Paradigm of Condensed Matter Theory

Theory of Quantum Magnetism

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Acknowledgement

In this lecture, I have used many pictures downloaded from Internet. I am very grateful to the authors of these pictures, although I do not even known their names in many cases.

Magnetism Is an Evergreen Tree of Science

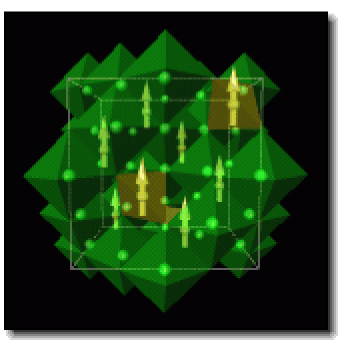
The study of magnetism as a cooperative phenomena has been responsible for the most significant advances in the theory of thermodynamic phase transitions. This has transformed statistical mechanics into one of the sharpest and most significant tools for the study of condensed matter.

Magnets: Ancient Gift

Han Dynasty
Chinese Compass

China
- 4000 BC magnetite 磁铁矿
- 3000-2500 BC meteoric iron

Greek
- 800 BC lodestone 磁石



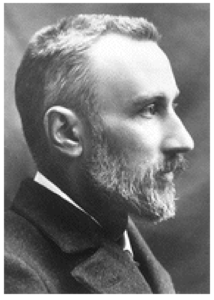
Fe_3O_4

Magnetic memory

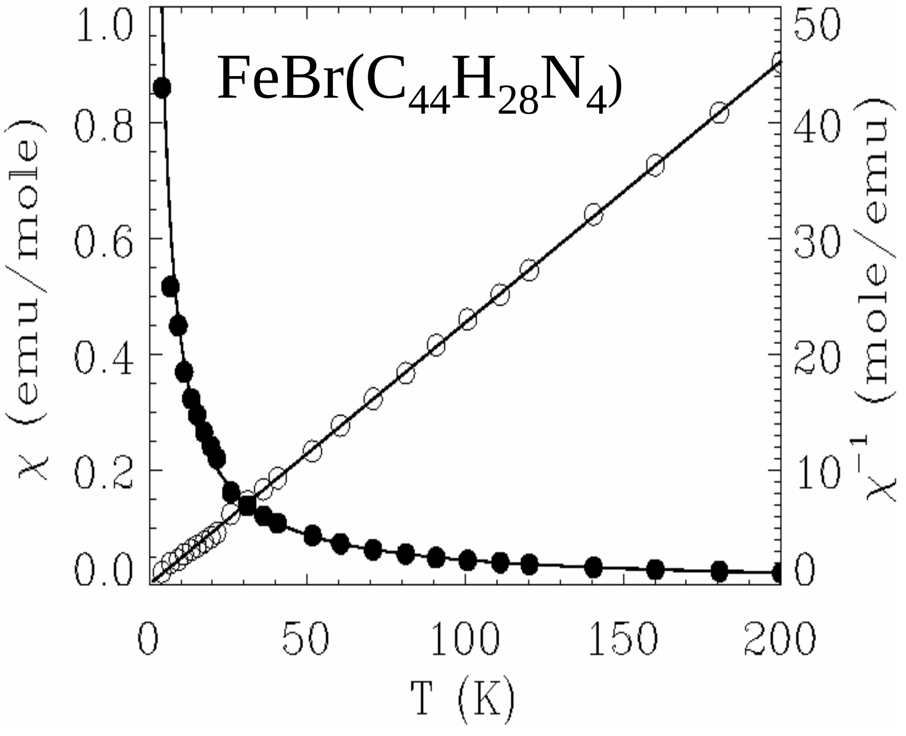
Outset of Modern Theory of Magnetism

- Pierre Curie discovered the Curie law of paramagnetic materials and Curie transition temperature

$$\chi = \frac{C}{T}$$



Pierre Curie
1903 Nobel Prize
1859-1906



Classical Theory of Paramagnetism

Energy of a dipole $$E = -\vec{\mu} \cdot \vec{H}$$

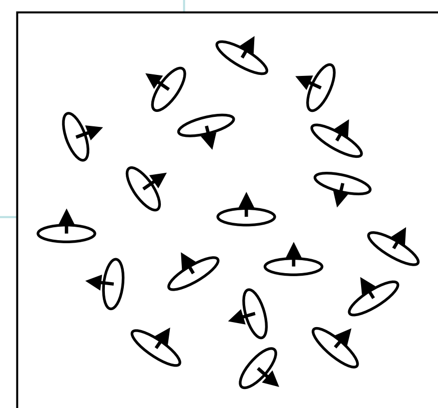
Probability of a dipole in energy E $$p(E) = e^{-E/k_B T}$$

Average of dipole orientation $$dn \propto d\theta \sin\theta e^{\mu H \cos\theta / k_B T}$$

Paul Langevin
1872-1946

Magnetization: $$M = N\mu \left(\coth \frac{\mu H}{k_B T} - \frac{k_B T}{\mu H} \right)$$

Susceptibility $$\chi = \frac{M}{H} \sim \frac{1}{T}$$



paramagnetic minerals

Olivine $(Fe,Mg)_2SiO_4$
橄榄石

Montmorillonite (clay)
蒙脱石（粘土）

Siderite $(FeCO_3)$
菱铁矿, 陨铁

Serpentinite
$Mg_3Si_2O_5(OH)_4$
蛇纹岩

Chromite $(FeCr_2O_4)$
铬铁矿

diamagnetic minerals

Quartz (SiO_2)
石英

Calcite $(CaCO_3)$
方解石

Graphite (C)
石墨

Halite (NaCl)
岩盐

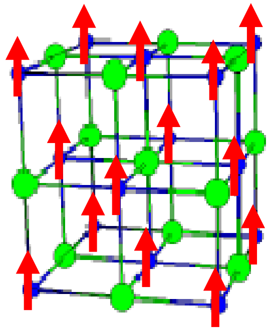
Sphalerite (ZnS)
闪锌矿

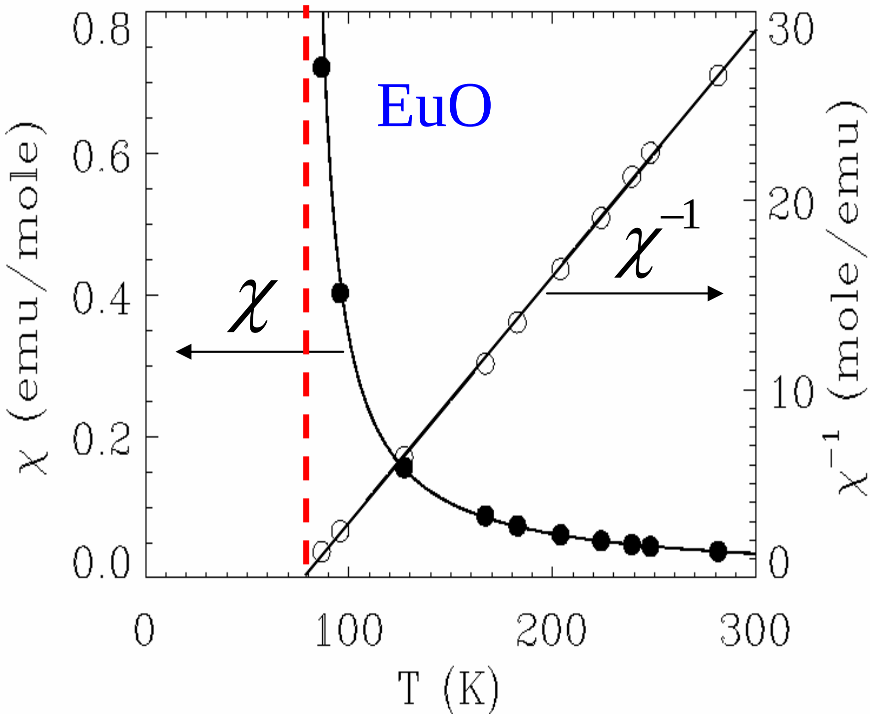
Theory of Molecular Field

- 1907 Pierre Weiss formulated the first modern theory of magnetism: molecular field
  --- first self-consistent mean-field theory

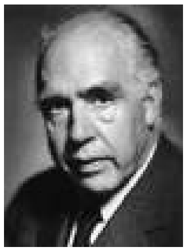
$$\chi = \frac{C}{T - T_c}$$

Pierre Weiss
1864-1940





Bohr-van Leeuwen Theorem



Niels Bohr
1885-1962

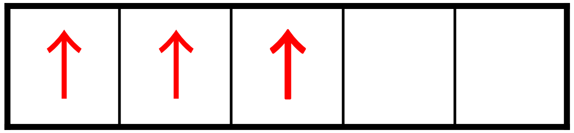
At any finite temperature, and in all finite applied electrical or magnetic fields, the net magnetization of a collection of electrons (orbital currents) in thermal equilibrium vanishes identically.

