The Abdus Salam
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1866-14

School on Pulsed Neutrons: Characterization of Materials

15 - 26 October 2007

Single Crystal Neutron Spectroscopy

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Switzerland

Single Crystal Spectroscopy

to probe the Physics of Low Dimensional Systems

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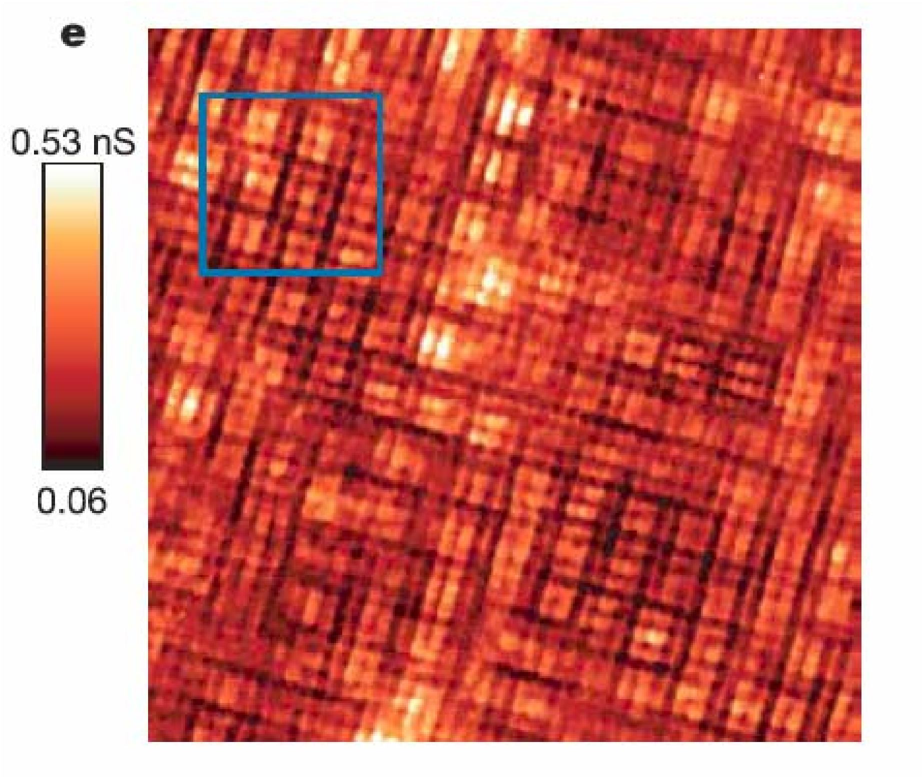
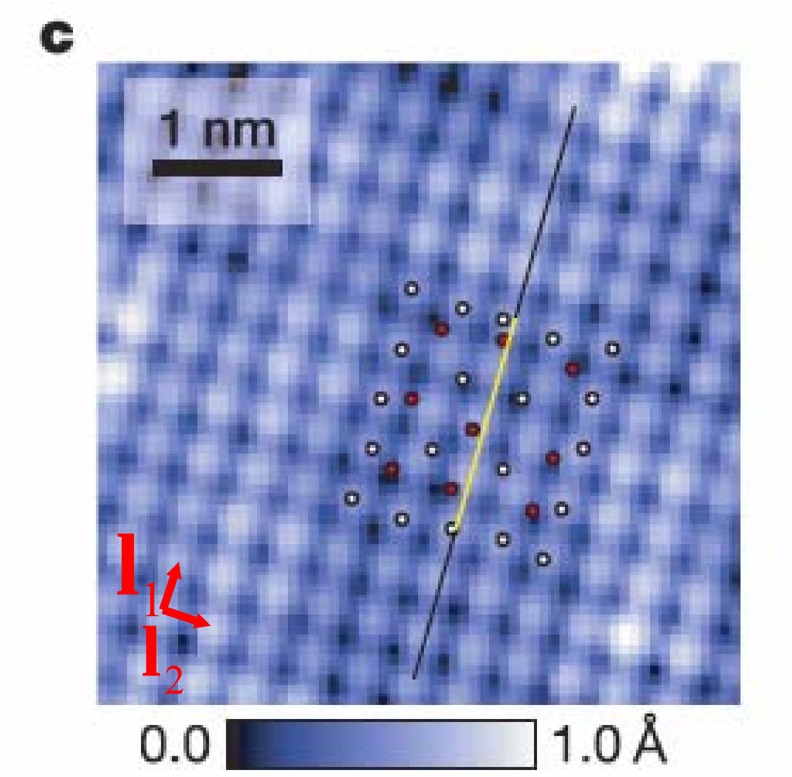
Layout:

1) Introduction to dynamics in crystals
2) Introduction to low-D systems
3) Neutron scattering on magnetic insulators
4) From zero to 2 dimensions

Periodic arrangement of atoms in a solid (STM Davis Nature 2004)





$$d = x_1\mathbf{l}_1 + x_2\mathbf{l}_2$$

n-atoms per unit cell

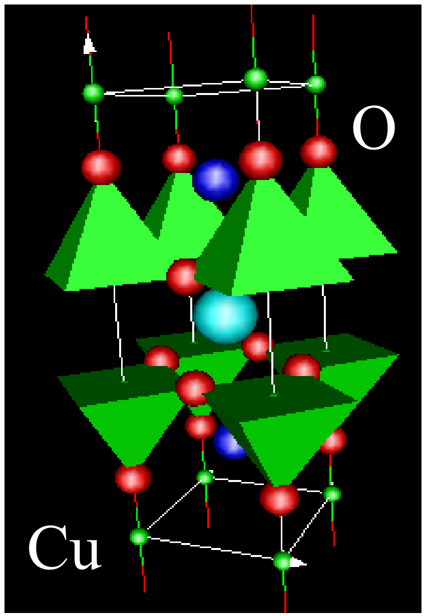
$\mathbf{d}_i = x_1\mathbf{l}_1 + x_2\mathbf{l}_2 + x_3\mathbf{l}_3$

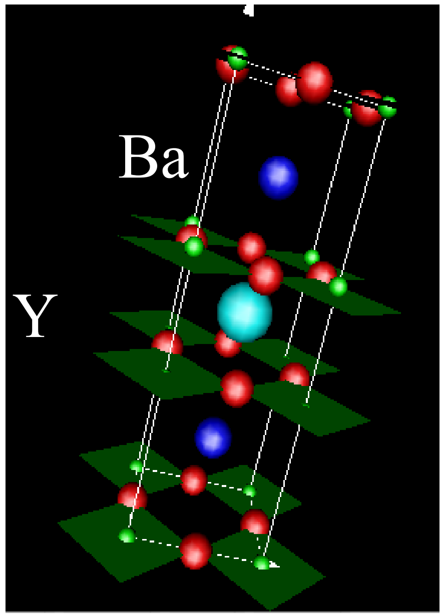
$(0 \leq x_i \leq 1)$

$YBa_2Cu_3O_6$

$P4/mmm,\ D^1_{4h}$

```
C 3.8920 3.8920 11.9909 90. 90. 90.
S GRUP P 4/m m m
A Ba1          0.50000 0.50000 0.19440
A Y1           0.50000 0.50000 0.50000
A Cu1          0.00000 0.00000 0.00000
A Cu2          0.00000 0.00000 0.36130
A O1           0.00000 0.00000 0.15010
A O2           0.00000 0.50000 0.37910
A O4   0.00000 0.50000 0.00000
```





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Real lattice: Basis vectors: $\mathbf{l}_1$, $\mathbf{l}_2$, $\mathbf{l}_3$

$$d = x_1\mathbf{l}_1 + x_2\mathbf{l}_2 + x_3\mathbf{l}_3 \qquad \left(d = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3\right)$$

Reciprocal lattice: Basis vectors: τ_1, τ_2, τ_3

$$\tau_{hkl} = h\tau_1 + k\tau_2 + l\tau_3 \qquad (\tau_{\mathrm{hkl}} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3)$$

$$\tau_1 = \frac{2\pi \;\; \mathbf{l}_2 \times \mathbf{l}_3}{\mathbf{l}_1(\mathbf{l}_2 \times \mathbf{l}_3)};\; \ldots \qquad \mathbf{b}_1 = \frac{2\pi\, \mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1\left(\mathbf{a}_2 \times \mathbf{a}_3\right)};\ldots$$

Distance between planes: $$d_{hkl} = \frac{2\pi}{\left|\tau_{hkl}\right|}$$

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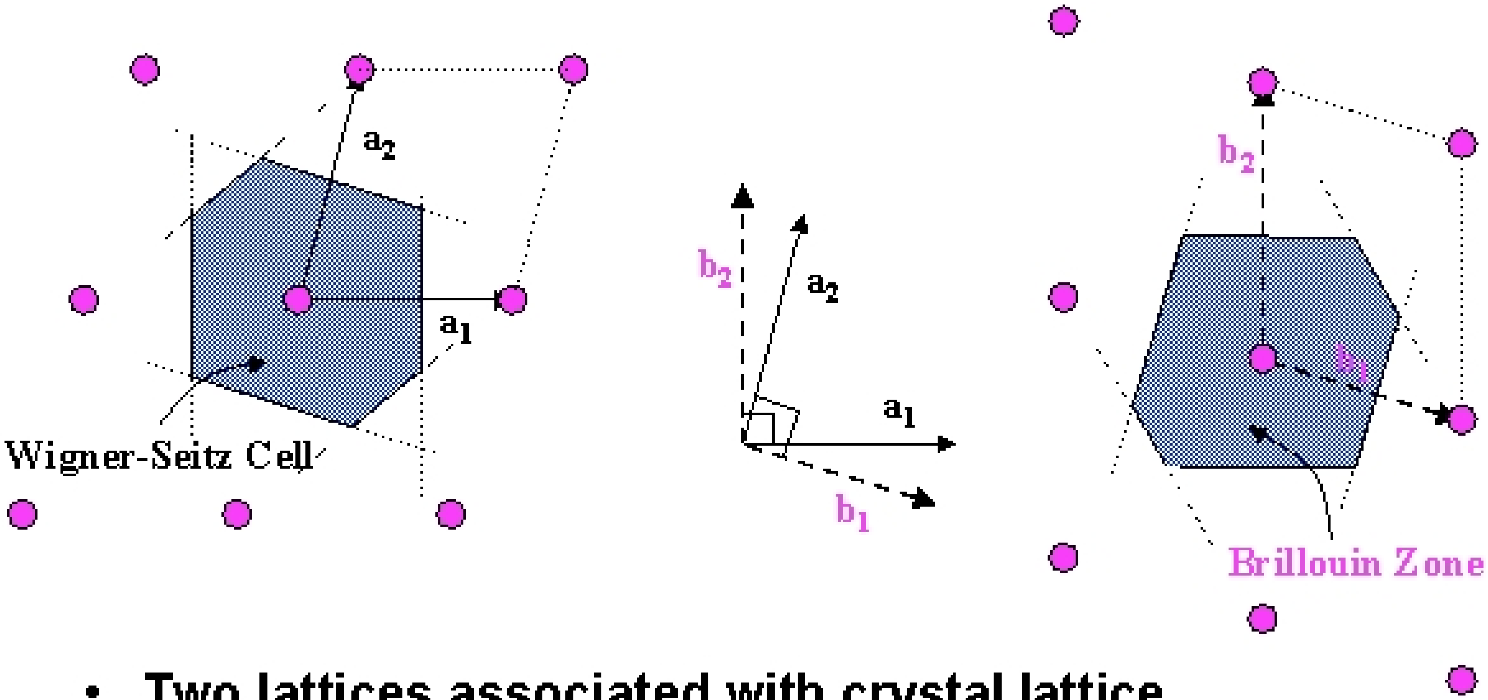
Real & Reciprocal lattices in 2 D



- Two lattices associated with crystal lattice
- b_1 perpendicular to a_2 , b_2 perpendicular to a_1
- Wigner-Seitz Cell of Reciprocal lattice called the "First Brillouin Zone" or just "Brillouin Zone"

Reciprocal Lattice in 3D

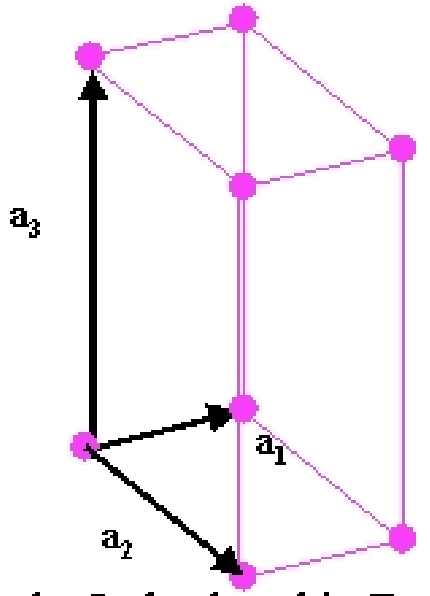
- The primitive vectors of the reciprocal lattice are defined by the vectors b_i that satisfy

  $$b_i \cdot a_j = 2\pi\, \delta_{ij}\, , \text{ where } \delta_{ij} = 1,\ \ \delta_{ij} = 0,\ i \neq j$$

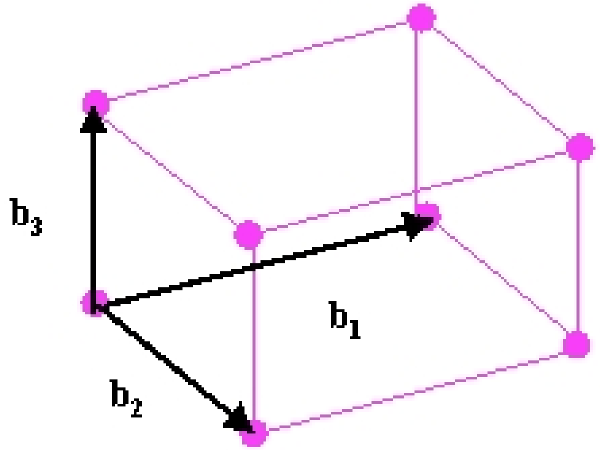
- How to find the b's?

- Note: b_1 is orthogonal to a_2 and a_3, etc.
- In 3D, this is found by noting that $(a_2 \times a_3)$ is orthogonal to a_2 and a_3
- Also volume of primitive cell $V = |a_1 \cdot (a_2 \times a_3)|$
- Then $b_i = (2\pi / V)\,(a_j \times a_k)$, where $i \neq j \neq k$

Three Dimensional Lattices
Simplest examples



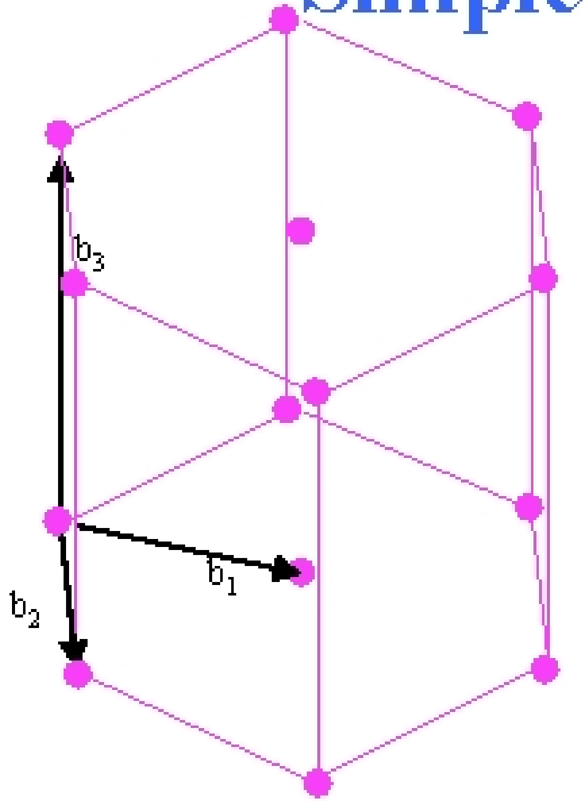
Simple Orthorhombic Bravais Lattice
with $a_3 > a_2 > a_1$



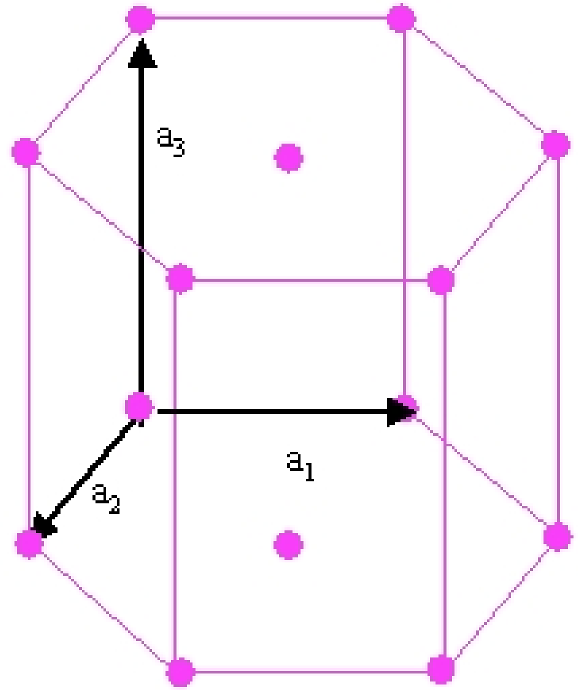
Reciprocal Lattice
Note: $b_1 > b_2 > b_3$

- **Long lengths in real space imply short lengths in reciprocal space and vice versa**

Three Dimensional Lattices
Simplest examples



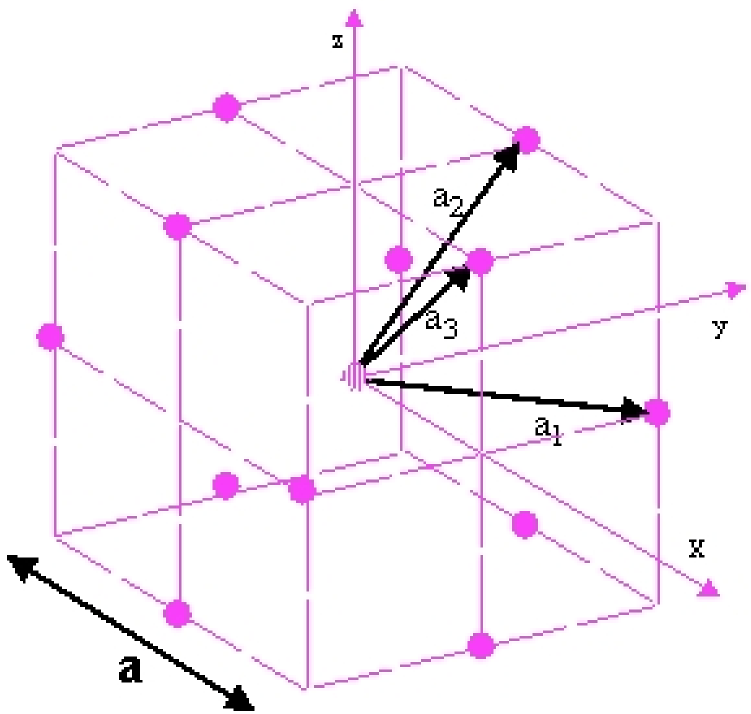
Reciprocal Lattice



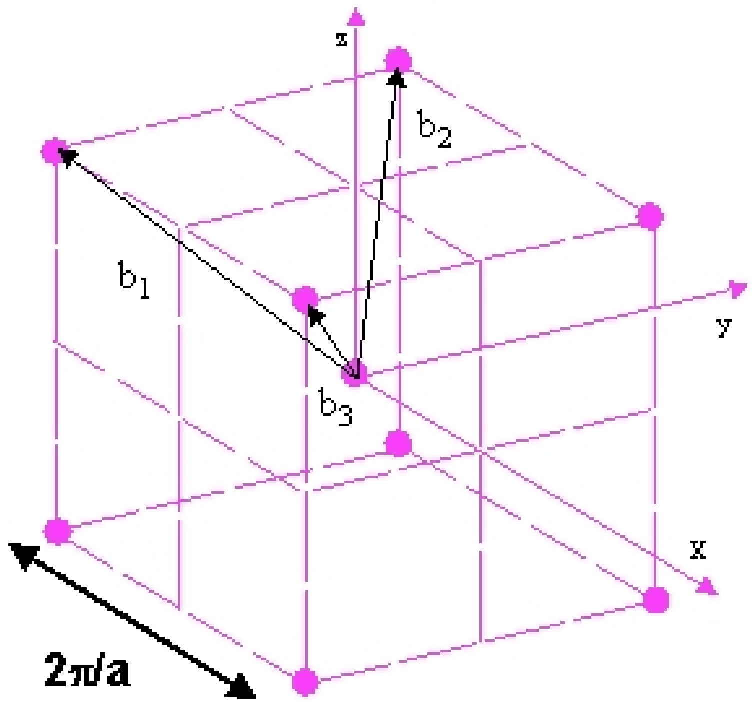
Hexagonal Bravais Lattice

- **Reciprocal lattice is also haxagonal, but rotated**
- **See homework problem in Kittel**

Face Centered - Body Centered Cubic Reciprocal to one another

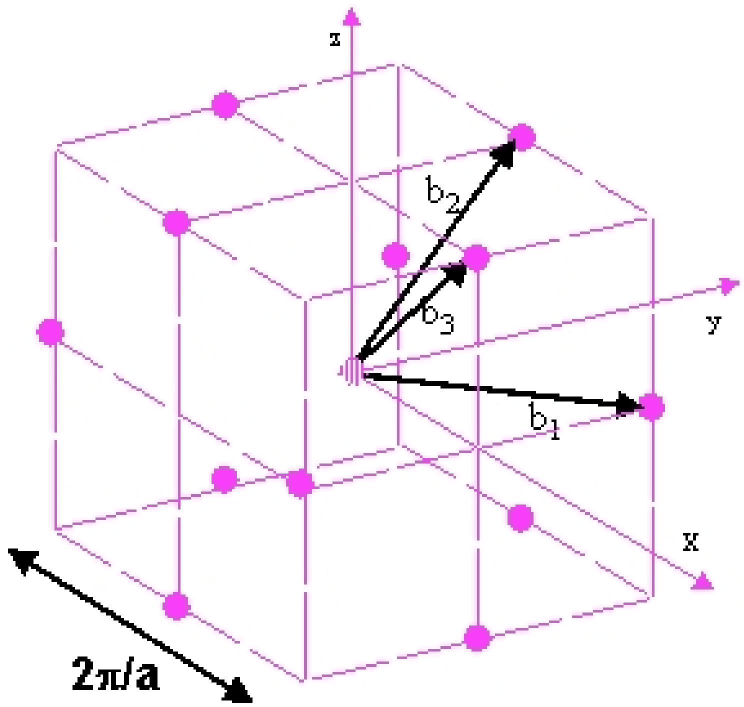


Primitive vectors and the conventional cell of fcc lattice

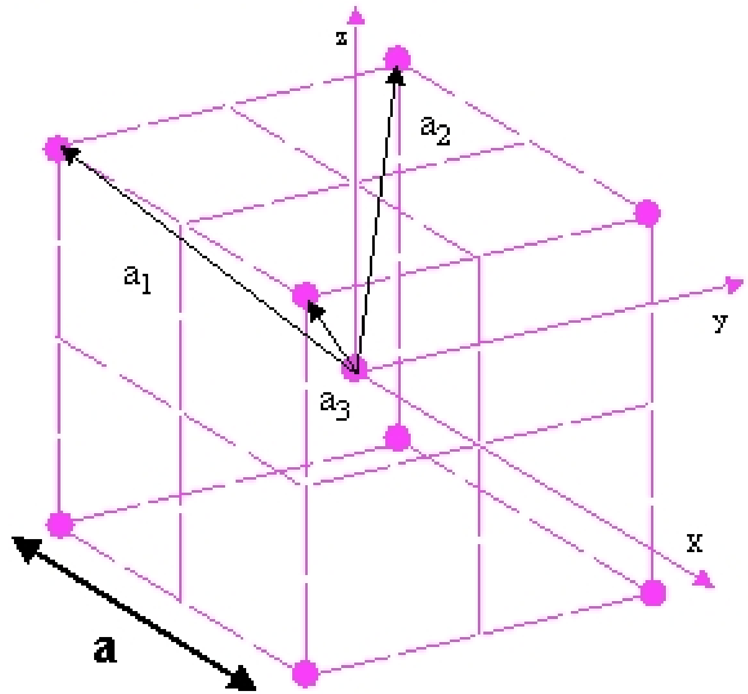


Reciprocal lattice is Body Centered Cubic

Face Centered - Body Centered Cubic Reciprocal to one another

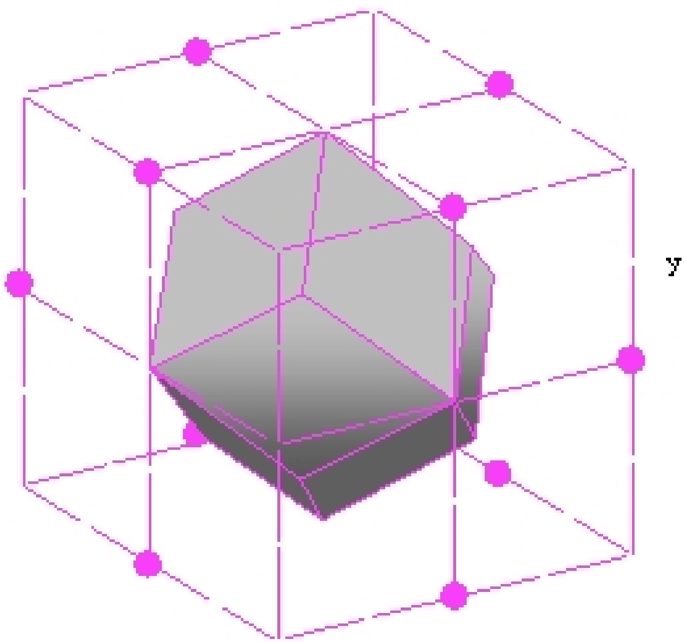


Reciprocal lattice is Face Centered Cubic

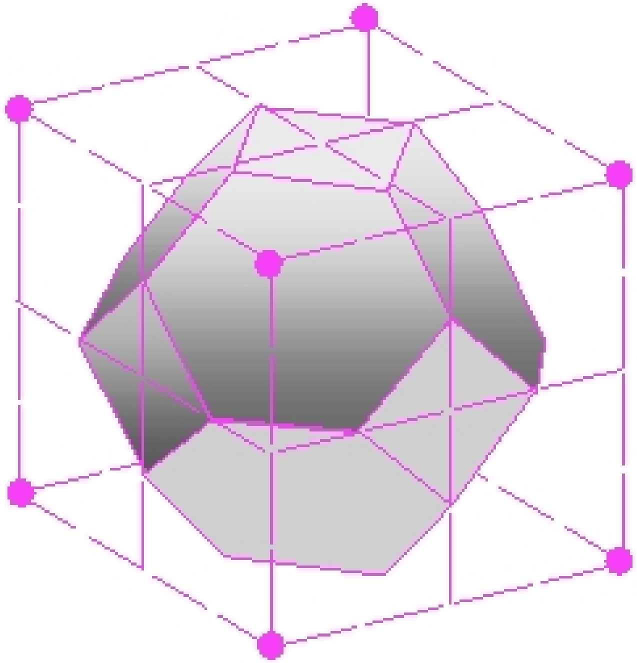


Primitive vectors and the conventional cell of bcc lattice

Face Centered Cubic

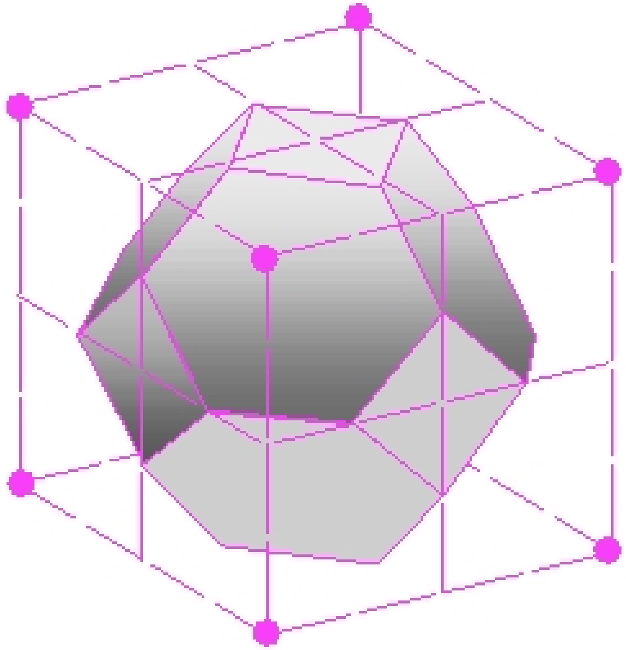


Wigner-Seitz Cell for
Face Centered Cubic Lattice

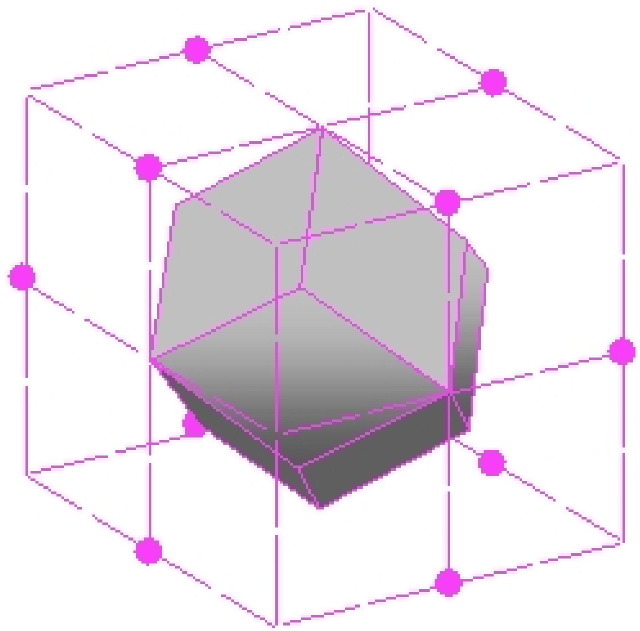


Brillouin Zone =
Wigner-Seitz Cell for
Reciprocal Lattice

Body Centered Cubic



Wigner-Seitz Cell for
Body Centered Cubic Lattice



Brillouin Zone =
Wigner-Seitz Cell for
Reciprocal Lattice

Why do we need reciprocal space at all?

--> because of coherent scattering cross-section

$$\left(\frac{d\sigma}{d\Omega}\right)_{inc} = \left[\langle b^2\rangle - \langle b\rangle^2\right]\sum_{j=j'} e^{-i\mathbf{Q}(\hat{\mathbf{R}}_{j'}-\hat{\mathbf{R}}_j)} = N\left[\langle b^2\rangle - \langle b\rangle^2\right]$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{coh} = N_0\frac{(2\pi)^3}{v_0}\sum_{\tau}|F_\tau|^2\,\delta(\mathbf{Q}-\tau);$$

τ=reciprocal lattice vector

Structure factor $F_\tau = \sum_d b_d e^{i\tau\mathbf{d}}$

d= position of atom d
in unit cell

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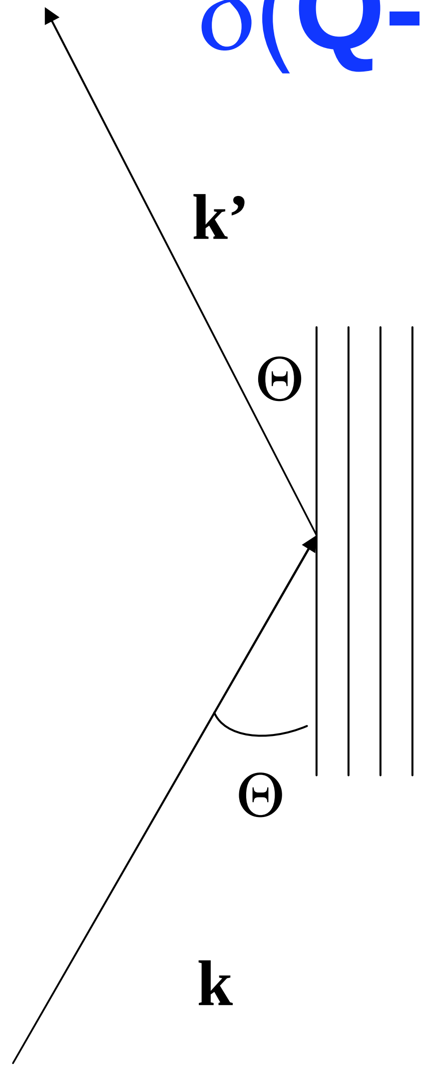
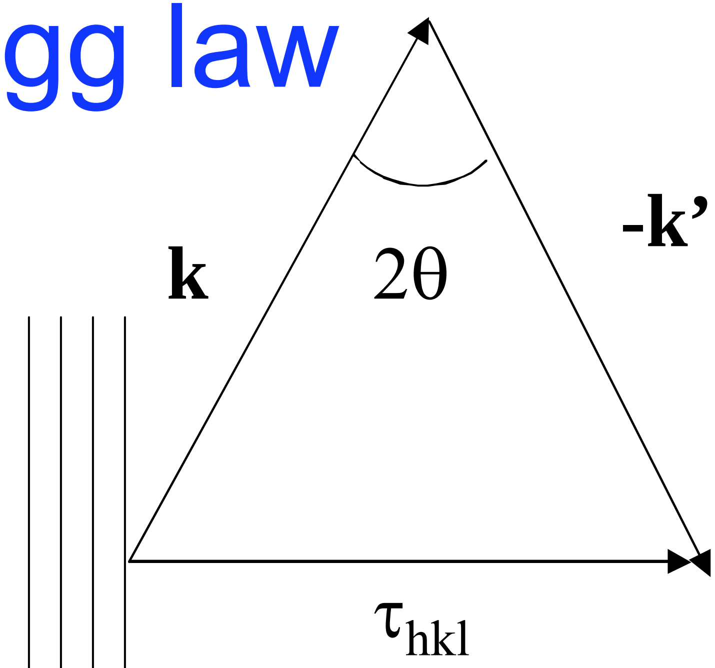
$\delta(\mathbf{Q}-\tau)$ = Bragg law



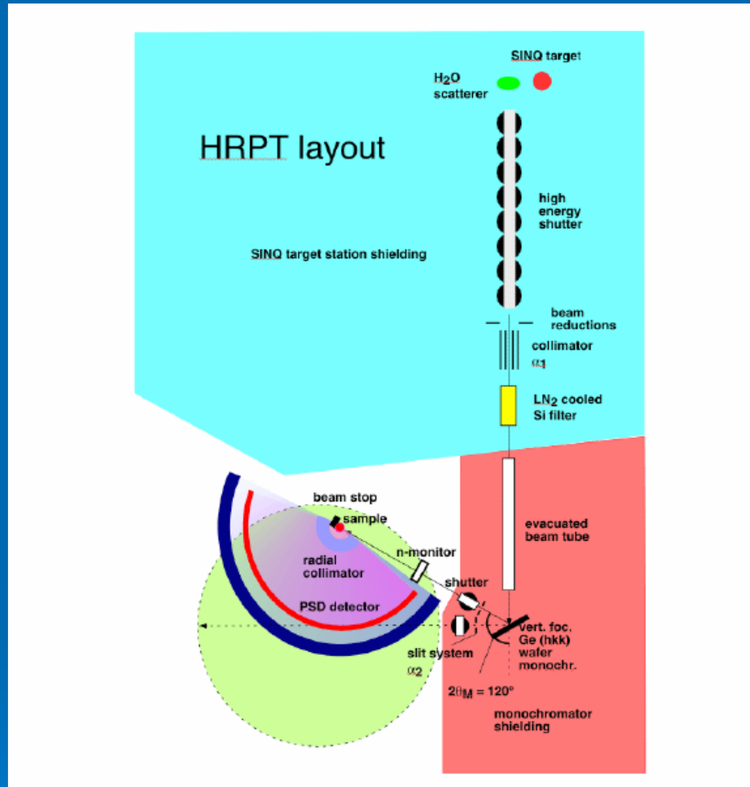


$$\frac{\tau}{2} = k\sin(\theta),\ \tau = \frac{2\pi}{d},\ k = \frac{2\pi}{\lambda}$$

$$\lambda = 2d\sin\theta$$

HRPT

HRPT

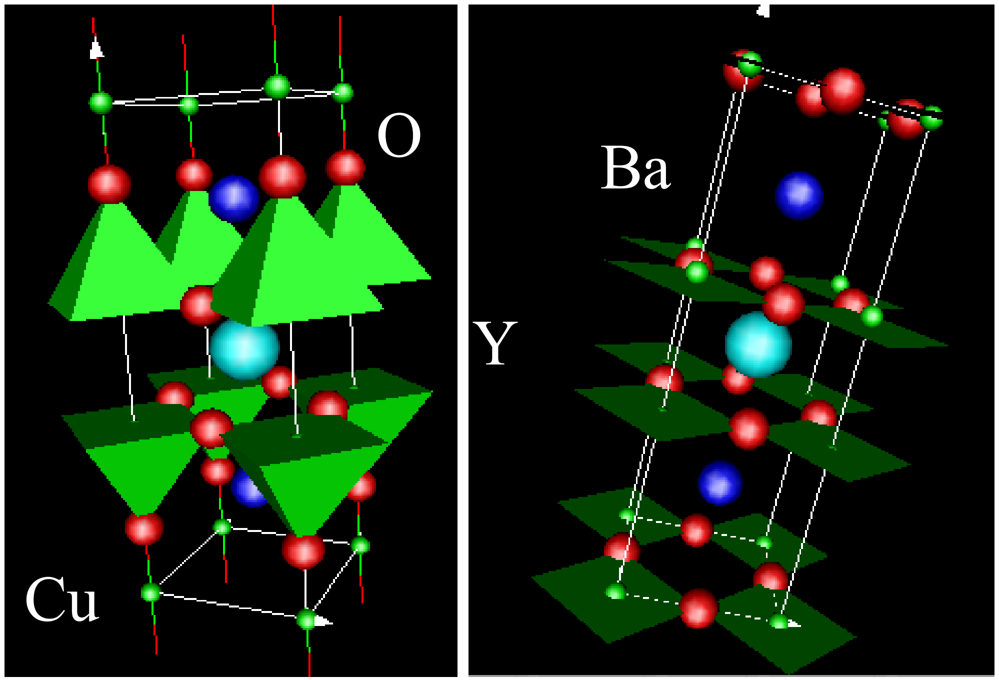


HRPT layout
SINQ target
H_2O scatterer
high energy shutter
SINQ target station shielding
beam reductions
collimator
α1
LN_2 cooled Si filter
beam stop
sample
radial collimator
n-monitor
shutter
PSD detector
evacuated beam tube
vert. foc. Ge (hkk) wafer monochr.
slit system
α2
$2\theta_M = 120°$
monochromator shielding

$YBa_2Cu_3O_6$

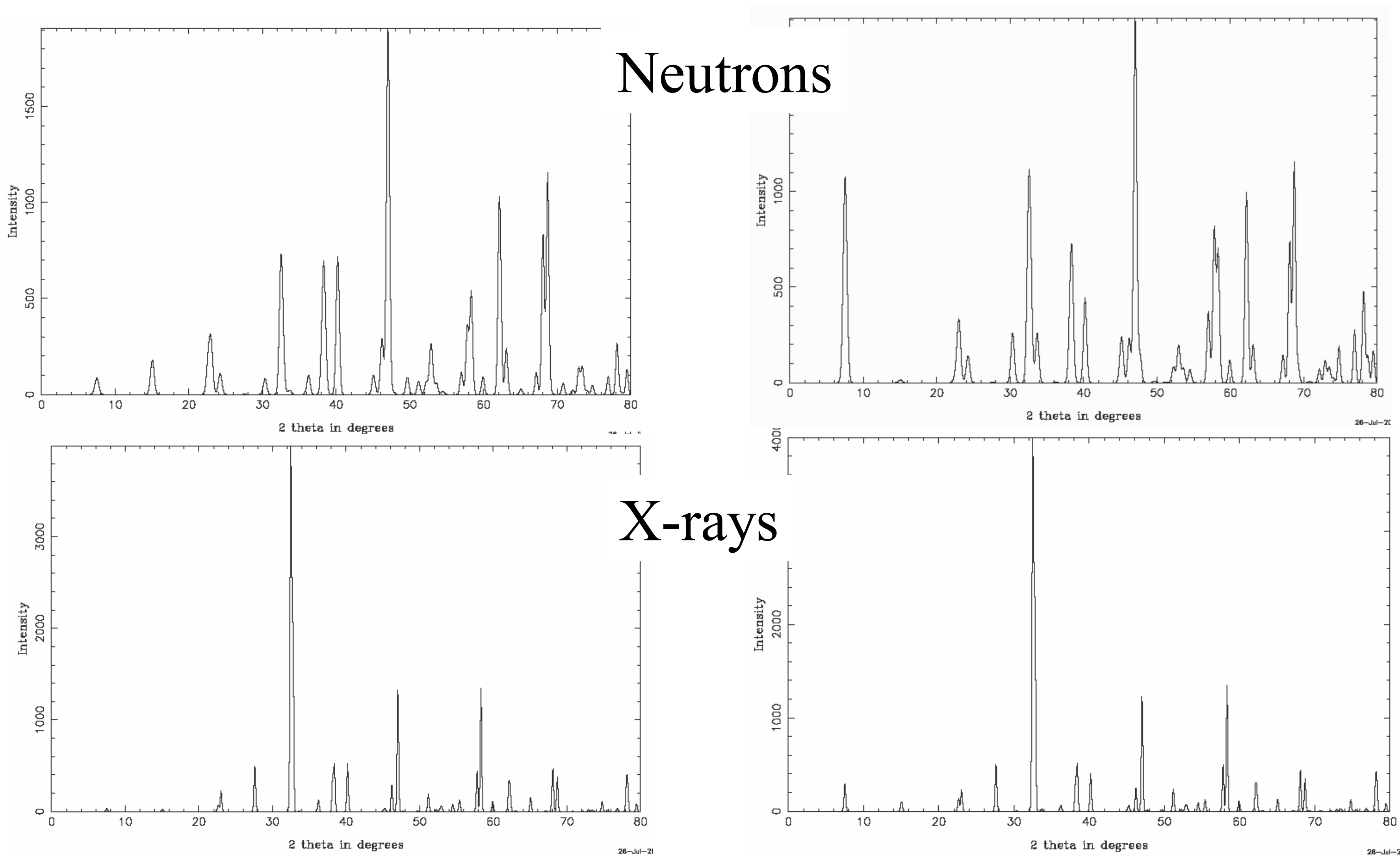
“Apex” model

“Plane” model



$YBa_2Cu_3O_6$

"Apex" model — "Plane" model



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Copper: crystallizes in a face cubic centered (fcc) structure.

