frac{\Gamma \cdot \omega}{\Gamma^2 + \omega^2}$$

$-\chi'(q_0, 0)$  and  $\Gamma$  and FWHM vary as function of T  
 - all indicate a close instability !



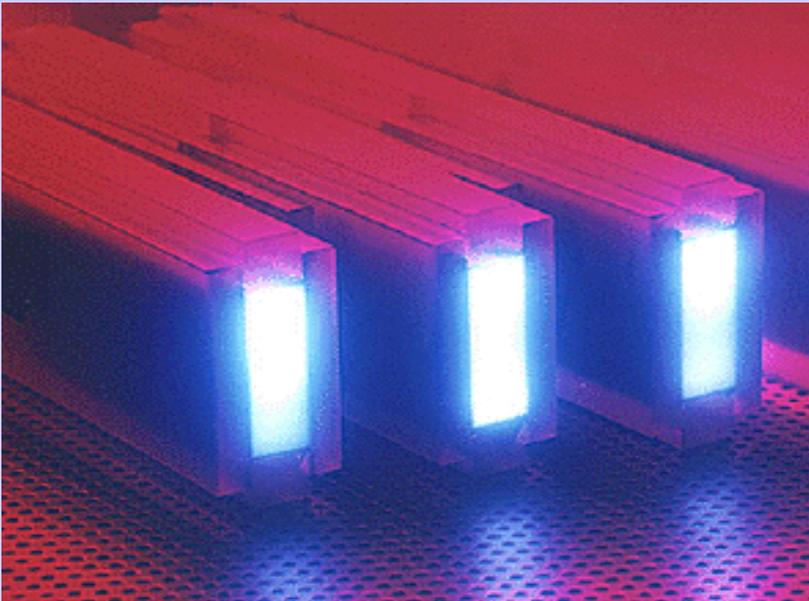
# V.4 Polarisierte Neutronenstreuung

## **-Erzeugung**

- a) magnetische Monochromatoren**
- b) Bender – Supermirror-Guides**
- c) He<sup>3</sup>-Spin-Filter**

# Neutron polarization

## Polarising mirrors and multilayers

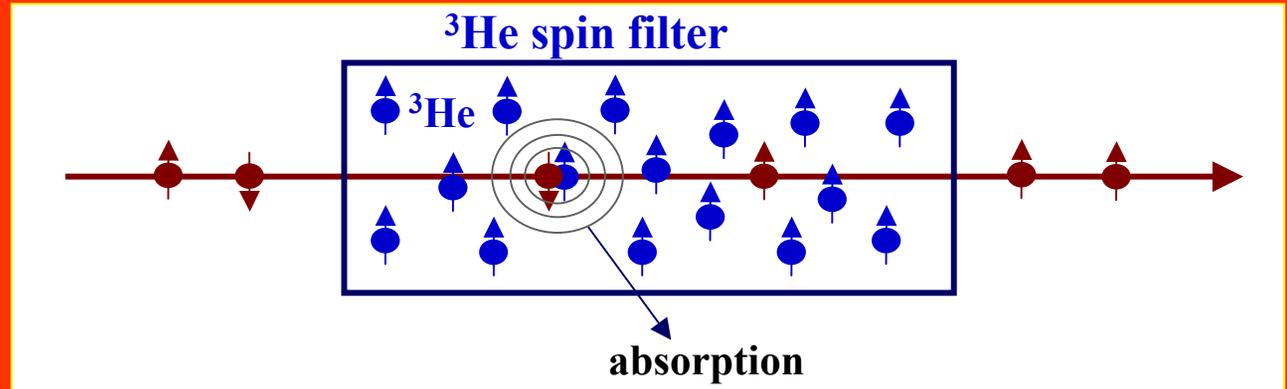


Like Bragg reflection, neutron refraction depends on the spin state.

Curved guides that allow the total reflection of only one spin state.

# Neutron polarization

$^3\text{He}$  spin filter



Neutrons with spin antiparallel to the one of  $^3\text{He}$  atoms are absorbed



# Polarisierte magnet. Neutronenstreuung

ein- und ausfallende Neutronen mit Spin-Zustand

$$\langle\langle \sigma | \vec{\sigma} \cdot \mathbf{S}_{\perp l}(0) | \sigma' \rangle \langle \sigma' | \vec{\sigma} \cdot \mathbf{S}_{\perp l'}(t) | \sigma \rangle \rangle =$$

$$\left\{ \begin{array}{l} + \rightarrow + \quad \langle S_{\perp l}^z(0) S_{\perp l}^z(t) \rangle \\ - \rightarrow - \quad \langle S_{\perp l}^z(0) S_{\perp l}^z(t) \rangle \\ + \rightarrow - \quad \langle S_{\perp l}^-(0) S_{\perp l}^+(t) \rangle \\ - \rightarrow + \quad \langle S_{\perp l}^+(0) S_{\perp l}^-(t) \rangle \end{array} \right.$$

Non spin flip:

$$\mathbf{S} \parallel \mathbf{H} \quad \mathbf{S} \perp \vec{k}$$

Spin flip:

$$\mathbf{S} \perp \mathbf{H} \quad \mathbf{S} \perp \vec{k}$$

# Erinnerung : Quantenmechanik : Pauli-Spinoperatoren

Für  $S=0.5$  nur 2  $S_z$ -Eigenfunktionen

$$|^{1/2},^{1/2}\rangle =:u$$

$$|^{1/2},^{-1/2}\rangle =:v$$

$$\langle u|u\rangle = \langle v|v\rangle = 1 \quad \text{und} \quad \langle u|v\rangle = \langle v|u\rangle = 0$$

$$S^+u=0 \quad S^+v=u \quad S^-u=v \quad S^-v=0$$

Pauli-Spinoperatoren :  $\sigma_x = 2S_x$  etc.  
werden nur für  $S = \frac{1}{2}$  benutzt