Van Vleck
1977 Nobel

Classic Theory of magnetism is irrelevant and Quantum Theory is needed!

Spin: Origin of Magnetic Moment

- Electron spin
- Ion spins: Hund's Rule



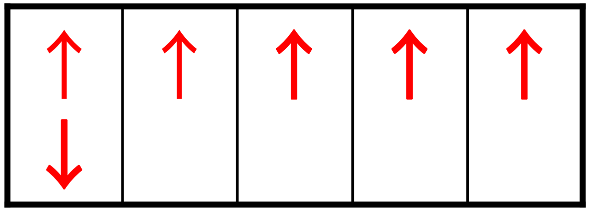
Cr3+: $3d^3$

1st rule: S=3/2
2nd rule: L=3
S-O coupling: J = 3/2

Paul Dirac

George Uhlenbeck

S.A. Goudsmit



Fe: 3d6

S = 2, L = 2, J = L+S = 4

79 elements are magnetic in atomic state

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

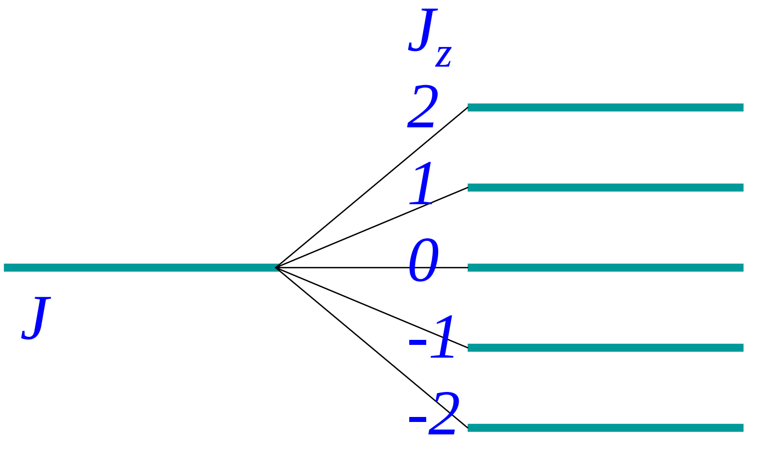
15 elements are magnetically ordered in the solid state

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
				Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu
				Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lw

Quantized Langevin Theory

$$M = N \frac{\sum_{J_z=-J}^{J} - g\mu_B J \exp\left(- g\mu_B JH / k_B T\right)}{\sum_{J_z=-J}^{J} \exp(-g\mu_B JH / k_B T)}$$

$$= N\mu_B gJ \; f\left(\frac{g\mu_B HJ}{k_B T}\right)$$



Curie Law: $\chi_m(T) = \frac{M}{H} \propto \frac{1}{T}$

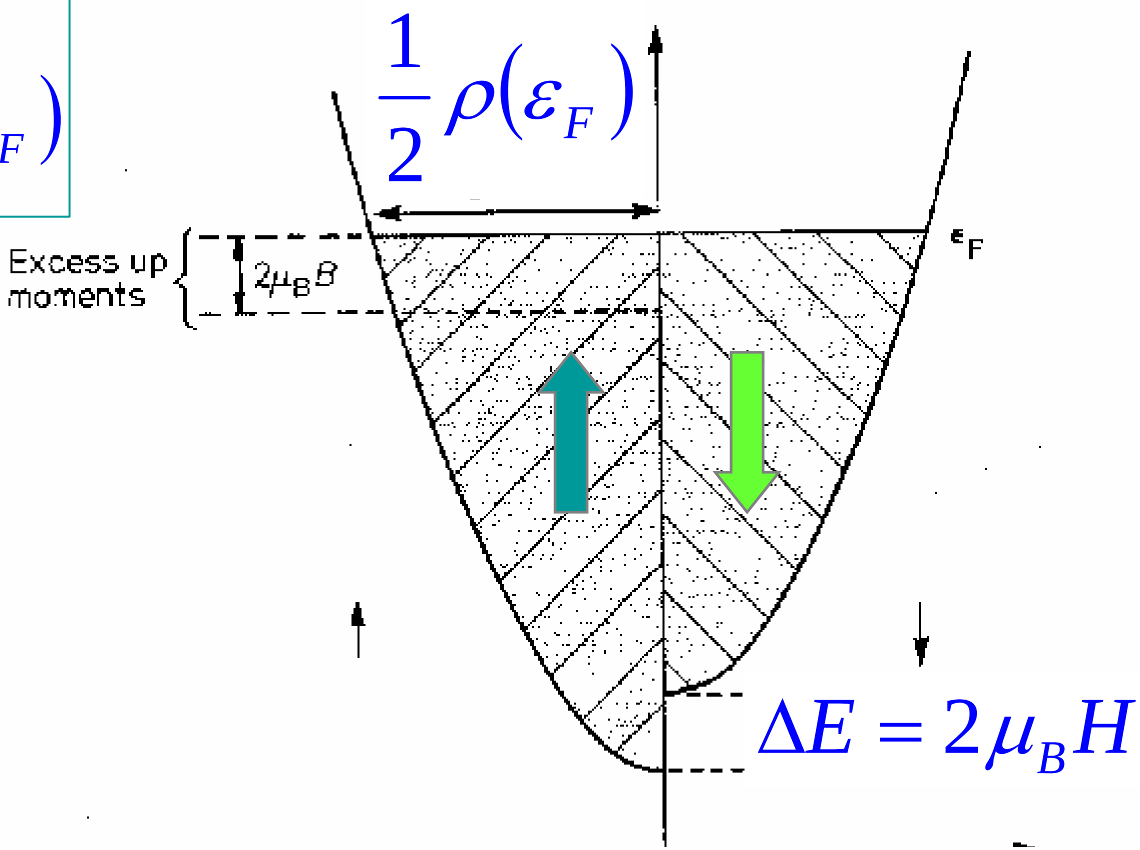
Pauli Paramagnetism of Metal

$$M \approx \mu_B \Delta n = \mu_B^2 \rho(\varepsilon_F) H$$

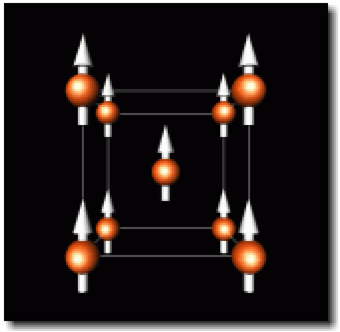
$$\chi(T) = \frac{M}{H} = \mu_0 \mu_B^2 \rho(\varepsilon_F)$$