$\mathbf{d}_1$=a(0,0,0), $\mathbf{d}_2$=a(1/2,1/2,0), $\mathbf{d}_3$=a(1/2,0,1/2), $\mathbf{d}_4$=a(0,1/2,1/2) τ_{hkl}=2π/a (h,k,l)

$$\mathrm{F}_\tau = \sum_d b_d e^{i\tau\mathbf{d}}$$

$$F_{100} = \exp\left\{\frac{2\pi}{a} i(1,0,0)a(0,0,0)\right\} + \exp\{2\pi i(1,0,0)(1/2,1/2,0)\}$$

$$+\exp\{2\pi i(1,0,0)(1/2,0,1/2)\} + \exp\{2\pi i(1,0,0)(0,1/2,1/2)\}$$

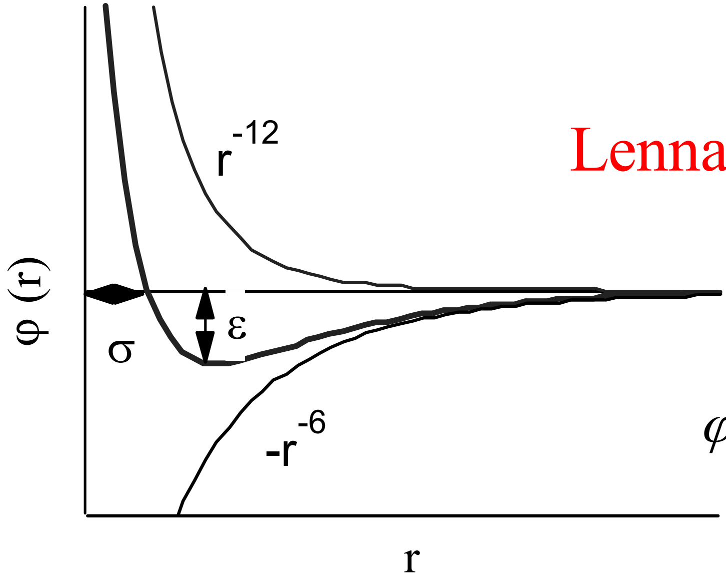
$$= 1 + \exp\{\pi i\} + \exp\{\pi i\} + 1 = \mathbf{0}$$

$$F_{200} = 1 + \exp\{2\pi i\} + \exp\{2\pi i\} + 1 = 4$$

$$F_{111} = 1 + \exp\{2\pi i\} + \exp\{2\pi i\} + \exp\{2\pi i\} = 4$$

Dynamics of periodic assembly of atoms

Interactions between particles (atoms, molecules)



Lennard-Jones 6-12 potential

$$\varphi(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

$$U = \frac{1}{2}\sum_{R,R'}\varphi(R-R') = \frac{1}{2}\sum_{R\neq 0}\varphi(R)$$

In a solid:

displacement from equilibrium position r =R+u(R)

$$\mathrm{U} = \frac{1}{2}\sum_{r,r'}\varphi(r-r') = \frac{1}{2}\sum_{R,R'}\varphi\big(R-R'+u(R)-u(R')\big)$$

Serie expansion

$$\mathrm{U} = \frac{N}{2}\sum_{R}\varphi(R) + \frac{1}{2}\sum_{R,R'}\big(u(R)-u(R')\big)\nabla\varphi(R-R')$$

$$+\frac{1}{4}\sum_{R,R'}\big(u(R)-u(R')\big)^2\nabla^2\varphi(R-R') + \dots$$

Harmonic term !

Force constant !

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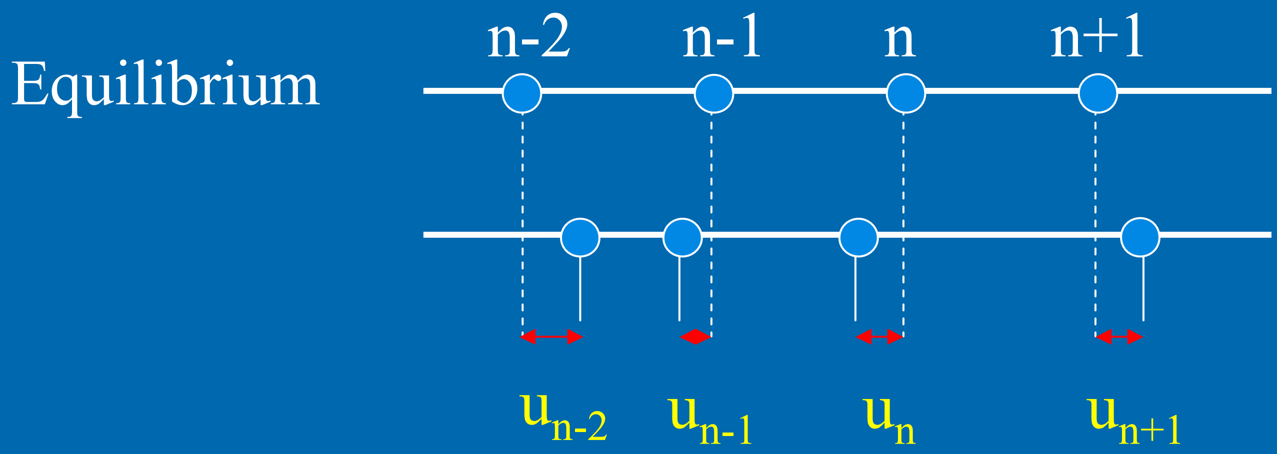
Linear chain of identical atoms



$$F_n = \beta(u_{n+1} - u_n) - \beta(u_n - u_{n-1})$$

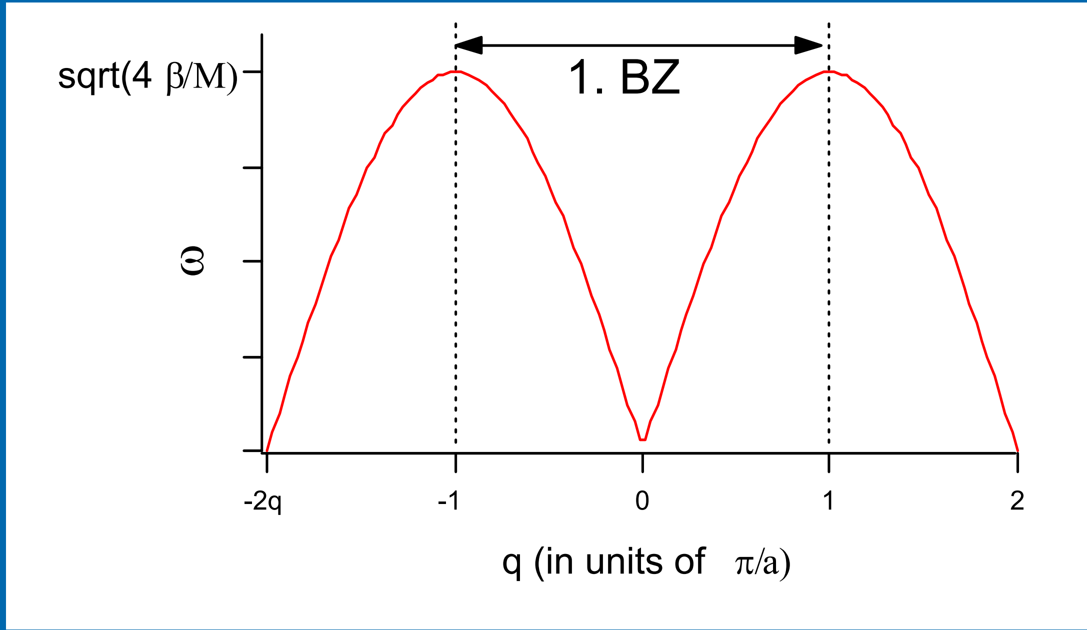
$$M\ddot{u}_n = F_n = \beta(u_{n+1} + u_{n-1} - 2u_n)$$

$$u_n = \xi e^{i(\omega t + qna)}$$

$$\omega = \pm\sqrt{\frac{4\beta}{M}}\sin\left(\frac{qa}{2}\right)$$

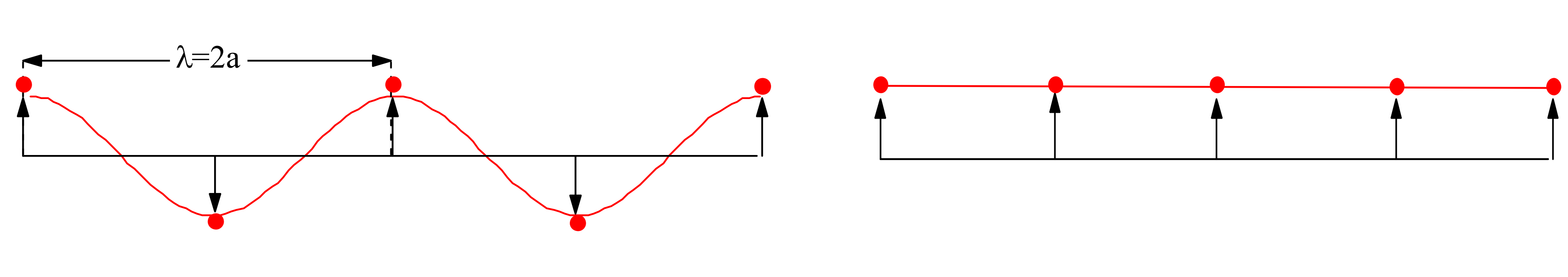
The coherent displacement of atoms can be visualized by the ratio:

$$u_n / u_{n+1} = e^{-iqa}$$



a) Zone-boundary: q=π/a

b) Zone center: q=0



$$u_n / u_{n+1} = -1$$

$$u_n / u_{n+1} = 1 \quad \lambda = \infty$$

Connection to "real world"

Debye-Modell for small q ($q \ll \pi/a$)

$$\sin\left(\frac{qa}{2}\right) \approx \frac{qa}{2} \qquad \omega \approx \sqrt{\frac{\beta}{M}}aq$$

"Density" $\rho = M/a$, elastic constant $c = \beta a$

$$\omega \approx \sqrt{\frac{\beta}{M}}aq = \sqrt{\frac{c}{\rho}}aq = \mathrm{v}q$$

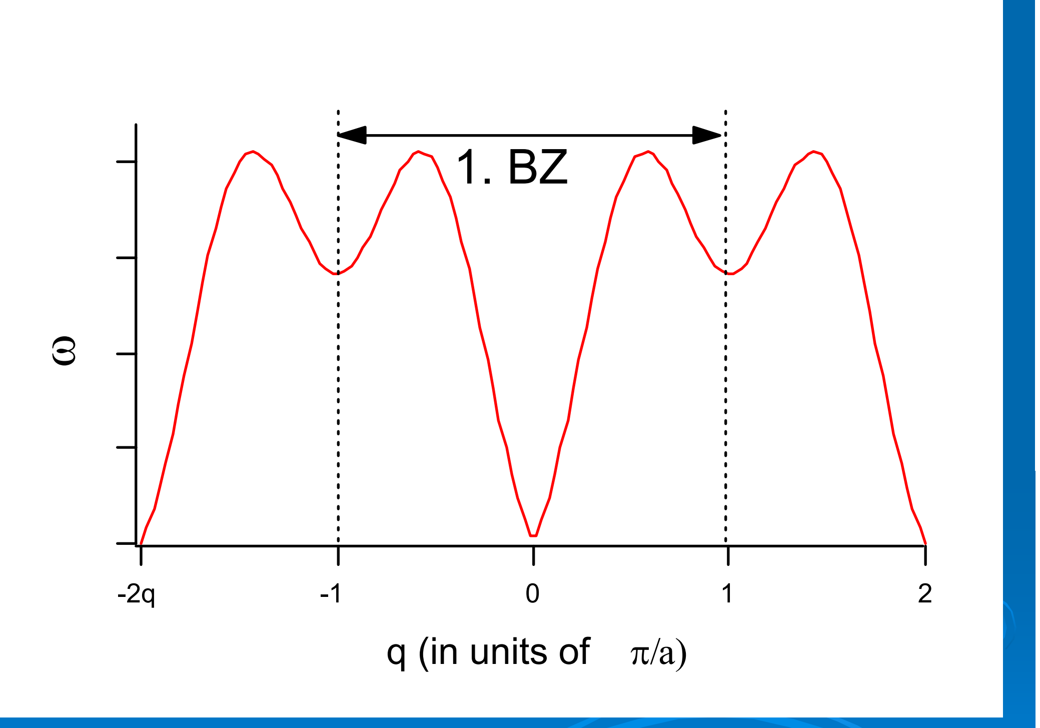
v= sound velocity

NN+NNN…

$$M\ddot{u}_n = F_n = \sum_j \beta_1 (u_{n+j} + u_{n-j}) + \beta_0 u_n$$

$$u_n = \xi e^{i(\omega t + qna)}$$

$$\omega^2 = \frac{4}{M}\sum_j \beta_j \sin^2\left(\frac{jqa}{2}\right)$$



$$\beta_1 = 2\beta_2$$
$$\beta_j = 0 \; if \; j > 2$$

Neutron Scattering

•Measures how particles scatter off of a sample

•Scattering depends on interaction between sample and particles

•Different scattering probes show different characteristics
- -Photons
- -Electrons
- -Helium atoms
- -Neutrons

Why Neutron Scattering ?

-Wavlength: $\lambda(\AA)=9.044/\sqrt{E\ (meV)}$

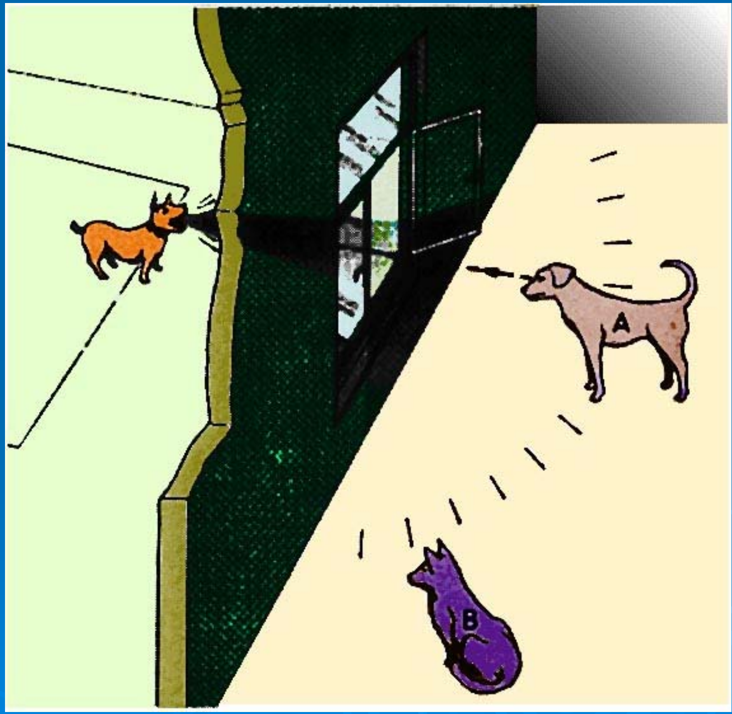
-At 10 meV, λ=2.86 Å

1) Neutron wavelength

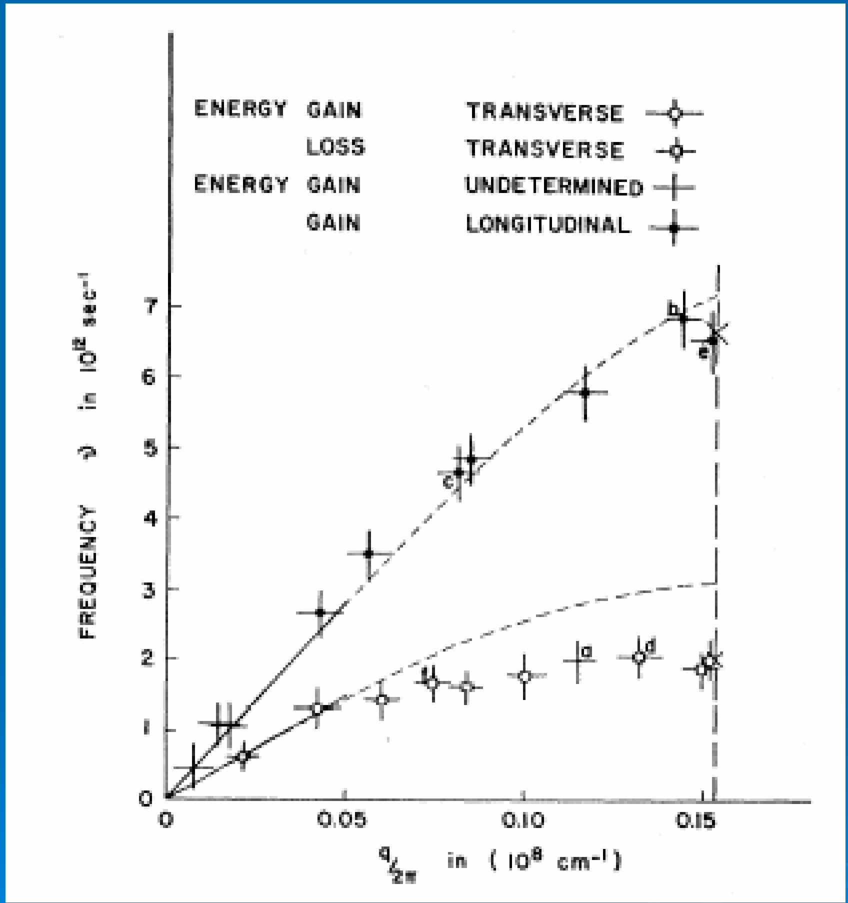
≈

Structures of interest

⇒ interference effects



Neutron energy



-Thermal sources ≈ 5-100 meV

-Cold sources ≈ 1-10 meV

⇒Comparable to excitation energies in solids and liquids

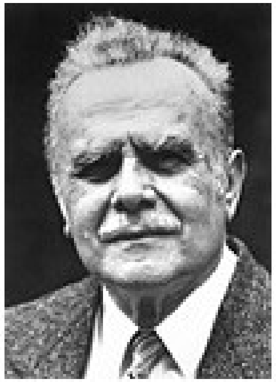
Brockhouse (1957)

Germanium

The Nobel Prize in Physics 1994

"for pioneering contributions to the development of neutron scattering techniques for studies of condensed matter"

"for the development of neutron spectroscopy"



Bertram N. Brockhouse

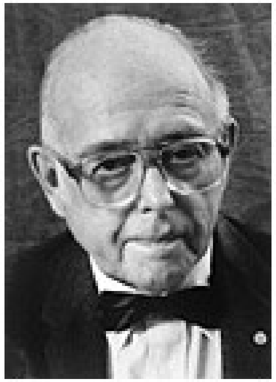
1/2 of the prize

Canada

McMaster University
Hamilton, Ontario, Canada

b. 1918
d. 2003

"for the development of the neutron diffraction technique"



Clifford G. Shull

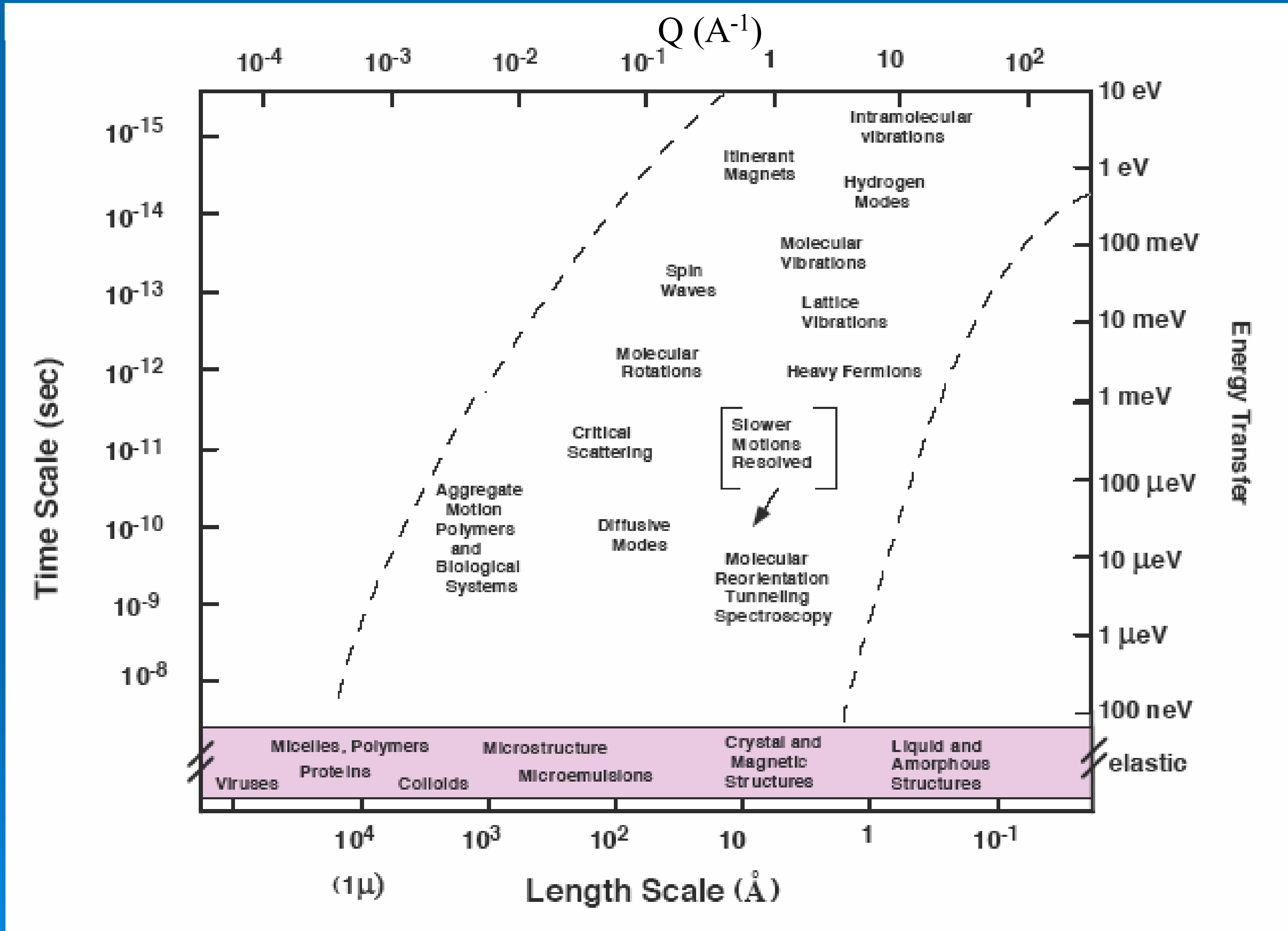
1/2 of the prize

USA

Massachusetts Institute of Technology (MIT)
Cambridge, MA, USA

b. 1915
d. 2001

Dynamics of Solids and Liquids



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Neutrons are … neutral

+

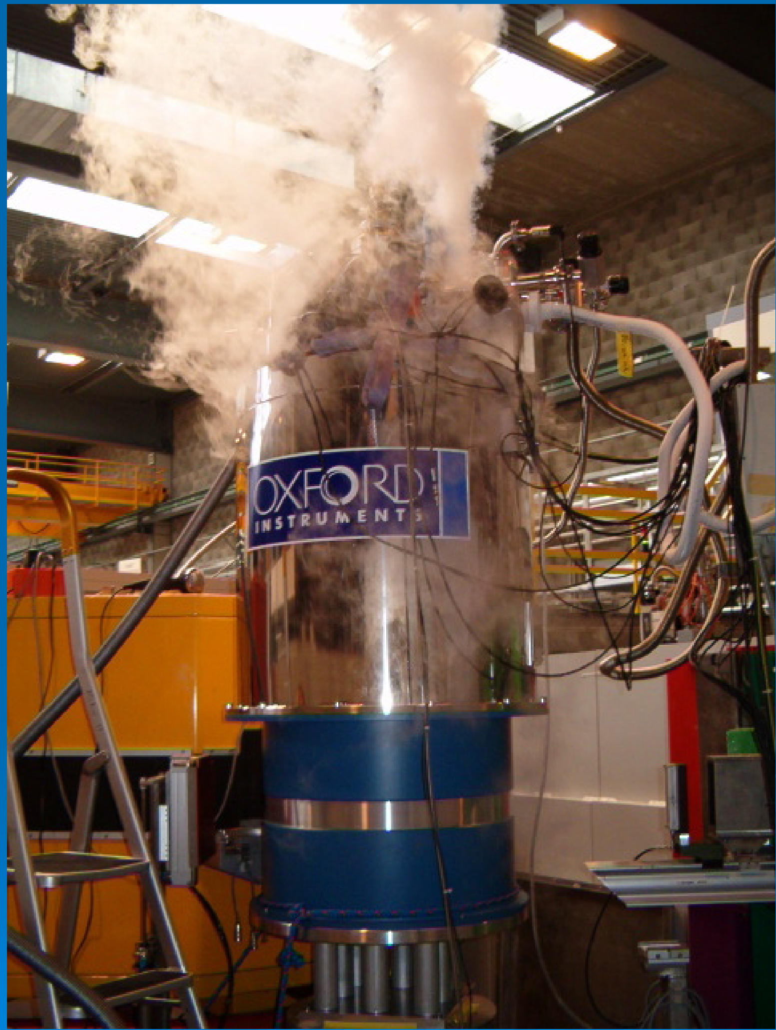
⇒ large penetration, measure bulk properties

⇒extreme sample environments

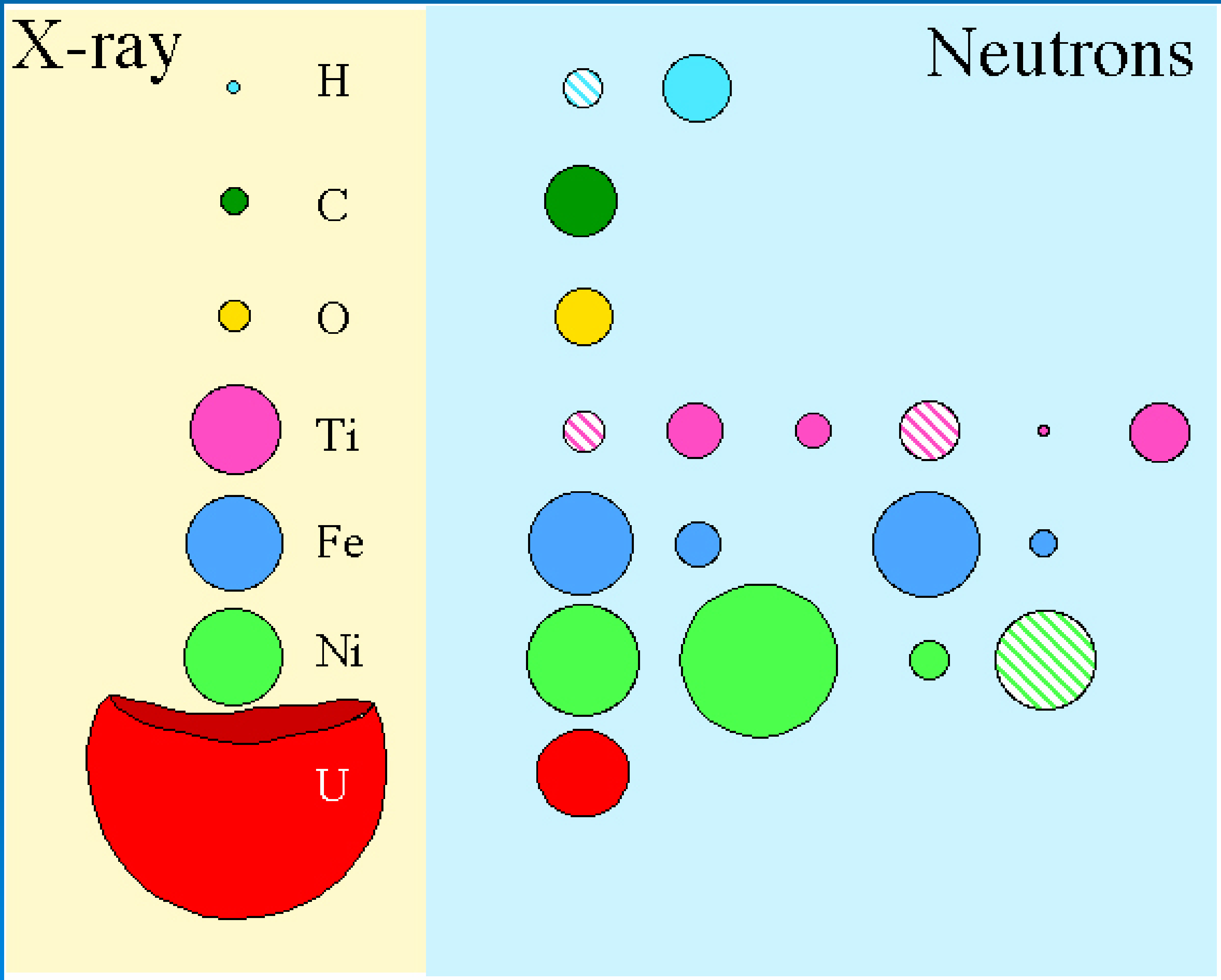
-

⇒No interactions with charge densities (electrons)

⇒Sample size is crucial



Scattering power



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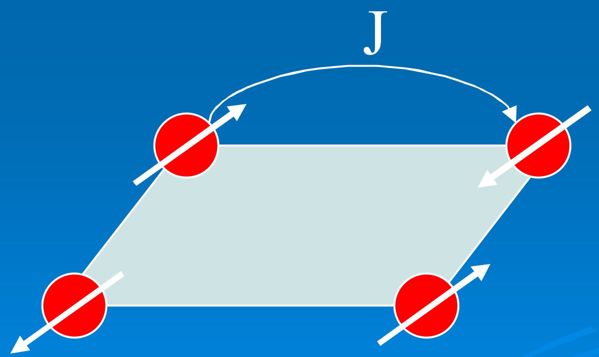
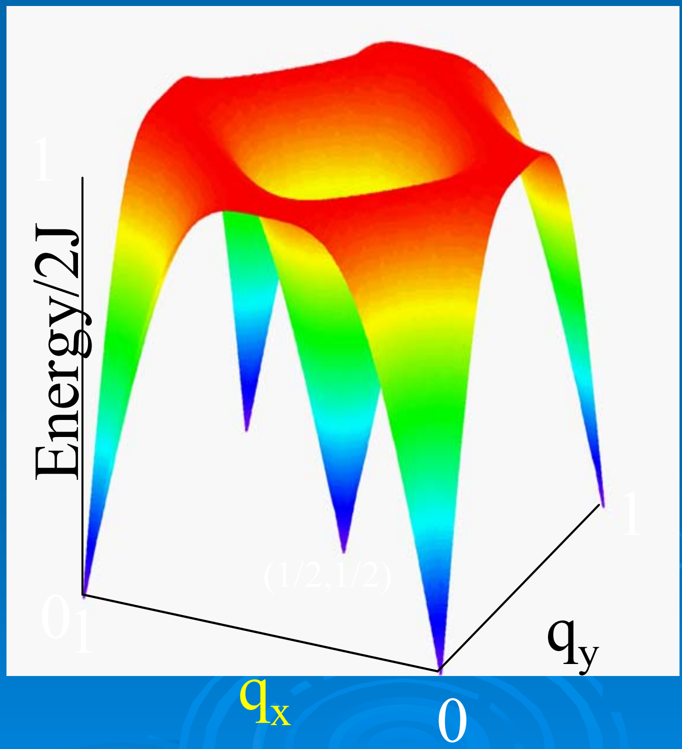
Neutrons possess a magnetic moment ($\mu_N = 1.04 \times 10^{-3}\ \mu_B$) !

⇒ magnetic structures
⇒ magnetic excitations

$$H = \sum_{\langle ij \rangle} J S_i S_j$$





Neutron Wave Properties

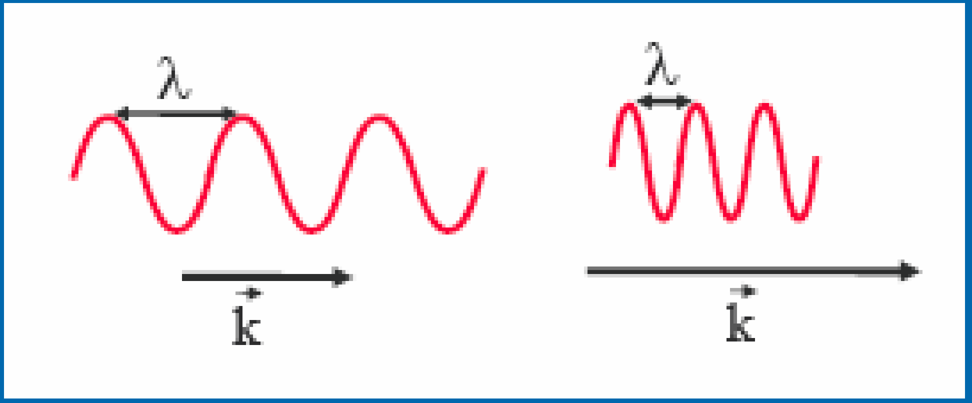
Quantum mechanics: particles show wave properties

Momentum:

$$m\mathbf{v} = \mathbf{p} = \hbar \mathbf{k}, \ \ |p| = \hbar \frac{2\pi}{\lambda}$$

Energy:

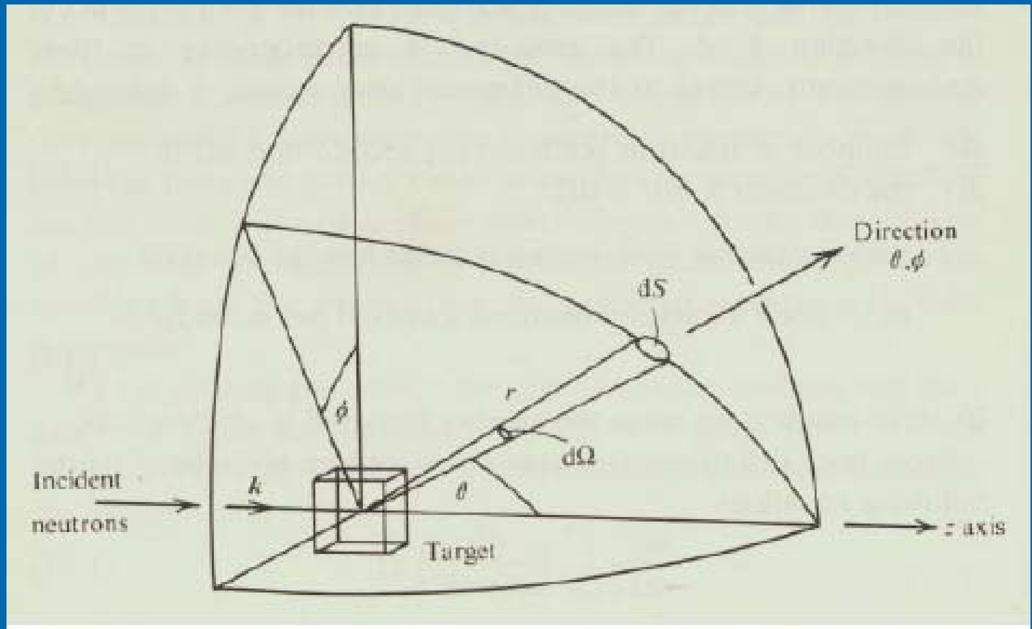
$$E = \frac{1}{2} m v^2 = \frac{\hbar^2}{2m} k^2 = \hbar\omega$$



Energy unit conversion:

1 meV ≈ 8 cm^{-1} ≈ 240 Ghz
≈ 12 K ≈ 0.1 kJ/mol

Total or differential cross-section



ϕ= number of incident neutrons per cm^2 per second

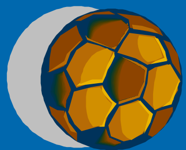
σ= total number of neutrons scattered per second / ϕ

$$\frac{d\sigma}{d\Omega} = \frac{\text{number of neutrons scattered per second into } d\Omega}{\phi d\Omega}$$

$$\frac{d\sigma}{d\Omega d\omega} = \frac{\text{number of neutrons scattered per second into } d\Omega \text{ \& } d\omega}{\phi d\Omega d\omega}$$

σ = Probability of hitting a target

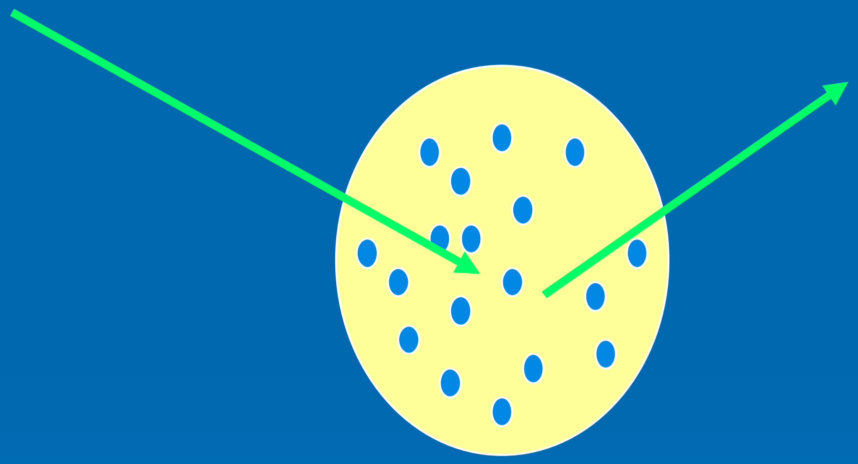
σ



=0.99

σ = Probability

… that a neutron scatters at an atom:



$$\sigma \approx 1 \text{ barn} = 10^{-24} cm^2$$

Surface of France:

$1000 \times 1000\ km^2$

$=10^6\ km^2 = 10^{12}\ m^2$

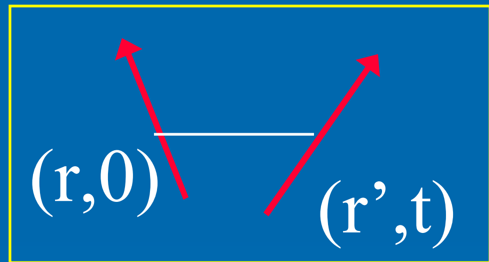
$=10^{18}\ mm^2 = 10^{24}\ \mu m^2$

Fourier transform

$$\frac{d^2\sigma}{d\Omega d\omega} \approx S(\mathbf{Q},\omega) = \text{FT in space and time of}$$

$$< S_{\mathbf{r}}^{\alpha}(t) S_{\mathbf{r'}}^{\beta}(0) > \text{ or } G(\mathbf{r},t)$$

S($\mathbf{Q}$,ω) is called the scattering function



$< S_{\mathbf{r}}^{\alpha}(t) S_{\mathbf{r'}}^{\beta}(0) >$ and G($\mathbf{r}$,t) are called space-time pair correlation functions

describe the Static and Dynamics of condensed matter at an atomic level.

S_{coh}(Q) and G_p(r) for simple liquids

- The peaks in g(r) represent atoms in “coordination shells”
- g(r) is expected to be zero for r < particle diameter
  – ripples are truncation errors from Fourier transform of S(Q)

Fig. 5.1 The structure factor $S(\kappa)$ for ^{36}Ar at 85 K. The curve through the experimental points is obtained from a molecular dynamics calculation of Verlet based on a Lennard-Jones potential. (After Yarnell *et al.*, 1973.)