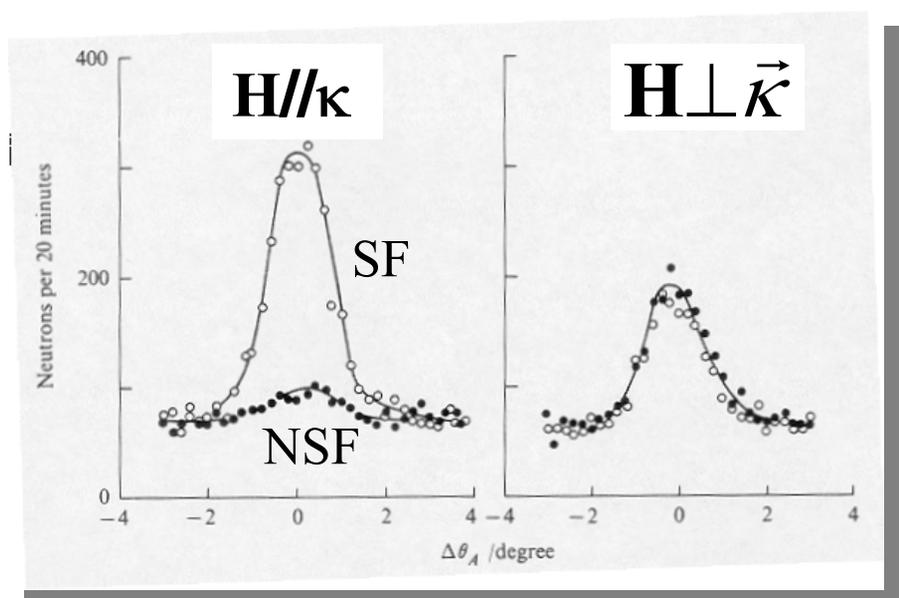
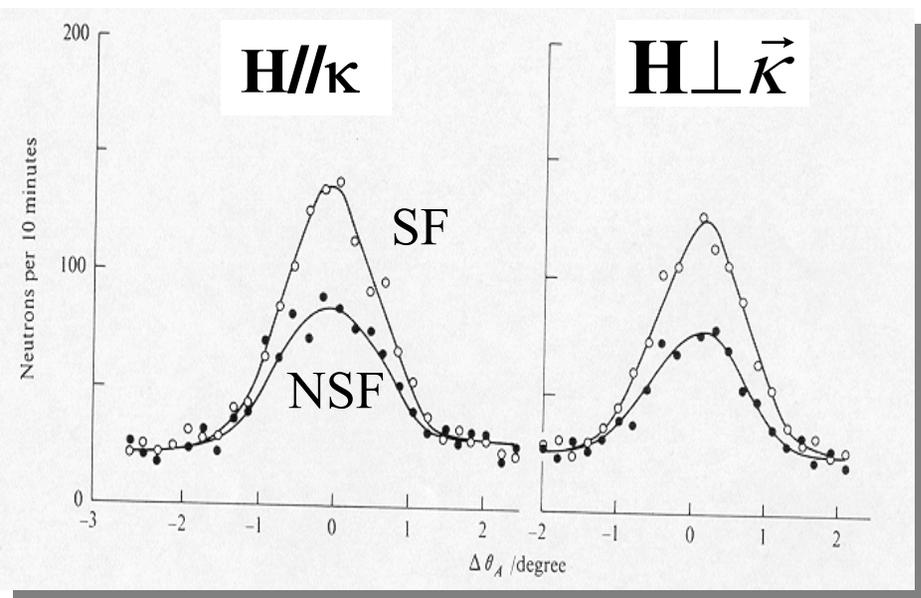
$$\sigma_x = S^+ + S^- \quad \sigma_y = -i(S^+ - S^-)$$

# Polarization : fixed through the guide fields

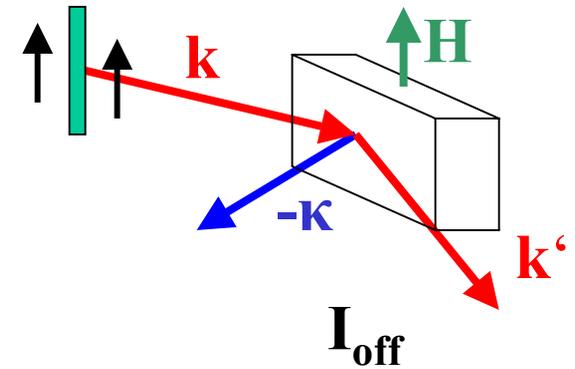
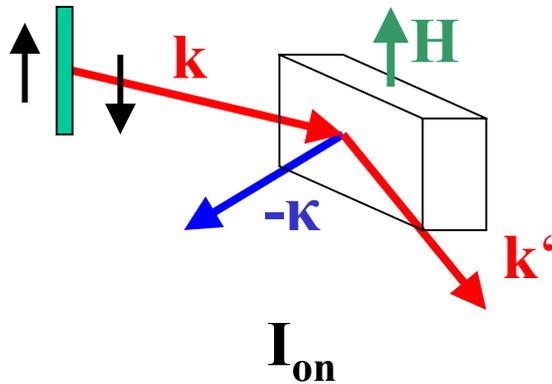
Type of scattering	H//κ		H perp κ	
	SF	NSF	SF	NSF
Nuclear coherent	0	1	0	1
Nuclear isotope incoherent	0	1	0	1
Nuclear spin incoherent	2/3	1/3	2/3	1/3
Magnetic	$S^{xx} + S^{yy}$	0	$S^{xx}$	$S^{yy}$