Density of states

Wolfgang Pauli

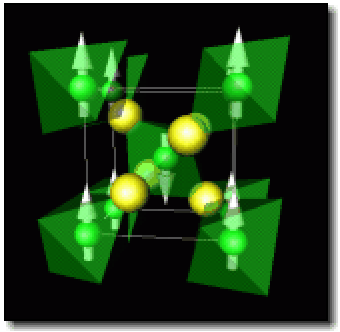


Different types of collective magnetism



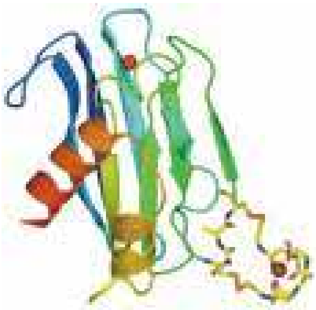
BCC Iron

Ferromagnet

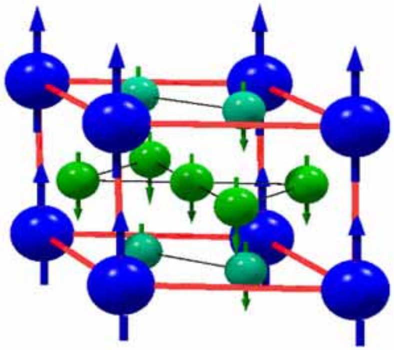


MnF_2

Antiferromagnet

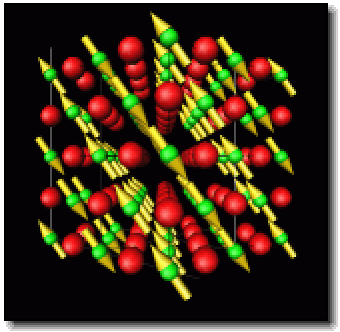


Paramagnet



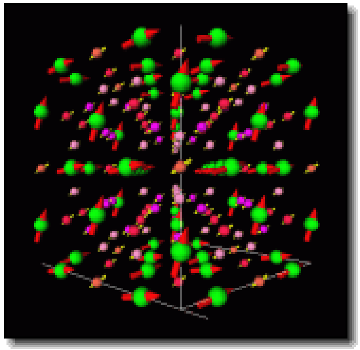
$GdCo_5$

Ferrimagnet



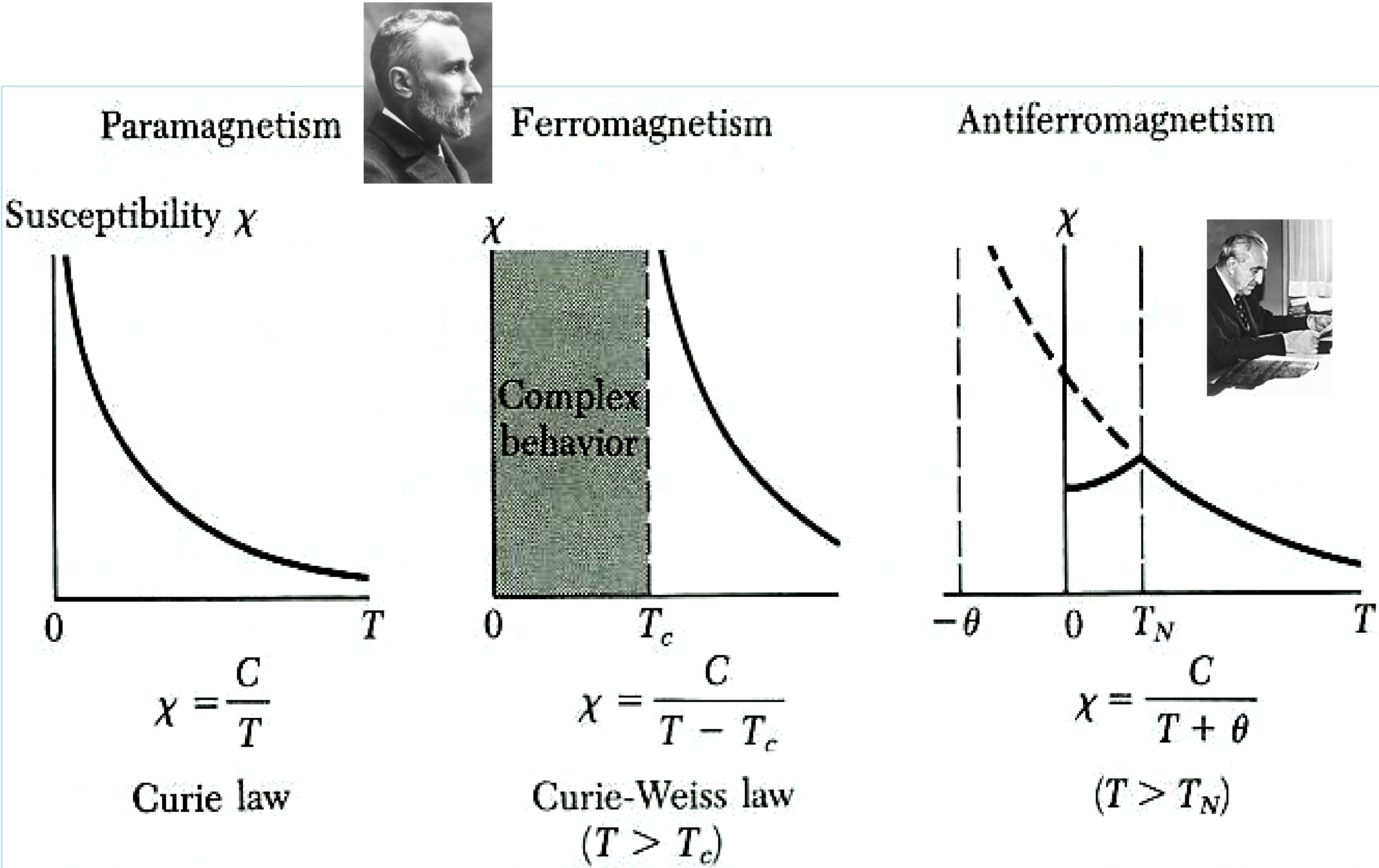
MnO

Antiferromagnet

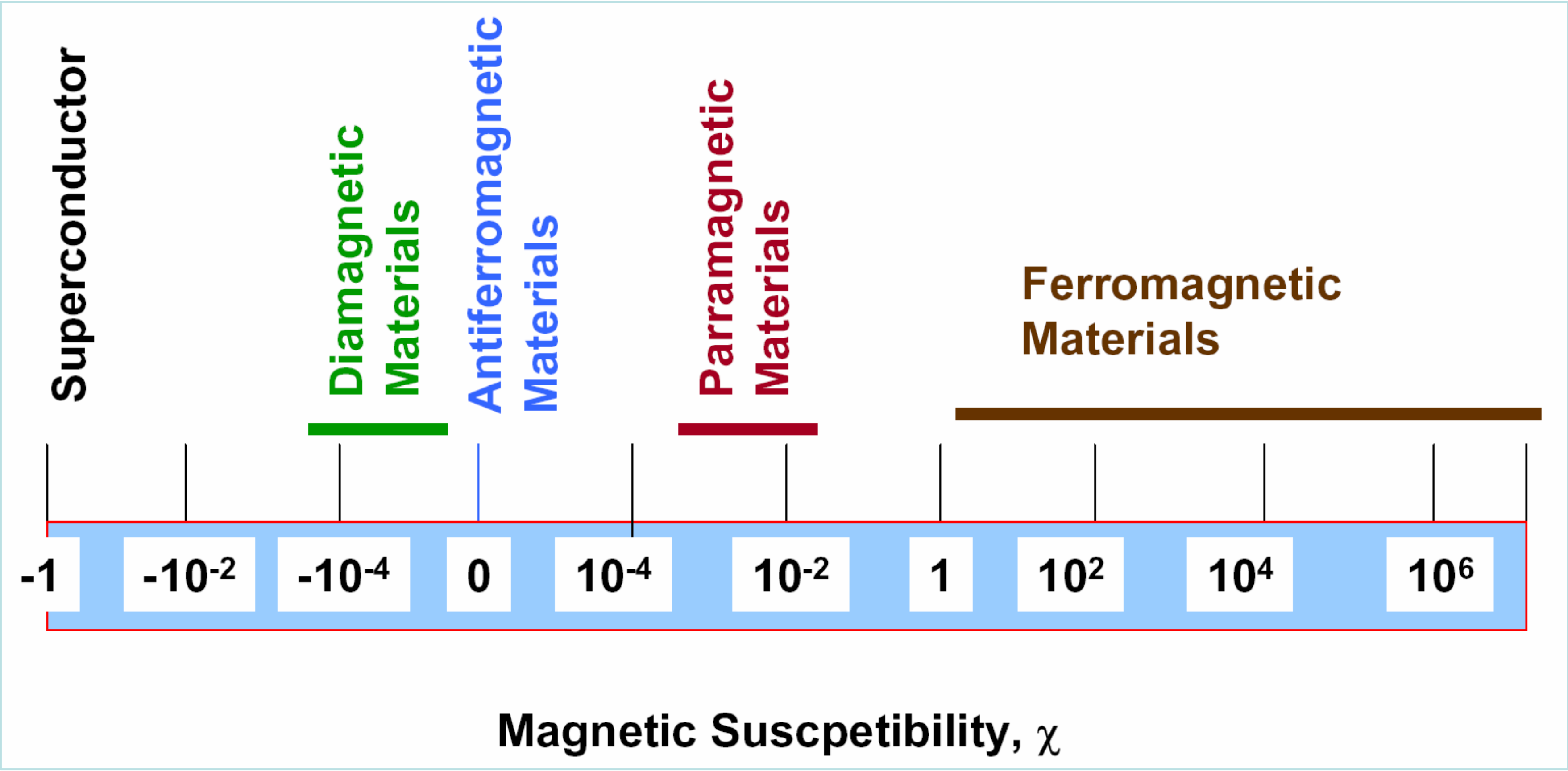


Er_6Mn_{23}

Different types of collective magnetism

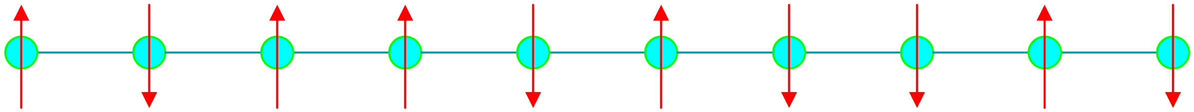


Susceptibility



Heisenberg Model

$$H = J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j$$



- J < 0 Ferromagnetic coupling (metal or insulator)
- J > 0 Antiferromagnetic coupling (insulator, freeze charge degrees of freedom)