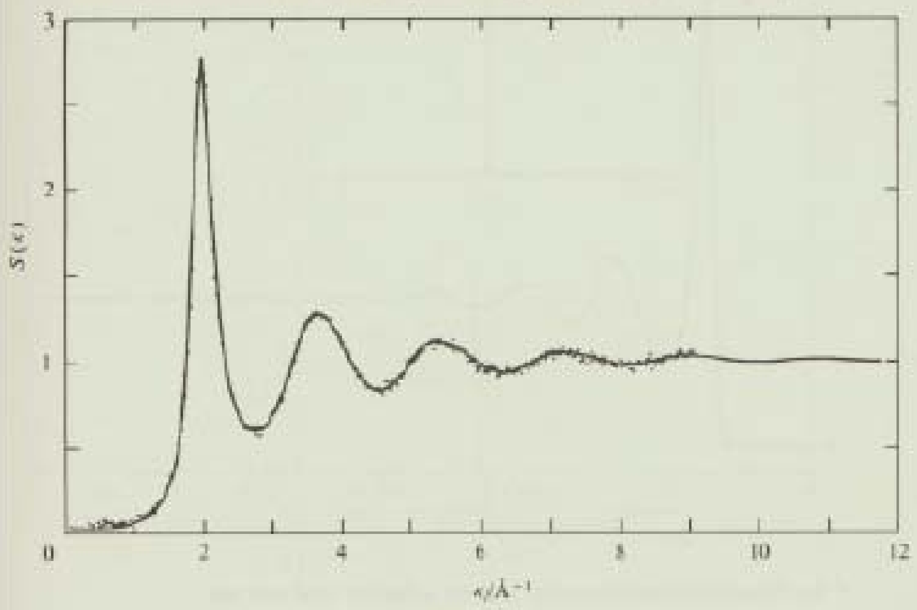
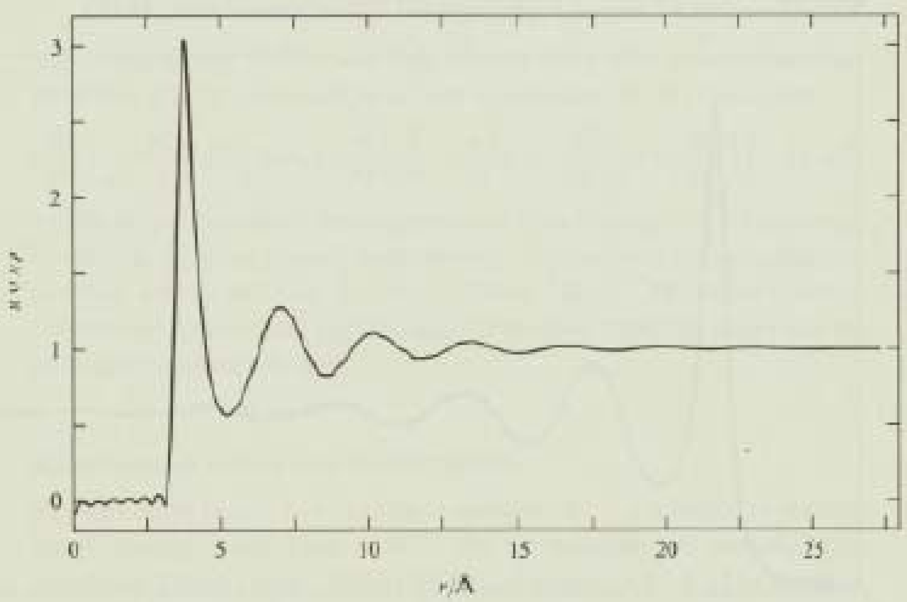


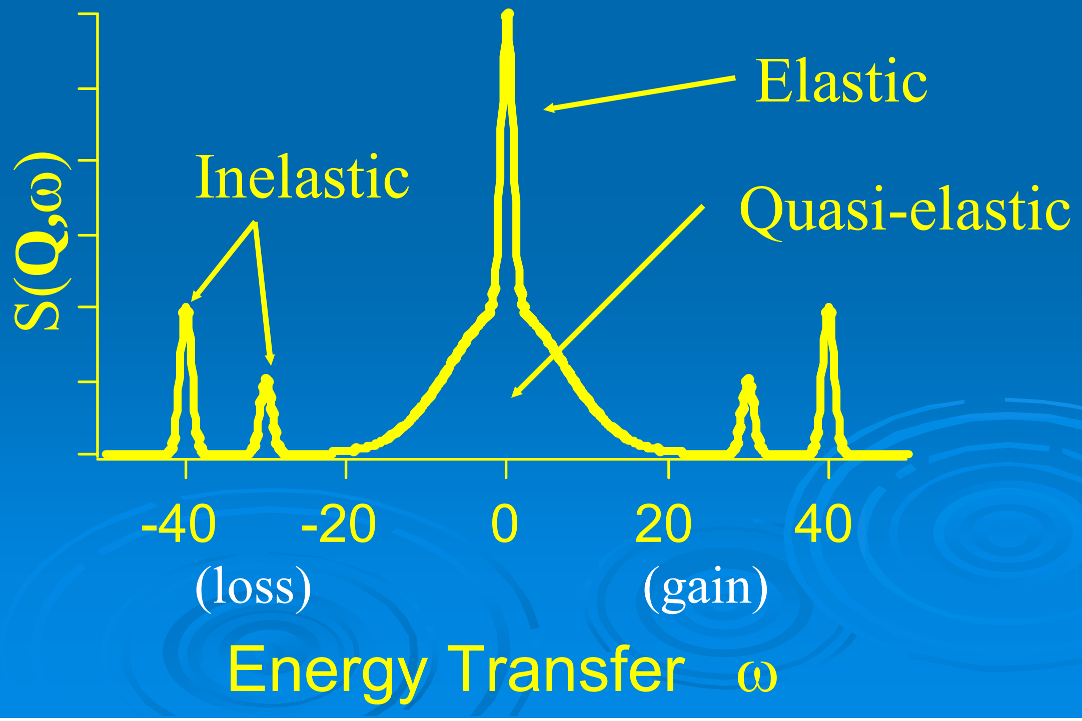
Fig. 5.2 The pair-distribution function $g(r)$ obtained from the experimental results in Fig. 5.1. The mean number density is $\rho = 2.13 \times 10^{28}$ atoms m^{-3}. (After Yarnell *et al.*, 1973.)



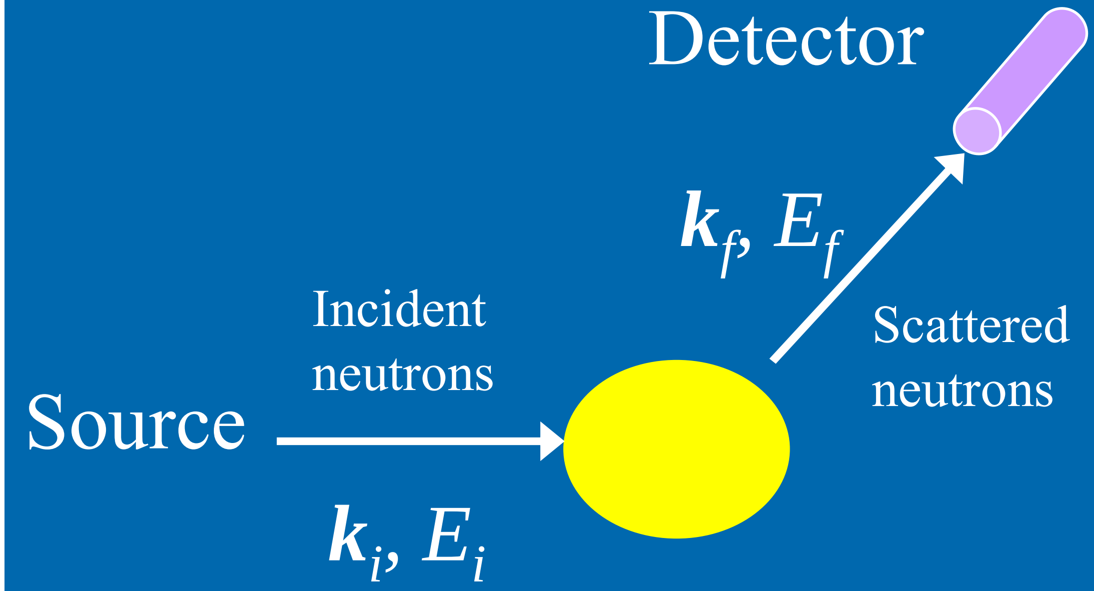
Scattering function S(Q,ω)

Intensity of scattered neutrons in detector is proportional to scattering function S(***Q***,ω):

- S(***Q***,ω) depends only on the sample, not on neutron instrument
- S(***Q***,ω) contains information about structure (***Q***) and dynamics (ω)



Neutron Scattering Experiment



Momentum Conservation

- $Q = k_i - k_f$

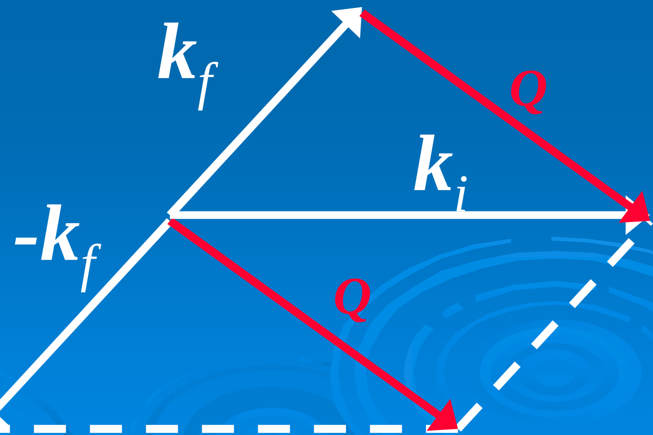
Q represents the momentum transferred to the sample.

In scattering plane:

4 independent parameters

k_x, k_y for initial and final neutrons
(E depends on k)

Scattering triangle:

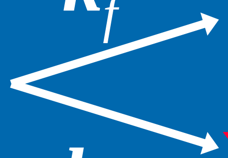


Elastic vs Inelastic Scattering

Energy conservation:

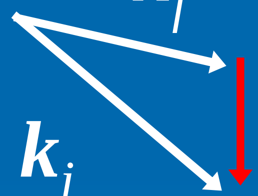
$$\Delta E_{neutron} = -\Delta E_{sample}$$

$$\Delta E_{sample} = E_i - E_f \equiv \hbar\omega = \frac{\hbar^2}{2m}\left(k_i^2 - k_f^2\right)$$



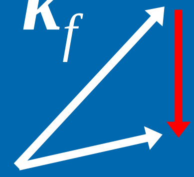
$k_i = k_f$

$\omega = 0$



$k_i > k_f$

$\omega > 0$



$k_i < k_f$

$\omega < 0$

Note: ω can vary independently of **Q** (here **Q**=cte, $|k_f|$=cte)

Paul Scherrer Institute

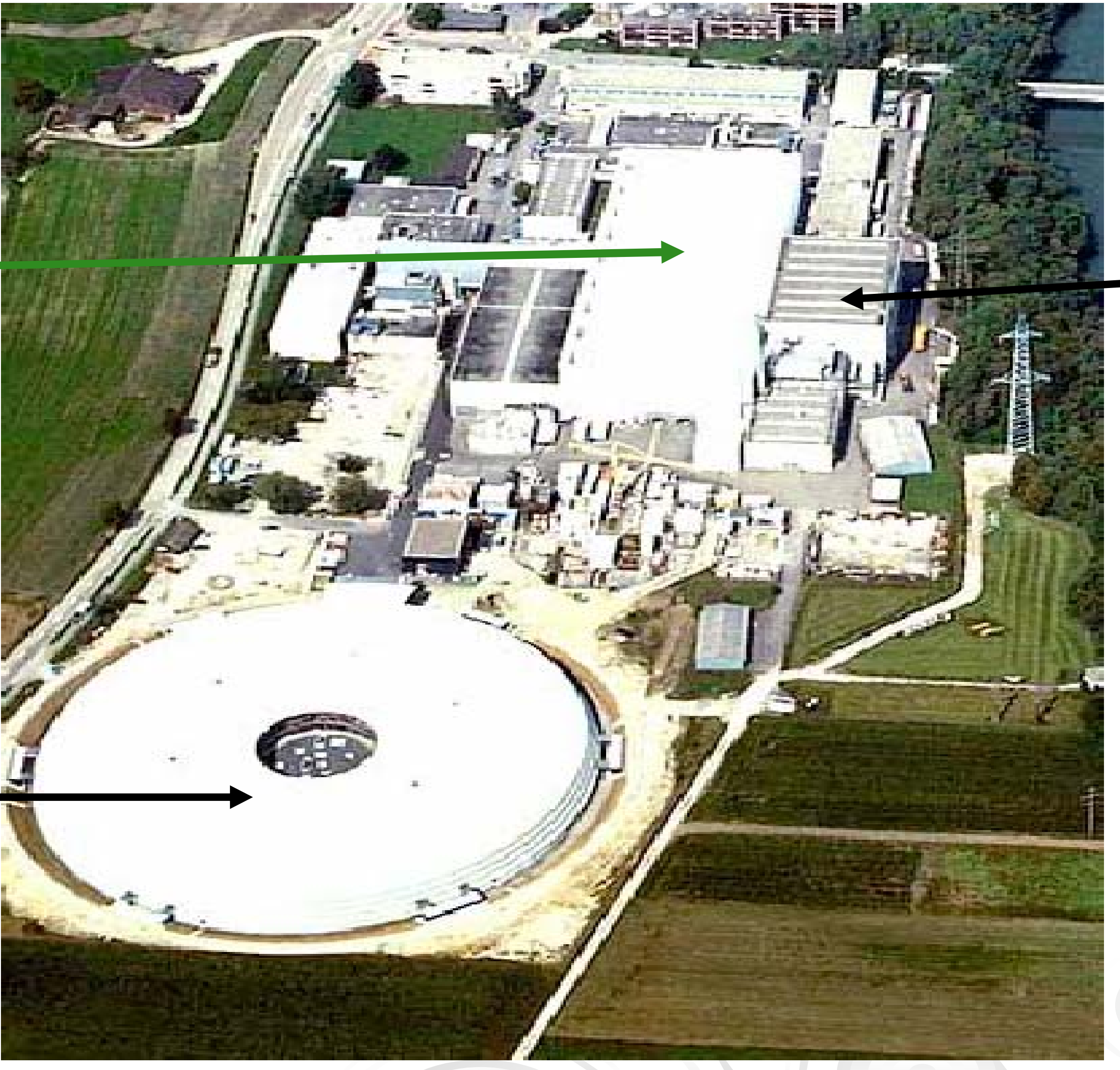
Bâle

Zurich

Muons

Neutrons

Photons



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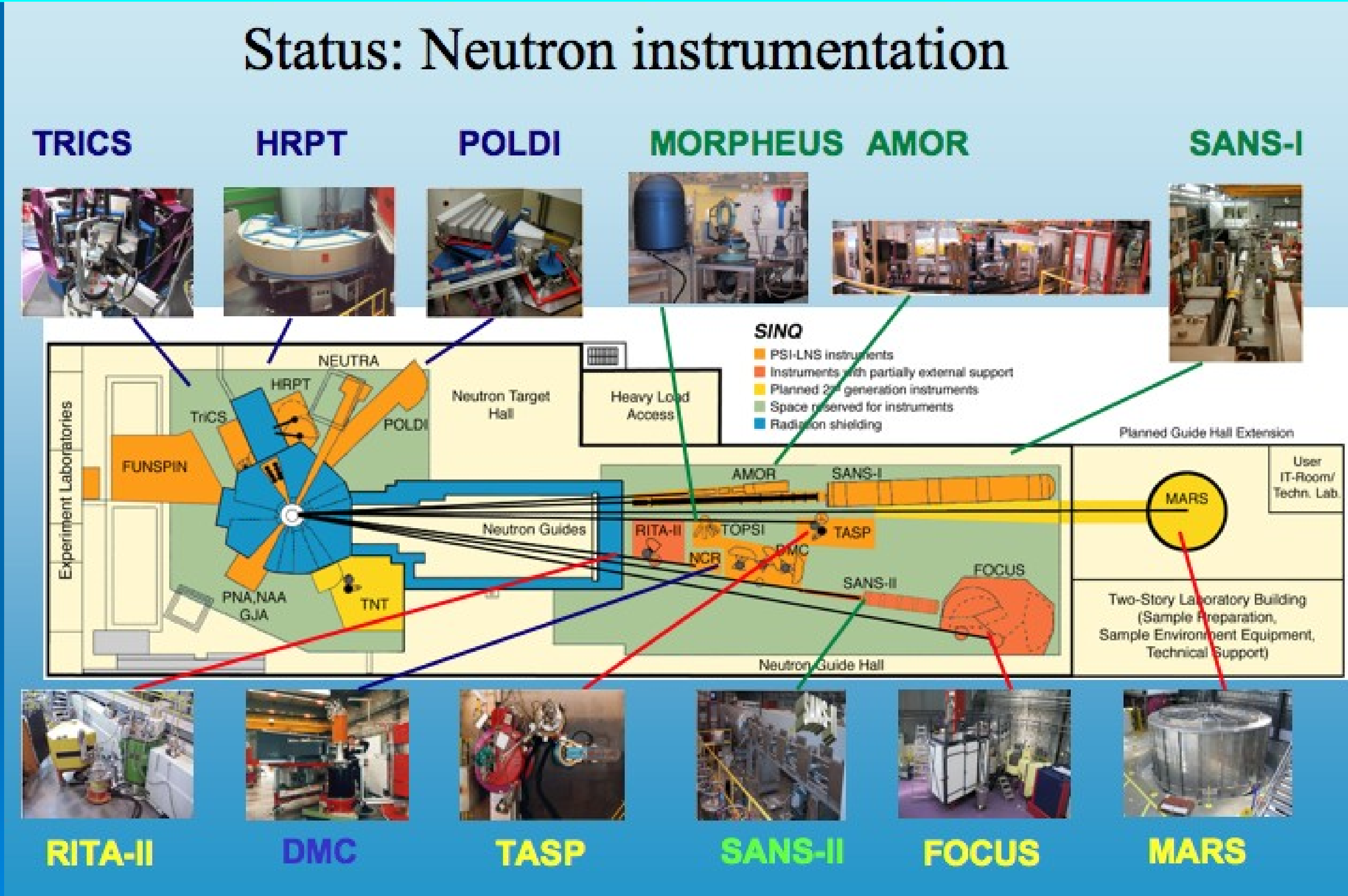
Neutron Scattering / Paul Scherrer Institute



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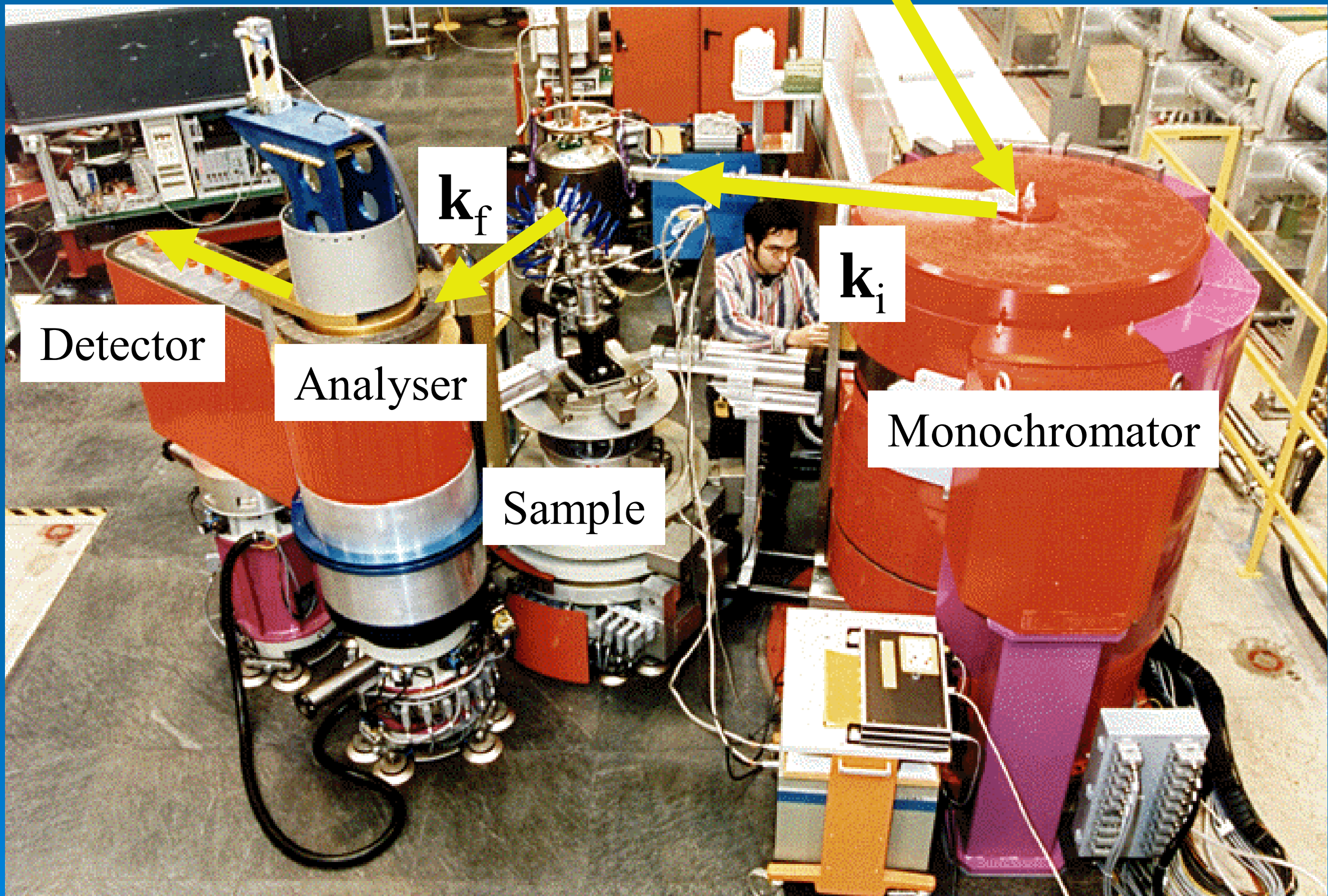
Triple-Axis Spectrometer TASP @ PSI



$$E(meV) = 2\left[\mathbf{k}\left(\AA^{-1}\right)\right]^2$$

Sample

Q=-(k$_f$-k$_i$)

$$\hbar\omega = -\left(E_f - E_i\right)$$

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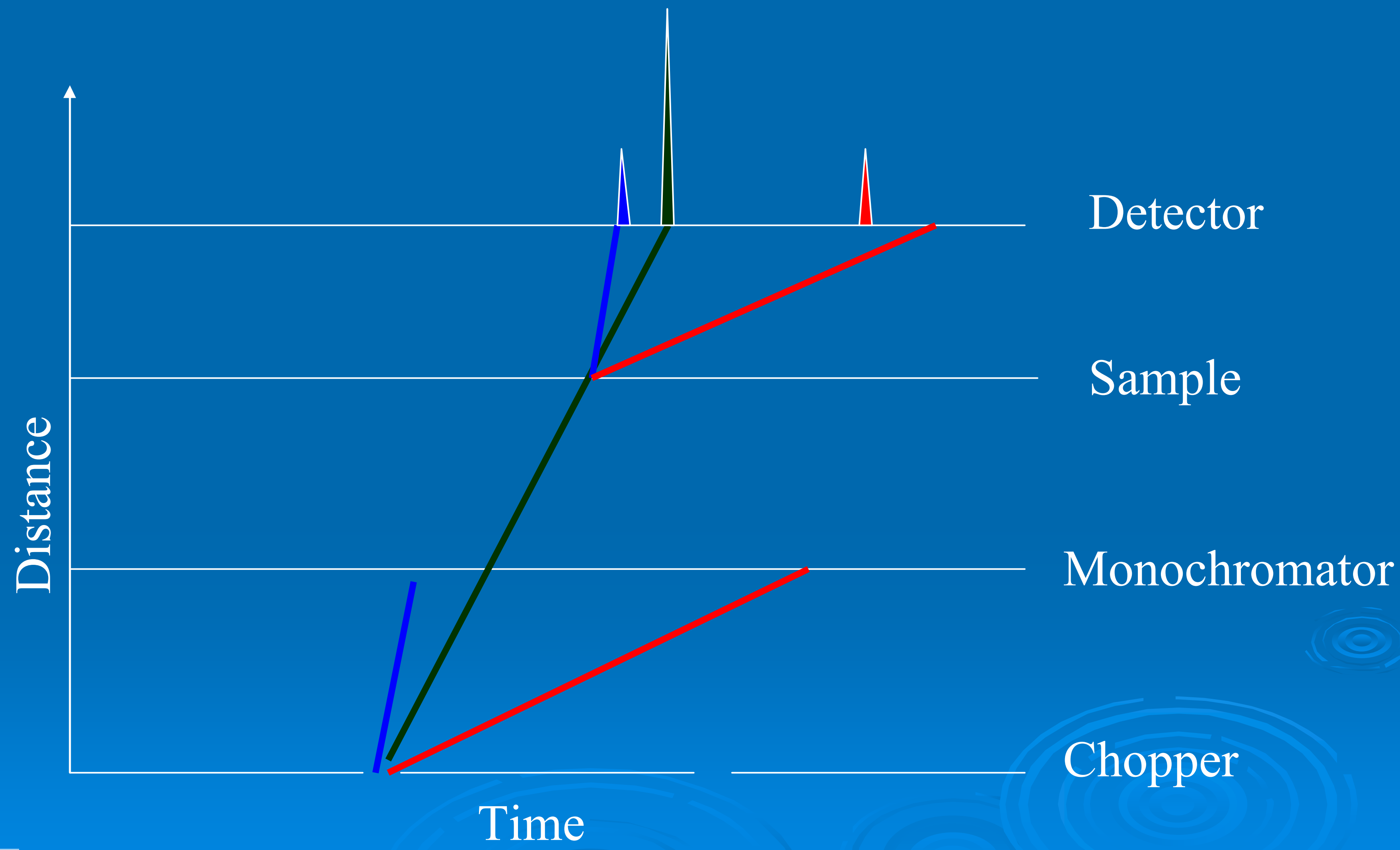
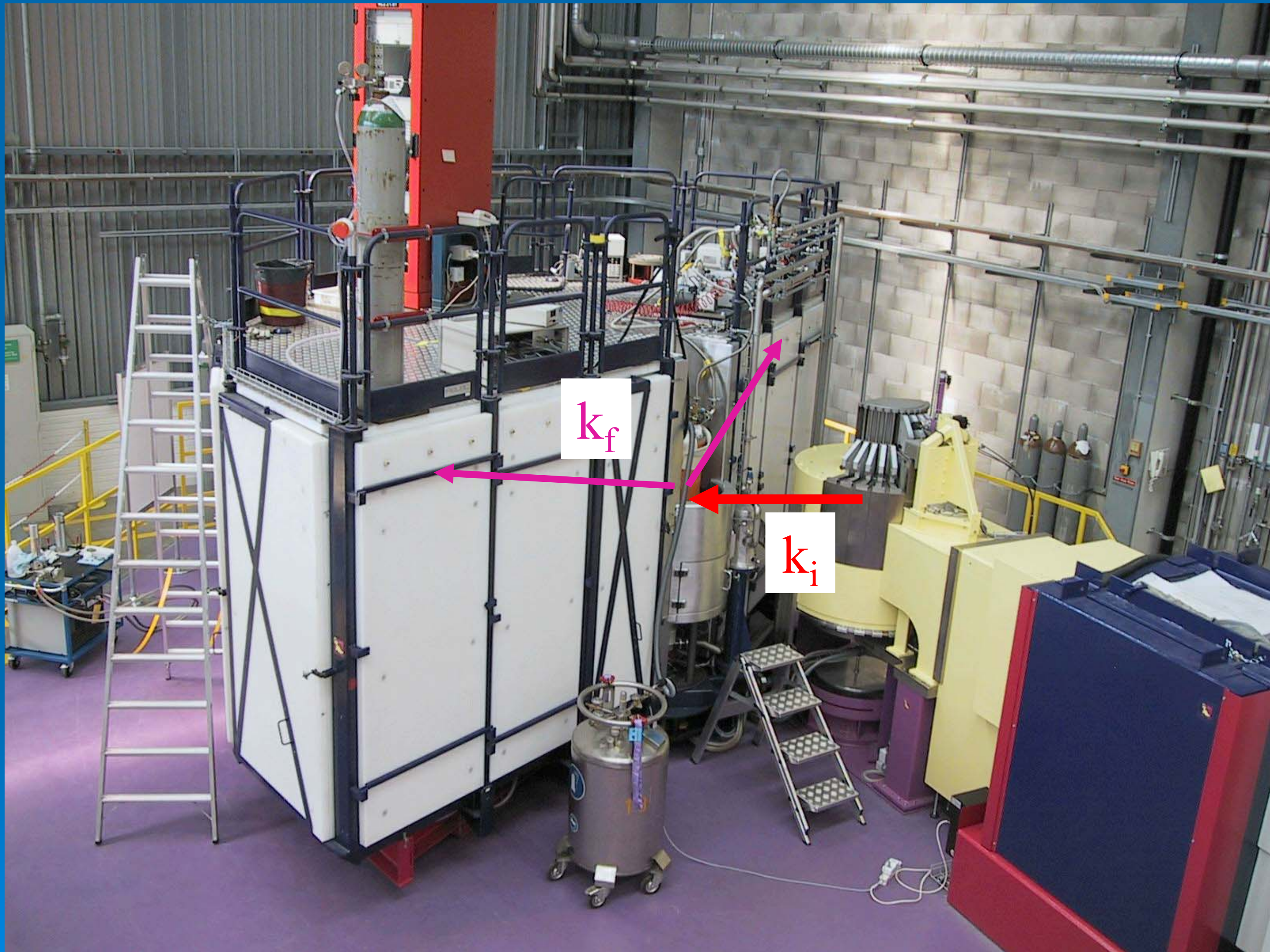
Time-of-flight technique



SINQ-FOCUS

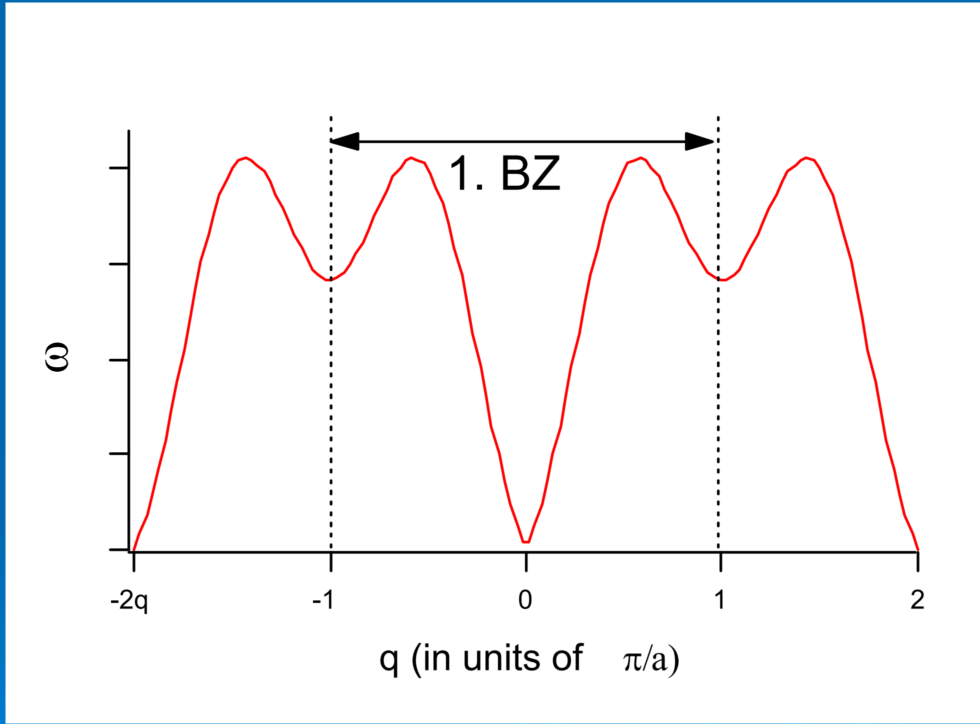


NN+NNN…

$$M\ddot{u}_n = F_n = \sum_j \beta_1(u_{n+j} + u_{n-j}) + \beta_0 u_n$$

$$u_n = \xi e^{i(\omega t + qna)}$$

$$\omega^2 = \frac{4}{M}\sum_j \beta_j \sin^2\left(\frac{jqa}{2}\right)$$

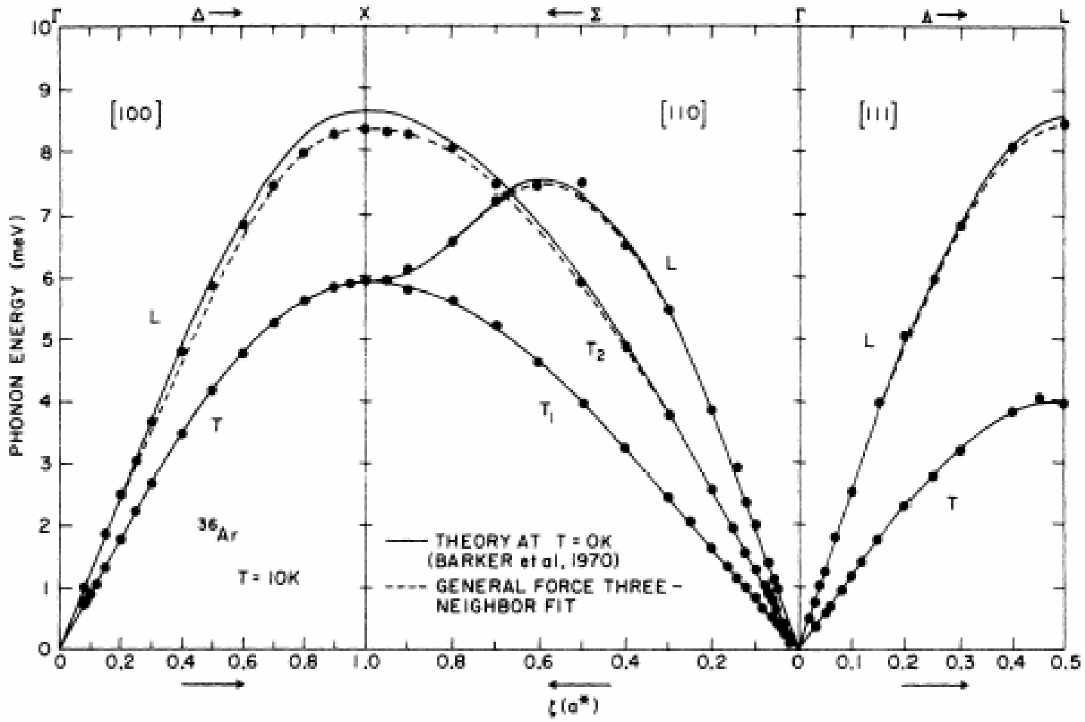


$$\beta_1 = 2\beta_2$$

$$\beta_j = 0 \; if \; j > 2$$

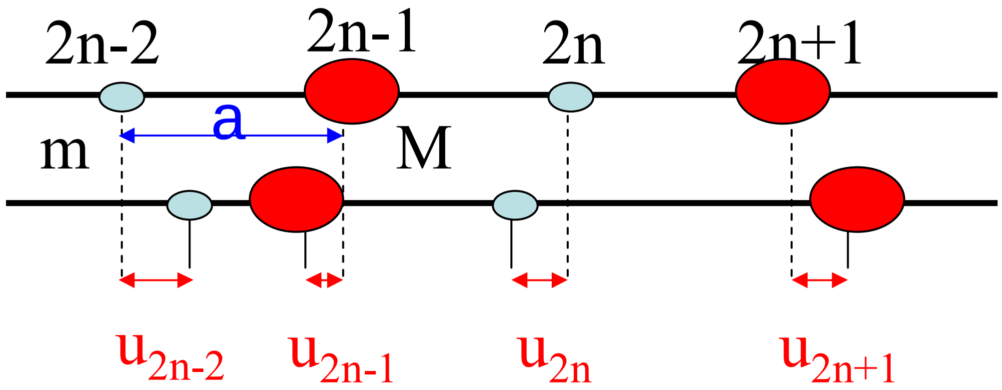
Phonons in Ar (FM-3M)

(Fujii PRB **10** (1974) 3647)



Force constant	Model 1	Model 2	Model 3	Batchelder *et al.* ($T = 4$ K)
$1XX$	609 ± 4	605 ± 5	605 ± 5	604
$1ZZ$	− 8 ± 3	5 ± 7	0 ± 7	− 7
$1XY$	617 ± 5	633 ± 9	633 ± 9	531
$2XX$	− 44 ± 4	− 24 ± 11	− 24 ± 11	− 60
$2YY$	− 2 ± 3	− 3 ± 4	− 1 ± 4	− 21
$3XX$	0 ± 2	− 5 ± 4	− 2 ± 4	···
$3YY$	0 ± 1	0 ± 1	0 ± 1	···
$3YZ$	0 ± 1	0 ± 2	− 1 ± 2	···
$3ZX$	0 ± 1	− 2 ± 2	− 1 ± 2	···
α	0	− 32 ± 12	− 28 ± 12	80
β	0	− 5 ± 5	0 ± 5	···
γ	0	− 3 ± 7	− 1 ± 7	···

Linear chain with 2 atoms



$$m\ddot{u}_{2n} \;\; = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n})$$

$$M\ddot{u}_{2n+1} = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1})$$

Solution:

$$u_{2n} = \xi e^{i(\omega t + 2nqa)}$$

$$u_{2n+1} = \eta e^{i(\omega t + [2n+1]qa)}$$

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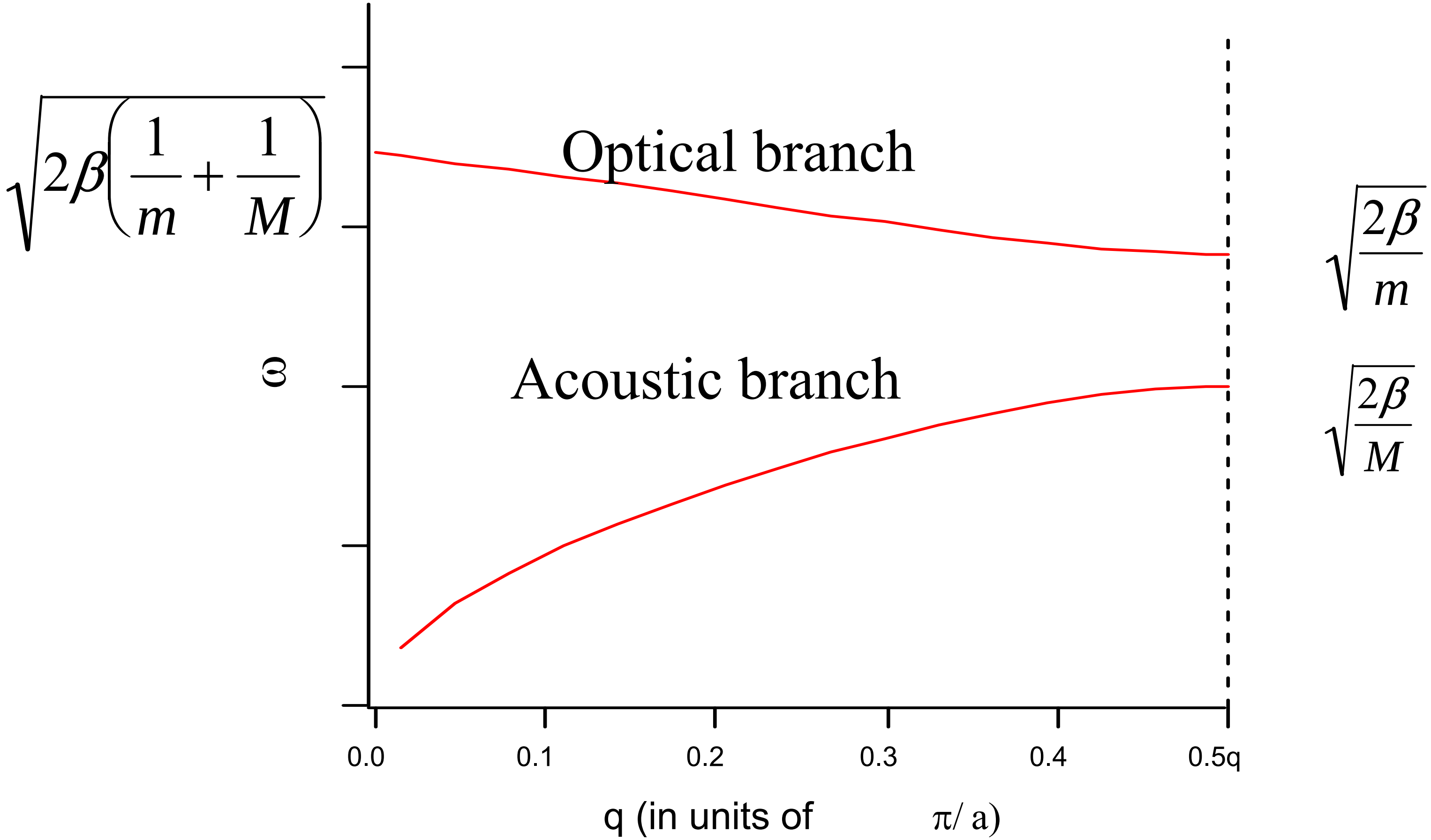
$$-\omega^2 m\xi = \beta\eta\left(e^{iqa} - e^{-iqa}\right) - 2\beta\xi$$

$$-\omega^2 M\eta = \beta\xi\left(e^{iqa} - e^{-iqa}\right) - 2\beta\eta$$

Non-trivial solution:

$$\begin{vmatrix} 2\beta - \omega^2 m & -2\beta\cos(\mathrm{qa}) \\ -2\beta\cos(\mathrm{qa}) & 2\beta - \omega^2 M \end{vmatrix} = 0$$

$$\omega^2 = \beta\left(\frac{1}{m} + \frac{1}{M}\right) \pm \beta\left[\left(\frac{1}{m} + \frac{1}{M}\right)^2 - \frac{4\ \sin^2(qa)}{m\ M}\right]^{\frac{1}{2}}$$



Visualization of atomic motions:

$$u_{2n}/u_{2n+1}=\frac{\xi}{\eta}e^{-iqa}$$

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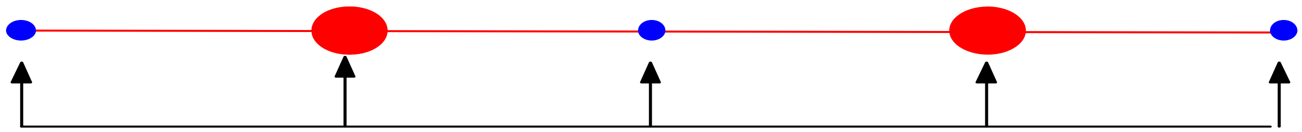
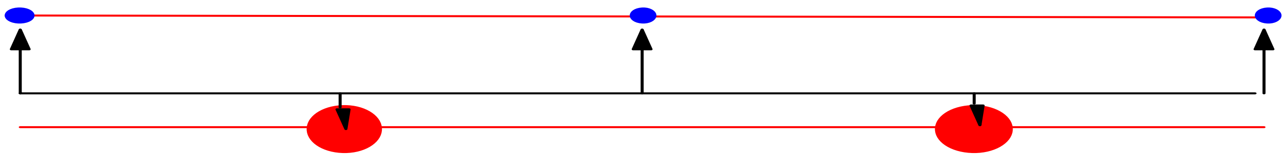
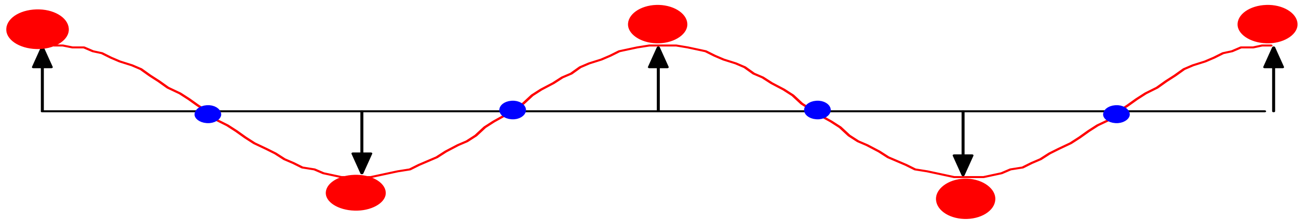
$q = 0$, akustisch