Nuclear isotope incoherent scattering

Paramagnetic scattering  $MnF_2$



# Polarisierte Elastische Neutronen–Streuung



$$I_{on} - I_{off} = 2(b^* m + bm^*)$$

-polarisierender Monochromator

ferromagnetische Substanz + Ausrichten der Domänen mit Feld

$$F_{ges} = F_N \pm F_{magn.}$$

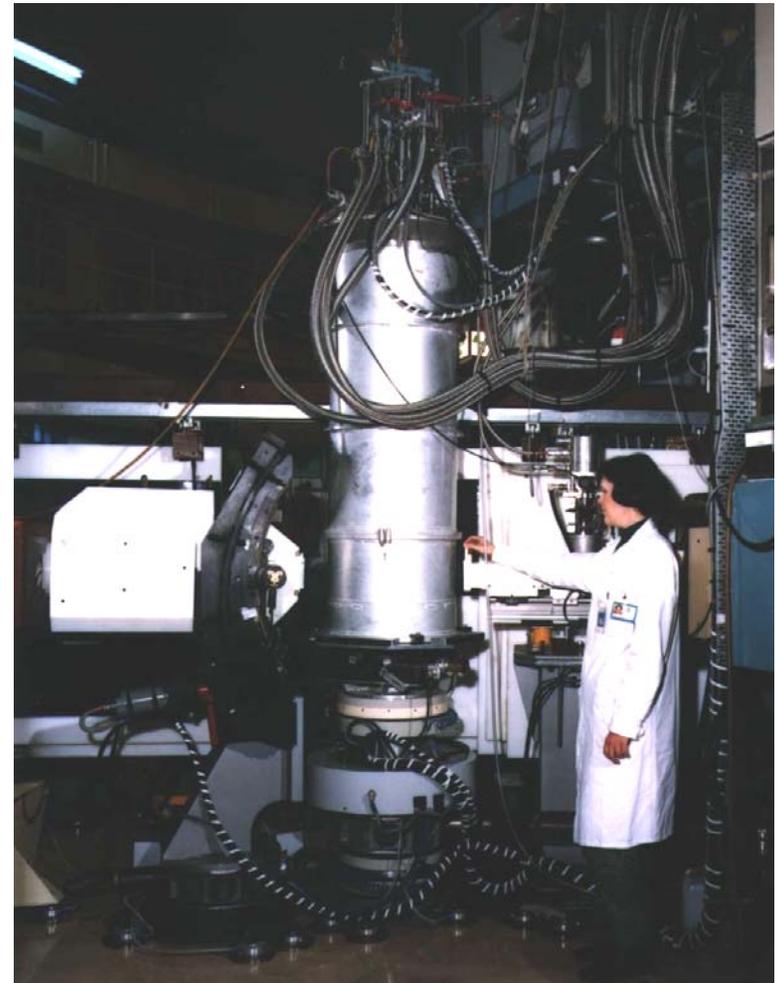
man benötigt ein Material mit  $|F_N| = |F_{magn.}|$

➔ Auslöschung einer Spin-Komponente

Beam tube .....	5 C1 Hot source
Monochromator .....	Heusler Cu <sub>2</sub> MnAl (111)
Collimation .....	Horizontal divergence before the monochromator 58', 28' or 14'
Type of instrument .....	two-axis; lifting arm detector polarized neutrons
Max. beam size at specimen .....	20 x 20 mm
Incident wavelength .....	$\lambda = 0.84 \text{ \AA}$
Angular ranges .....	Detector : 0, 120° in the horizontal plane -5, + 18° in the vertical plane
Minimum step size scan .....	0.01°
Detector .....	<sup>3</sup> He counter
Data collection and instrument control system .....	PC Data are transferred to a SUN computer for further treatment.