Heisenberg
Nobel 1932

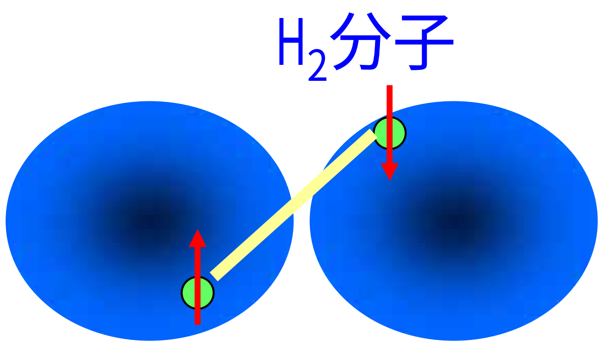
$$S_i = c_i^+ \frac{\sigma}{2} c_i$$

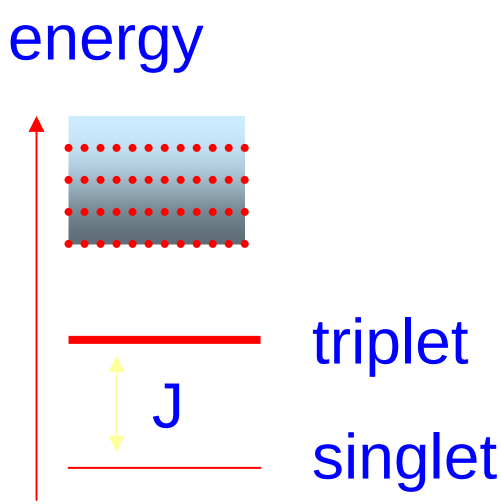
$$\hat{\boldsymbol{S}}_i^2 = S(S+1)\,\hbar^2$$

$$[\hat{S}_j^x, \hat{S}_j^y] = i\hbar\,\hat{S}_j^z$$

Hint from Hydrogen molecule

- Direct Coulomb prevents two electrons to form a chemical bond
- H_2 or chemical bond is formed by the exchange interaction of electrons





Exchange Interaction of Electrons

$$\Psi_+(1,2)=\left[\psi_1(r_1)\psi_2(r_2)-\psi_1(r_2)\psi_2(r_1)\right]\chi_S(1,2)$$ E_0 ground state, spin singlet

$$\Psi_-(1,2)=\left[\psi_1(r_1)\psi_2(r_2)+\psi_1(r_2)\psi_2(r_1)\right]\chi_T(1,2)$$ E_1 1st excitation, spin triplet

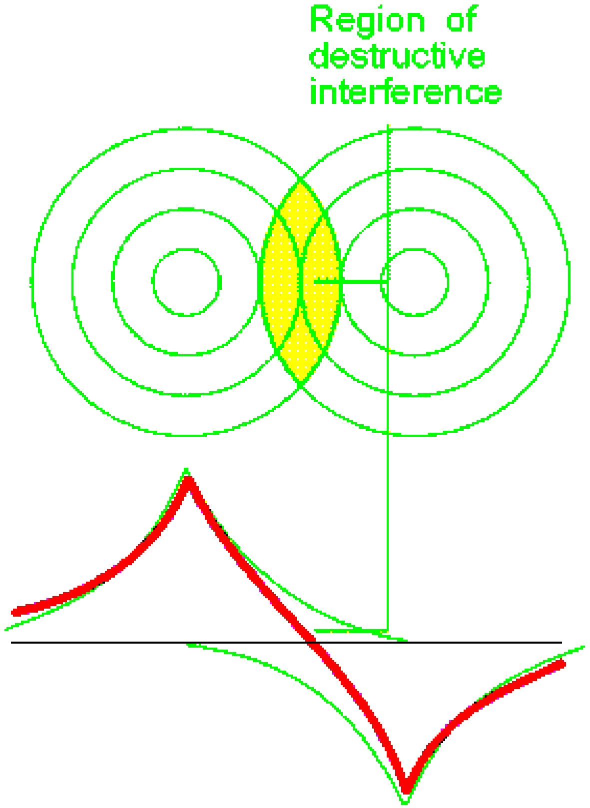
W Heitler F London

Z. Physik, 44， 455 (1927)

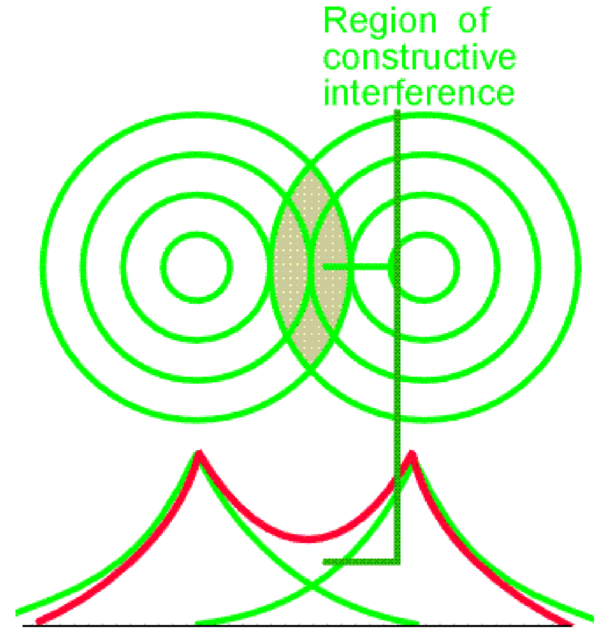
$$\chi_S(1,2)=\frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2-\downarrow_1\uparrow_2\right)$$

$$\chi_P(1,2)=\begin{cases}\uparrow_1\uparrow_2\\ \frac{1}{\sqrt{2}}\left(\uparrow_1\downarrow_2+\downarrow_1\uparrow_2\right)\\ \downarrow_1\downarrow_2\end{cases}$$

Exchange interactions



S=1 wave function antisymmetric

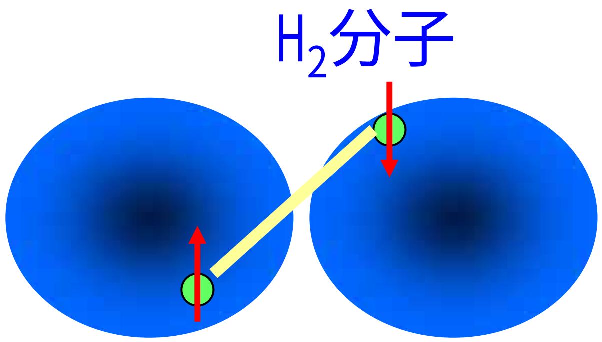


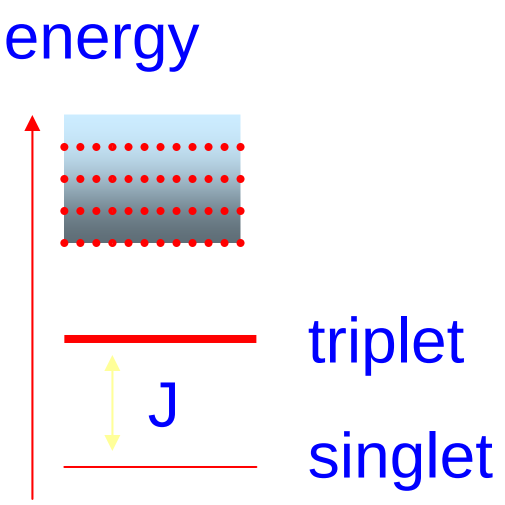
S=0 wave function symmetric

Effective description of low energy states of H_2

- Heisenberg exchange interaction

$$J\vec{S}_1\cdot\vec{S}_2=\begin{cases}-\dfrac{3}{4}J & \text{Singlet}\\[2ex] \dfrac{1}{4}J & \text{Triplet}\end{cases}$$