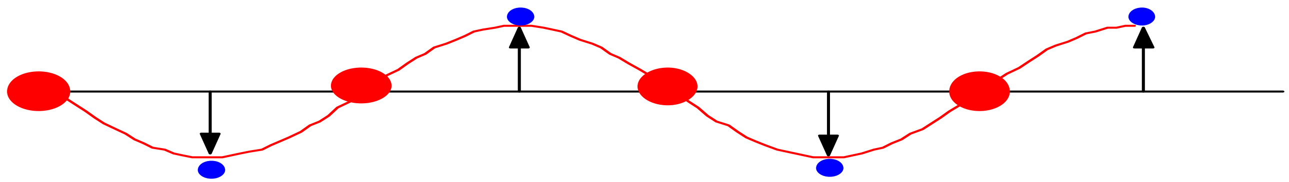
$q = 0$, optisch



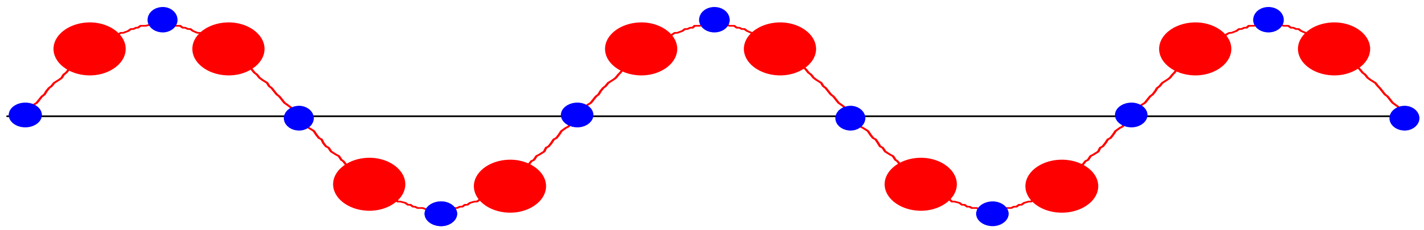
$q = \frac{\pi}{2a}$, akustisch



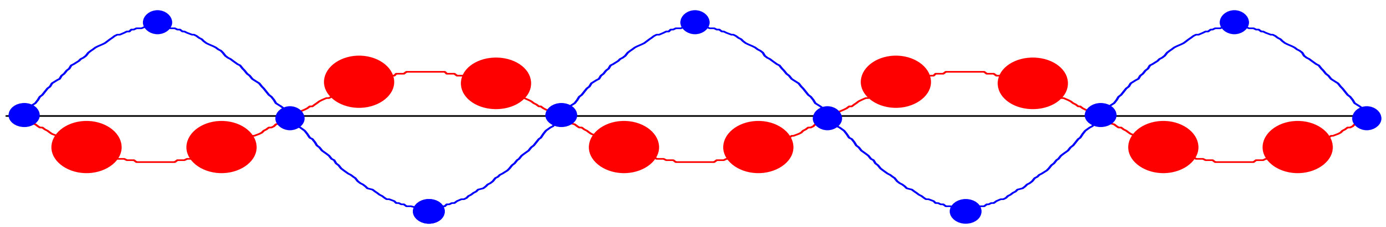
$q = \frac{\pi}{2a}$, optisch



$$0 \le q \le \frac{\pi}{2a}, \text{ acoustic}$$



$$0 \le q \le \frac{\pi}{2a}, \text{ optical}$$



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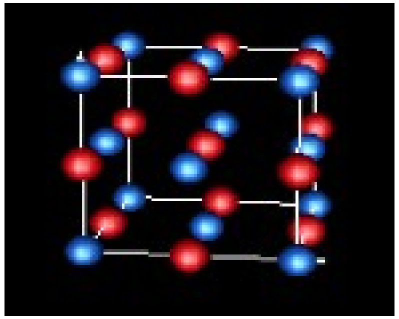
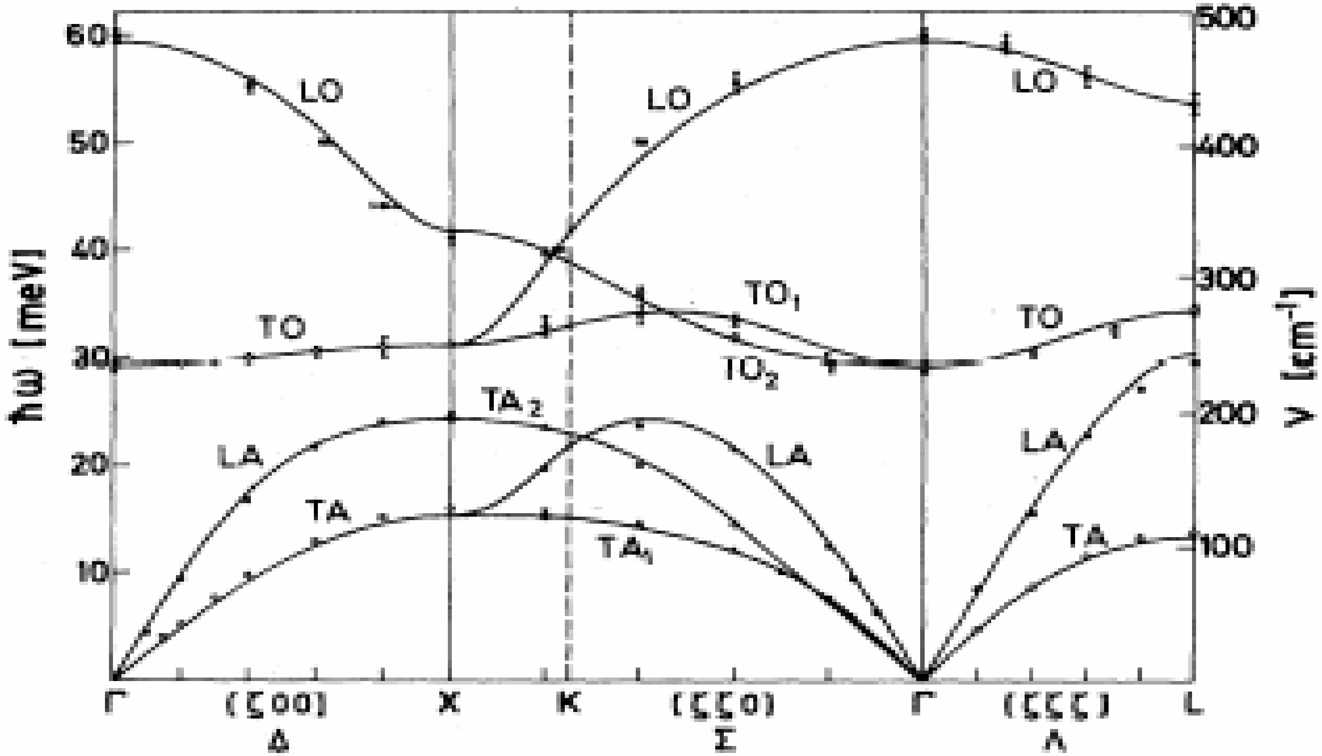


SrO (NaCl Structure)

Rieder, PRB **12** (1975) 3374



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Low Dimension: what for?

•Quantum fluctuations become increasingly important as the dimension is reduced.

ABSENCE OF FERROMAGNETISM OR ANTIFERROMAGNETISM IN ONE- OR TWO-DIMENSIONAL ISOTROPIC HEISENBERG MODELS*

N. D. Mermin† and H. Wagner‡
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York
(Received 17 October 1966)

It is rigorously proved that at any nonzero temperature, a one- or two-dimensional isotropic spin-S Heisenberg model with finite-range exchange interaction can be neither ferromagnetic nor antiferromagnetic. The method of proof is capable of excluding a variety of types of ordering in one and two dimensions.

➢ A challenge on all length scales

Maybe the “Big Bang” was powered by “Vacuum Quantum Fluctuations” ? (Hawkins *et al.*)

De plus l'inflation possède, comme toute forme de matière, des fluctuations quantiques (résultat de l'inégalité de Heisenberg). Une des conséquences inattendues de l'inflation est que ces fluctuations initialement de nature quantique évoluent durant la phase d'expansion accélérée pour devenir des variations classiques ordinaires de densité. Par ailleurs le calcul du spectre de ces fluctuations effectué dans le cadre de la théorie des perturbations cosmologiques montre qu'il suit précisément les contraintes du spectre de Harrison-Zeldovitch.

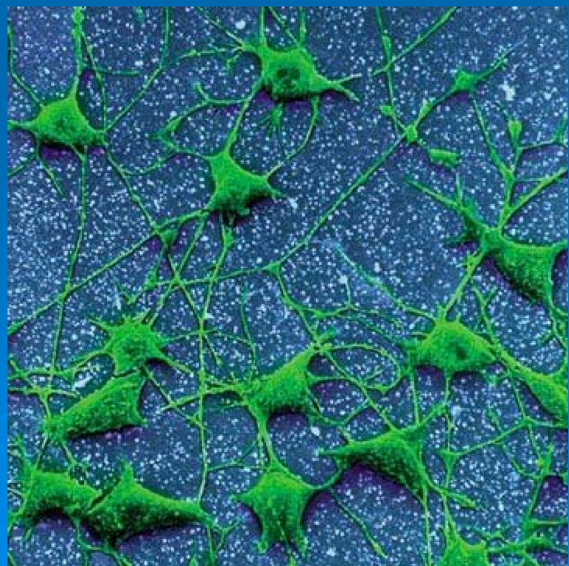
Neural networks ⇒

PHYSICAL REVIEW A VOLUME 34, NUMBER 4 OCTOBER 1986

Spin-glass models of a neural network

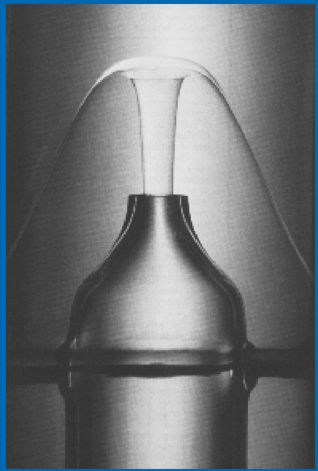
J. L. van Hemmen
Sonderforschungsbereich 123 der Universität Heidelberg, D-6900 Heidelberg 1, Federal Republic of Germany
(Received 1 November 1985)

A general theory of spin-glass-like neural networks with a Monte Carlo dynamics and finitely many attractors (stored patterns) is presented. The long-time behavior of these models is determined by the equilibrium statistical mechanics of certain infinite-range Ising spin glasses, whose thermodynamic stability is analyzed in detail. As special cases we consider the Hopfield and the Little model and show that the free energy of the latter is twice that of the former because of a *duplication* of spin variables which occurs in the Little model. It is also indicated how metastable states can be partly suppressed or even completely avoided.



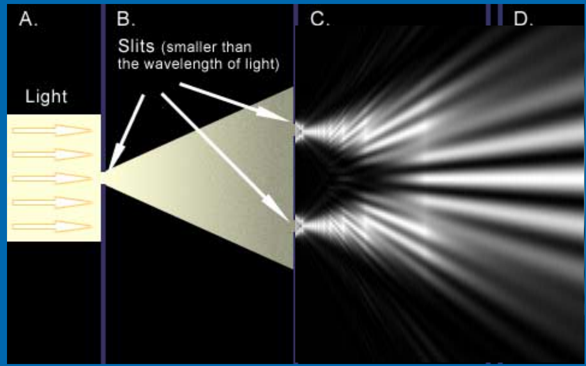
Quantum Matter

Quantum Order

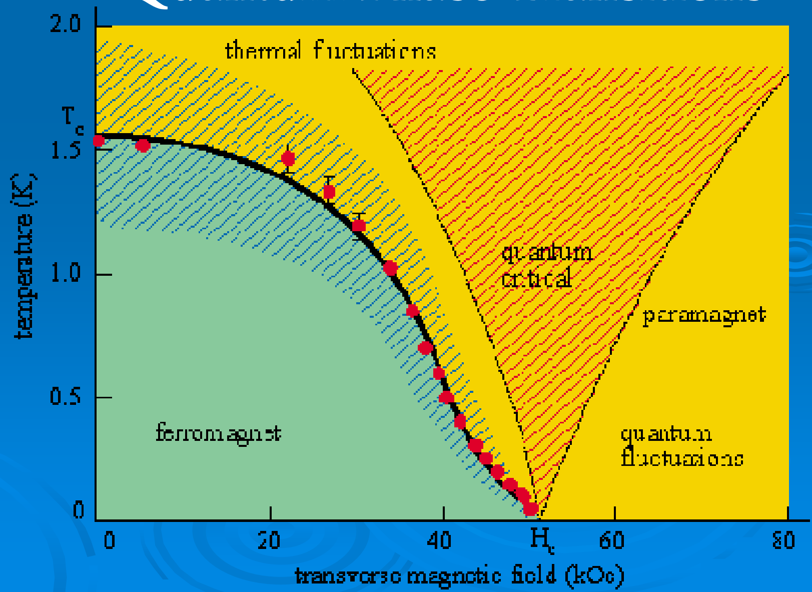


Classical Order

Entanglement



Quantum Phase Transitions



Classical Phase Transitions

New Phases of Matter

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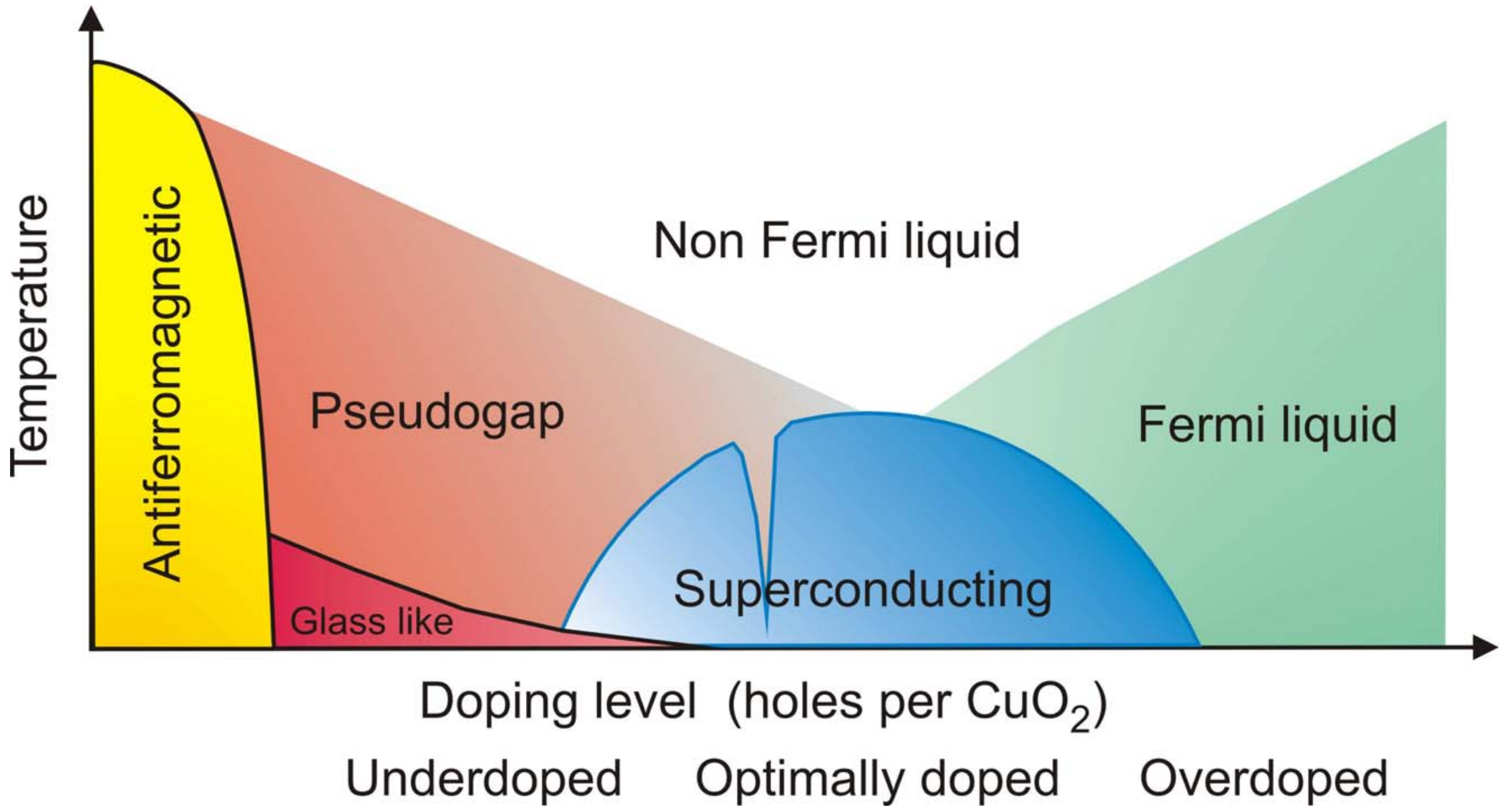
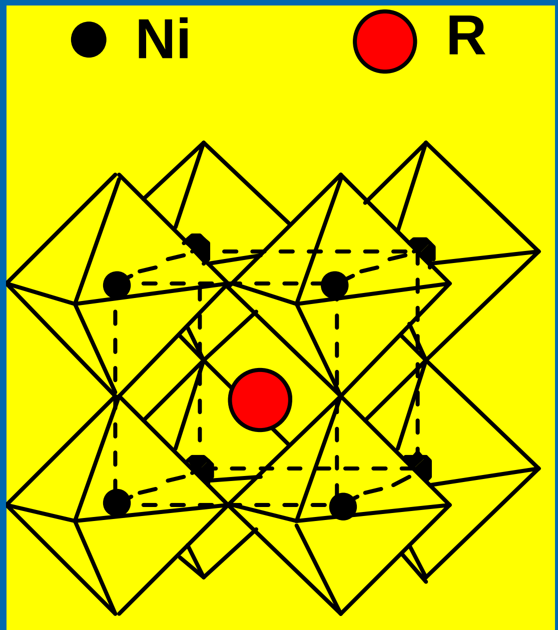
$La_{2-x}Sr_xCuO_4$



Low Dimensional Systems



3D ($RNiO_3$)

Isotropic properties

($\rho_a \approx \rho_b$, ρ_c)

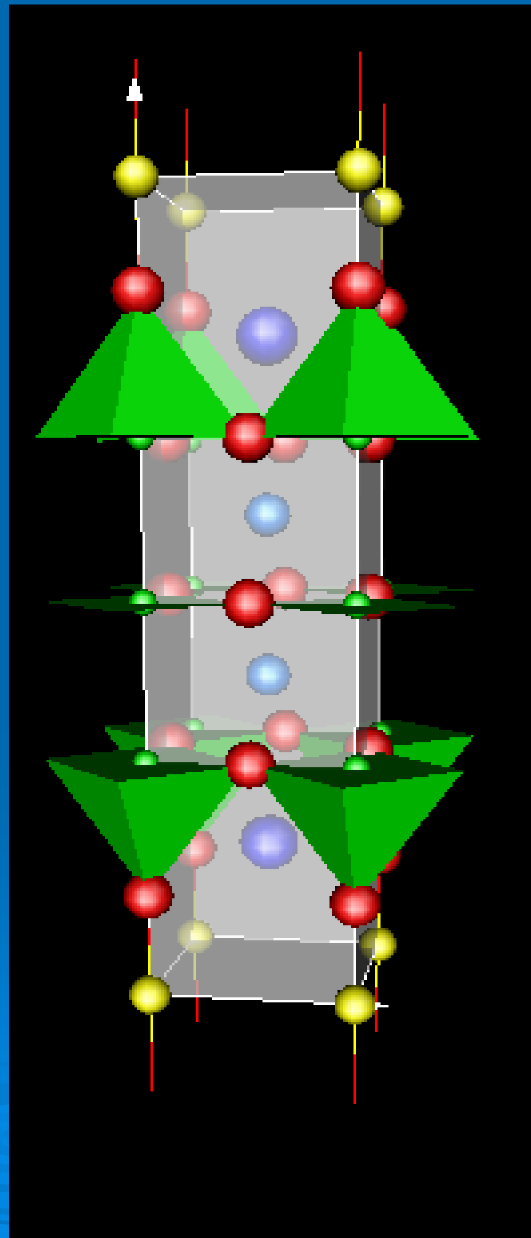
2D

Manganites

Cuprates

Anisotropic properties

($\rho_a \approx \rho_b << \rho_c$)



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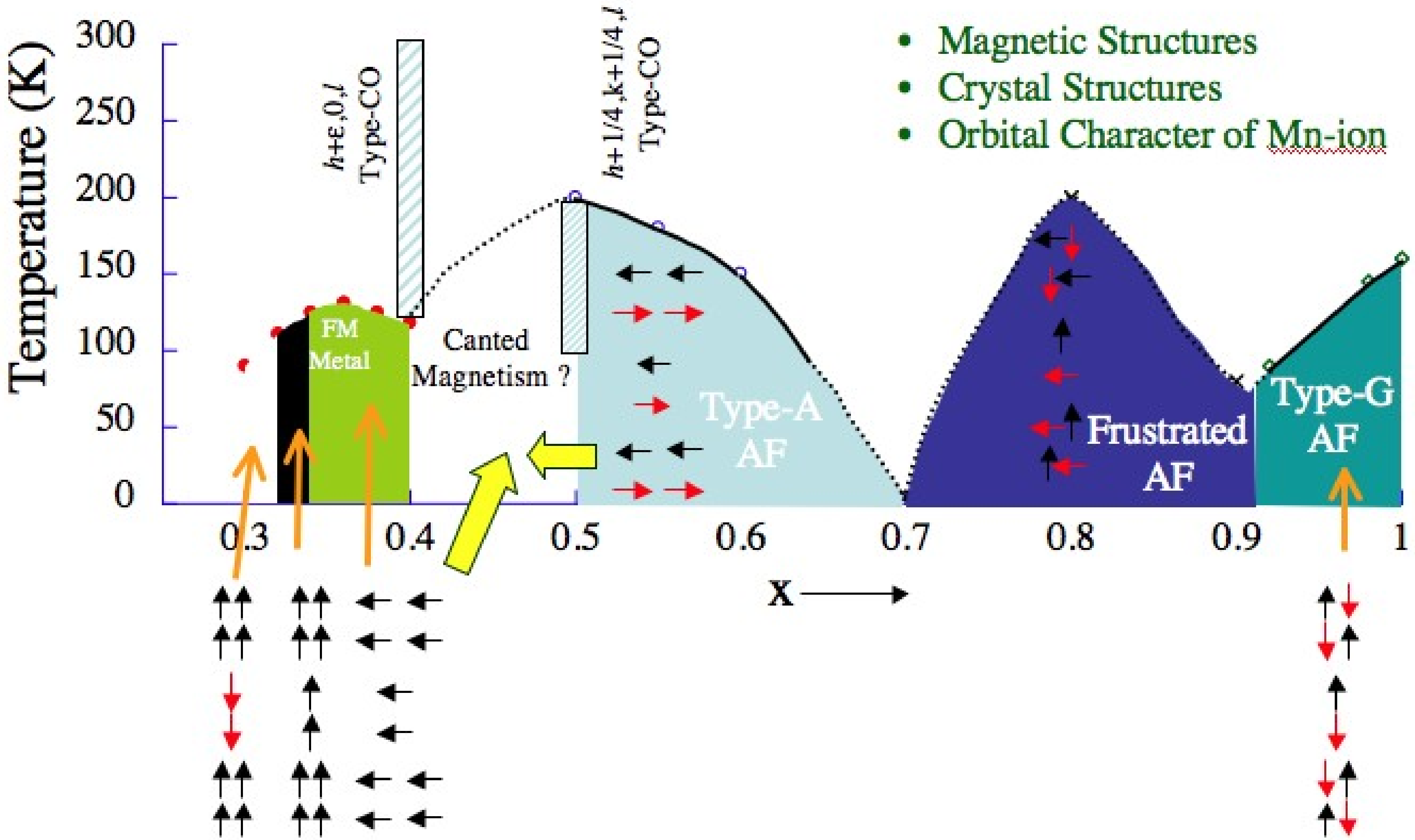
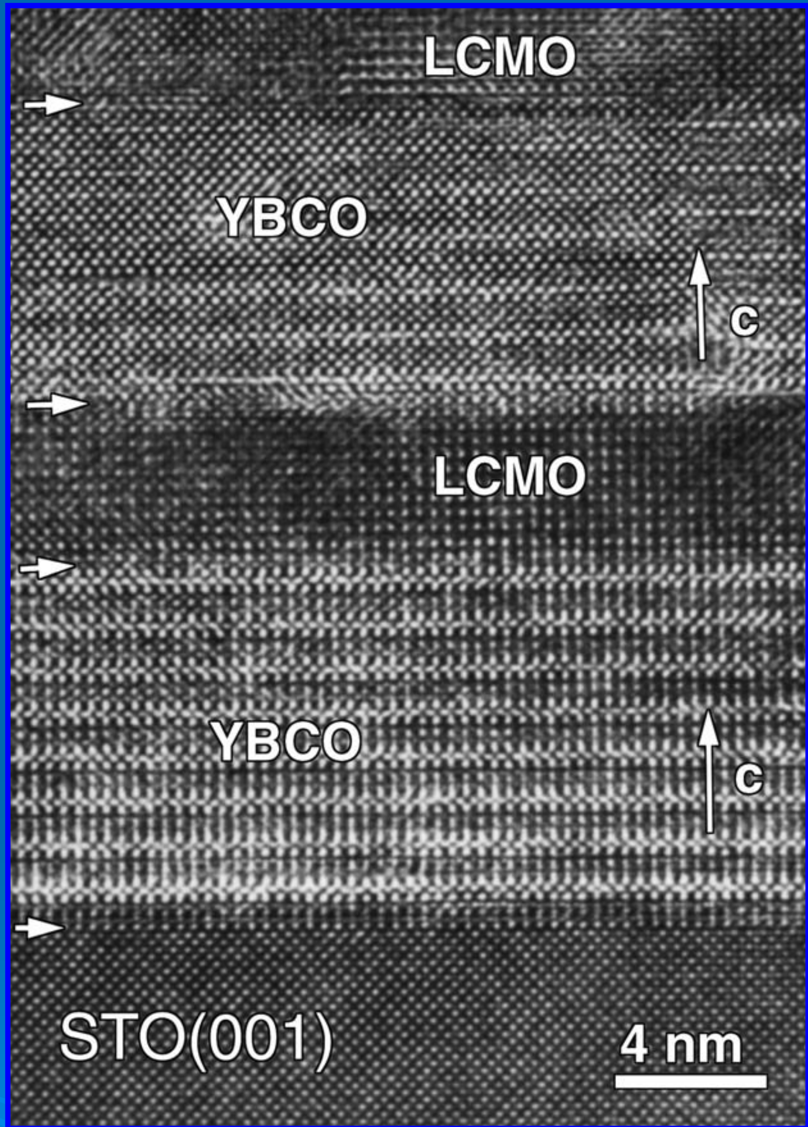
$La_{2-2x}Sr_{1+2x}Mn_2O_7$



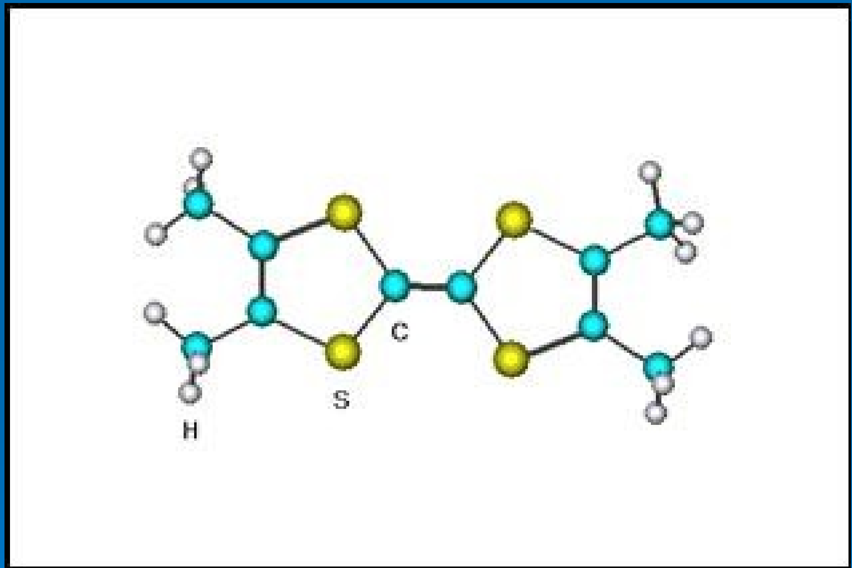
Artificial multliayers

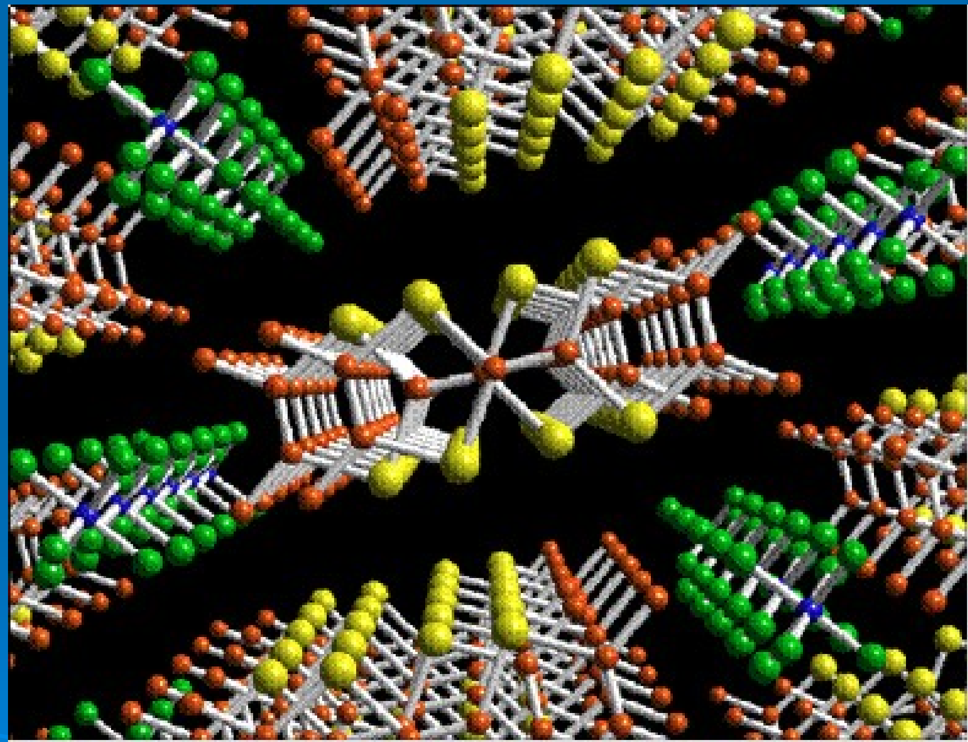
Habermeier
MPI, Stuttgart



What about 1 Dimension?

Organic conductors $(TMTSF)_2PF_6$
Bechgaard's salt $(TM)_2X$





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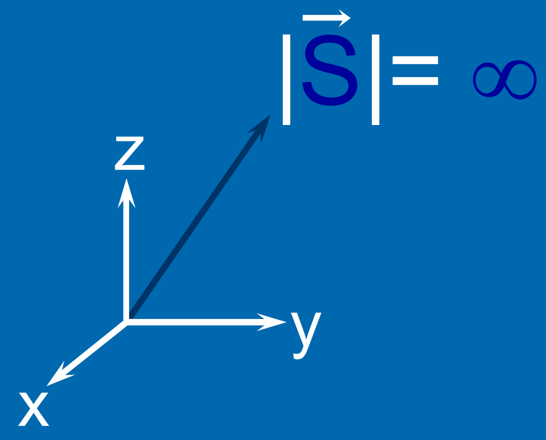
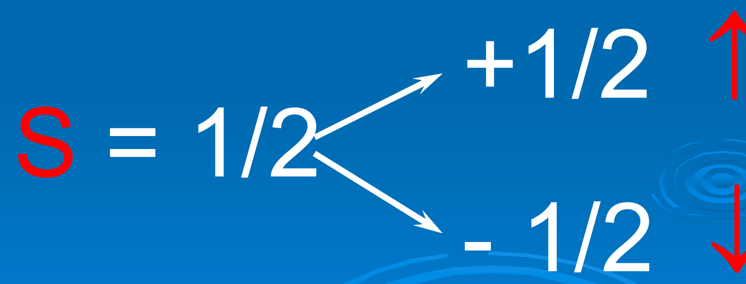
Alternative: Physics of Spins

- "Atomic scale bar-magnets"
- S = *n*/2, the archetype of quantisation.
- Classical magnetic moments, |S| = ∞, are vectors that point in some specified direction.



- Quantum spins, S = 1/2, only have two states, neither of which reveals the full moment $\sqrt{S(S+1)}$



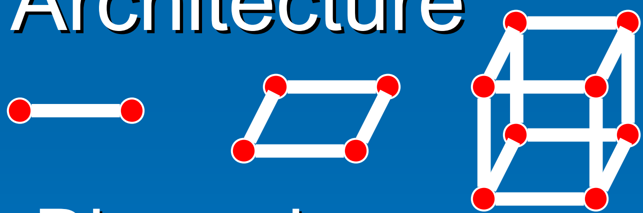
Building models

- Spins

  Length: |S|=1/2 … ∞
  Quantum / classical

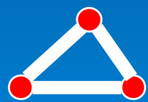
  Dimension: Ising, XY, Heisenberg

- Architecture



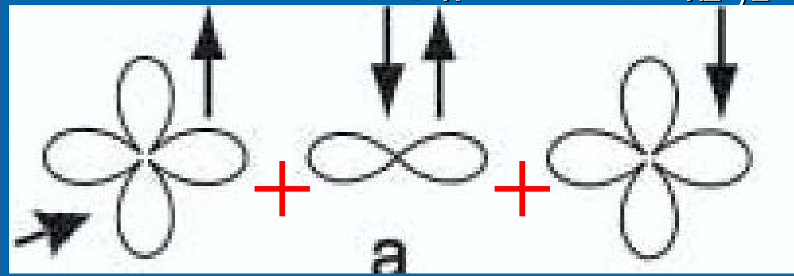
  Dimension

  Connectivity



- Interactions

  Cu^{2+} O $2p_x$ Cu $3d_{x2-y2}$



  ☞ $= -2J \sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j$

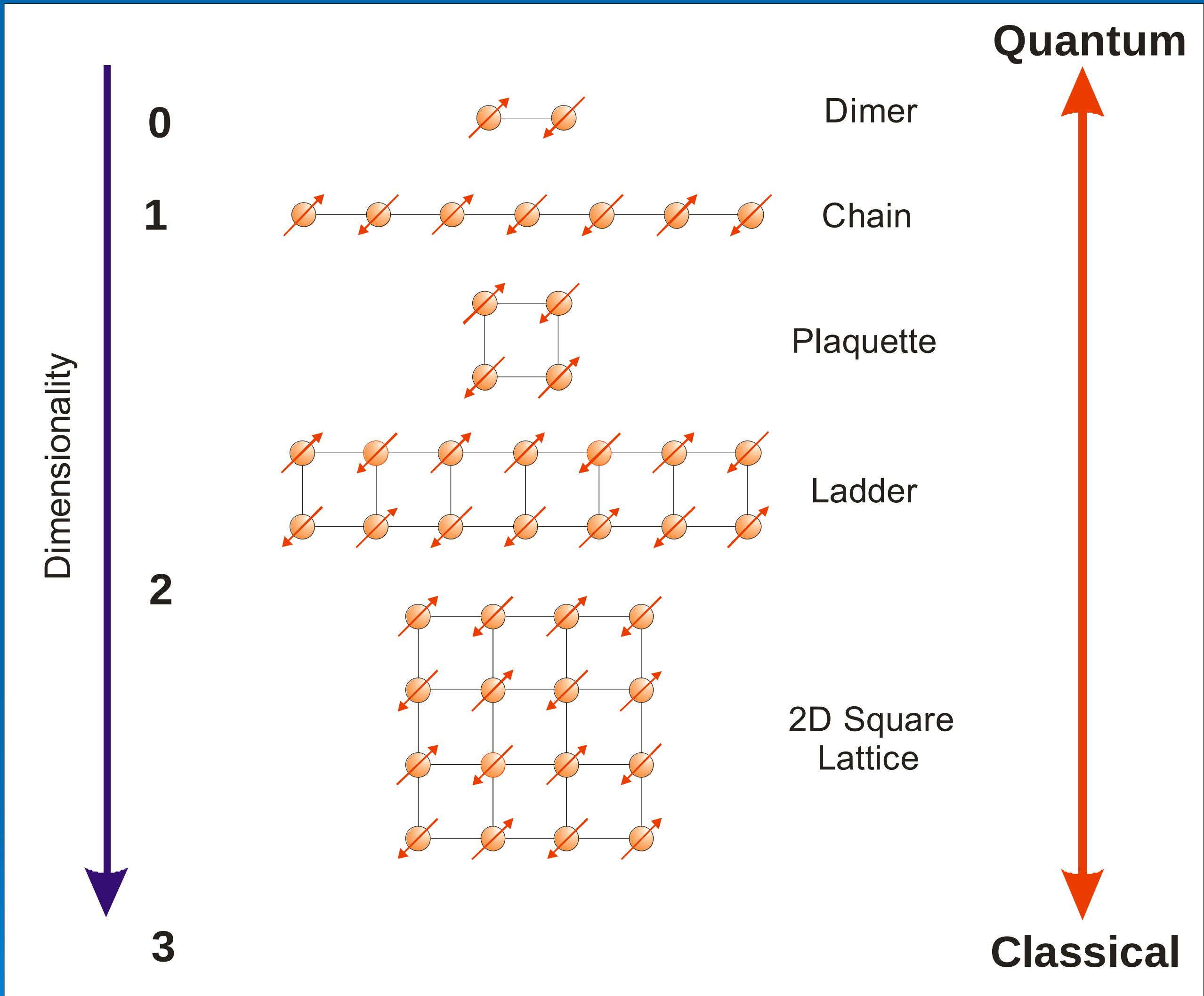
  Anti-/Ferromagnetic

- Extensions

  Randomness

  Charge, orbit, lattice...

Magnetic Architecture



Two dimensions: border between classical and quantum world

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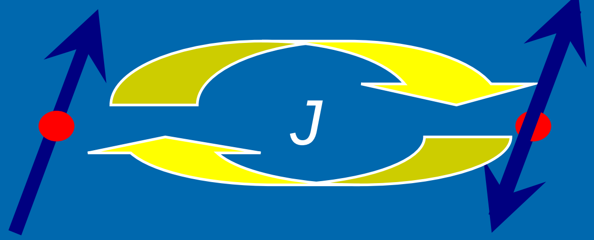
Example: Spin=1/2 Dimer

$\mathcal{H} = -2J \sum \boldsymbol{S}_i \cdot \boldsymbol{S}_j$



Ferromagnet: $J > 0$

$|GS\rangle = |\uparrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$

"Classical"

Antiferromagnetic: $J < 0$

$E = 3/4J$ — $S_{tot}=1$: $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$

J

$-1/4J$ — $S_{tot}=0$: $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$

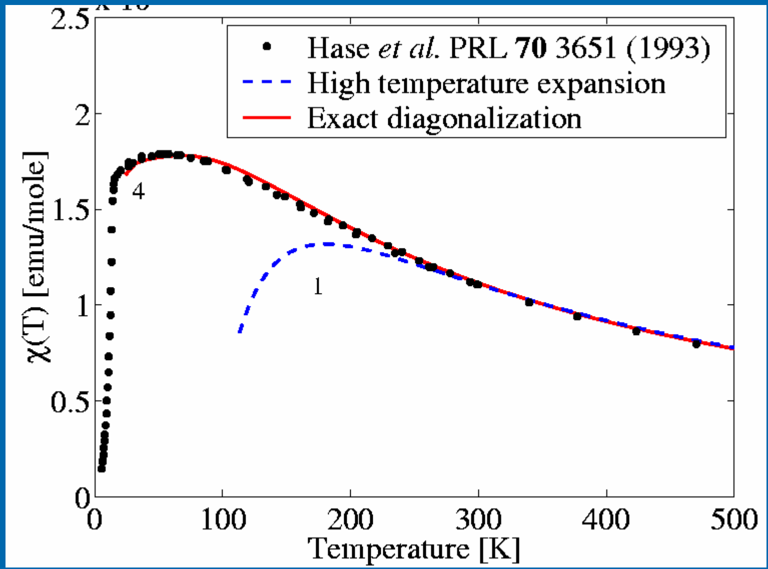
Singlet ground state: prototype of entanglement

$\langle S^z{}_1\rangle = \langle S^z{}_2\rangle = 0$

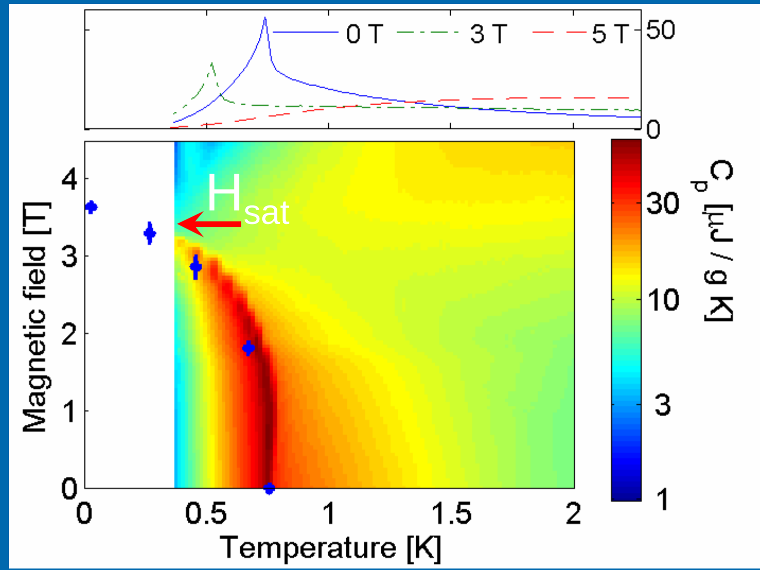
How to investigate such magnetic states?