Auxiliary equipment

- \* Crystal from 1.5 K → 300 K.
- \* Cryomagnet H < 7.8 Tesla



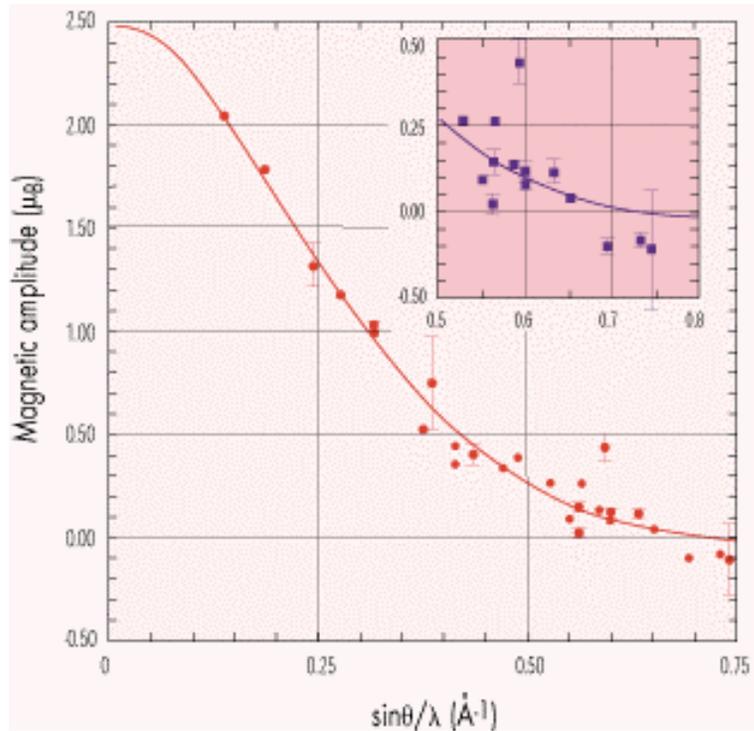


Figure 1: The experimental values of the magnetic form-factor measured at the  $h0$ . Bragg reflections of  $\text{Cr}_2\text{O}_3$ . The smooth curve is the spin-only free ion form-factor for  $\text{Cr}^{3+}$  normalised to  $2.5 \mu_B$ .