Exchange interactions

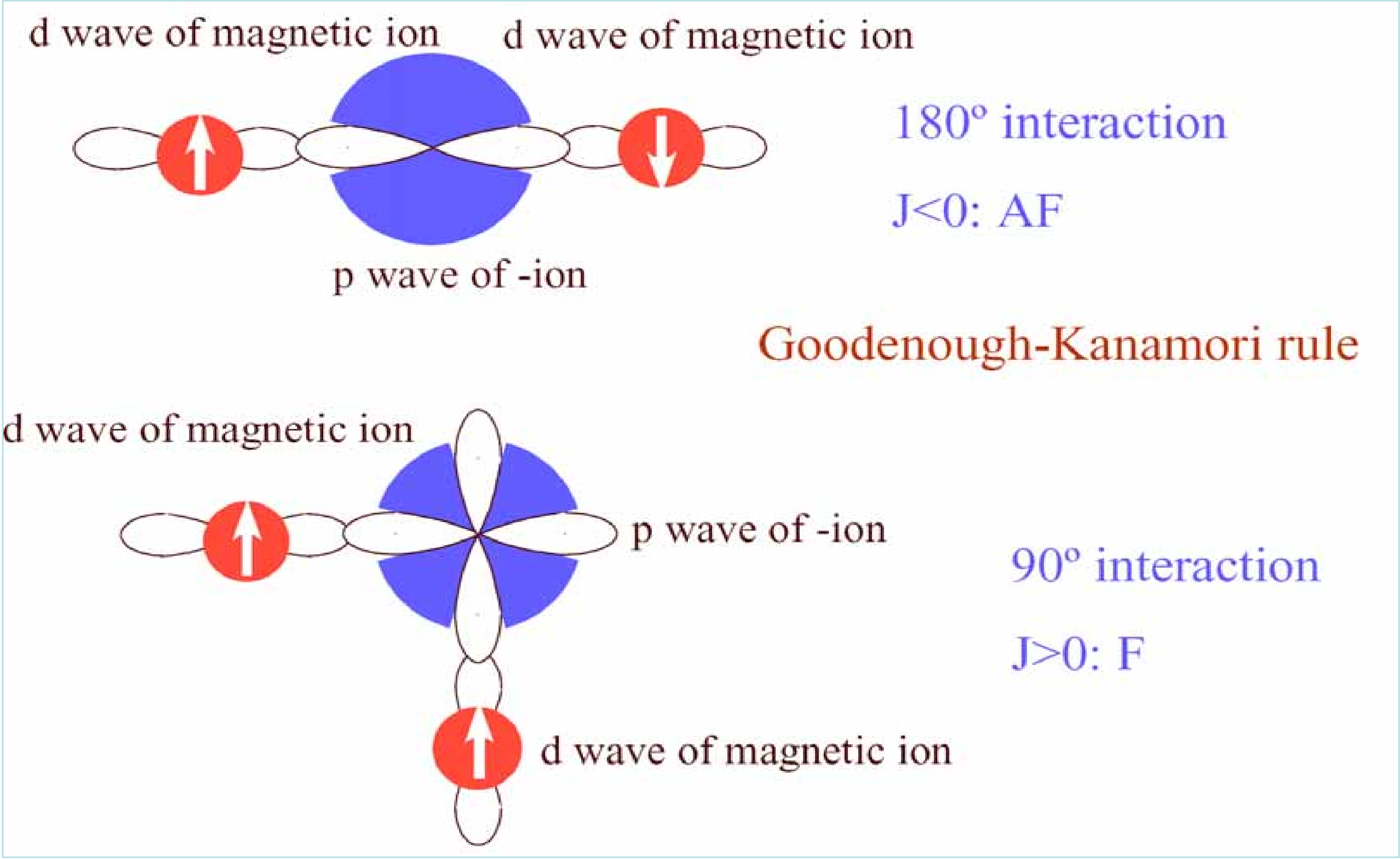
In solids: direct exchange is present but small because d and f orbitals are localized:

$$J_{12} \propto \int dr_1 dr_2 \Phi_1^*(r_1)\Phi_2(r_2)V(r_{12})\Phi_1^*(r_2)\Phi_2(r_1)$$

Indirect mecanisms are usually larger:

- Superexchange (short range, ferro or AF)
- RKKY (long range, oscillating sign)
- Double exchange (ferro)
- Itinerant magnetic systems

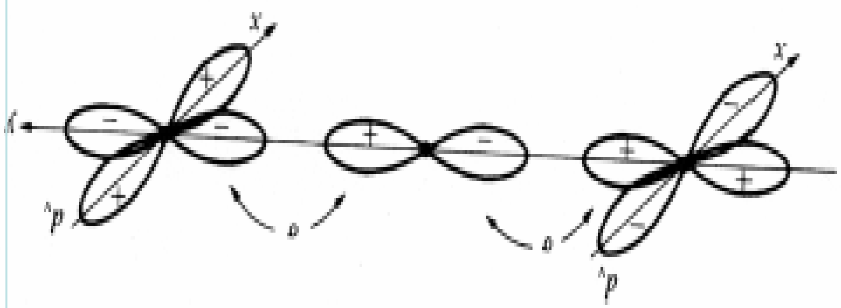
Superexchange



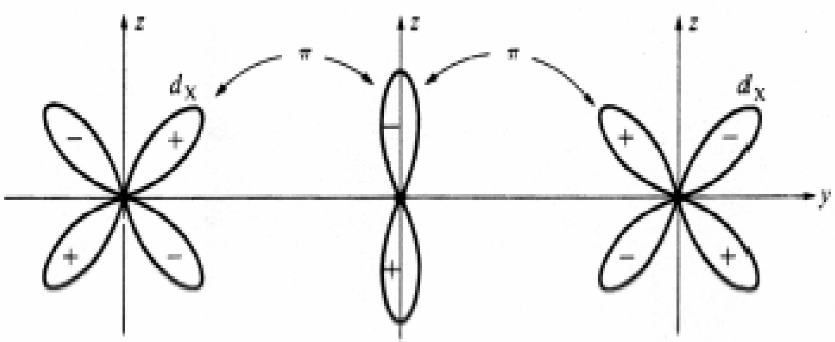
More Examples of Superexchange interactions

Antiferromagnetic

Strong:

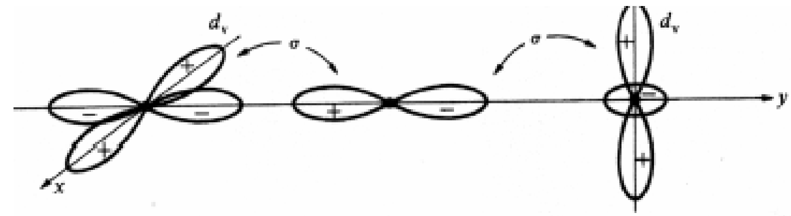


weak:

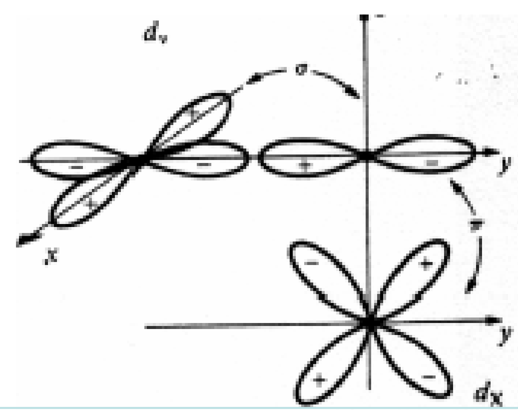


Ferromagnetic

2 different orbitals



90 ° coupling

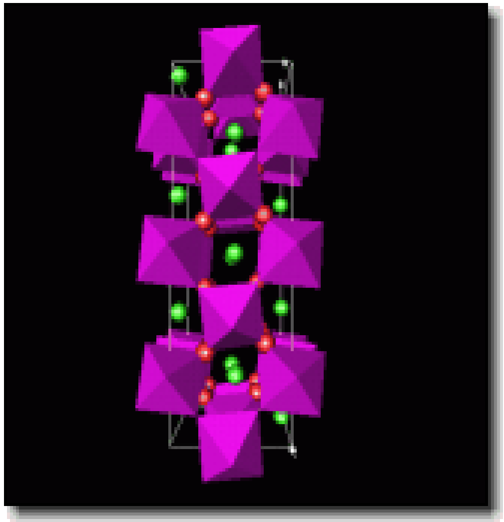


Double exchange

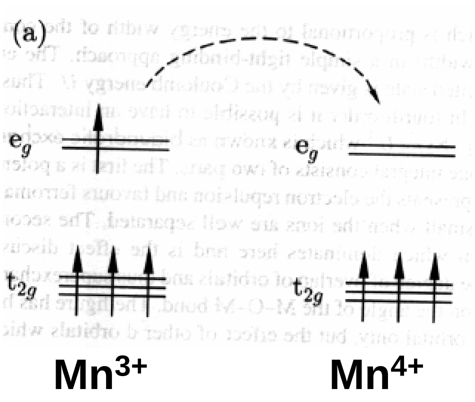
La1-xCaxMnO3

Colossal Magnetoresistance

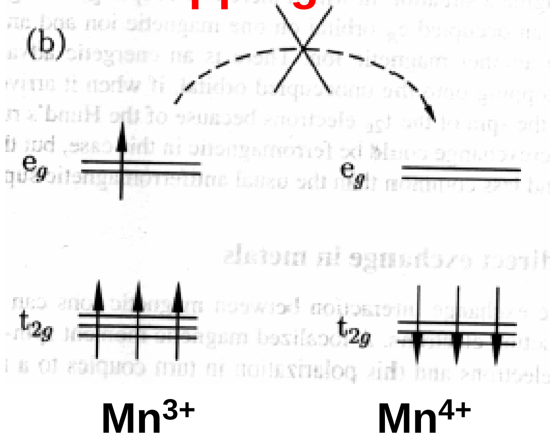
Mn^{4+} (S=3/2) and Mn^{3+} (S=2)



Ferro: possible hopping



AF: no hopping



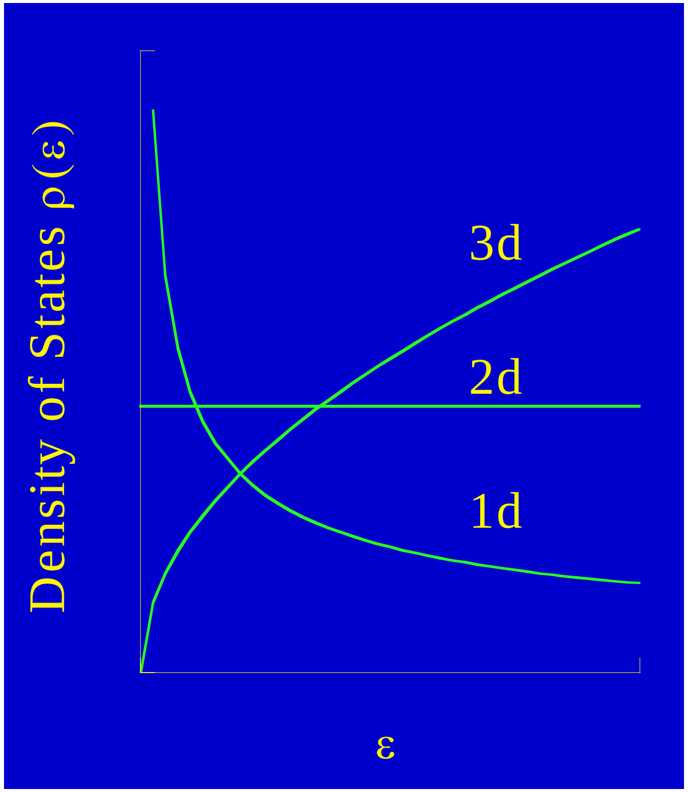
Mermin-Wagner Theorem

No long range magnetic ordering for Heisenberg spins with short range interactions at finite temperature in 1-D and 2-D

$$\varepsilon = \frac{1}{2m} p^2$$

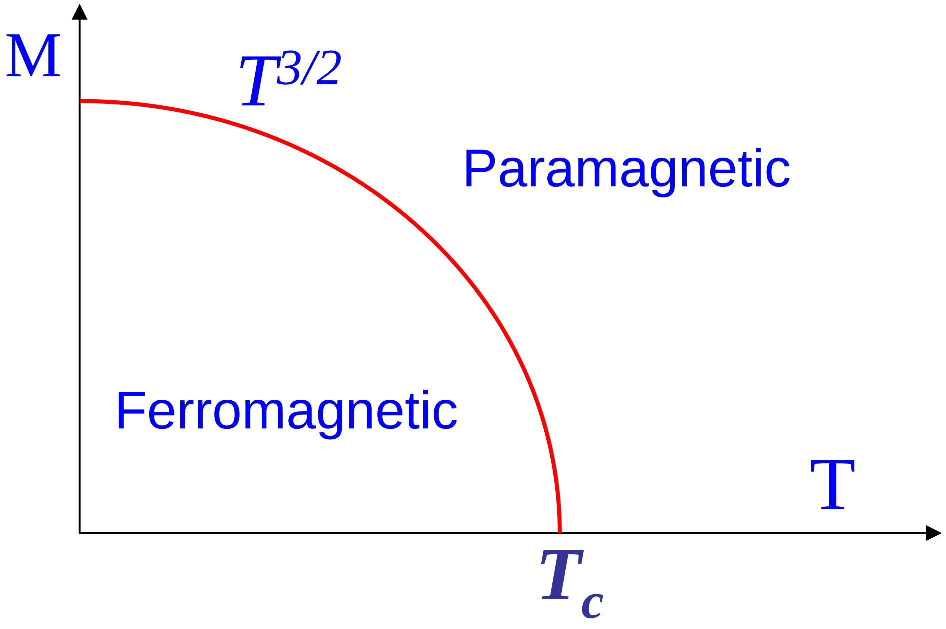
$$\rho(\varepsilon) \sim \varepsilon^{\frac{d}{2}-1}$$

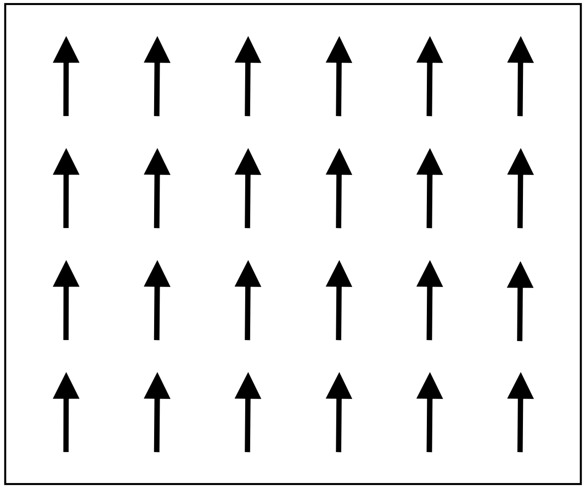
$$N \propto \int \frac{\rho(\varepsilon)}{\exp(\varepsilon / T) - 1} d\varepsilon$$