Magnetic measurements

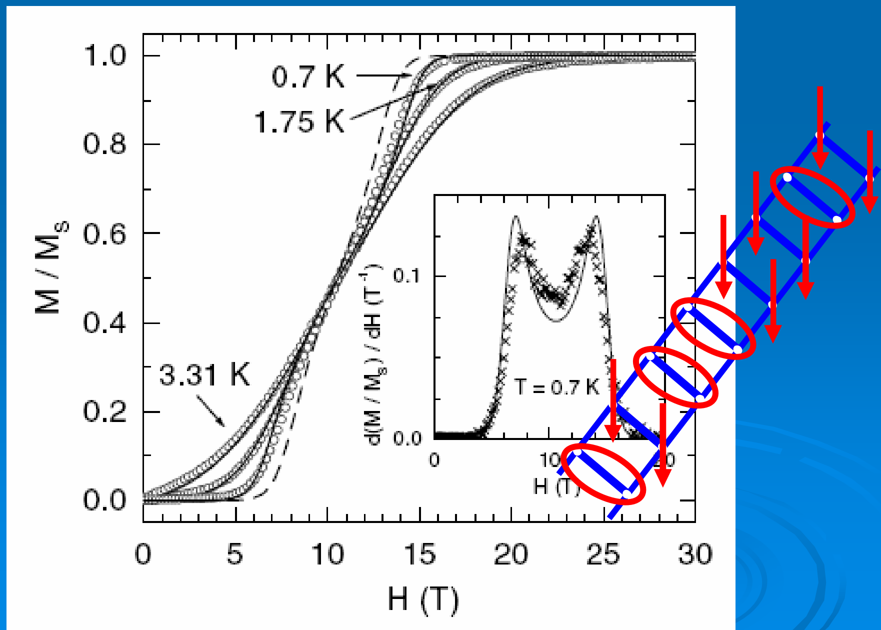
Susceptibility



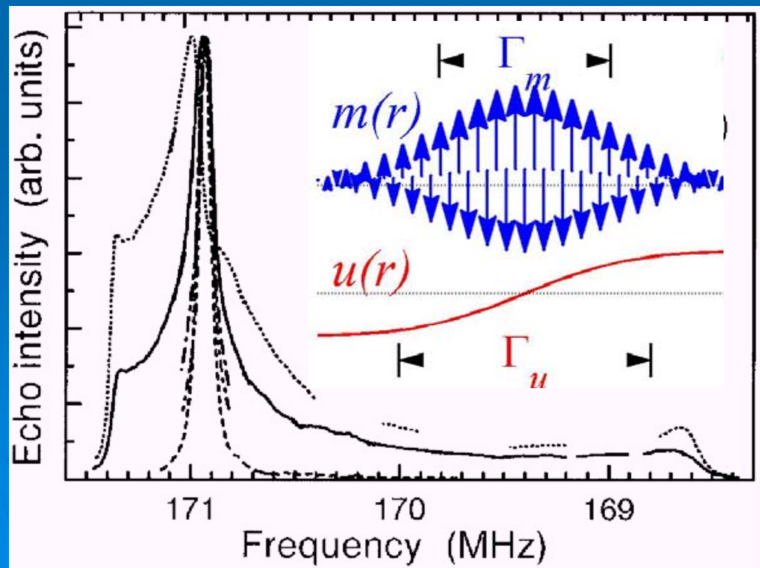
Specific heat

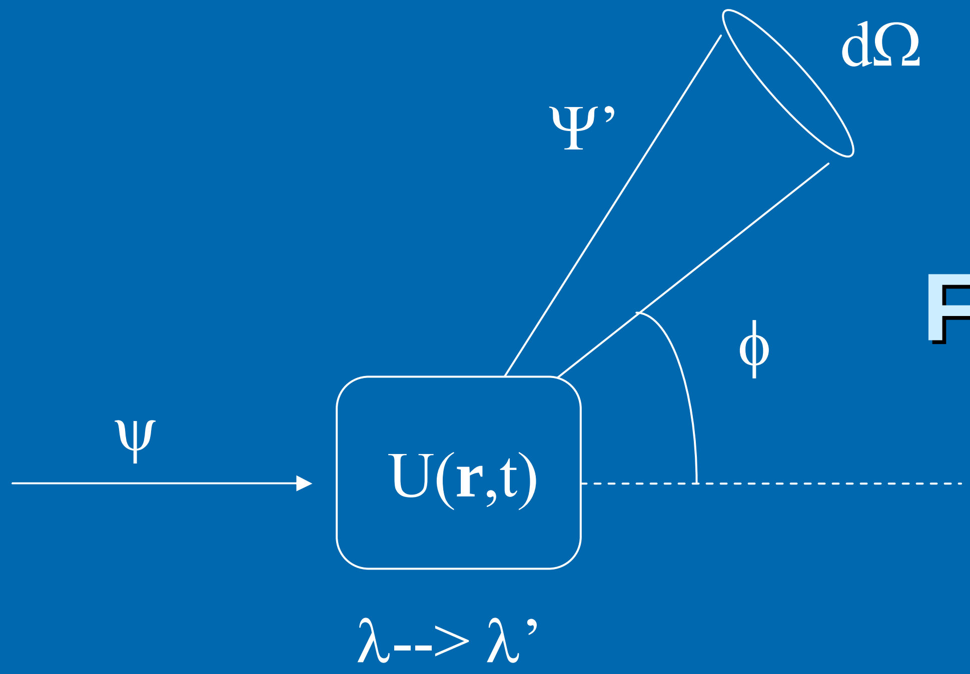


Magnetization



NMR, (μSR,…)





Fermi’s Golden Rule

$$\frac{d^2\sigma}{d\Omega d\omega} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 \sum_{\lambda} p_{\lambda} \sum_{\lambda'} \left| \langle \mathbf{k}'\lambda' | \hat{H} | \mathbf{k}\lambda \rangle \right|^2 \delta\left\{\hbar\omega + E_{\lambda} - E_{\lambda'}\right\}$$

Neutron-spin interaction

$$\hat{H} = -\hat{\mu}\hat{\mathbf{H}} \qquad \hat{\mathbf{H}} = \mathbf{rot}\left\{\frac{\hat{\mu}_e \times \mathbf{R}}{|\mathbf{R}|^3}\right\} - \frac{e}{m_e c}\frac{\hat{\mathbf{p}}_e \times \mathbf{R}}{|\mathbf{R}|^3},$$

Dipolmoment

Orbital moment (Biot-Savart)

$$\hat{\mu} = \gamma \mu_k \hat{\sigma}, \qquad \gamma = -1.913; \qquad \mu_k = \frac{e\hbar}{2mc}$$

$$\hat{\mu}_e = -2\mu_B \hat{\mathbf{s}}, \qquad \mu_B = \frac{e\hbar}{2m_e c}$$

Identical magnetic ions, Spin only

$$\frac{d^2\sigma}{d\Omega d\omega} = (\gamma r_o)^2 \frac{k'}{k} F^2(\mathbf{Q}) \exp\{-2W(\mathbf{Q})\} \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \frac{Q_\alpha Q_\beta}{Q^2} \right) S^{\alpha\beta}(\mathbf{Q},\omega)$$

Magnetic Scattering Function

$$S^{\alpha\beta}(\mathbf{Q},\omega) = \sum_{j,j'} e^{i\mathbf{Q}\left(\mathbf{R}_j - \mathbf{R}_{j'}\right)}$$

- $\sum_{S,M,S',M'} p_{S,M} \langle SM | \hat{\mathbf{S}}_j^\alpha | S'M' \rangle \langle S'M' | \hat{\mathbf{S}}_{j'}^\beta | SM \rangle$
- $\delta\left(\hbar\omega + E_{SM} - E_{S'M'}\right)$

Looks complicated? Maybe not…

$$\frac{1}{2}\left(\hat{S}^{+}+\hat{S}^{-}\right)=\hat{S}^{x}$$

$$\frac{1}{2i}\left(\hat{S}^{+}-\hat{S}^{-}\right)=\hat{S}^{y}$$

$$\hat{S}^{+}|M\rangle=\sqrt{(S-M)(S+M+1)}\,|M+1\rangle$$

$$\hat{S}^{-}|M\rangle=\sqrt{(S+M)(S-M+1)}\,|M-1\rangle$$

Elastic Scattering

$$\frac{d\sigma}{d\Omega} \approx S^{zz}(\mathbf{Q},\omega) = \sum_{j,j'} e^{i\mathbf{Q}(\mathbf{R}_j - \mathbf{R}_{j'})} \sum_{S,M} p_{S,M} \langle SM | \mathbf{S}^z_j | SM \rangle \langle SM | \mathbf{S}^z_{j'} | SM \rangle$$

$$\langle \mathbf{S}^z \rangle \approx \textit{Magnetization}$$

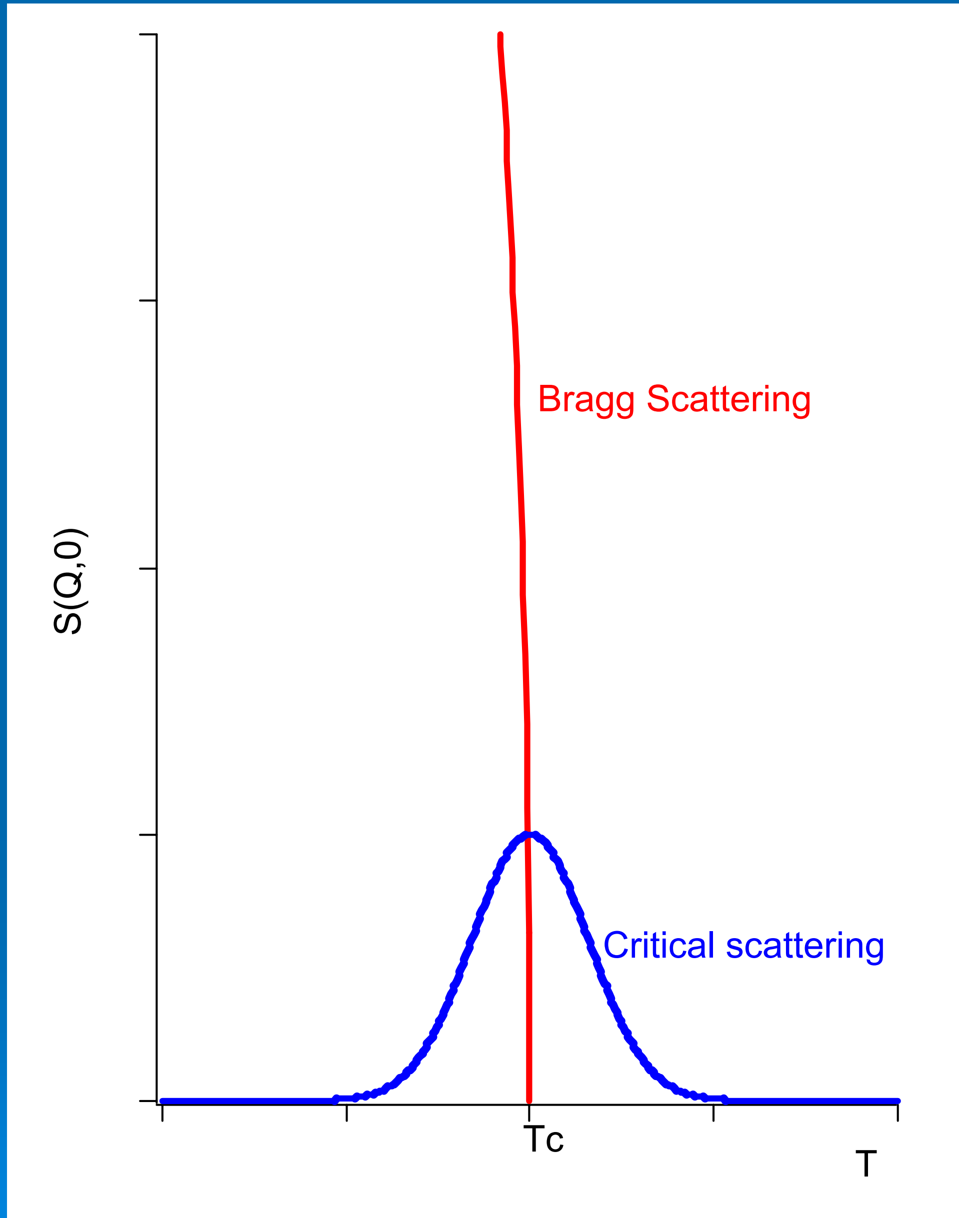
$$\mathbf{S}^z_j = \langle \mathbf{S}^z \rangle + \left(\mathbf{S}^z_j - \langle \mathbf{S}^z \rangle \right) = \langle \mathbf{S}^z \rangle + \Delta \mathbf{S}^z_j$$

$$-- >$$

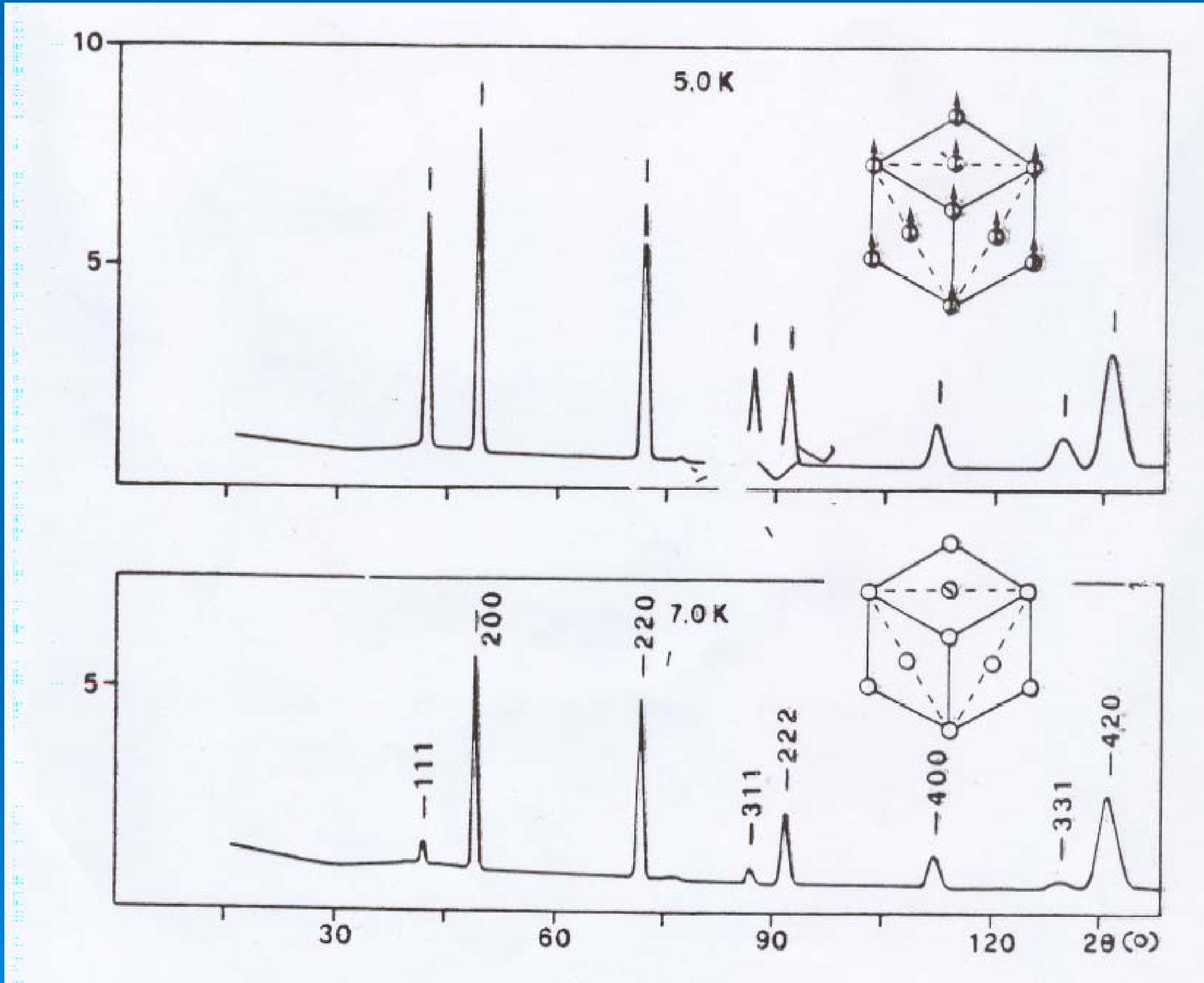
$$\frac{d\sigma}{d\Omega} \approx \delta(Q-\tau) \langle \mathbf{S}^z \rangle^2 + \langle \Delta \mathbf{S}^z_Q \Delta \mathbf{S}^z_{-Q} \rangle \approx M^2 + kT\chi(Q)$$

$$\frac{d\sigma}{d\Omega}_{Bragg} + \frac{d\sigma}{d\Omega}_{Critical}$$

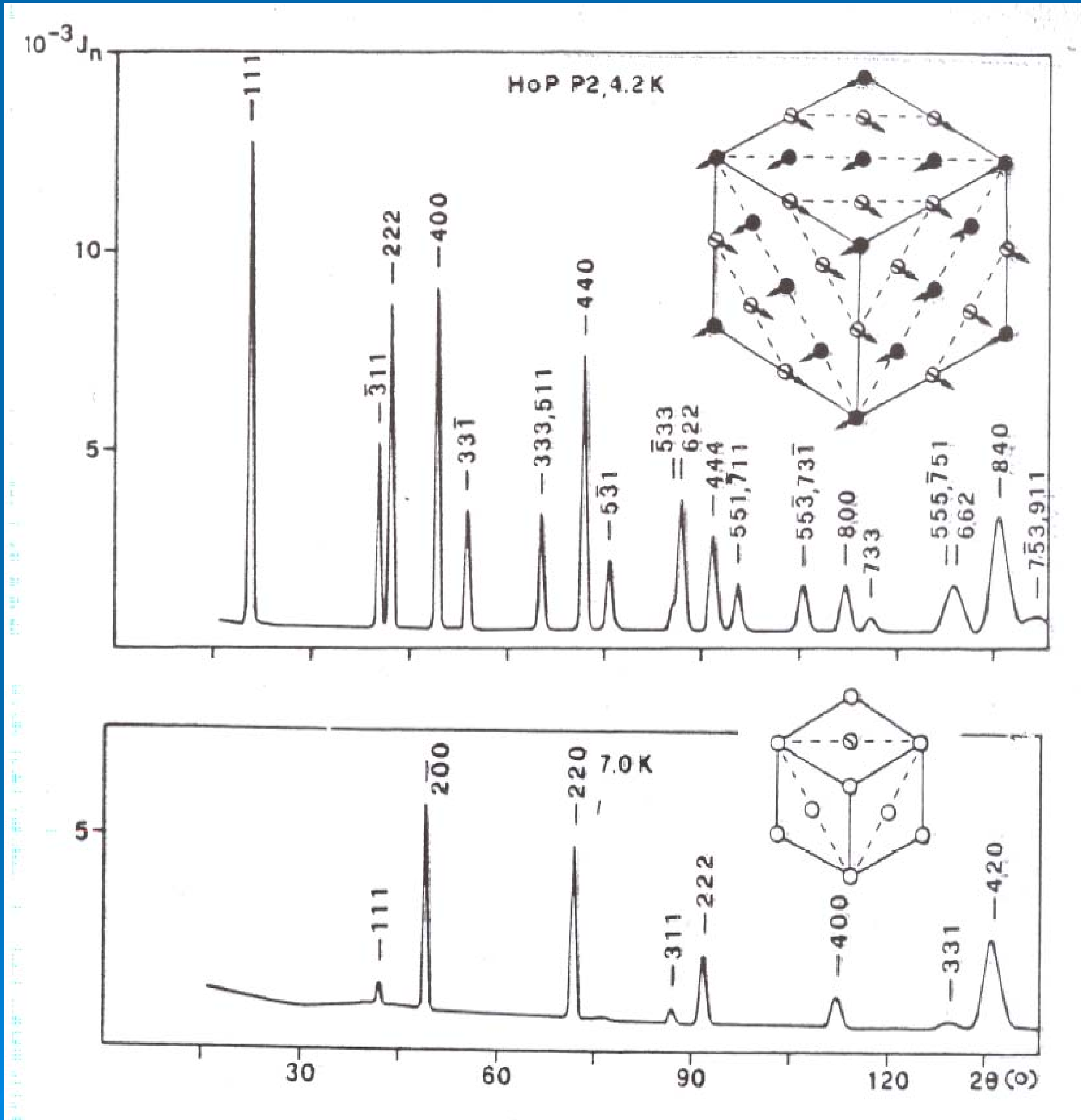
J. Mesot, 07


S(Q,0)
Bragg Scattering
Critical scattering
Tc
T

Bragg Scattering: HoP

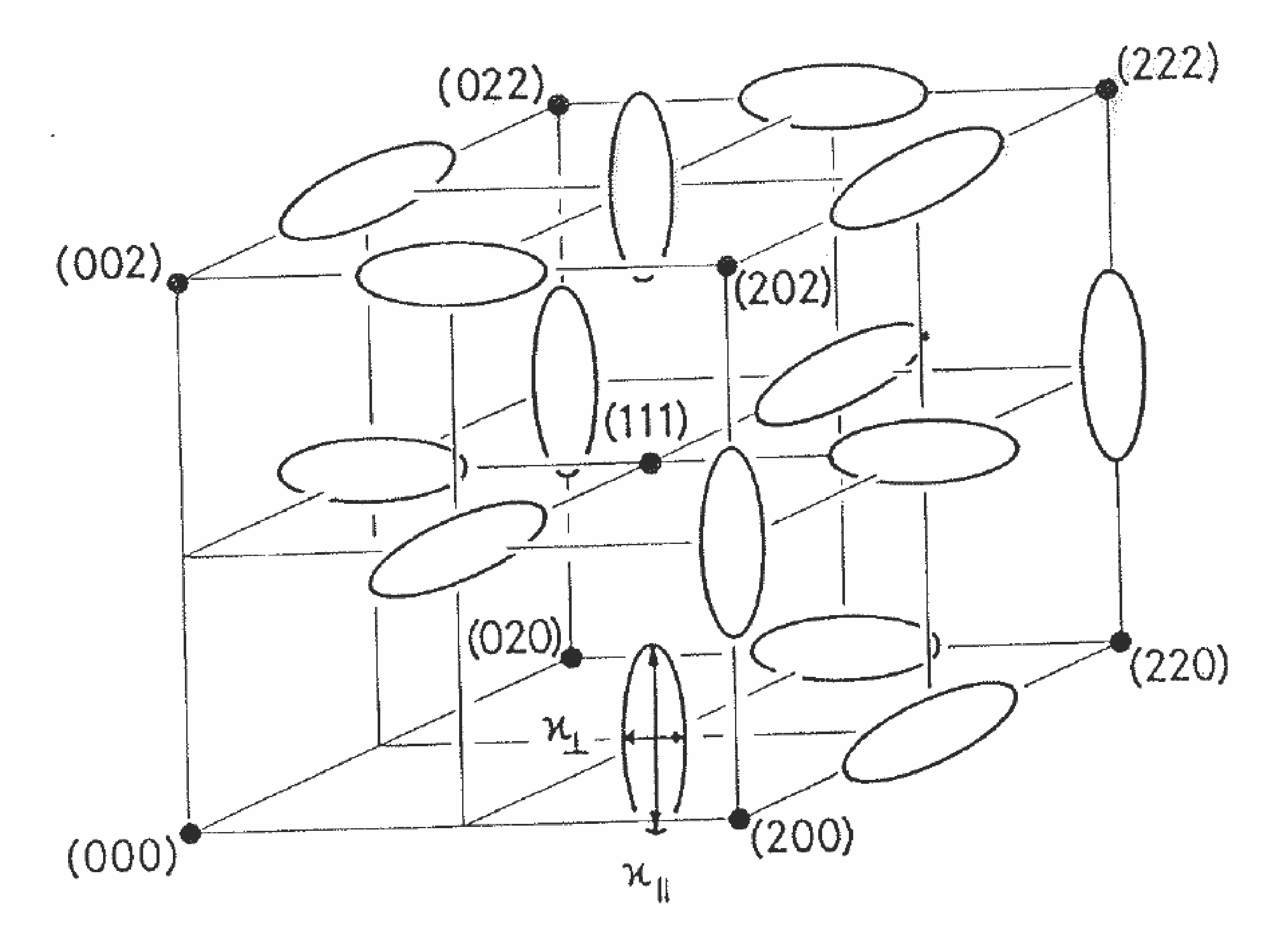


HoP, T=4.2 K

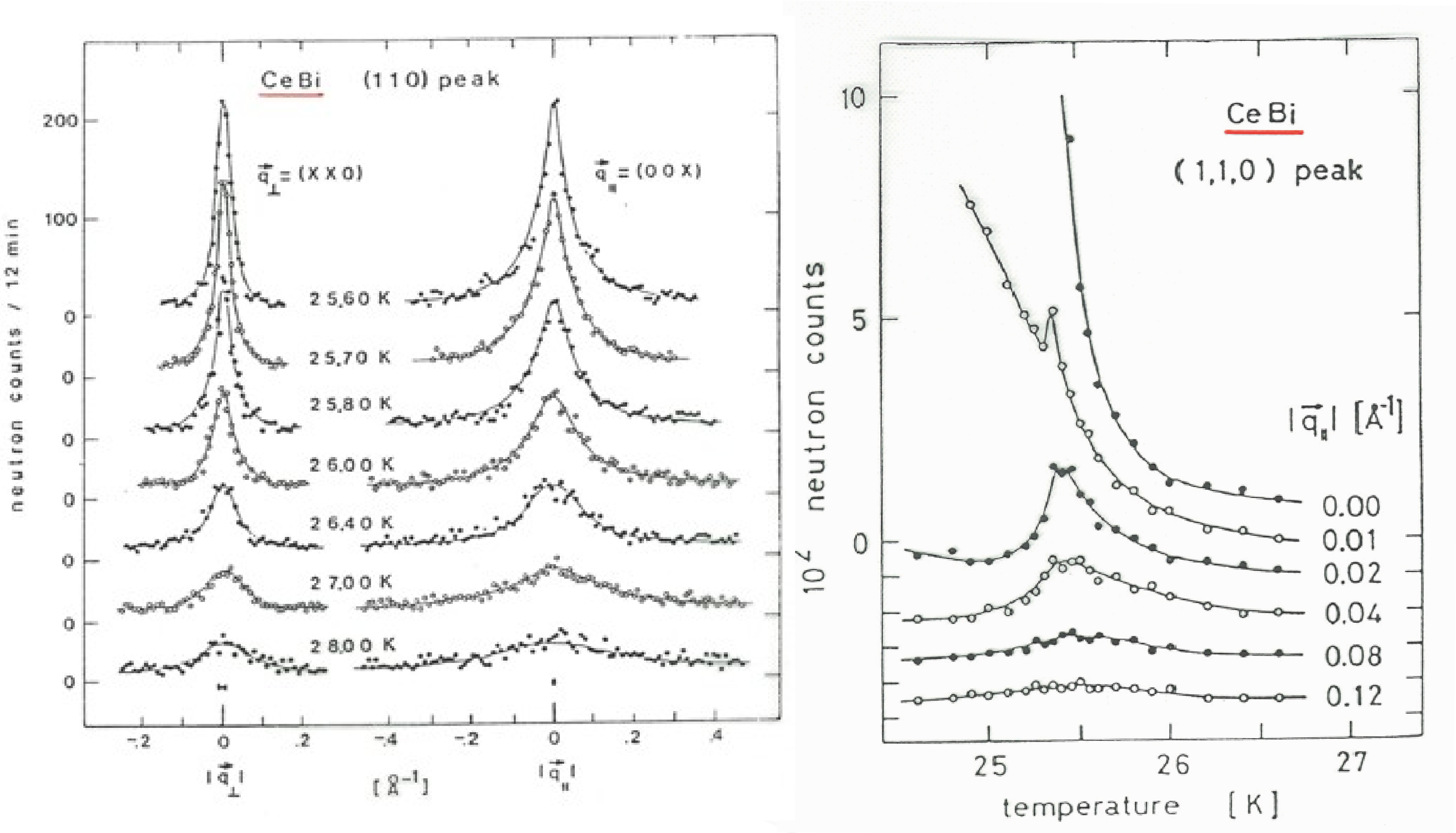


$10^{-3} J_n$
HoP P2, 4.2 K
7.0 K
111
$\bar{3}11$
222
400
$33\bar{1}$
333, 511
440
$5\bar{3}1$
$\bar{5}33$
622
444
$551, \bar{7}11$
$55\bar{3}, 73\bar{1}$
800
733
$555, \bar{7}51$
662
840
$7\bar{5}3, 911$
$\bar{2}00$
220
311
331
420
10
5
30
60
90
120
2θ (o)

CeBi, T_N=25.35 K



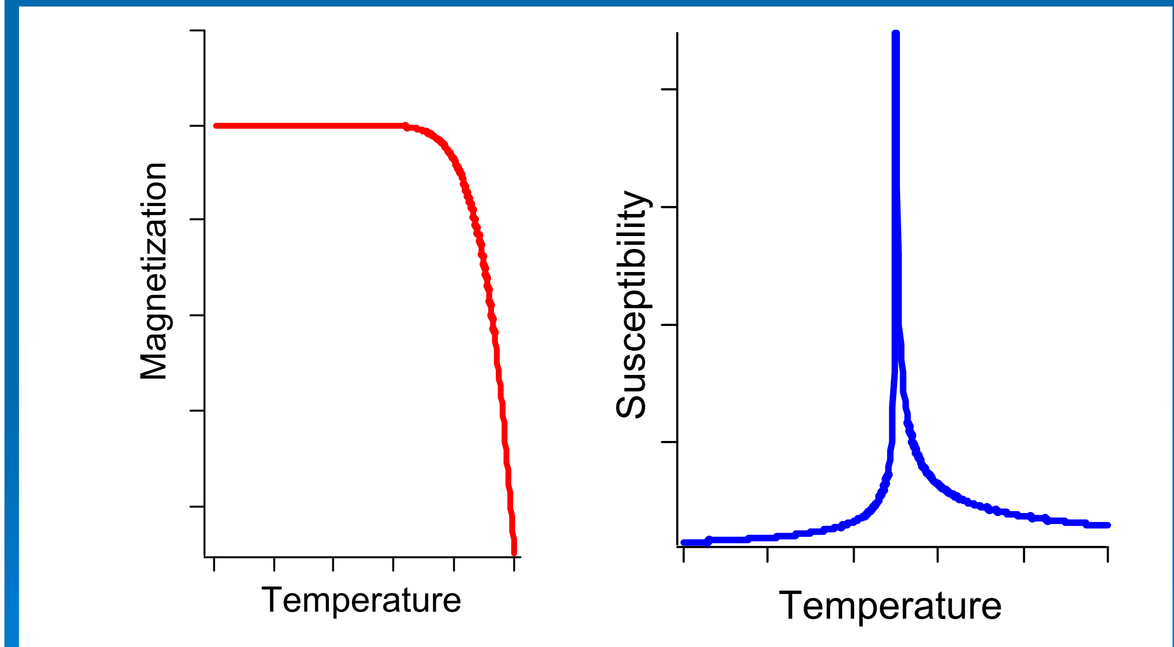
Hälg et al., JMMM 29 (82) 151


CeBi (110) peak
$\vec{q}_\perp$ = (X X 0)
$\vec{q}_\parallel$ = (0 0 X)
25.60 K
25.70 K
25.80 K
26.00 K
26.40 K
27.00 K
28.00 K
neutron counts / 12 min
$|\vec{q}_\perp|$
[Å^{-1}]
$|\vec{q}_\parallel|$
CeBi
(1,1,0) peak
$|\vec{q}_\parallel|$ [Å^{-1}]
0.00
0.01
0.02
0.04
0.08
0.12
10^4 neutron counts
temperature [K]

J. Mesot, 07

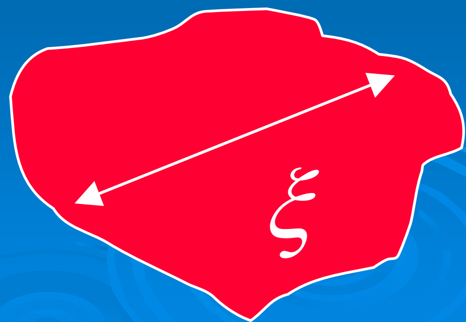
Critical exponents: $\mathbf{x} \propto \left(\pm \frac{T - T_c}{T_c} \right)^{\lambda} = (\pm t)^{\lambda}$

$$M \propto (-t)^{\beta} \qquad \chi \propto (\pm t)^{\gamma} \qquad \chi_Q \propto \frac{\chi}{\kappa^2 + Q^2}, \kappa \approx t^{\nu}$$



$$< \mathbf{S}_{\mathbf{r}}^{\alpha} \mathbf{S}_{\mathbf{r}'}^{\beta} > \approx \exp(-(\mathbf{r} - \mathbf{r}')\kappa)$$

$$\kappa = 1/\xi$$

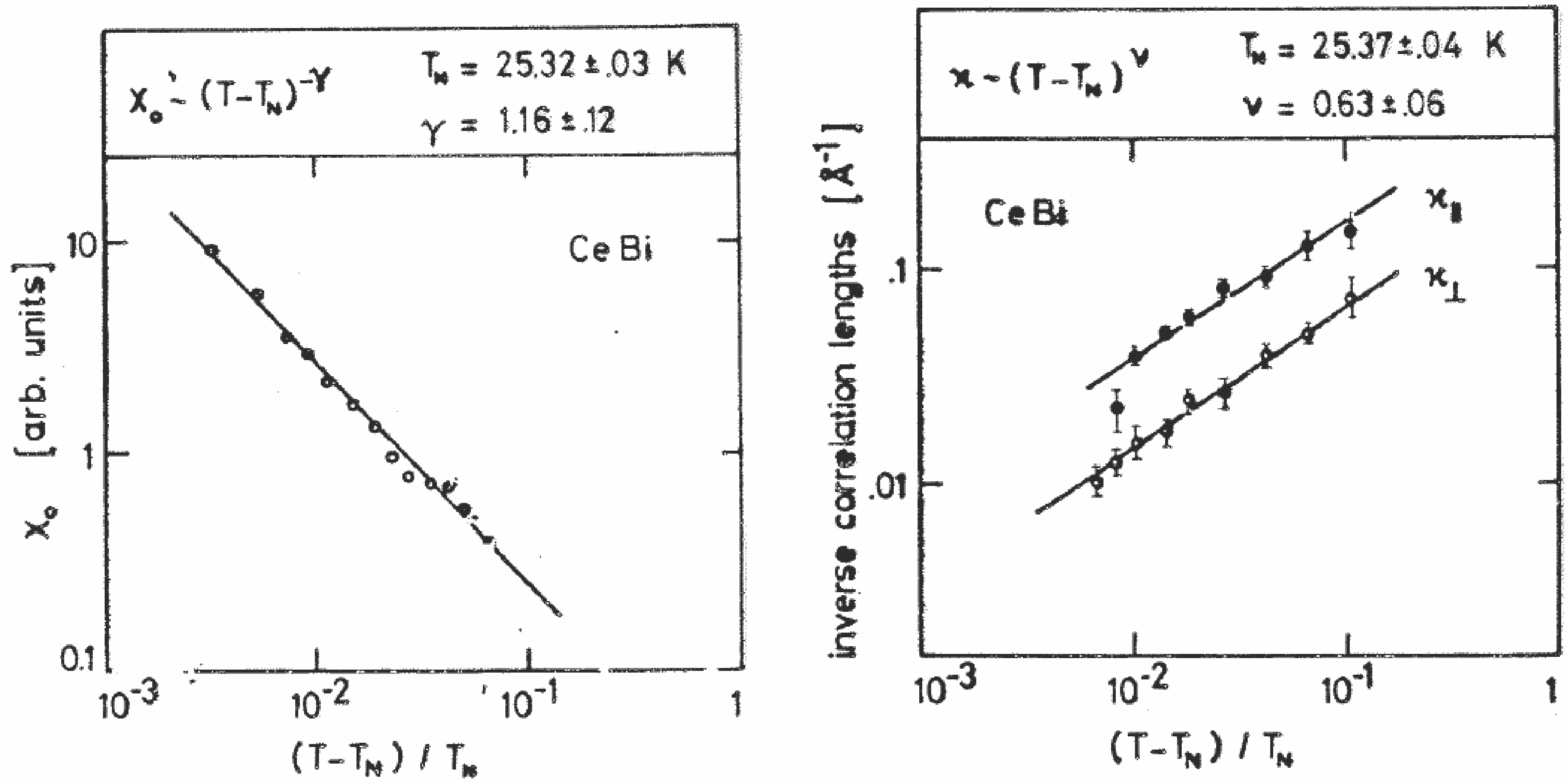


J. Mesot, 07

Exponents depend on — dim of order parameter n; dim of space d

$$\hat{H} = -J_{ij}\left(\left(1-A\right)\left(S_i^x S_j^x + S_i^y S_j^y\right) + A S_i^z S_j^z\right)$$

			β	$-\gamma$	ν
Mean field			0.5	1	0.5
Ising	n=1	d=2	1/4	7/4	1
A=1		d=3	0.313	5/4	0.638
XY (A=0)	n=2	d=3	1/3	1.32	0.675
Heisenberg (A=1/2)	n=3	d=3	0.345	1.4	0.7



Χ₀ ~ (T−T_N)^−γ
T_N = 25.32 ± .03 K
γ = 1.16 ± .12
Ce Bi
Χ₀ [arb. units]
10
1
0.1
10^-3
10^-2
10^-1
1
(T−T_N) / T_N
κ ~ (T−T_N)^ν
T_N = 25.37 ± .04 K
ν = 0.63 ± .06
Ce Bi
κ_∥
κ_⊥
inverse correlation lengths [Å^-1]
.1
.01
10^-3
10^-2
10^-1
1
(T−T_N) / T_N

M —–> β=0.317 (0.005)

Spin dynamics

$$S^{\alpha\beta}(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\,\frac{1}{N}\sum_{\vec{R}\vec{R}'} e^{i\vec{Q}\cdot(\vec{R}-\vec{R}')} < S^{\alpha}_{\vec{R}}(t)\, S^{\beta}_{\vec{R}'}(0) >$$

Question: how will the spin dynamics be affected by dimensionality and quantum fluctuations?

Fluctuation-dissipation theorem

$$S^{\alpha\beta}(\mathbf{Q},\omega)=\frac{N\hbar}{\pi}\left(1-e^{-\frac{\hbar\omega}{k_B T}}\right)^{-1} Im\,\chi^{\alpha\beta}(\mathbf{Q},\omega)$$

Generalized Magnetic Suscept.

$$M^{\alpha}(\mathbf{Q},\omega)=\chi^{\alpha\beta}(\mathbf{Q},\omega)H^{\beta}(\mathbf{Q},\omega)$$

Connection to microscopic models

Hamiltonian with eigenvalues E_i and eigenstates Γ_i

Z=partition function

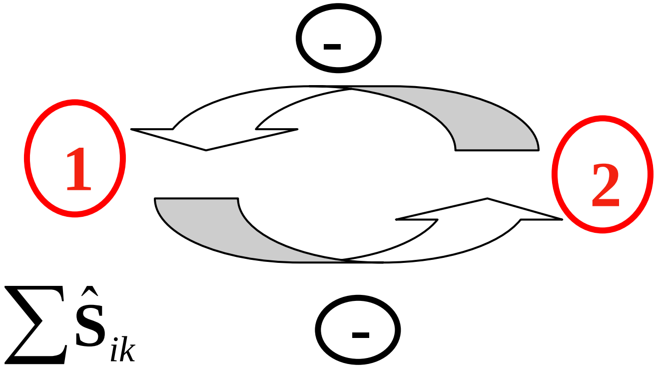
$$M_\alpha = \frac{1}{k_B T}\frac{\partial \ell n Z}{\partial H_\alpha} \qquad \left(= g\mu_B \sum_i p_i \langle \Gamma_i | S_\alpha | \Gamma_i \rangle \right)$$

$$\chi_{\alpha\alpha} = \frac{\partial M_\alpha}{\partial H_\alpha} \qquad = \left(g^2 \mu_B^2 \left[\sum_i \frac{\left|\langle \Gamma_i | S_\alpha | \Gamma_i \rangle\right|^2}{k_B T} p_i + \sum_{i\neq j} \frac{\left|\langle \Gamma_j | S_\alpha | \Gamma_i \rangle\right|^2}{E_i - E_j} (p_j - p_i) \right] \right)$$

$$p_i = \frac{1}{Z}\exp\left(-\frac{E_i}{k_B T} \right)$$

Type of Hamiltonians

Heisenberg & Dirac (1929) $\hat{H} = -2J\hat{S}_1\hat{S}_2$



Van Vleck (1932) $\hat{H} = -2\sum_{i>j} J_{ij}\hat{S}_i\hat{S}_j, \quad \hat{S}_i = \sum_k \hat{S}_{ik}$

Neel (1936) J<0 ; Antiferromagnetismus

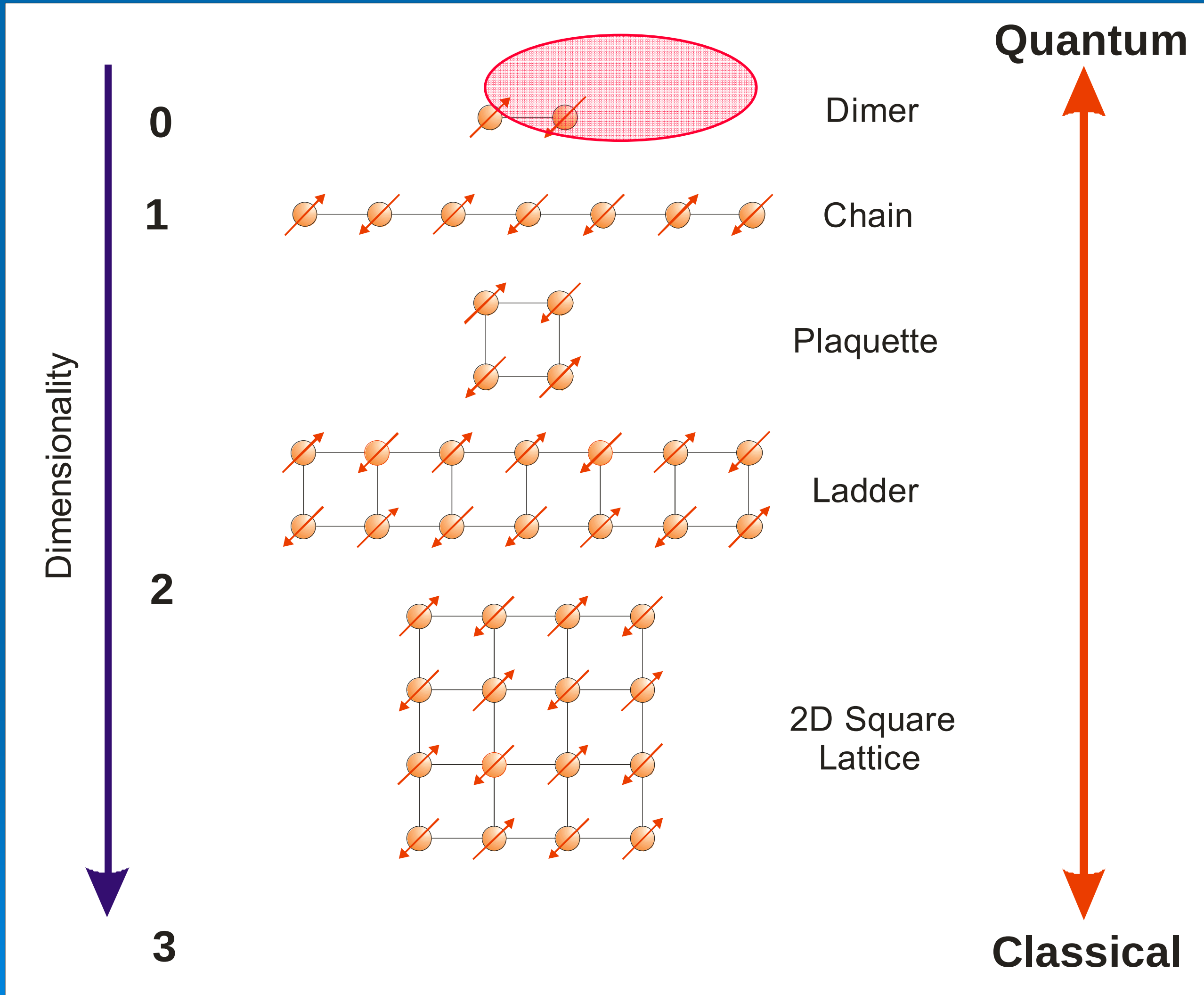
Further generalizations

$$\hat{H} = -2\sum_{i>j}\sum_{\alpha,\beta} J_{ij}^{\alpha\beta}\hat{S}_i^{\alpha}\hat{S}_j^{\beta}, \quad (anisotropy)$$

$$-\sum_{i>j} K_{ij}\left(\hat{S}_i\hat{S}_j\right)^2, \quad (higher-order\ exchange)$$

$$-\sum_{i>j} L_{ijl}\left(\hat{S}_i\hat{S}_j\right)\left(\hat{S}_j\hat{S}_l\right) \quad (three-body\ exchange)$$

Magnetic Architecture



J. Mesot, 07

Coupled system: Cr^{3+}-Cr^{3+}, $S_{1,2}=3/2$, distance r apart.