# Formfaktor- messungen

-Bestimmung der **Flippingratios**

Feld senkrecht

bestimme  $I_{\text{up}}$  and  $I_{\text{down}}$

$$I_{\text{up}} = (F_N + F_M)^2$$

$$I_{\text{down}} = (F_N - F_M)^2$$

$$I_{\text{up}}/I_{\text{down}} = (F_N + F_M)^2 / (F_N - F_M)^2$$

$$= (1 + \gamma)^2 / (1 - \gamma)^2$$

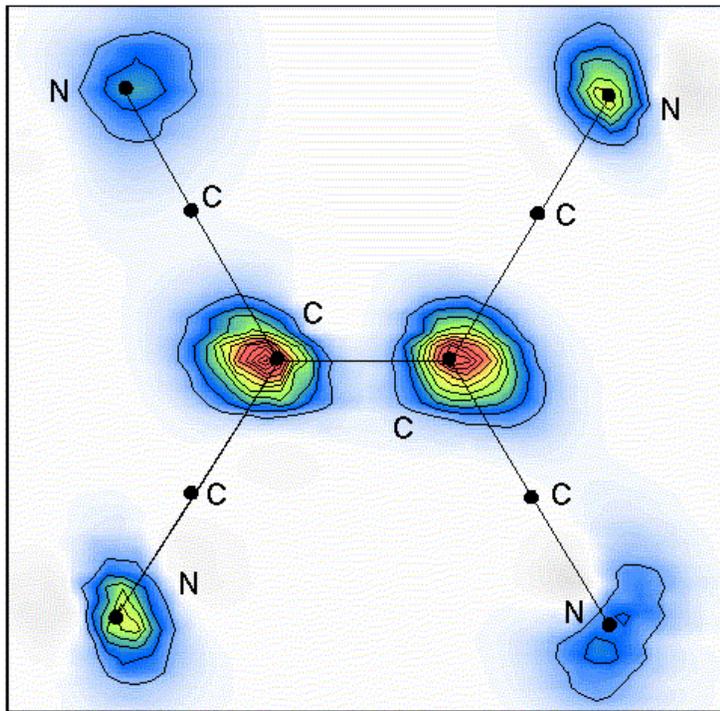
$$\text{mit } \gamma = F_N / F_M$$

$$I_{\text{up}}/I_{\text{down}} \sim 1 + 4\gamma$$

wenn Magnetismus schwach

# Organic Magnets

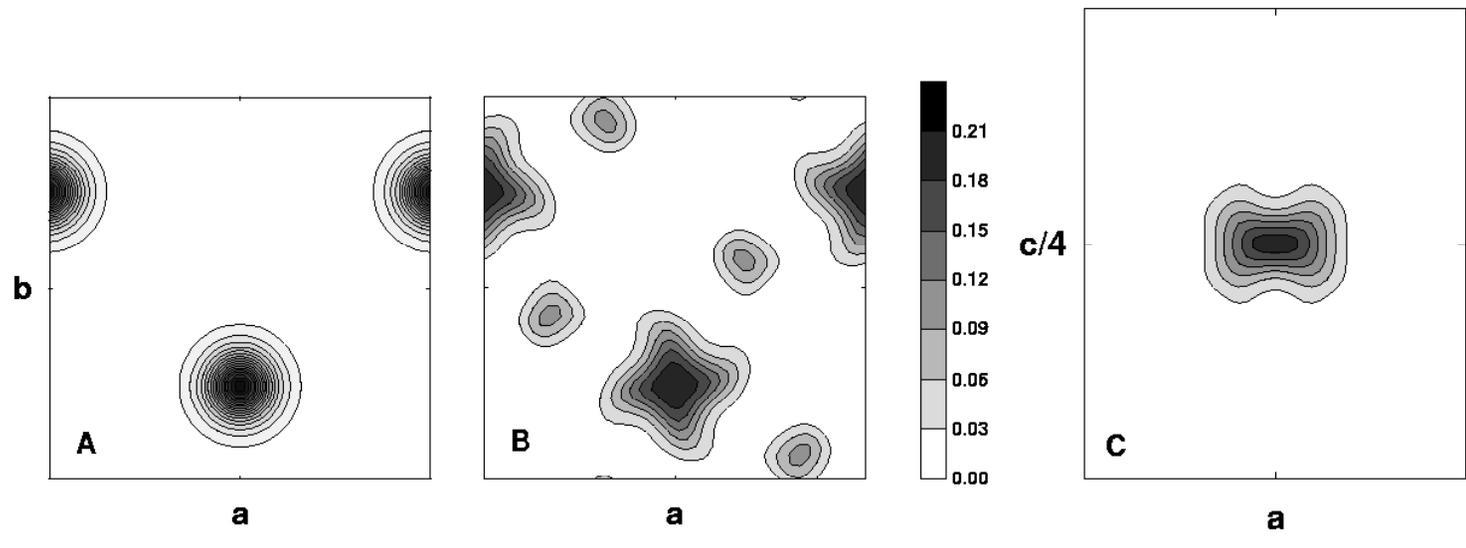
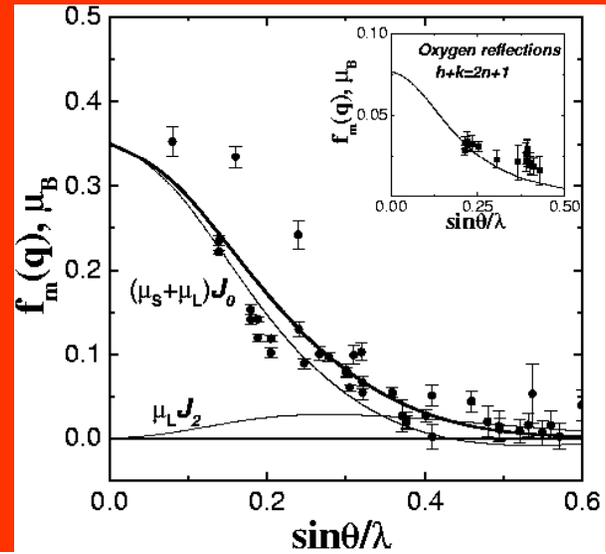
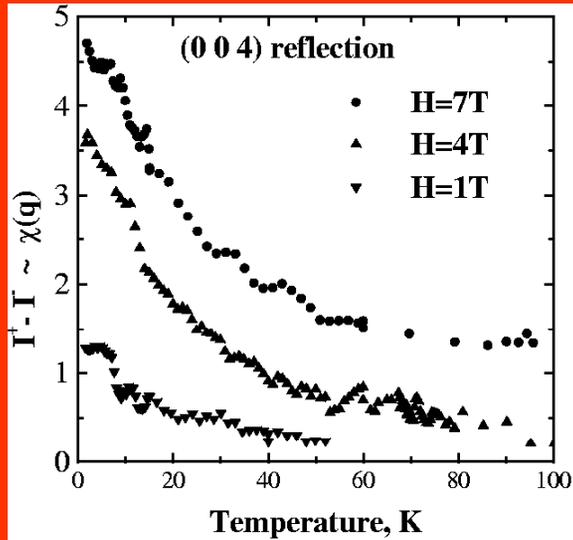
if  $L=0$ , then  $F(\kappa)$  is the Fourier transform of the spin density



Experimental spin density in the Tetracyanoethylene organic free radical-ion. Fourier data were obtained in polarized neutron diffraction experiments. Real-space density maps were then reconstructed with model-enhanced Maximum Entropy method.

A. Zheludev, et. al. *J. Am. Chem. Soc.* **116**, 7243-7249 (1994).

# Which band is responsible for magnetism in $\text{Ca}_{1.5}\text{Sr}_{0.5}\text{RuO}_4$ ?



take-off angle  $7^\circ < 2\theta_M < 38^\circ$

wavelength  $0.42 \text{ \AA} < \lambda < 0.843 \text{ \AA}$

high-flux,  $\text{Cu}_2\text{MnAl}$  (111)

low resolution  $d = 3.362 \text{ \AA}$

$1 \times 10^7 \text{ n.cm}^{-2}.\text{s}^{-1}$

less-flux,  $\text{Co}_{0.92}\text{Fe}_{0.08}$  (200)