Ferromagnetism

magnetic moments are spontaneously aligned





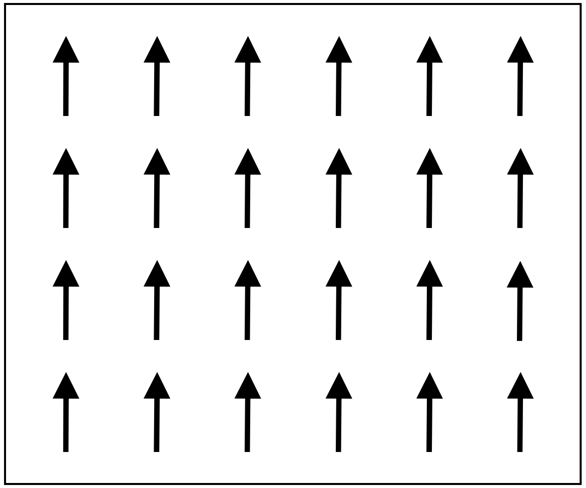
Curie temperature

Holstein-Primakoff Transformation

$$S_i^+ = b_i^+ \sqrt{2S - b_i^+ b_i}$$

$$S_i^- = \sqrt{2S - b_i^+ b_i}\, b_i$$

$$S_{iz} = b_i^+ b_i - S$$



$$b_i^+ b_i \le 2S$$

Spin Wave Expansion

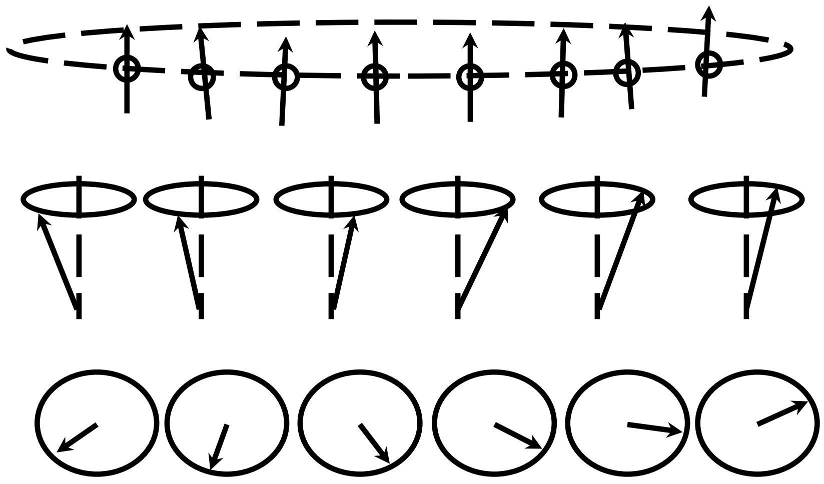
Low temperature excitations are dominated by spin waves

$$\langle b_i^+ b_i \rangle << S$$

$$\sqrt{2S - b_i^+ b_i} = \sqrt{2S}\left(1 - \frac{b_i^+ b_i}{4S} - \frac{\left(b_i^+ b_i\right)^2}{32S^2} \dots\right)$$

Spin wave:

Harmonic motion of
Holstein-Primakoff bosons



Ferromagnetic Spin Wave

$$S_i^+ = b_i^+ \sqrt{2S - b_i^+ b_i}$$

$$S_i^- = \sqrt{2S - b_i^+ b_i}\, b_i$$

$$S_{iz} = b_i^+ b_i - S$$

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$= -J \sum_{\langle ij \rangle} \left[\frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) + S_{iz} S_{jz} \right]$$

$$\approx -J \sum_{\langle ij \rangle} \left[S \left(b_i^+ b_j + b_j^+ b_i \right) - 2S b_i^+ b_i + S^2 \right]$$

Ferromagnetic Spin Wave

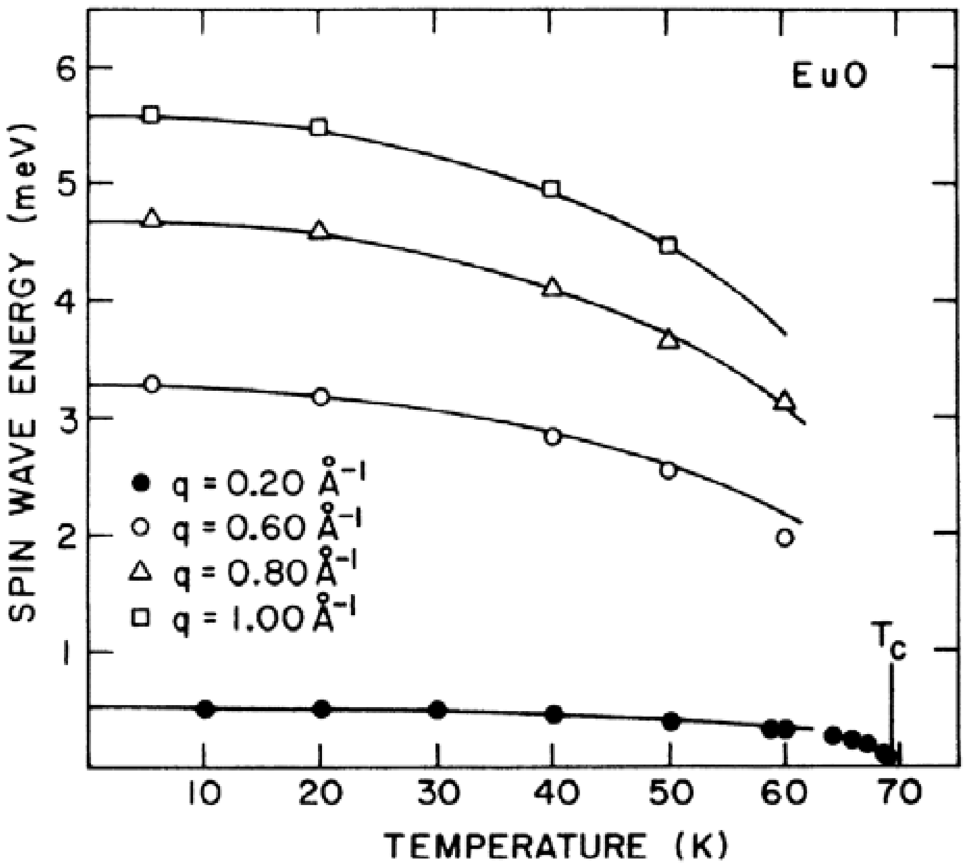
$$H \approx -J\sum_{\langle ij\rangle}\left[S\left(b_i^+ b_j + b_j^+ b_i\right) - 2Sb_i^+ b_i + S^2\right]$$

$$= \sum_{\langle ij\rangle}\omega_k b_k^+ b_k - JNdS^2$$

$$\omega_k = 2SdJ\left(1 - \frac{1}{d}\sum_{\alpha=1}^{d}\cos k_\alpha\right) \sim k^2$$