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2 \; --> \; \hat{\mathbf{S}}_1\hat{\mathbf{S}}_2 = \frac{1}{2}\left[\hat{\mathbf{S}}^2 - \hat{\mathbf{S}}_1^2 - \hat{\mathbf{S}}_2^2\right]$$

$E(S)=-J[S(S+1)-2S_1(S_1+1)$, $0<S<2S_1$,

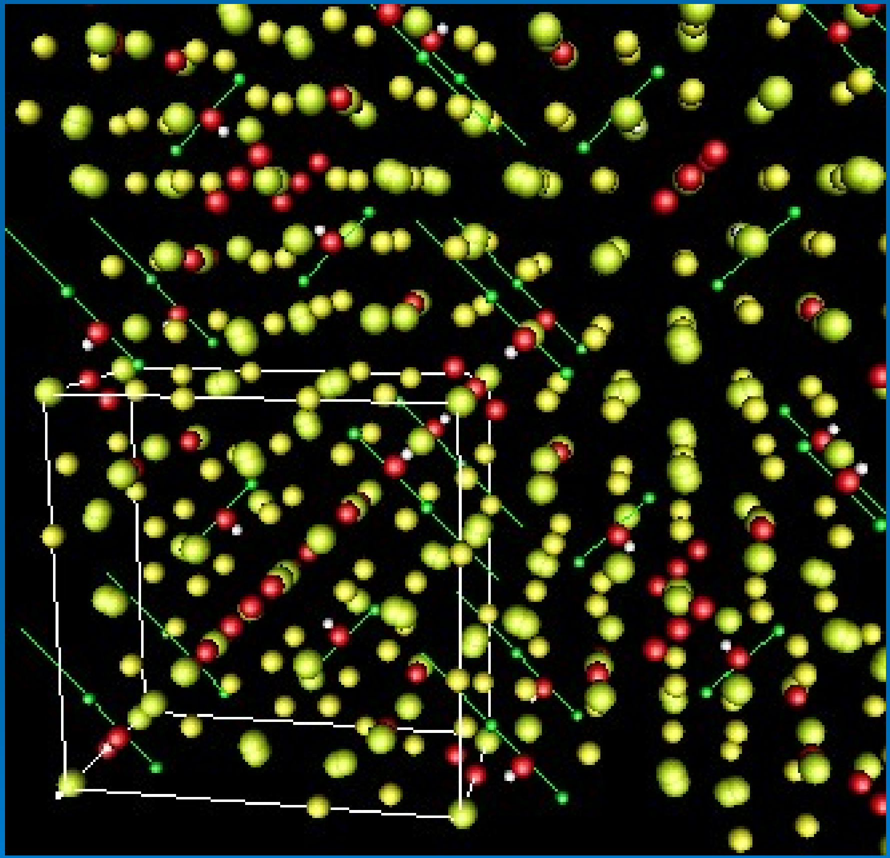
S		E(S)/|J|
3	(7)	12
2	(5)	6
1	(3)	2
0	(1)	0

$$\mathbf{S}^{\alpha\beta}(\vec{Q},\omega) = F^2(Q) \bullet \left[1 - \frac{\sin(Qr)}{Qr}\right] \bullet \delta\left(\omega - \left(E_j - E_i\right)\right) \bullet \delta\left(S_j - S_i \pm 1,0\right) \bullet p\left(E_i\right)$$

N *-((NH3)5CrOHCr(NH3)5)Cl5H2O-[P42/MNM]-
C 16.259 16.259 7.411 90. 90. 90.
S GRUP P 42/M N M

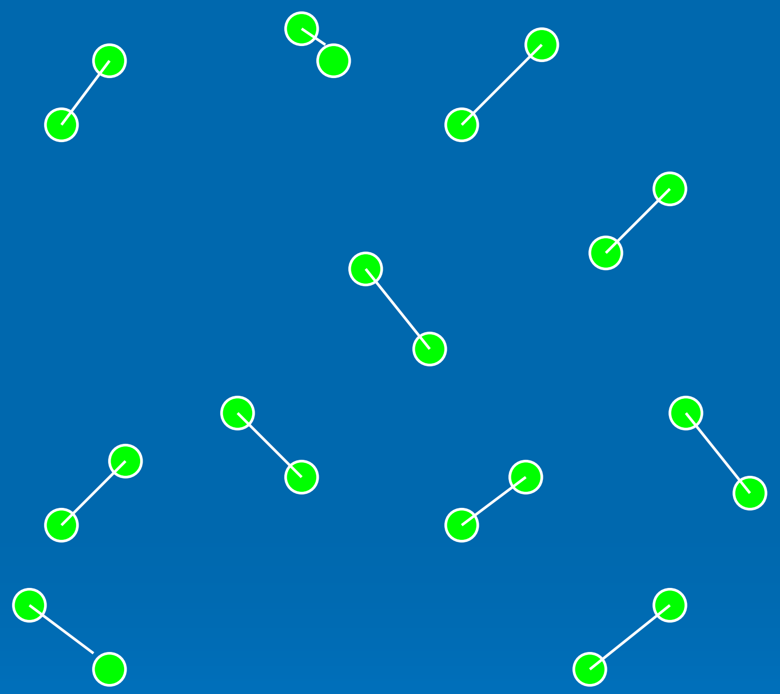
A Cr1		0.24210	0.07450	0.00000	0.00000	1.00000	
A N1		0.19090	0.99770	0.19690	0.00000	1.00000	
A N2		0.14420	0.29720	0.20080	0.00000	1.00000	
A N3		0.34850	0.99580	0.00000	0.00000	1.00000	
A O1		0.14780	0.14780	0.00000	3.85000	1.00000	
A O2		0.00000	0.00000	0.50000	12.3000	0.50000	
A O3		0.31020	0.31020	0.38420	13.8000	0.25000	
A O4		0.44880	0.44880	0.00000	6.50000	0.25000	
A Cl1		0.49950	0.13500	0.00000	2.70000	0.50000	
A Cl2		0.34720	0.99250	0.50000	4.70000	0.50000	
A Cl3		0.31060	0.31060	0.50000	6.10000	1.00000	
A Cl4		0.13480	0.13480	0.50000	4.80000	1.00000	
A Cl5		0.32740	0.32740	0.00000	2.80000	0.50000	
A Cl6		0.50000	0.50000	0.43430	3.60000	0.50000	
A H1		0.11900	0.11900	0.00000	6.50000	1.00000	
T Cr1	4	0.00160	0.00160	0.01480	0.00000	0.00000	0.00040
T N1	4	0.00550	0.00350	0.01960	0.00040	0.00450	-0.0012
T N2	4	0.00530	0.00450	0.02110	-0.0025	0.00060	-0.0023
T N3	4	0.00310	0.00310	0.12660	0.00000	0.00000	0.00230

Cr-dimer

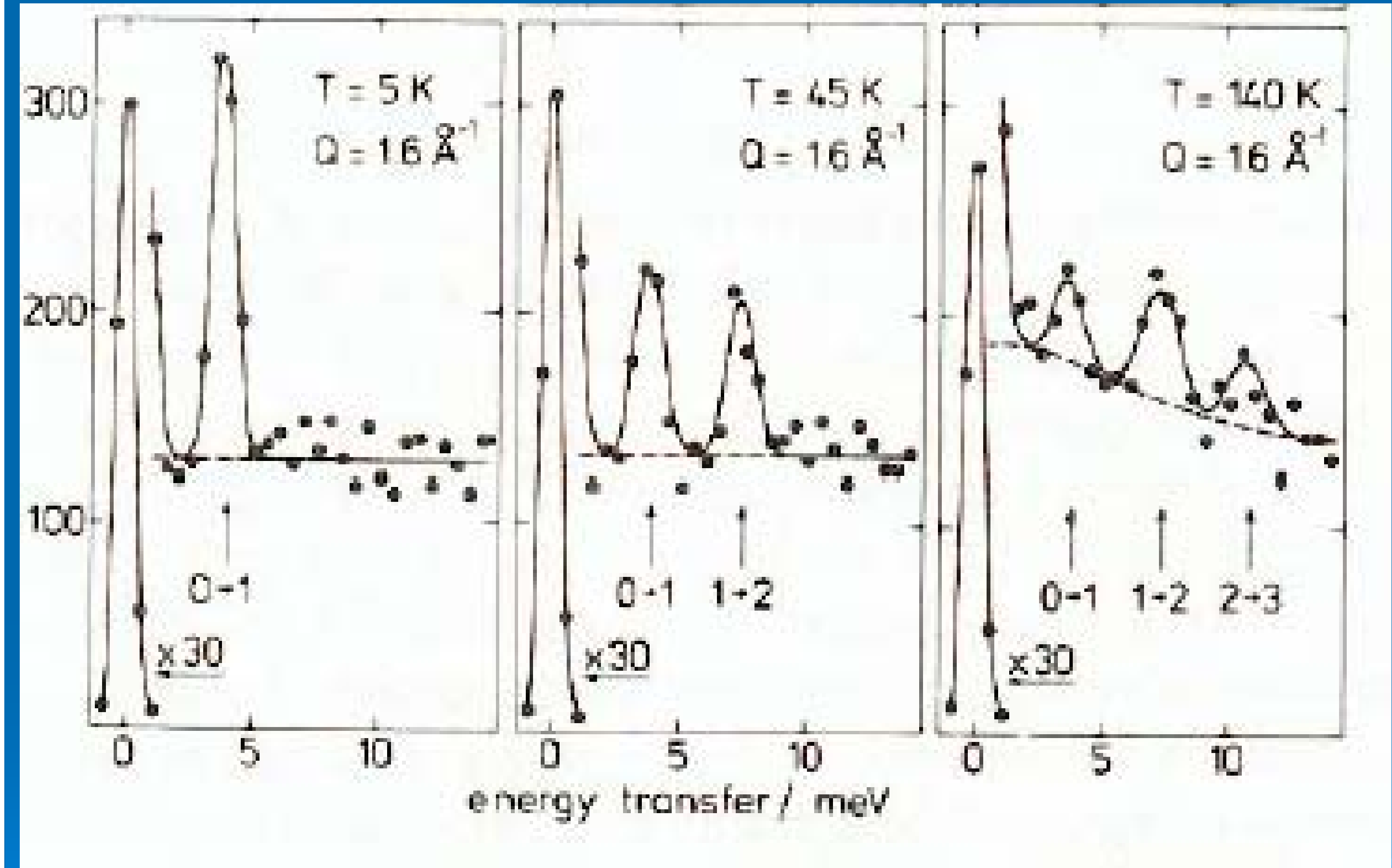


J. Mesot, 07

Cr-dimer

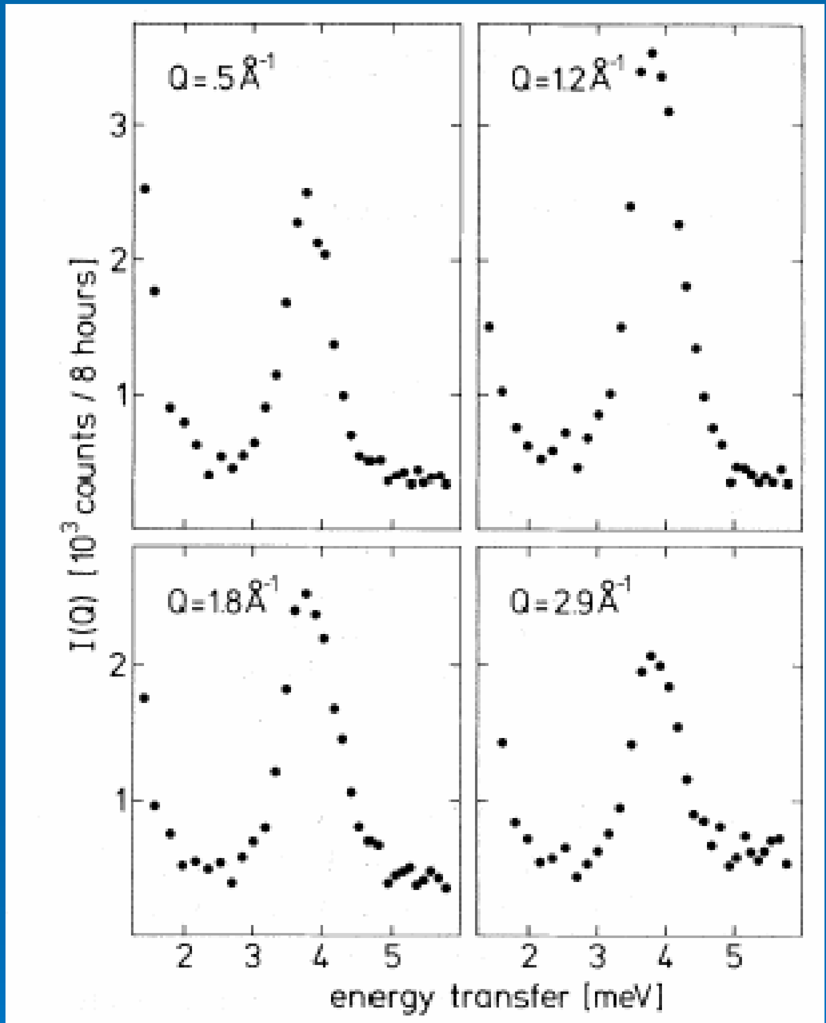


$(NH_3)_5Cr(OH)Cr(NH_3)_5$

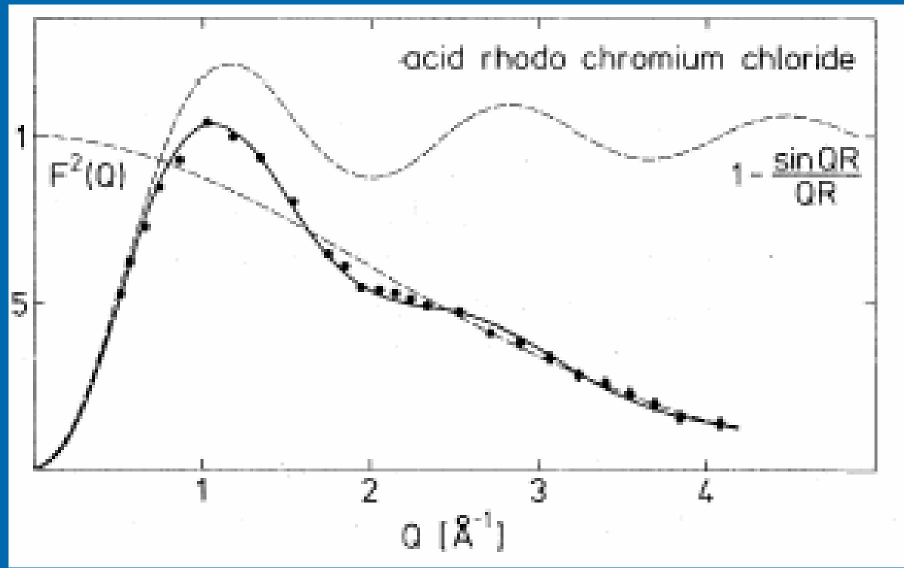


S	E(S)/|J|
3	12
2	6
1	2
0	0

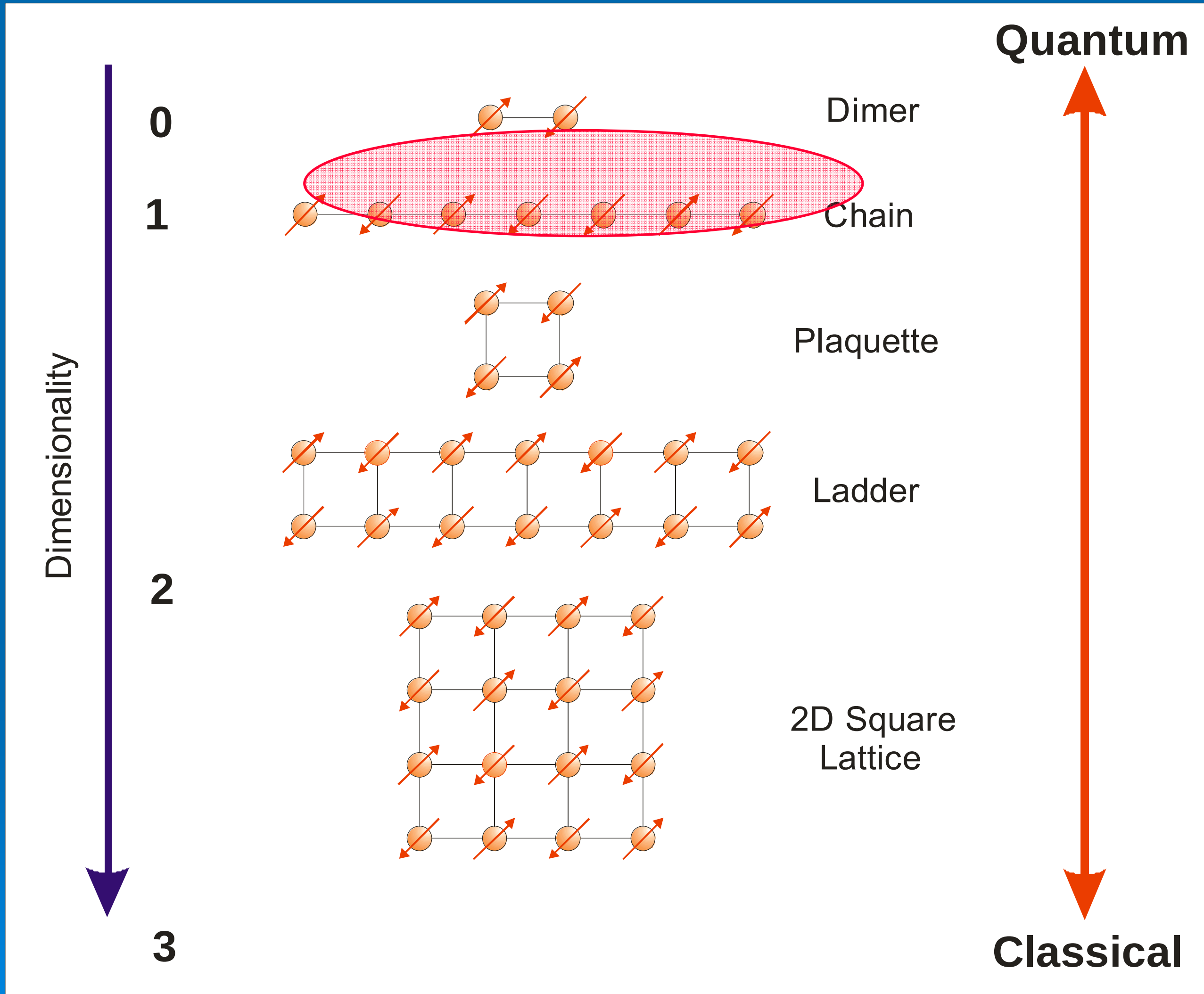
J. Mesot, 07


Q=.5Å-1
Q=1.2Å-1
Q=1.8Å-1
Q=2.9Å-1
I(Q) [10^3 counts / 8 hours]
energy transfer [meV]

I(Q)/exp(-2W)

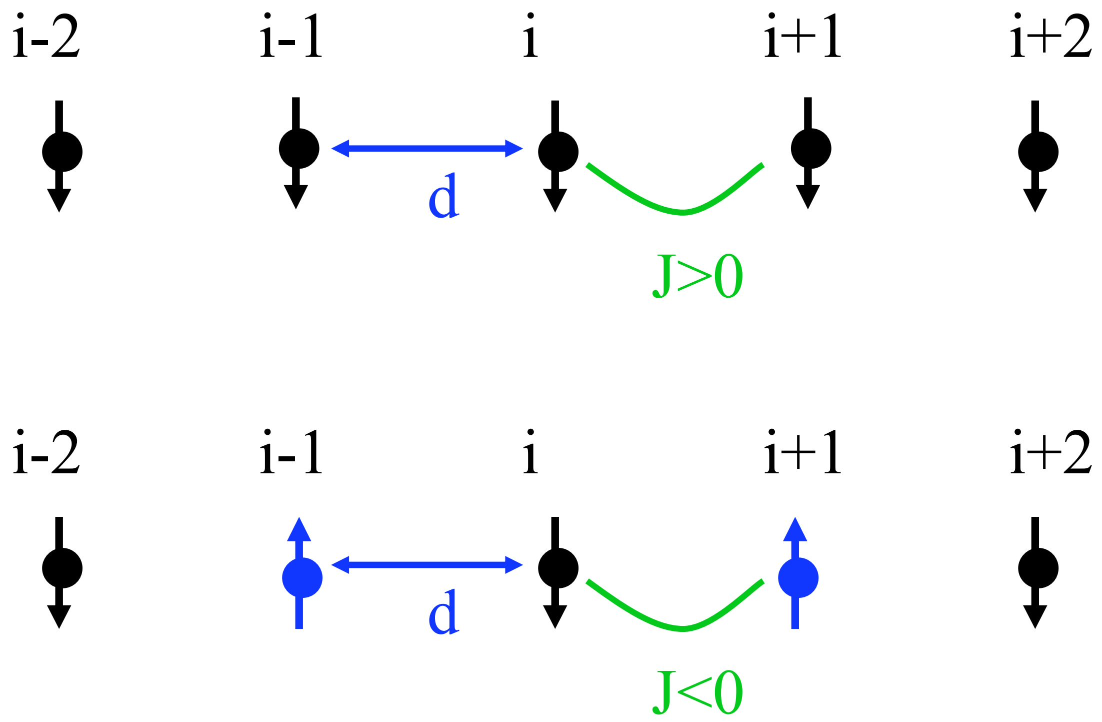

acid rhodo chromium chloride
F^2(Q)
1 - sinQR / QR
Q [Å^-1]

Magnetic Architecture

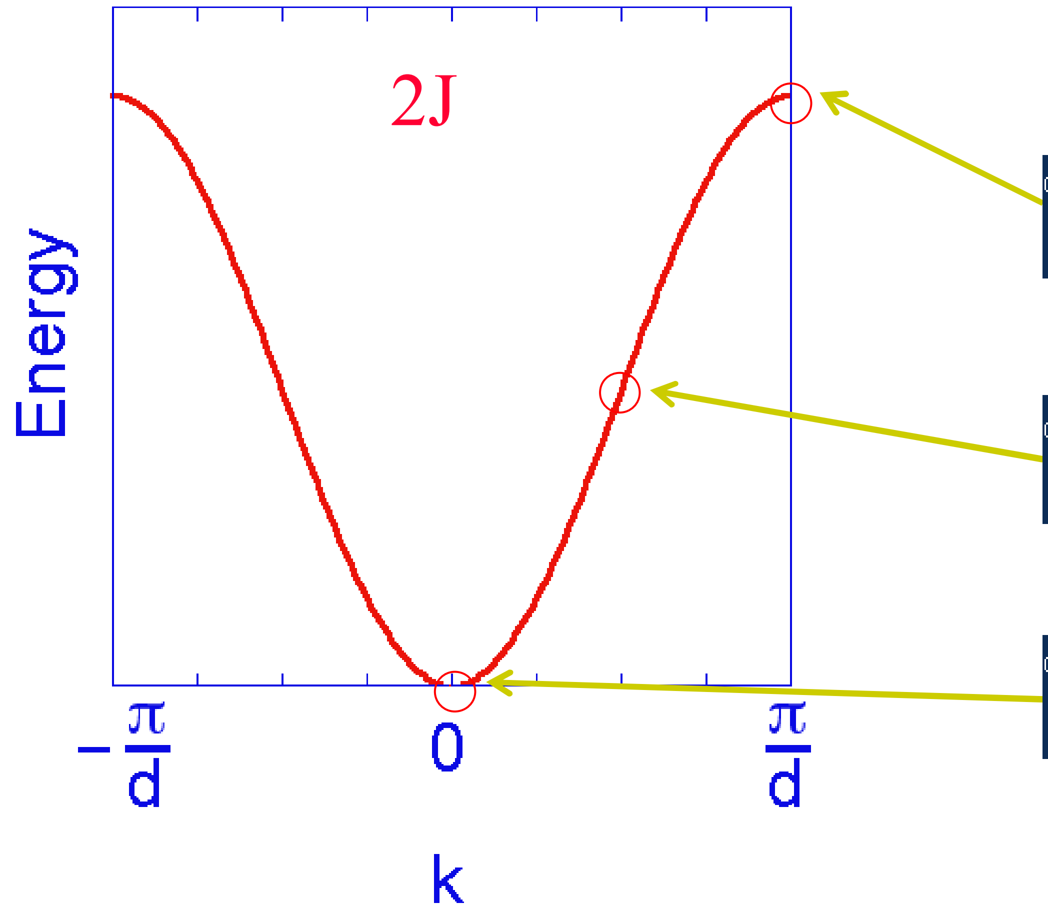


1-D Heisenberg chain

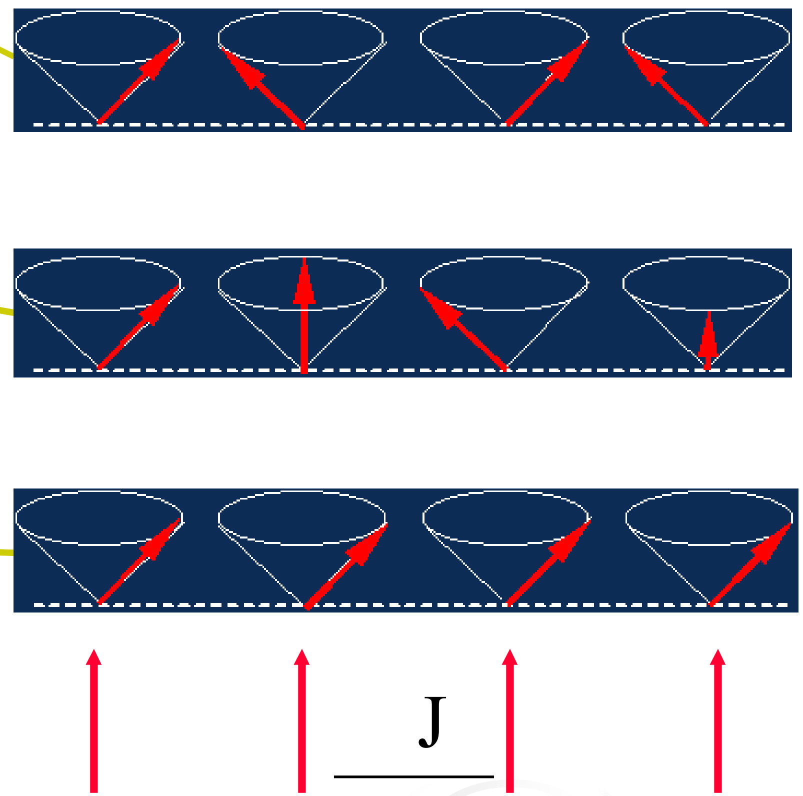
$$\hat{H} = -2J\sum_{i} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_{i+1}$$



Classical Spin Waves

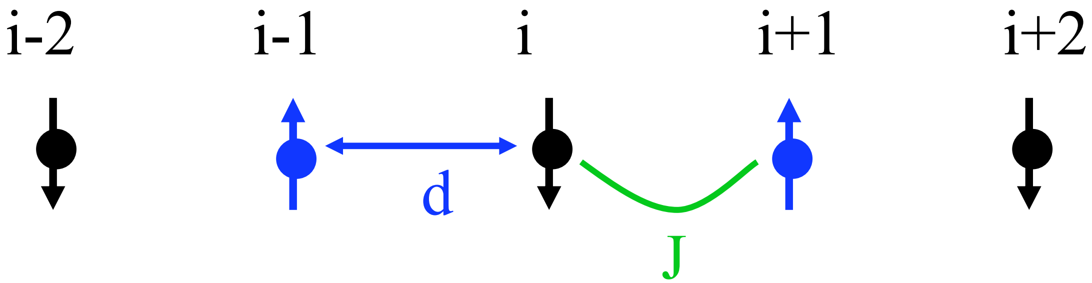


Excitations/Precessions:



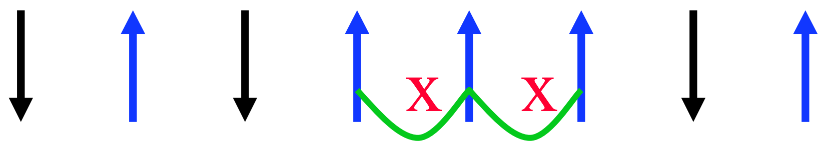
Well-defined S=1 excitations ⇒ sharp dispersion
Excitations are "transverse"

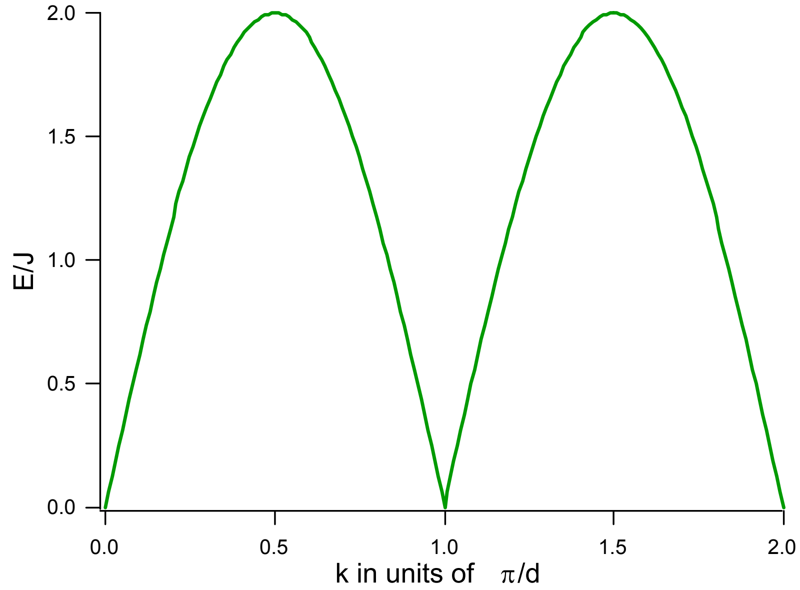
“Classical” Antiferromagnet



$$\hat{H} = -2J\sum_{i} \hat{\mathbf{S}}_{\mathrm{i}} \cdot \hat{\mathbf{S}}_{\mathrm{i+1}}$$

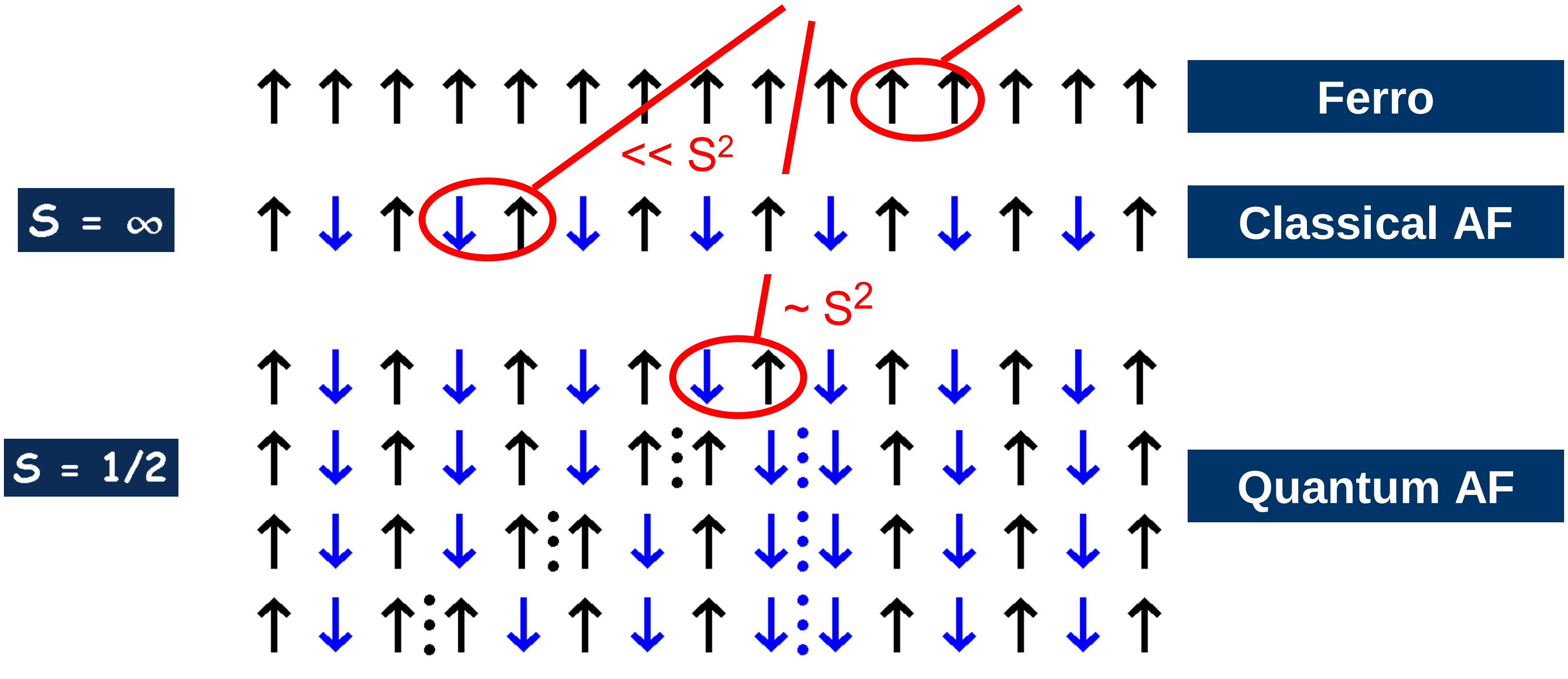
$$\omega = -2JS\left|\sin\left(kd\right)\right|$$





Well-defined S=1 excitations ⇒ sharp dispersion

$$\mathcal{H} = -J \sum S_n^z S_{n+1}^z + \frac{1}{2}\left(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+\right)$$



Ground state (Bethe 1931) disordered by quantum fluctuations

S=1/2 AF chain

Elementary excitations:

– “Spinons”: spin S = ½ domain walls with respect to local AF ‘order’

– Need 2 spinons to form S=1 excitation we can see with neutrons

↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑ ↓ ↑

↑ ↓ ↑ ↓ ↑ ↓ ↑⁝↑ ↓⁝↓ ↑ ↓ ↑ ↓ ↑

↑ ↓ ↑ ↓ ↑⁝↑ ↓ ↑ ↓⁝↓ ↑ ↓ ↑ ↓ ↑

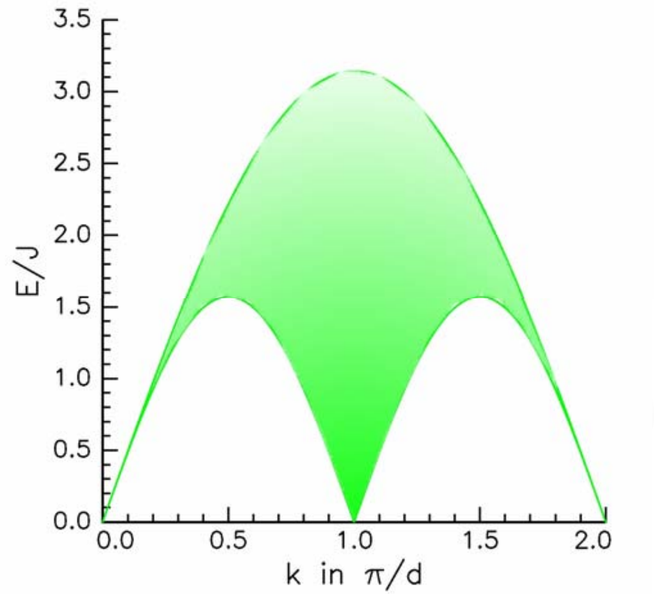
↑ ↓ ↑⁝↑ ↓ ↑ ↓ ↑ ↓⁝↓ ↑ ↓ ↑ ↓ ↑

Energy: $E(q) = E(k_1) + E(k_2)$

Momentum: $q = k_1 + k_2$

Spin: $S = \frac{1}{2} \pm \frac{1}{2}$

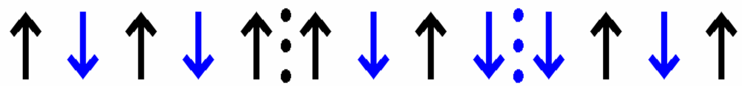
Continuum of scattering =

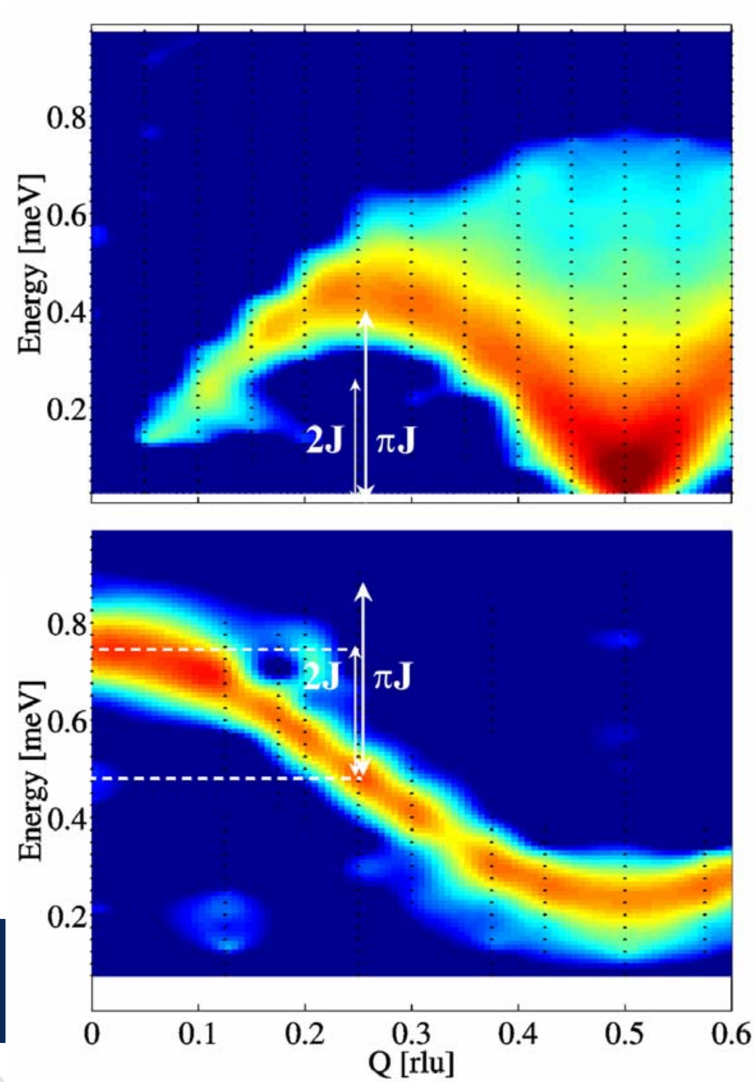


Switching off quantum mechanics !