better resolution  $d = 1.771 \text{ \AA}$

$2 \times 10^6 \text{ n.cm}^{-2}.\text{s}^{-1}$

## D3-Diffraktometer ILL

### Zero-field option

Cryopad

$40\text{mK} < T < 300\text{K}$

$^3\text{He}$  spin analyser

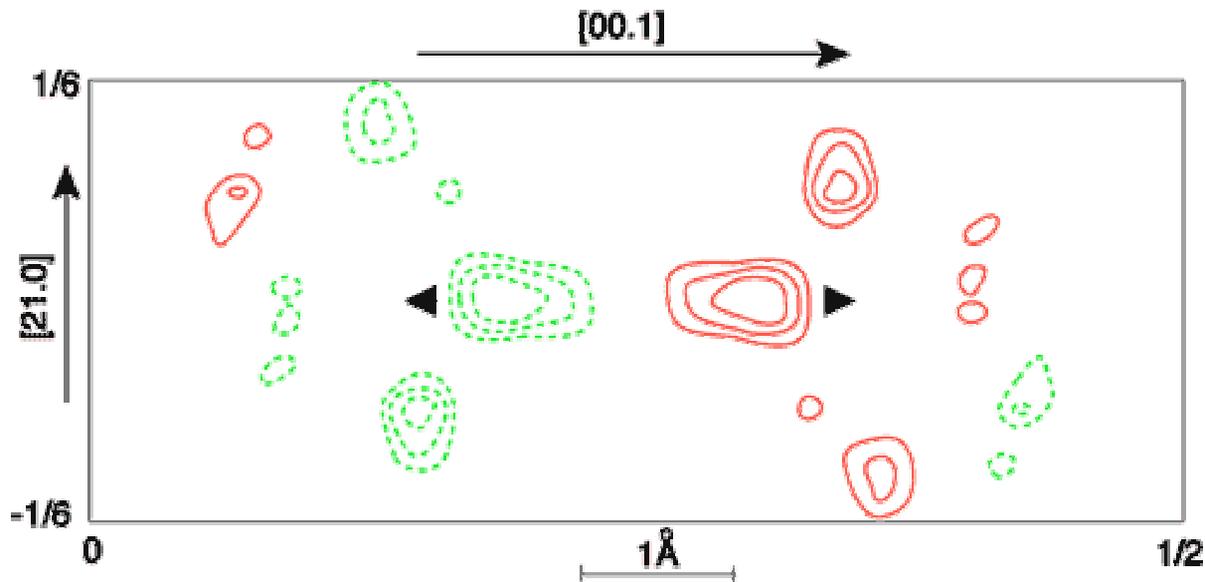
$P_{^3\text{He}}(0) = 70\%$

$60\text{h} < T_1 < 120\text{h}$



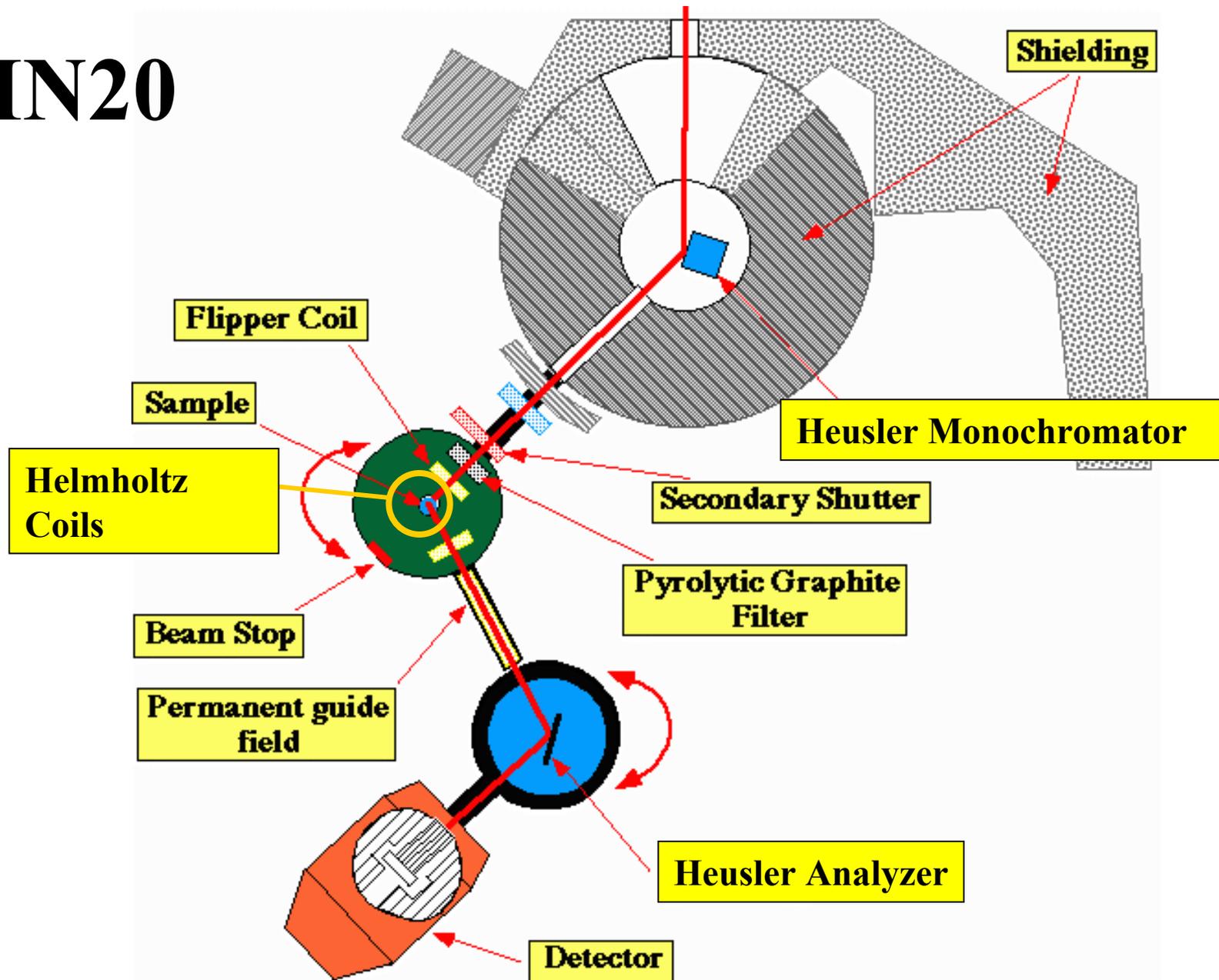
# Determination of the magnetization distribution in $\text{Cr}_2\text{O}_3$ using spherical neutron polarimetry