copper sulphate
$CuSO_4{\cdot}5D_2O$

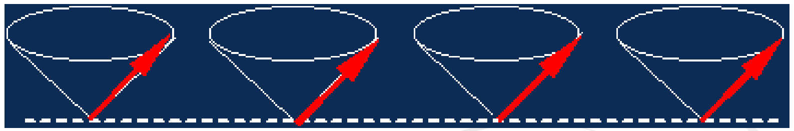
Spinon pair continuum





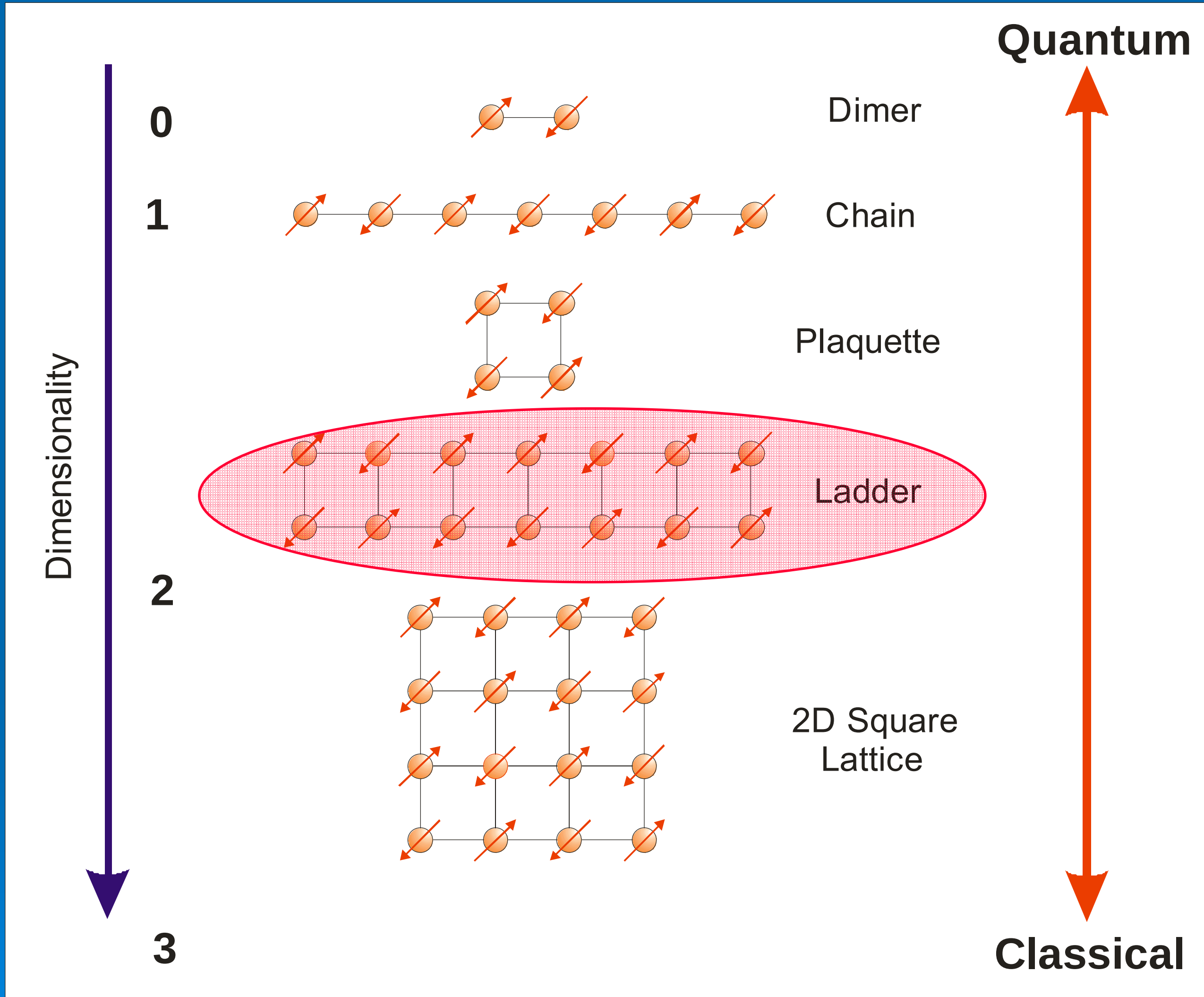
Strong magnetic field forces antiferromagnet into ferromagnet

spin wave dispersion ⇒

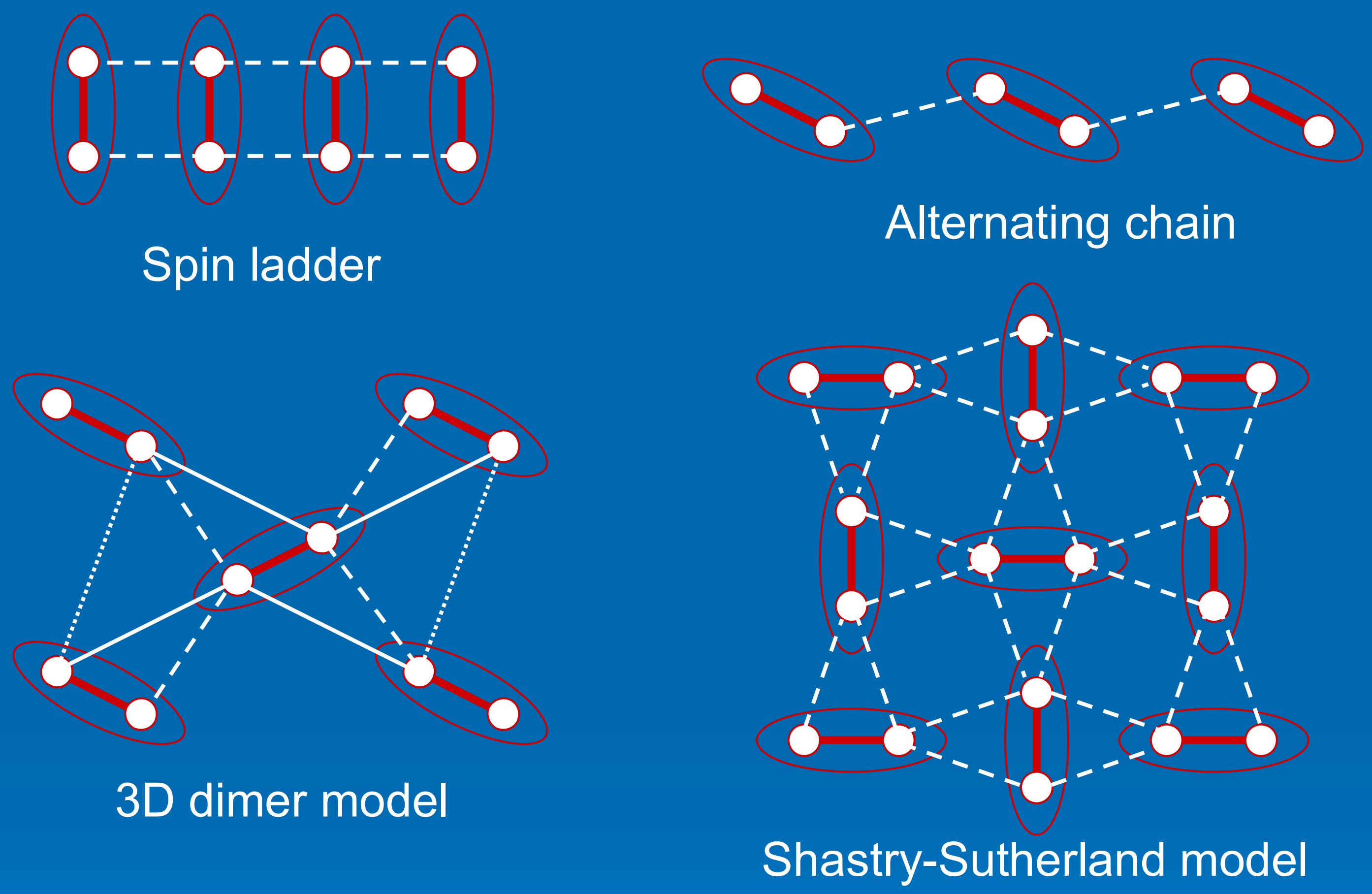


Rønnow et al.

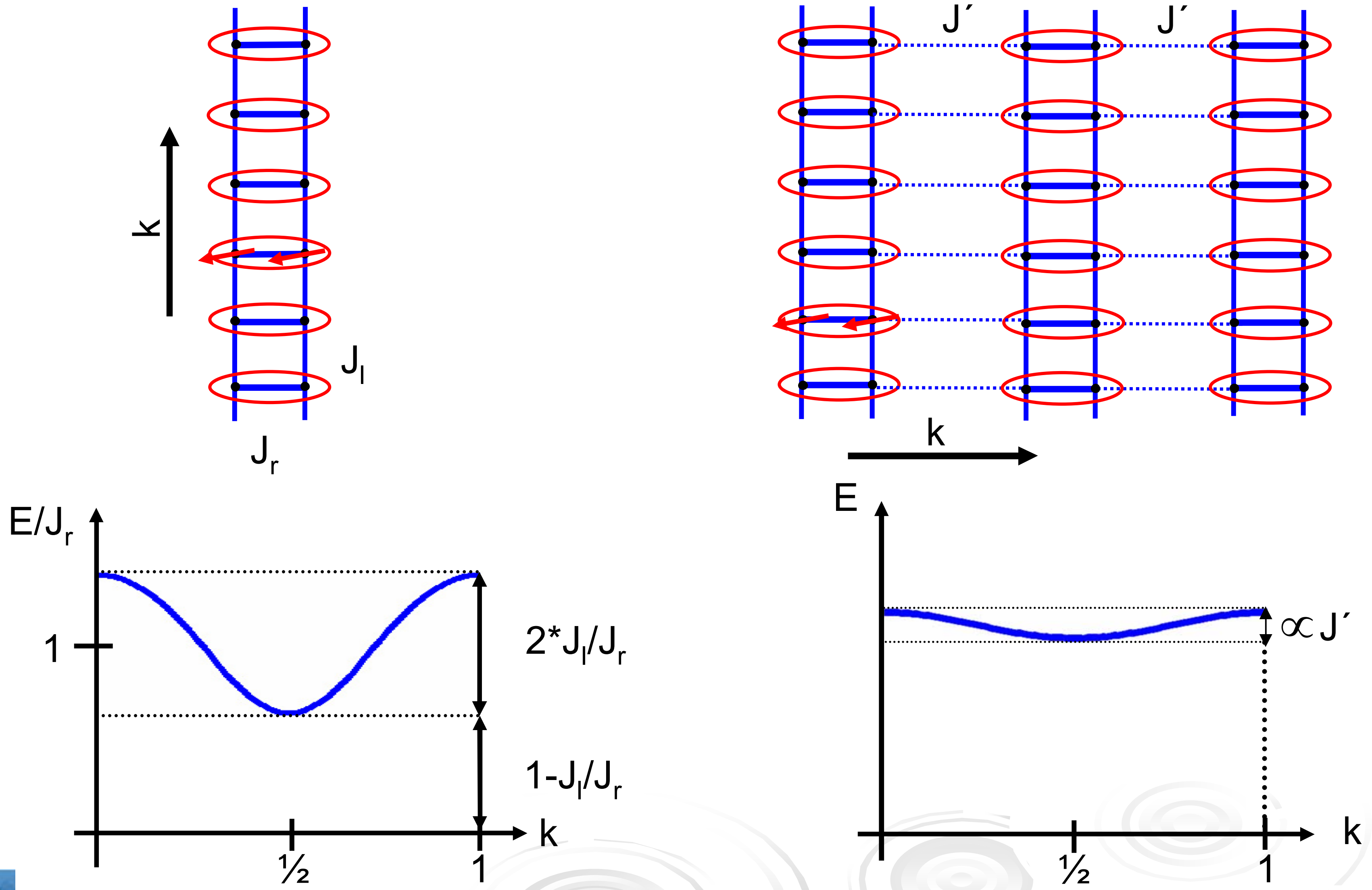
Magnetic Architecture



Model Quantum Spin Systems

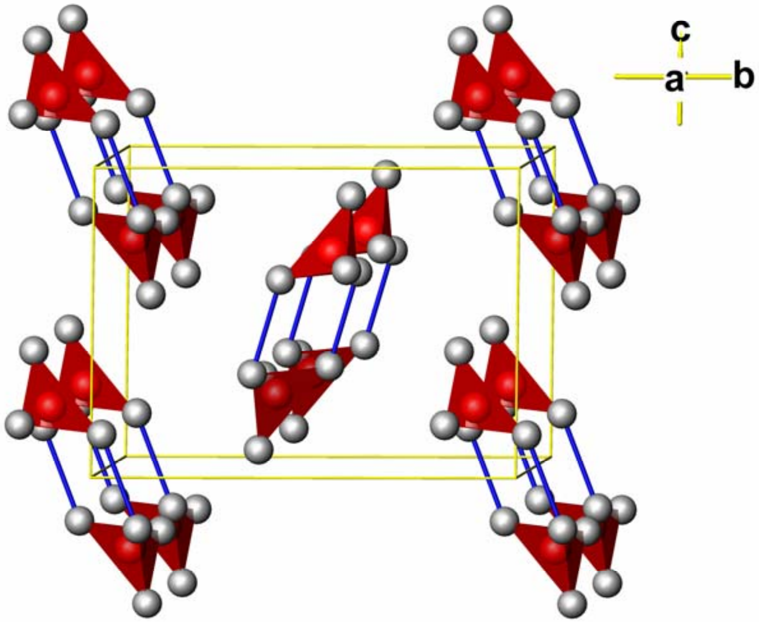


Spin ladders



T. Barnes et al., PRB 47, 3196 (1993)

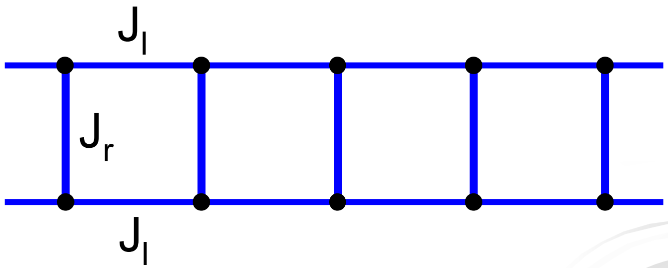
$(C_5H_{12}N)_2CuBr_4$

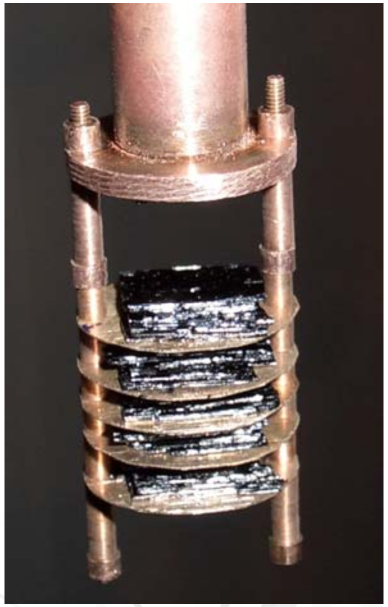


(PhD B. Thielemann)

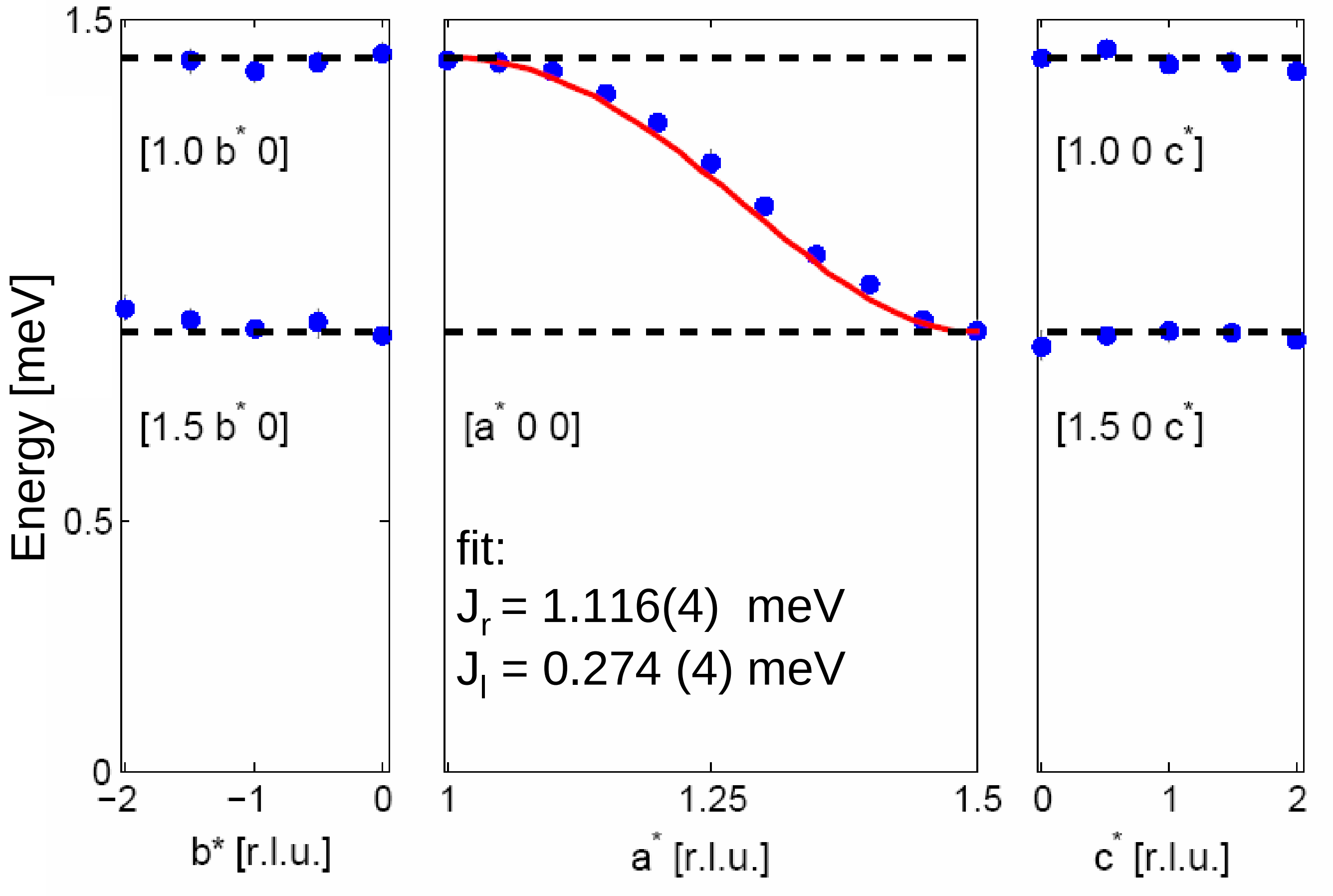
suggested spin model:

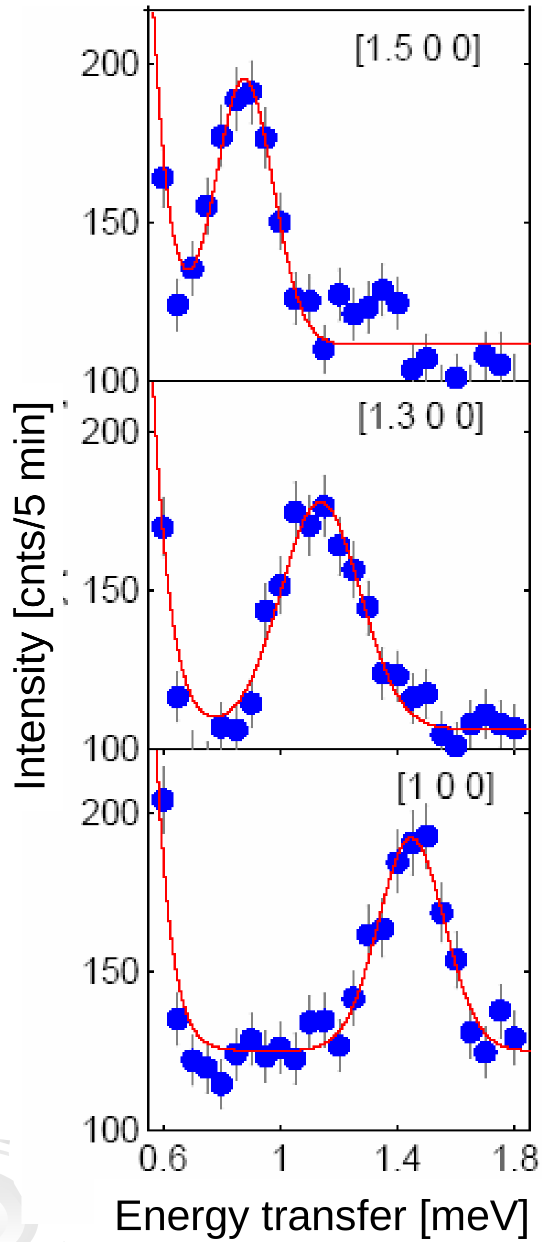
AFM ladder, $J_r/J_l>>1$





T = 50 mK





$J_r/J_l = 4.07(2) >> 1$ $\Rightarrow$ strong coupling limit

J` < 0.05 meV $\Rightarrow$ very 1D spin-ladder

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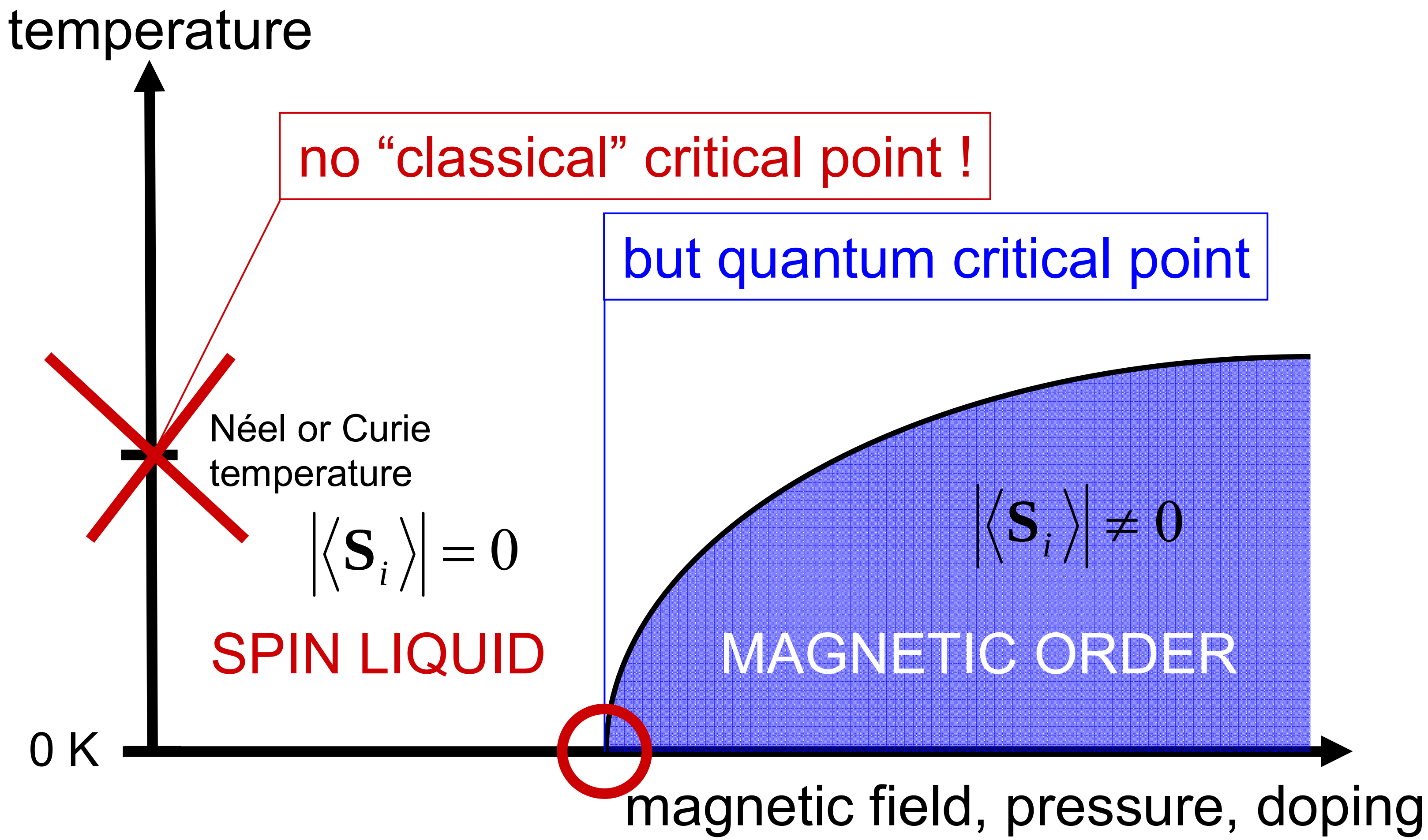
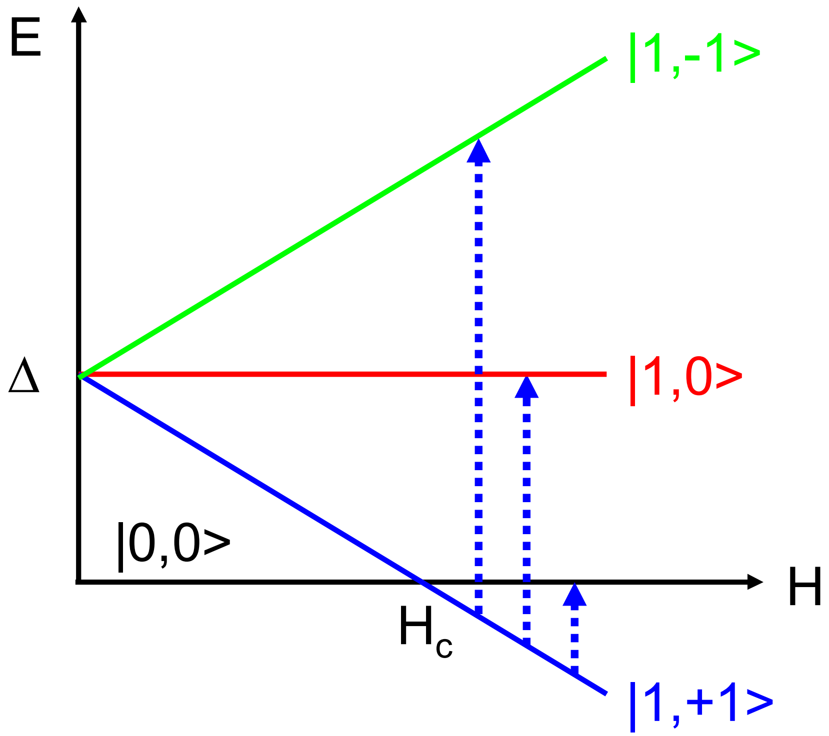
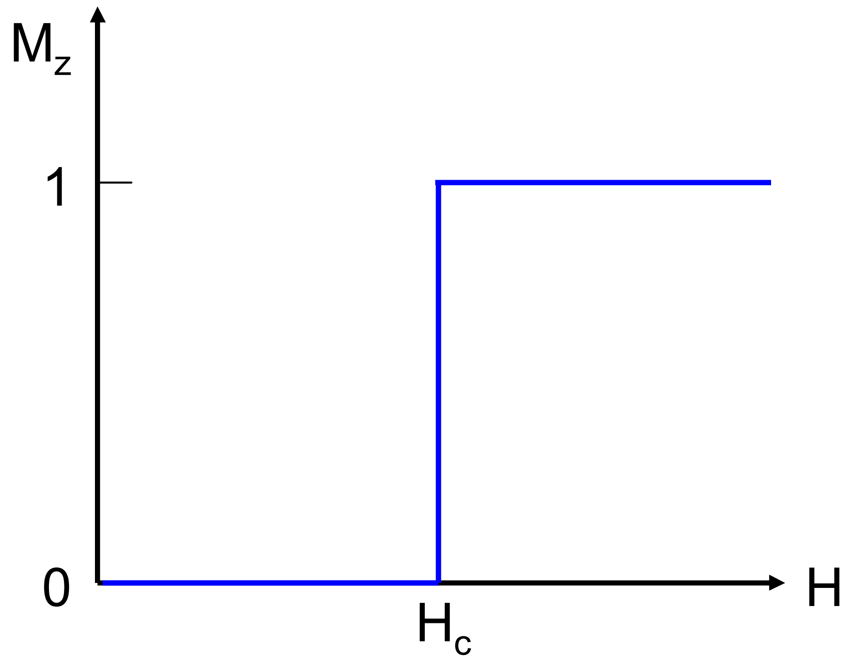
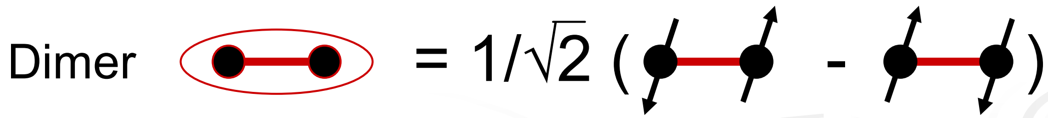

temperature
no “classical” critical point !
but quantum critical point
Néel or Curie
temperature
$\left|\langle \mathbf{S}_i \rangle\right| = 0$
$\left|\langle \mathbf{S}_i \rangle\right| \neq 0$
SPIN LIQUID
MAGNETIC ORDER
0 K
magnetic field, pressure, doping

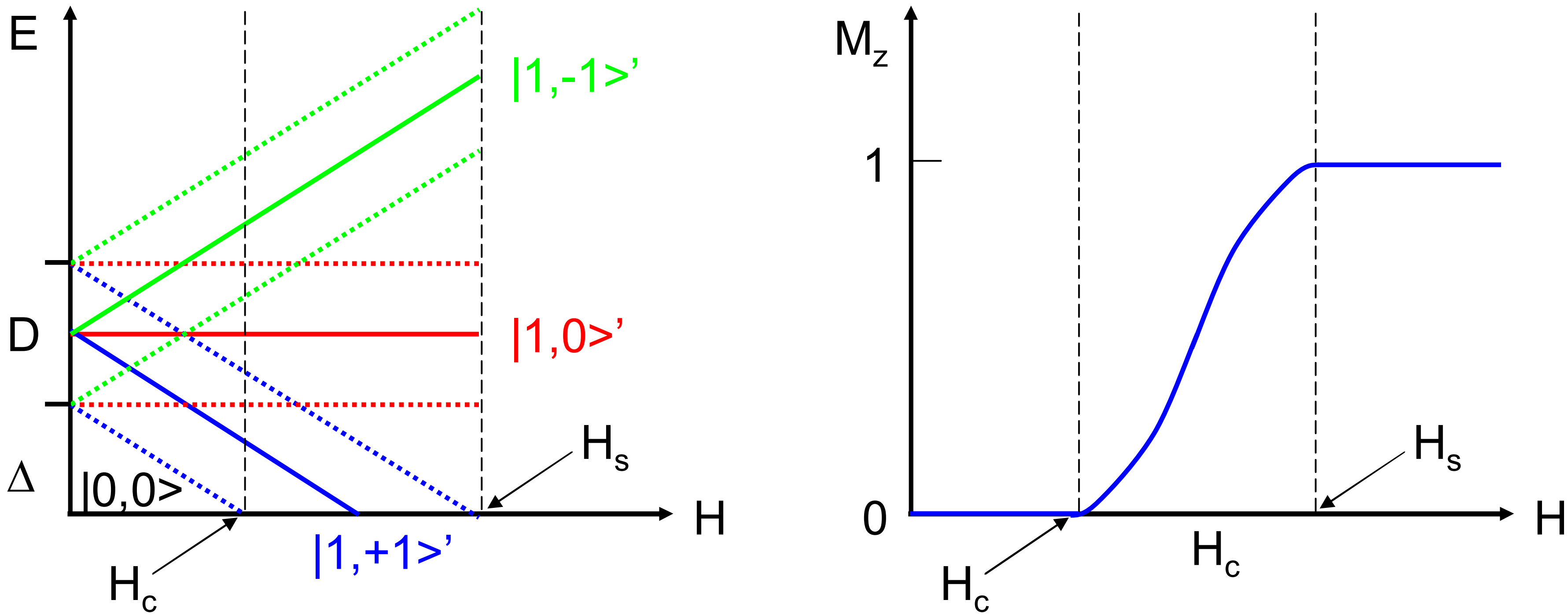
Quantum Phase Transition for Isolated Dimers



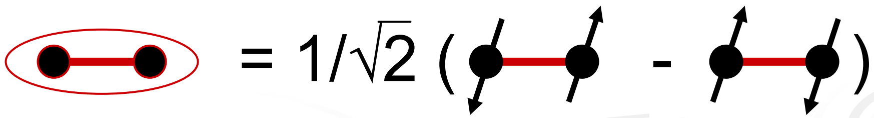




Quantum Phase Transition for Interacting Dimers



Dimer



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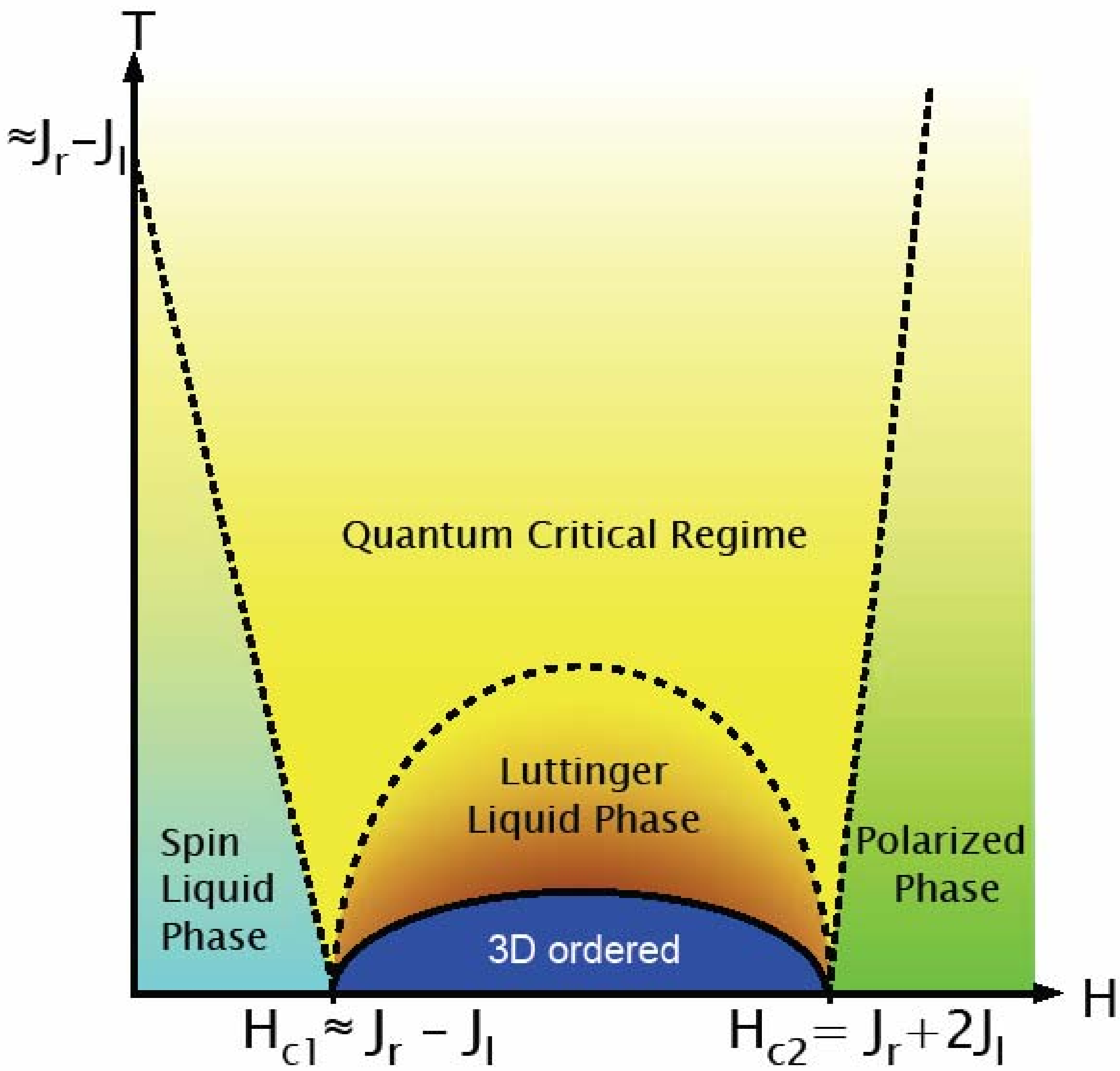
T
≈J_r−J_l
Quantum Critical Regime
Luttinger
Liquid Phase
Spin
Liquid
Phase
Polarized
Phase
3D ordered
H
H_c1≈ J_r − J_l
H_c2= J_r+2J_l

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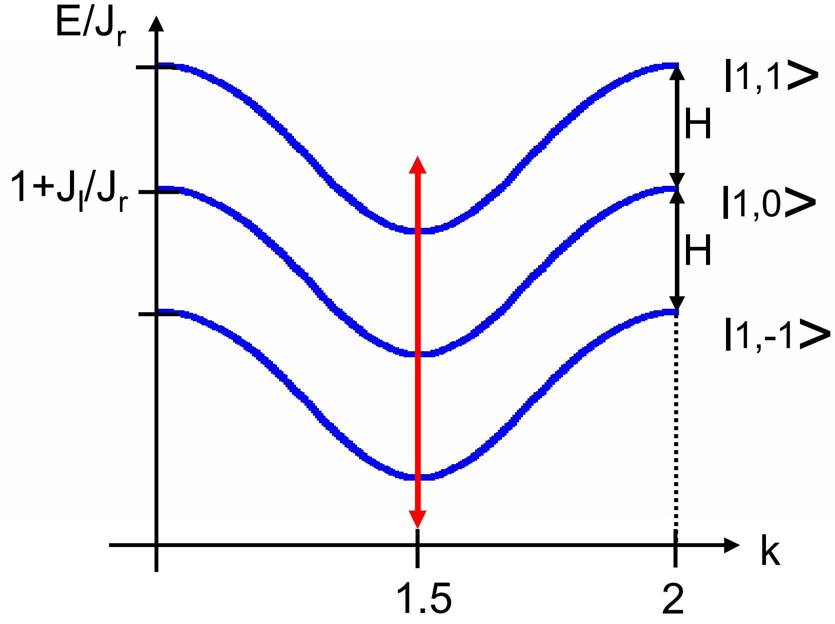
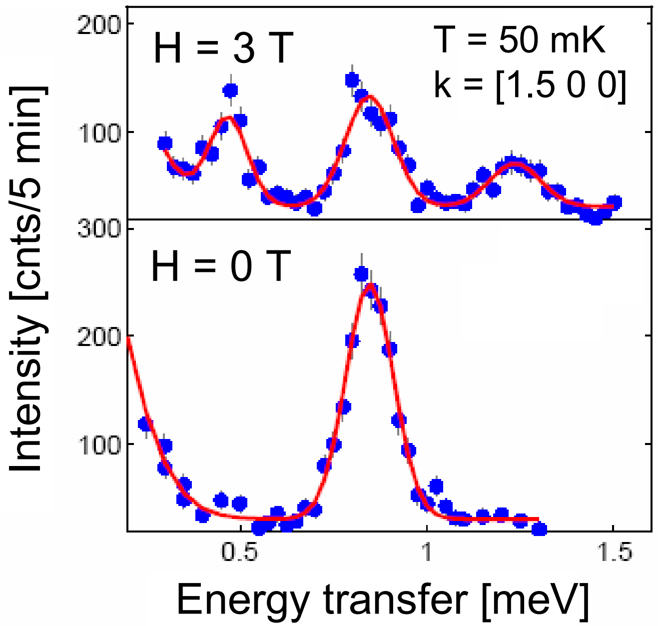
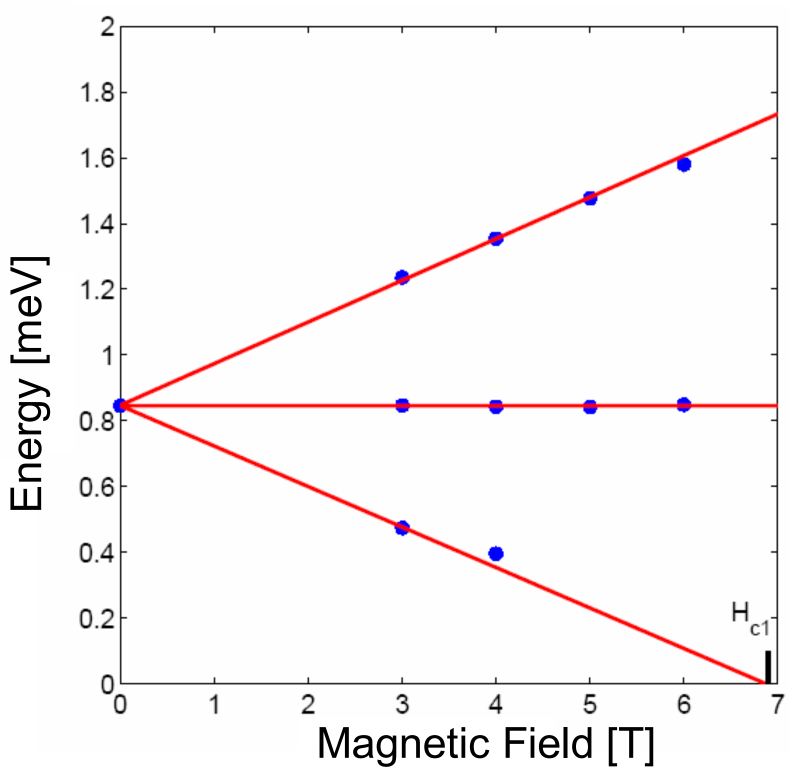
Excitations of the spin-liquid at H > 0T



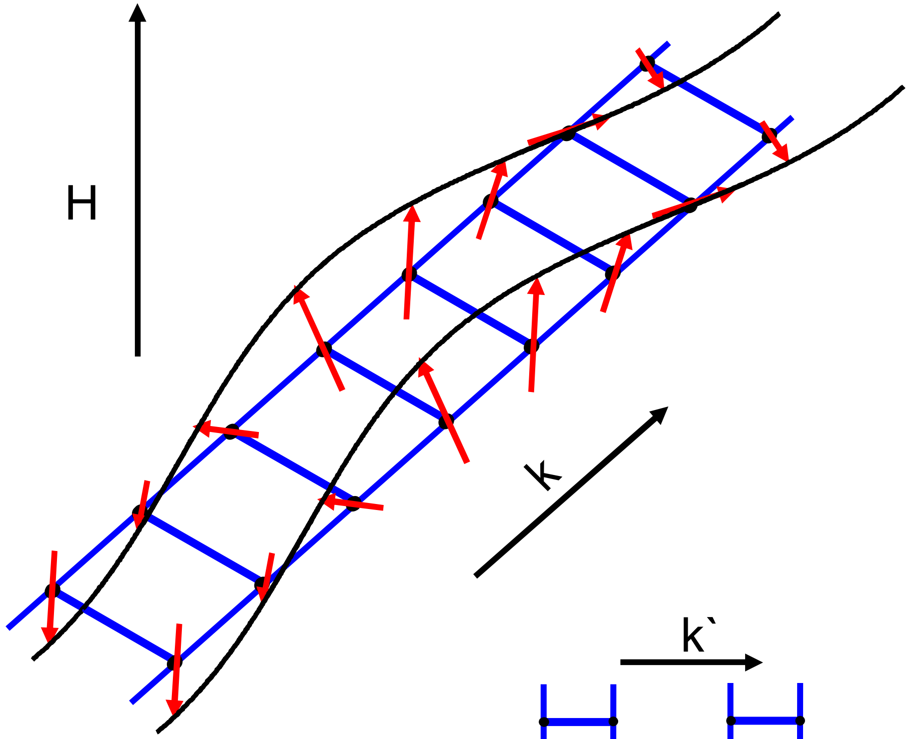


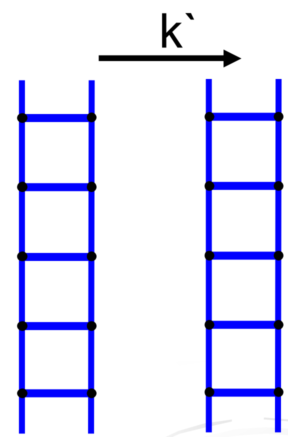


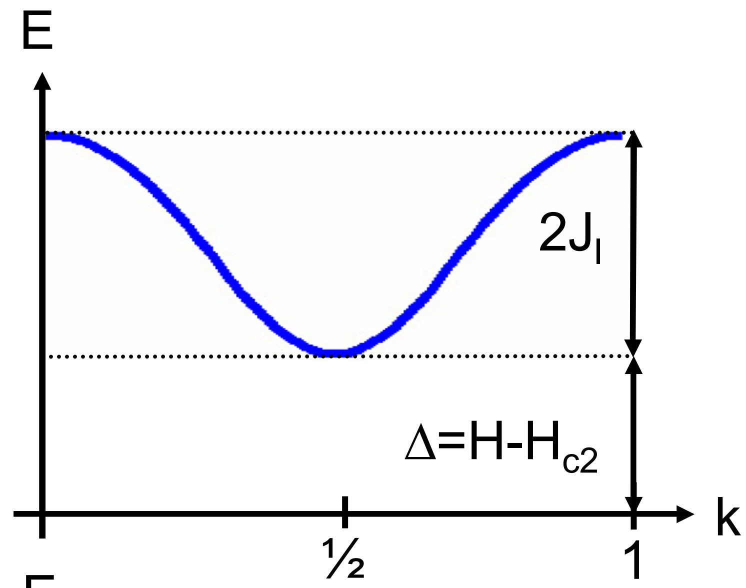
$\Rightarrow$ triplet excitation

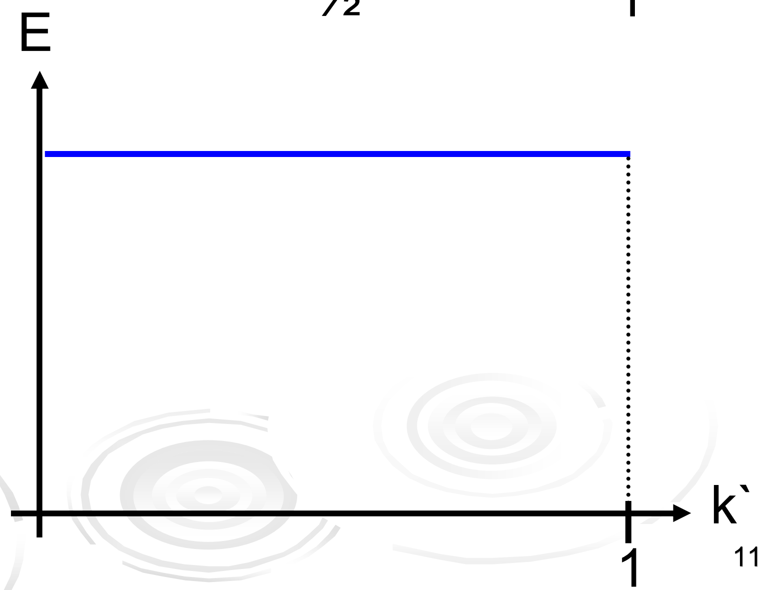
INS dispersion:	H_{c1}= 6.74(6) T
INS Zeeman split:	H_{c1}= 6.79(7) T
magnetisation:	H_{c1}= 6.6 T

Ferromagnetic spin waves in the saturated phase



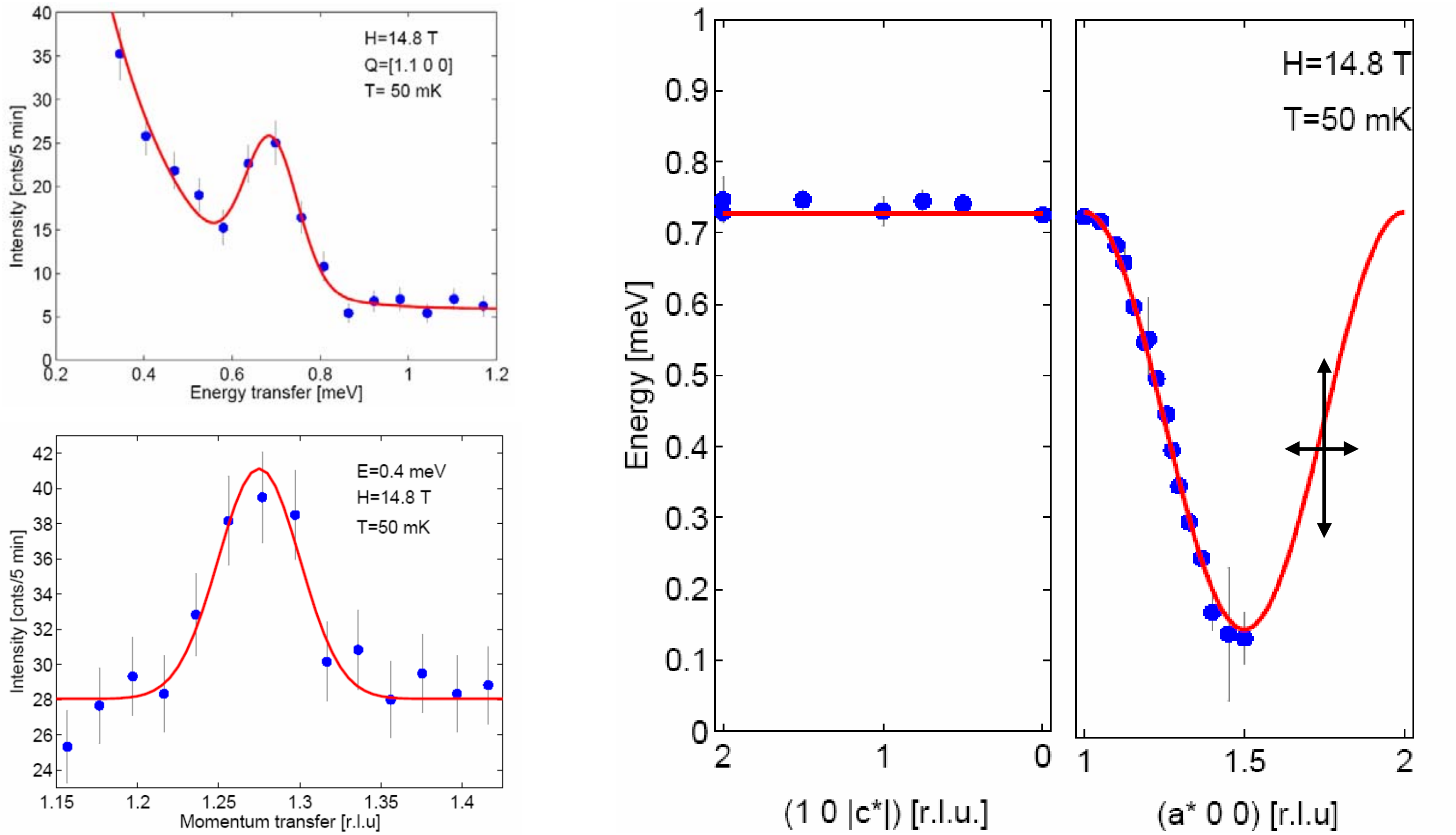






B. Normand, Acta Physica Polonica B 31, 3005

INS data in the saturated phase



exchange parameters: J_r = 1.116(3) meV, J_l = 0.290(4) meV
J' < 0.05 meV

Independent determination of $\hat{\mathcal{H}}$ $\Rightarrow$ excellent ladder behaviour

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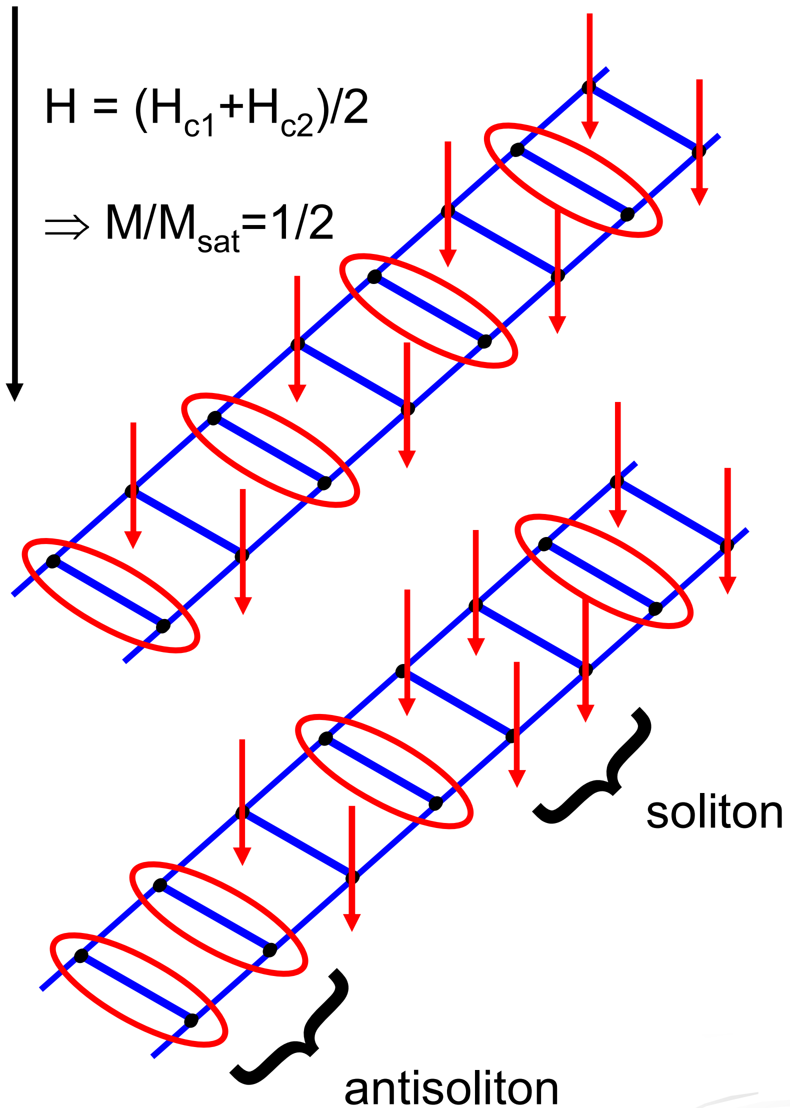
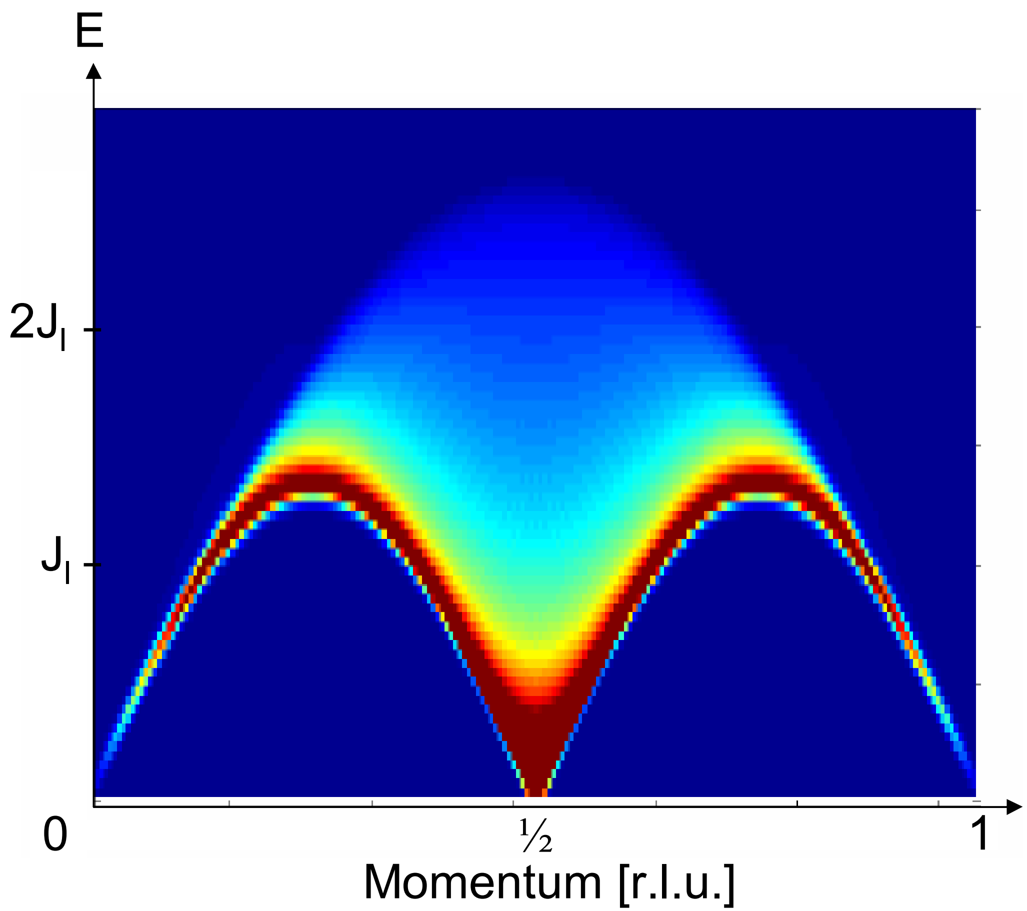
Excitations in the Luttinger phase





J. S. Caux, private communication

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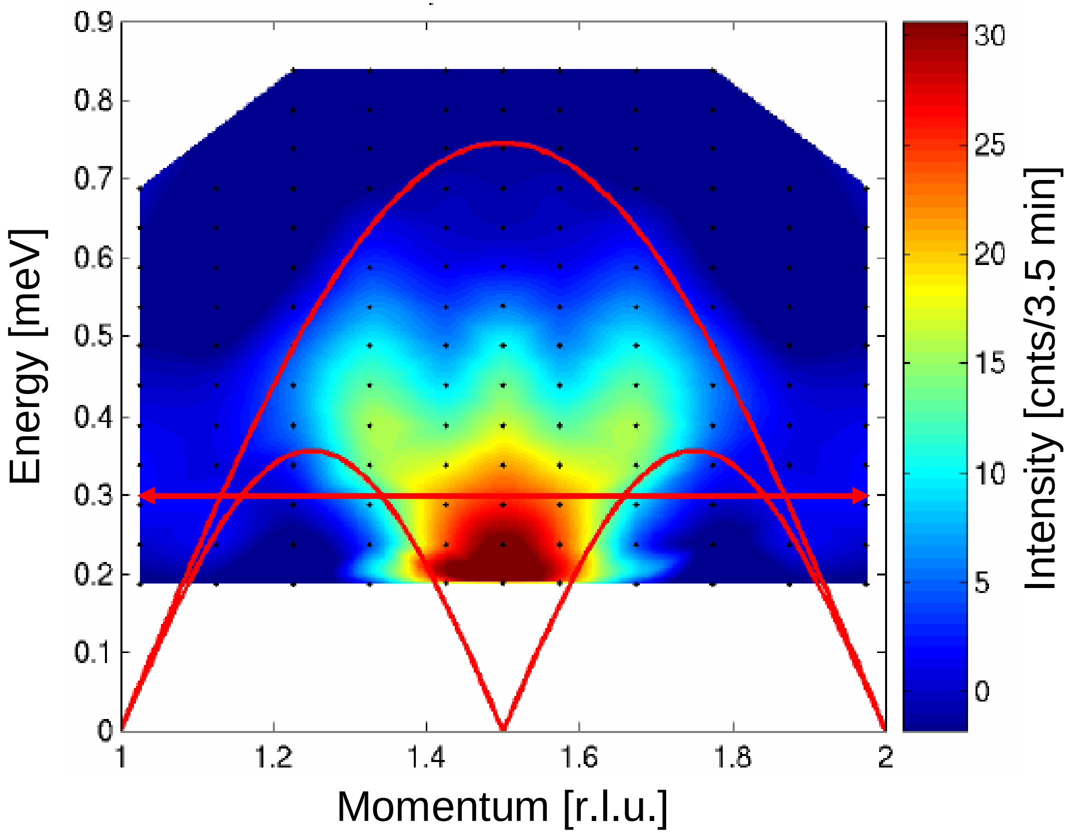
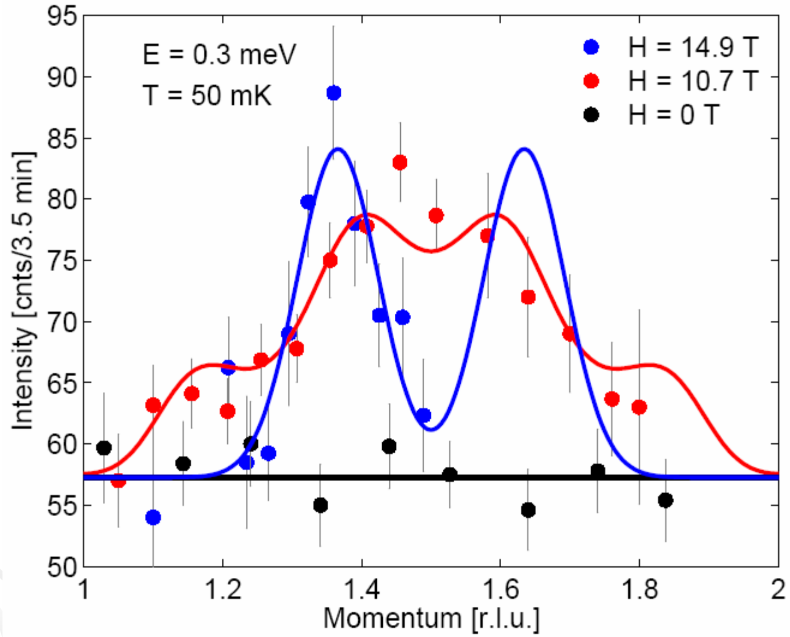
pairs of elementary excitations ⇒ Continuum

INS data in the Luttinger phase





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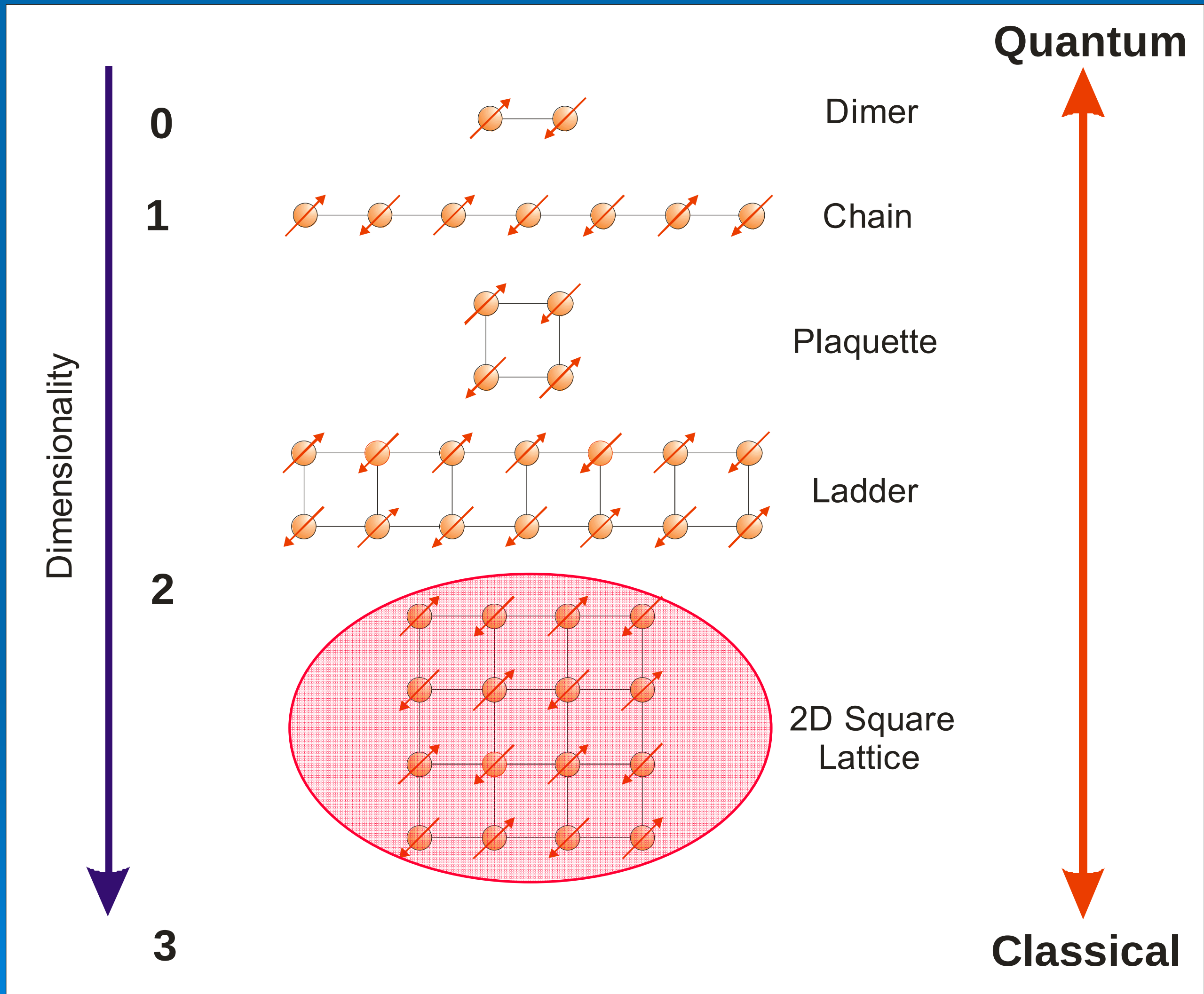
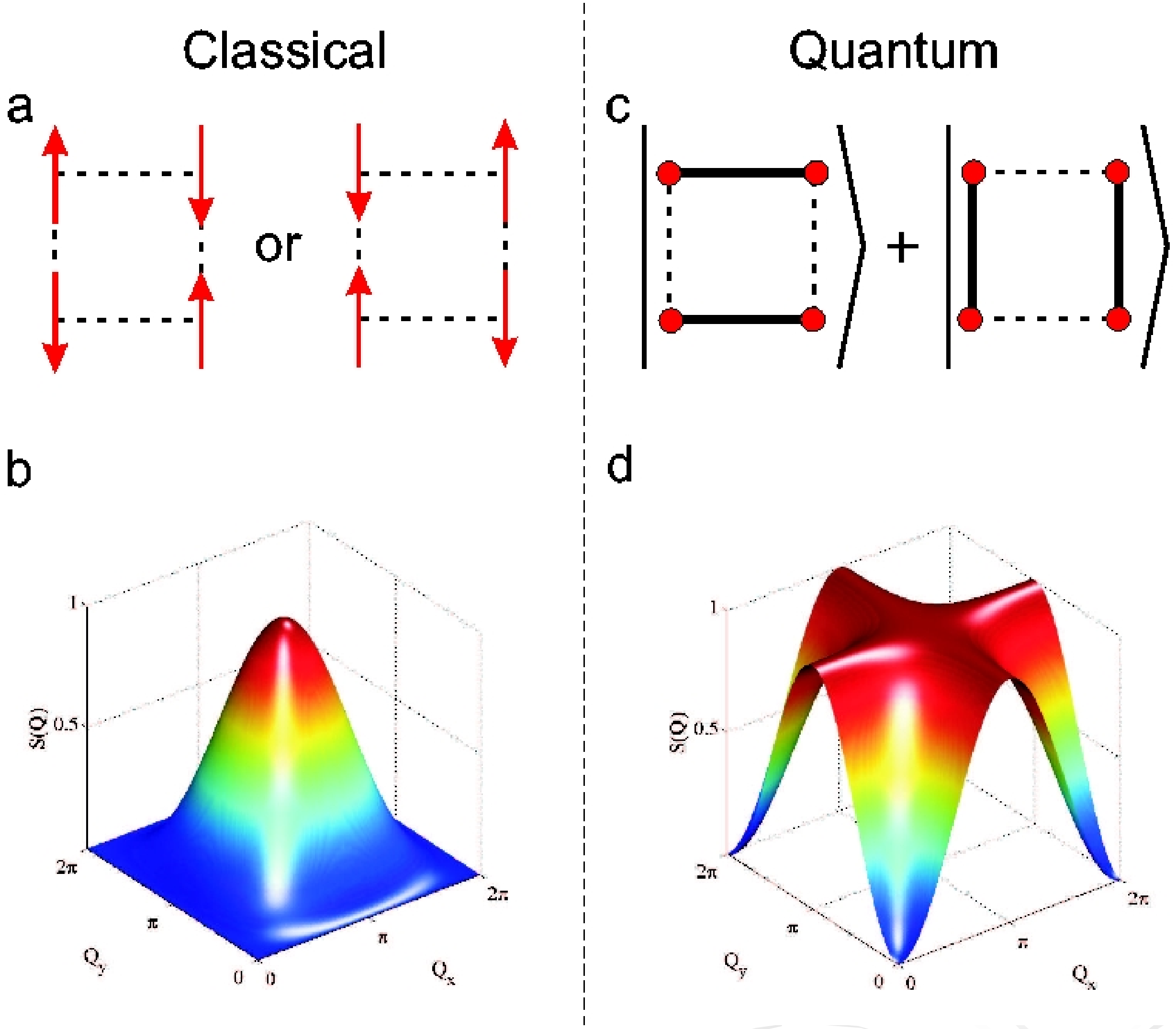
Magnetic Architecture



The Plaquette and the Valence Bond



Singlet

$$|d\rangle \equiv |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$$

Plaquette

$$\left|\begin{matrix} d_1 \\ d_2 \end{matrix}\right\rangle + |d_1 d_2\rangle =$$

$$\left(|\uparrow\downarrow\rangle_1 - |\downarrow\uparrow\rangle_1\right) \otimes \left(|\uparrow\downarrow\rangle_2 - |\downarrow\uparrow\rangle_2\right)$$

$$+\left(\left|\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right\rangle_1 - \left|\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right\rangle_1\right) \otimes \left(\left|\begin{matrix}\uparrow\\ \downarrow\end{matrix}\right\rangle_2 - \left|\begin{matrix}\downarrow\\ \uparrow\end{matrix}\right\rangle_2\right)$$

$$= -2\left|\begin{matrix}\uparrow\downarrow\\ \downarrow\uparrow\end{matrix}\right\rangle - 2\left|\begin{matrix}\downarrow\uparrow\\ \uparrow\downarrow\end{matrix}\right\rangle$$

$$+\left|\begin{matrix}\downarrow\uparrow\\ \downarrow\uparrow\end{matrix}\right\rangle + \left|\begin{matrix}\uparrow\downarrow\\ \uparrow\downarrow\end{matrix}\right\rangle + \left|\begin{matrix}\uparrow\uparrow\\ \downarrow\downarrow\end{matrix}\right\rangle + \left|\begin{matrix}\downarrow\downarrow\\ \downarrow\downarrow\end{matrix}\right\rangle$$

$$= |G\rangle$$

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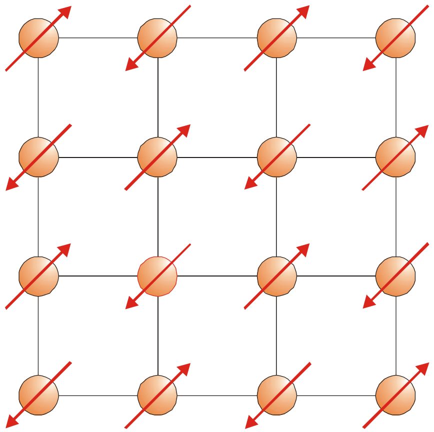
2D-Quantum Magnetism

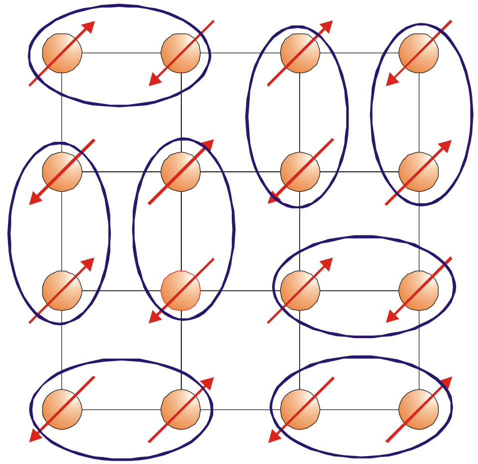
2D Heisenberg antiferromagnet on a square lattice

Long-range
Néel Order

$\langle S \rangle = 1/2$



v. s.



Spin-liquid
Resonating Valence Bond (RVB)

$\langle S \rangle = 0$

2D: ordered, but only 60% of full moment, and only at T=0

$\Downarrow$ Spin-waves

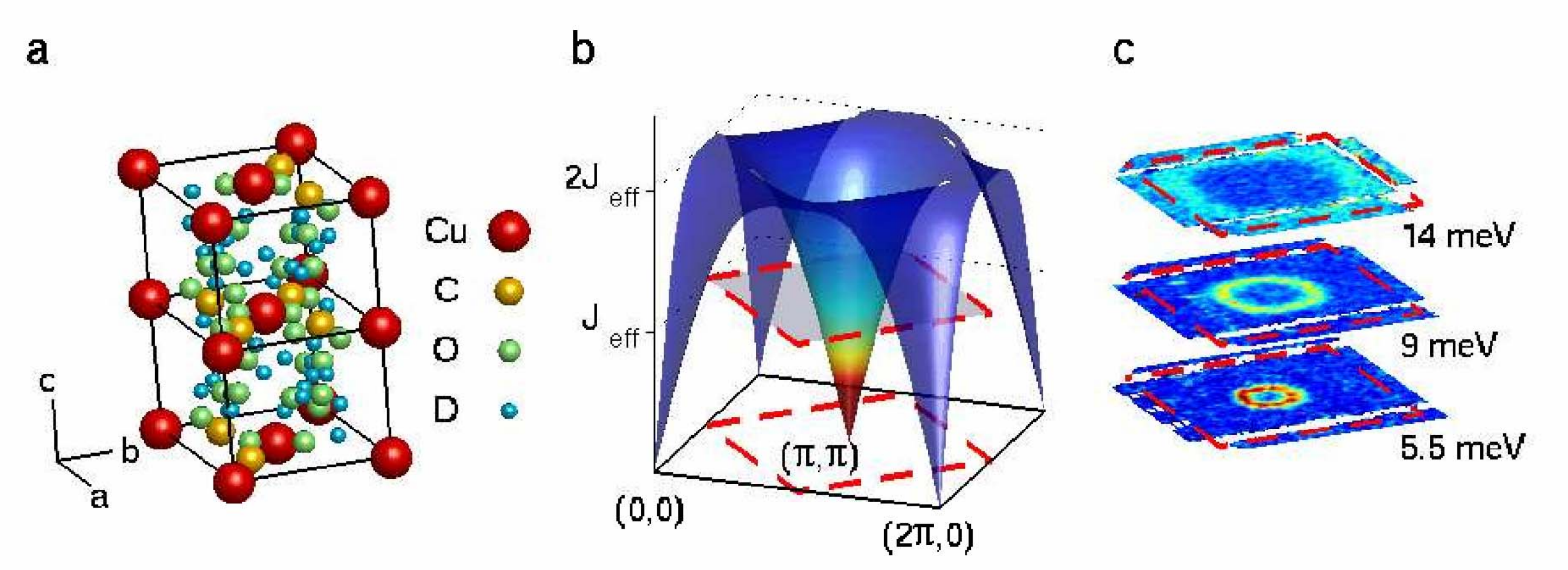
$\Uparrow$ Quantum fluctuations

- Are there other types of 'correlations' ?
  - Resonating valence bonds (RVB)
  - Gutzwiller-projected BCS

} Investigate excitations with neutron scattering

A model 2D quantum magnet

Copper formate tetra-deuterate (CFTD)



Crystal structure in real-space

Spin-wave dispersion in reciprocal space

Slices of neutron scattering intensity

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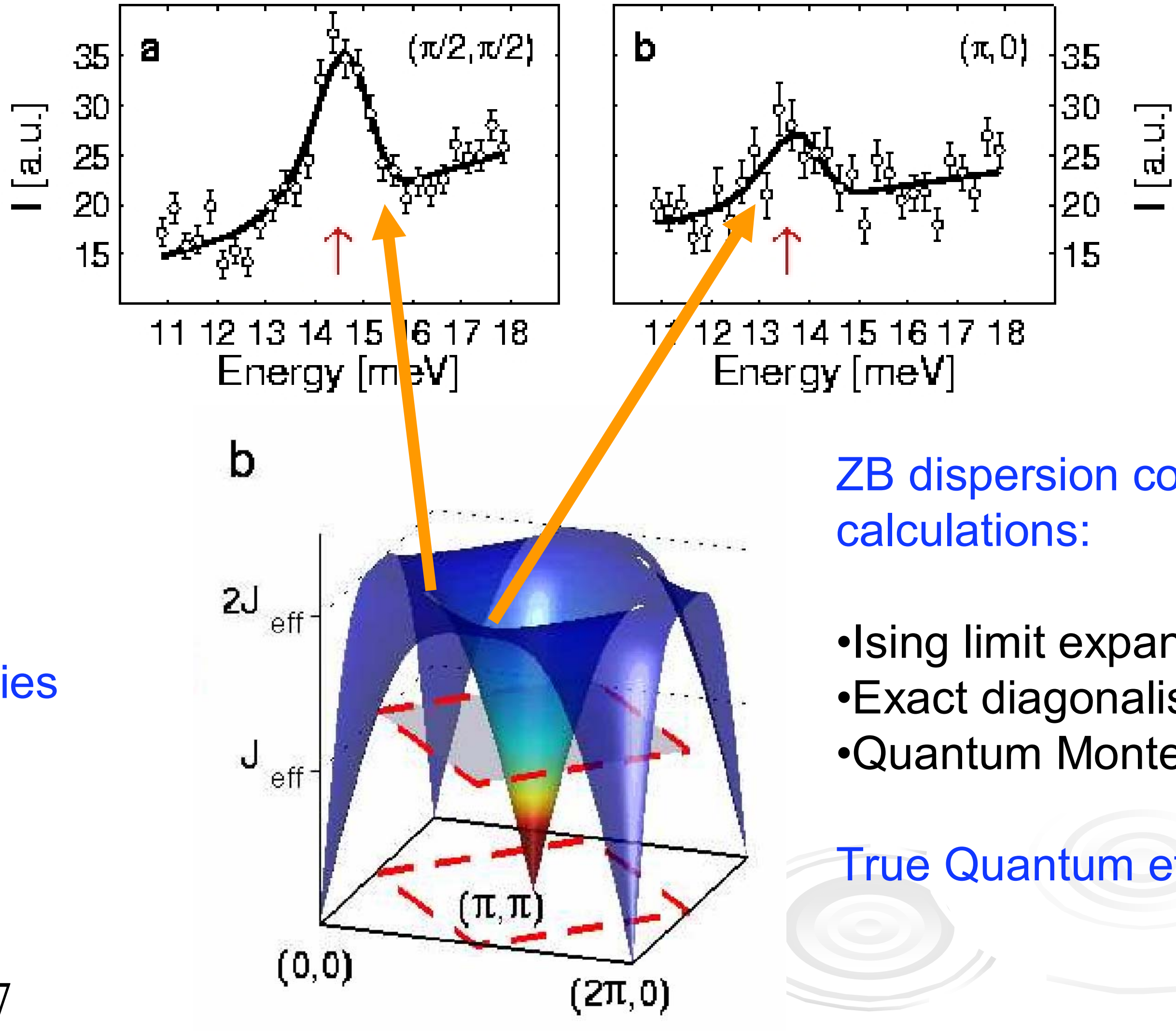
Surprise !

Anomalies at the Zone Boundary



Expected small uniform renormalisation of classical spin wave energies

Ronnow et al.

ZB dispersion confirmed by calculations:

- Ising limit expansion
- Exact diagonalisation
- Quantum Monte Carlo

True Quantum effect

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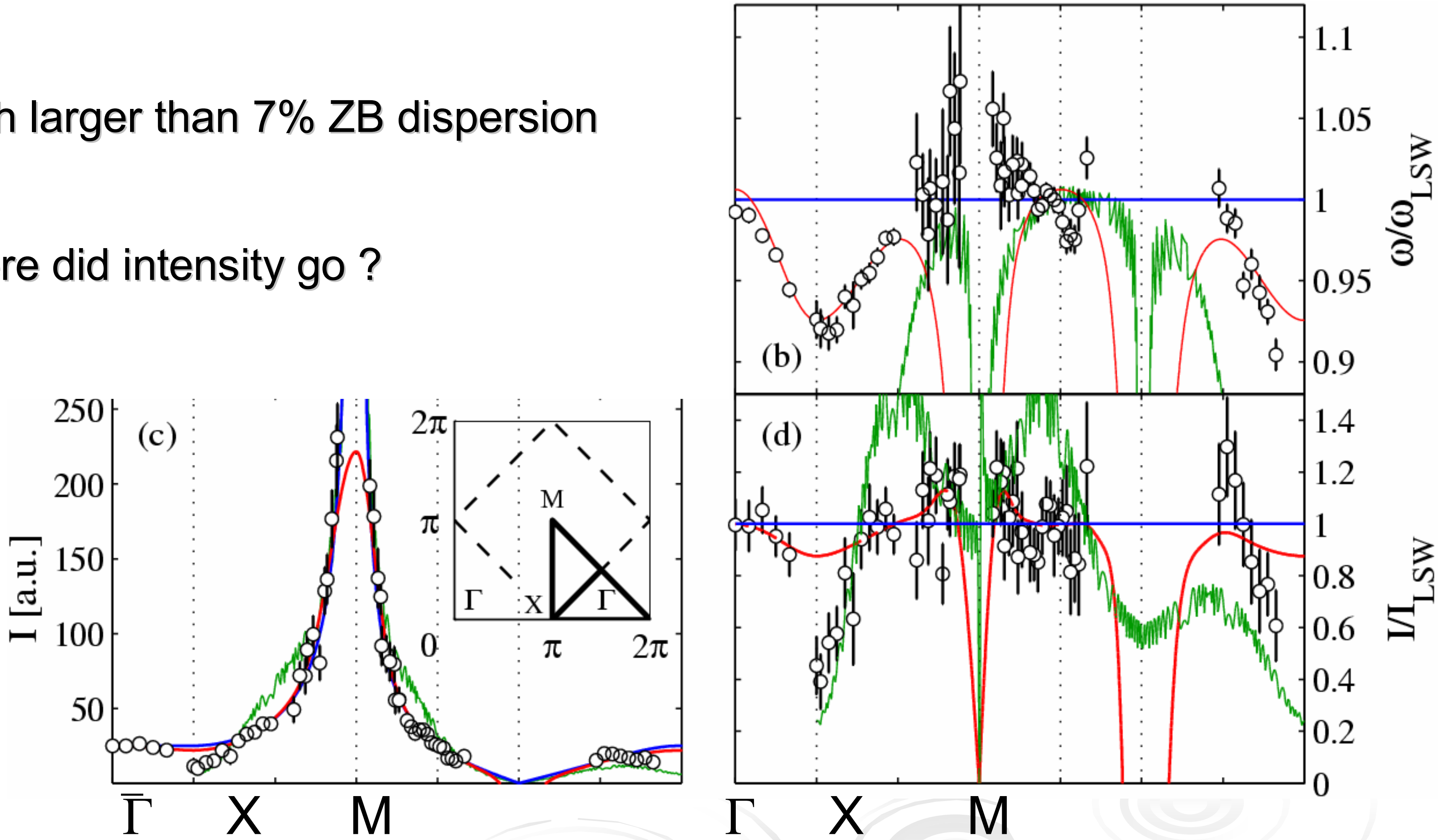
Magnon intensities

Giant 50% intensity effect at (π,0)

Much larger than 7% ZB dispersion

Where did intensity go ?



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Christensen, Rønnow *et al.* PNAS 2007