P. J. Brown, J. B. Forsyth, E. Lelièvre-Berna and F. Tasset  
*J. Phys.: Condens. Matter* **14** (2002) 1957–1966

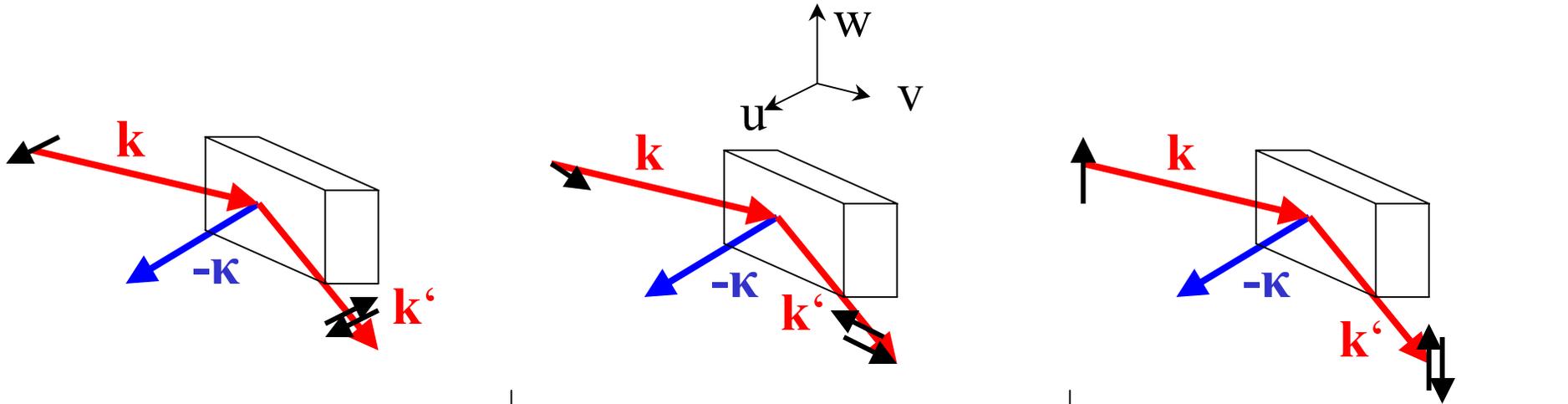


**Maximum-entropy reconstruction** of the density corresponding to the difference between the observed magnetization distribution and that calculated from the multipole model. The section shown is perpendicular to  $[0\ 1\ 0]$  and passes through the origin. The contours are logarithmically spaced with a factor of two between successive levels. The **highest contour is at  $1.0\ \mu\text{B}\ \text{\AA}^3$** ; negative contours are dashed. The filled triangles mark the  $\text{Cr}^{3+}$  ion positions; the one farthest to the right in the diagram has positive spin.

# IN20



# Polarisierte Neutronen+ Polarisationsanalyse



**$P \parallel k, P \parallel u$**

$$I_u^{SF} = \frac{2}{3} I_{inc}^{spin} + I_{magn}^v + I_{magn}^w$$

$$I_u^{NSF} = \frac{1}{3} I_{inc}^{spin} + I_{inc}^{isot} + I_{coh}^{nuc}$$

**$P \perp k, P \parallel v$**

$$I_v^{SF} = \frac{2}{3} I_{inc}^{spin} + I_{magn}^w$$

$$I_v^{NSF} = \frac{1}{3} I_{inc}^{spin} + I_{inc}^{isot}$$

$$+ I_{coh}^{nuc} + I_{magn}^v + \sqrt{I_{coh}^{nuc} I_{magn}^v}$$

**$P \perp k, P \parallel w$**

$$I_w^{SF} = \frac{2}{3} I_{inc}^{spin} + I_{magn}^v$$

$$I_w^{NSF} = \frac{1}{3} I_{inc}^{spin} + I_{inc}^{isot} +$$

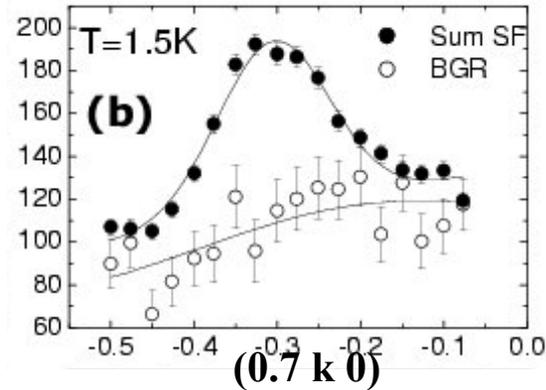
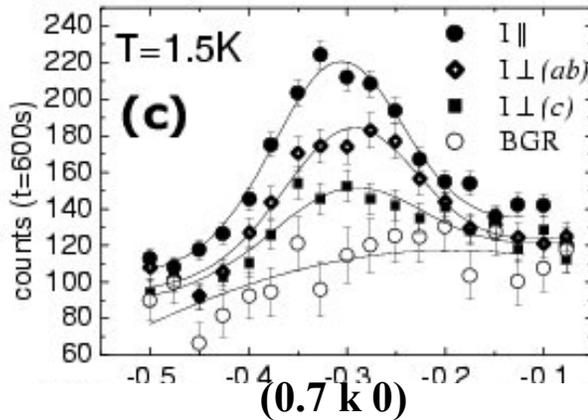
$$+ I_{coh}^{nuc} + I_{magn}^w + \sqrt{I_{coh}^{nuc} I_{magn}^w}$$

# polarized neutrons (IN20 at ILL)

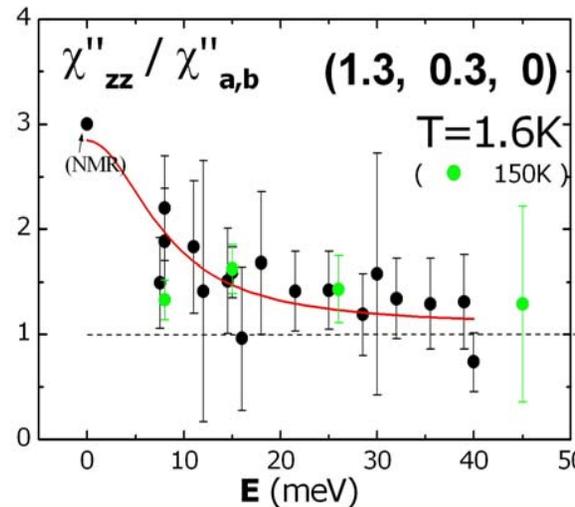
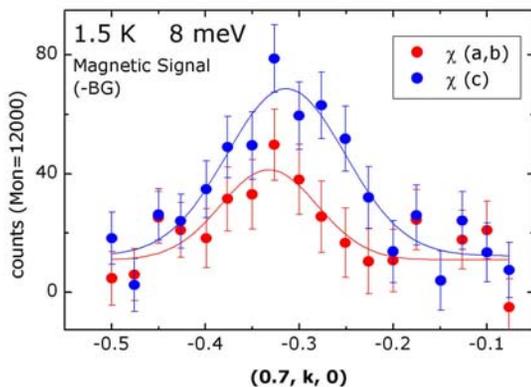
~10g of superconducting crystals



M. Braden et al.,  
PRL 2004



**importance of the anisotropy** : Eremin et al. (2002), Sato and Komoto (2000), Kuwabara and Ogata (1999), experiment : Servant et al., Kawano et al.



$\Gamma_{zz} \sim 8 \text{ meV}$

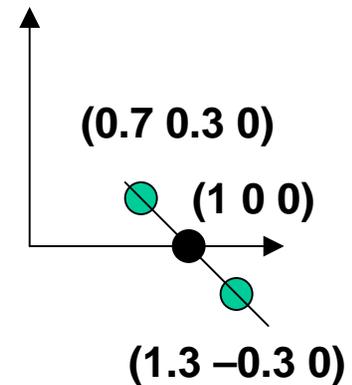
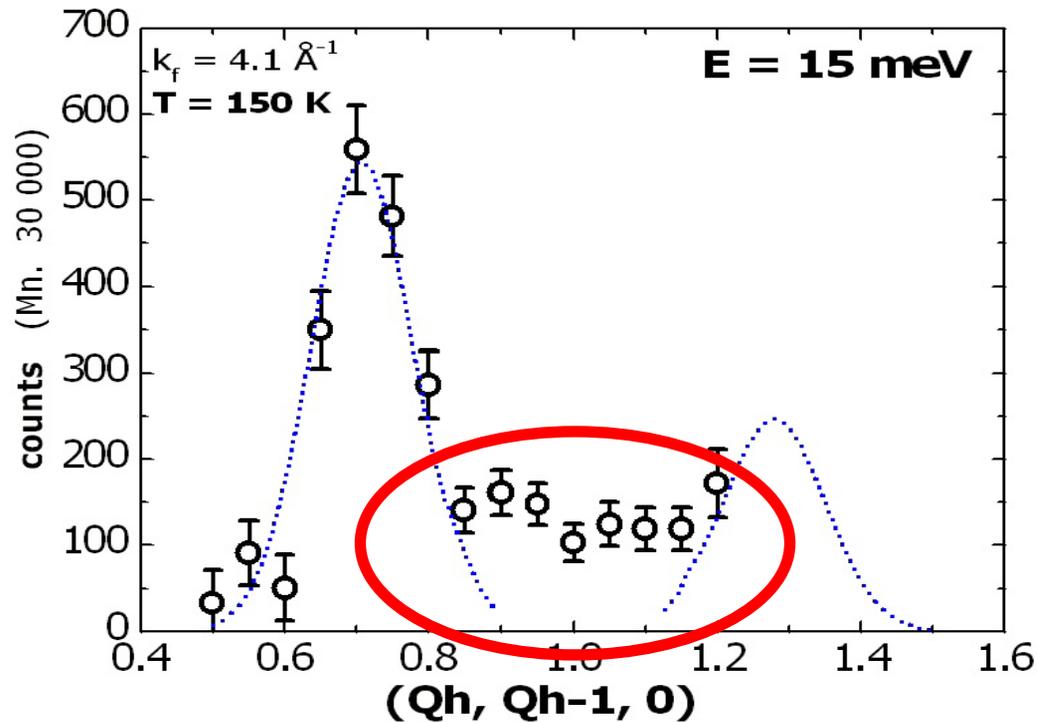
$\chi'_{zz}(\mathbf{q}_i, \omega=0) \sim 220 \mu_B^2/eV$

$\Gamma_{ab} \sim 13 \text{ meV}$

$\chi'_{ab}(\mathbf{q}_i, \omega=0) \sim 140 \mu_B^2/eV$

**- there is sizeable anisotropy : a factor 2 !!!**

# polarized neutrons (IN20 at ILL)



-first clear INS evidence for a – still weak - quasi-ferromagnetic contribution !

# Literatureempfehlungen :

Marshall & Lovesey **Theory of thermal neutron scattering** (Oxford)

G.L. Squires **Thermal neutron scattering** (Dover)

Shirane, Shapiro, Tranquada  
**Neutron scattering with a triple-axis-spectrometer** (Cambridge)

Bacon **Neutron diffraction** (Oxford)



***ENDE***