dimension

Comparison with Experimental Result



Bloch Law of Magnetization

$$M = -\langle S_{iz} \rangle = \langle S - b_i^\dagger b_i \rangle$$

$$= S - \frac{1}{N}\sum_k \frac{1}{e^{\beta\omega_k} - 1}$$

$$= S - \int d\omega \frac{\rho(\omega)}{e^{\beta\omega} - 1}$$

$$\sim -T^{3/2}$$

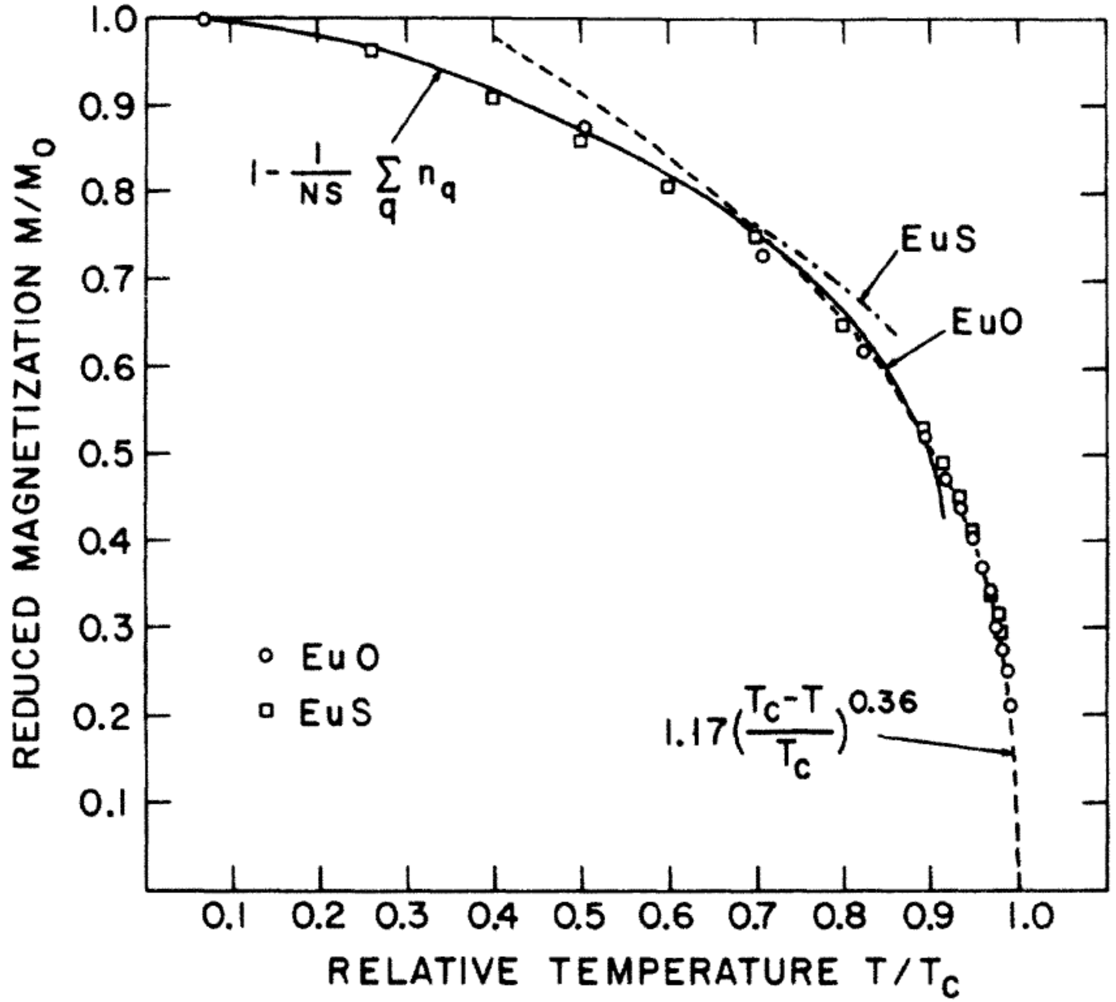
$$\omega \sim k^2$$

$$d\omega \sim k dk$$

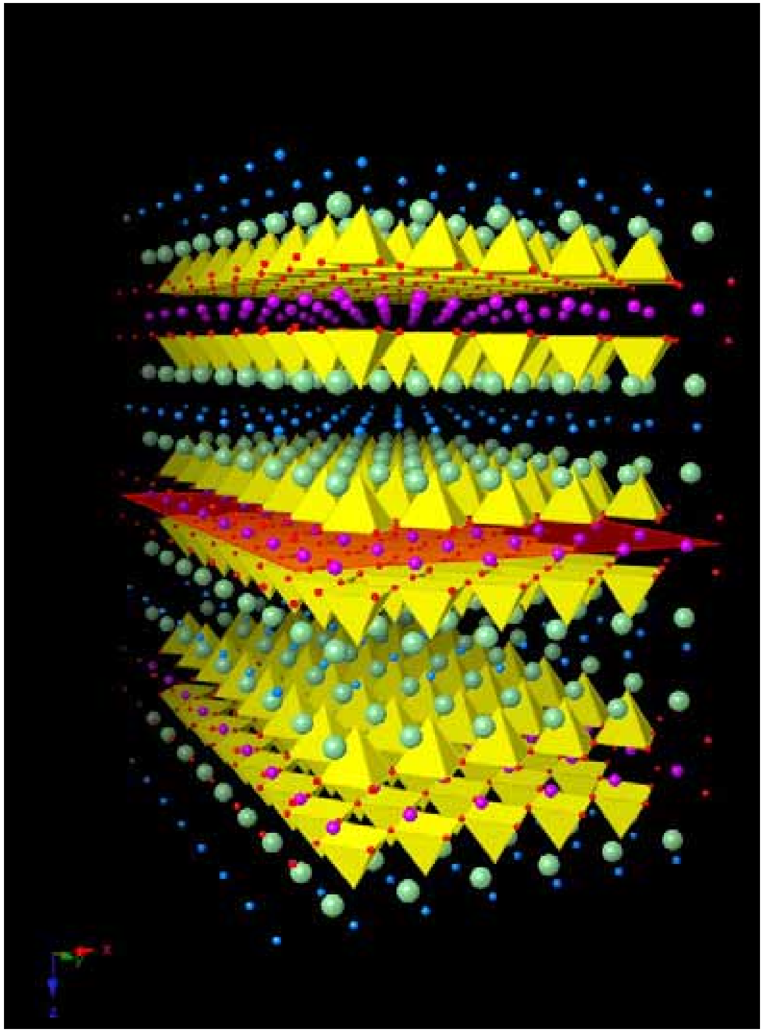
$$\rho(\omega) d\omega \sim k^2 dk \sim \omega^{1/2} d\omega$$

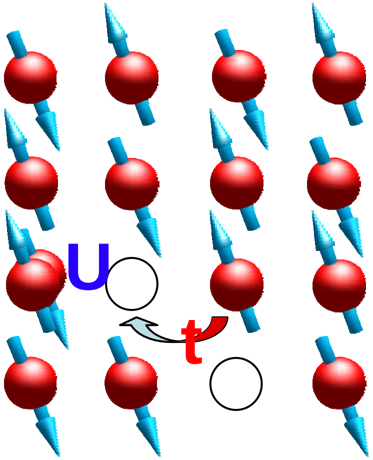
$$\rho(\omega) \sim \omega^{1/2}$$

Experiment vs Self-Consistent Spin Wave



Antiferromagnetism

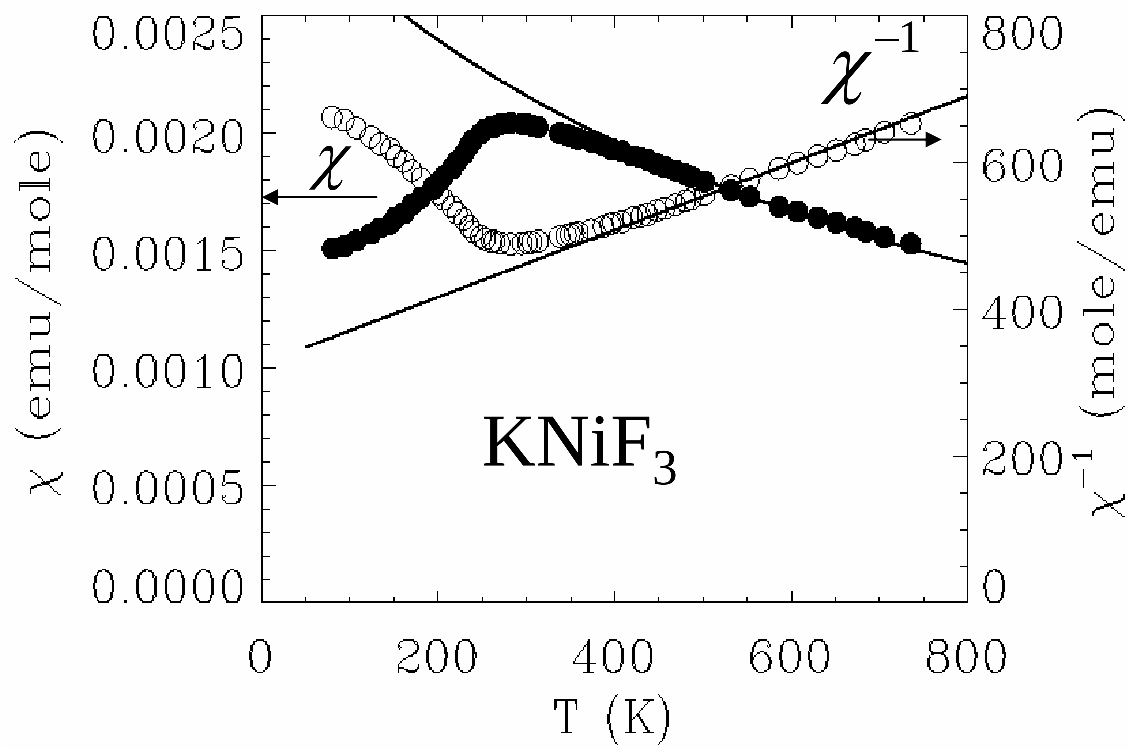


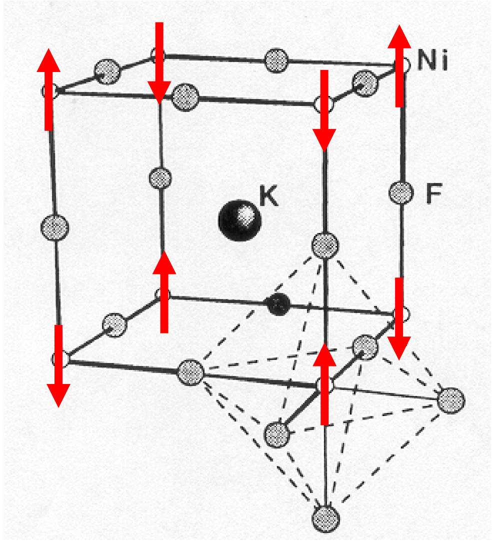


Neel
Nobel 1970

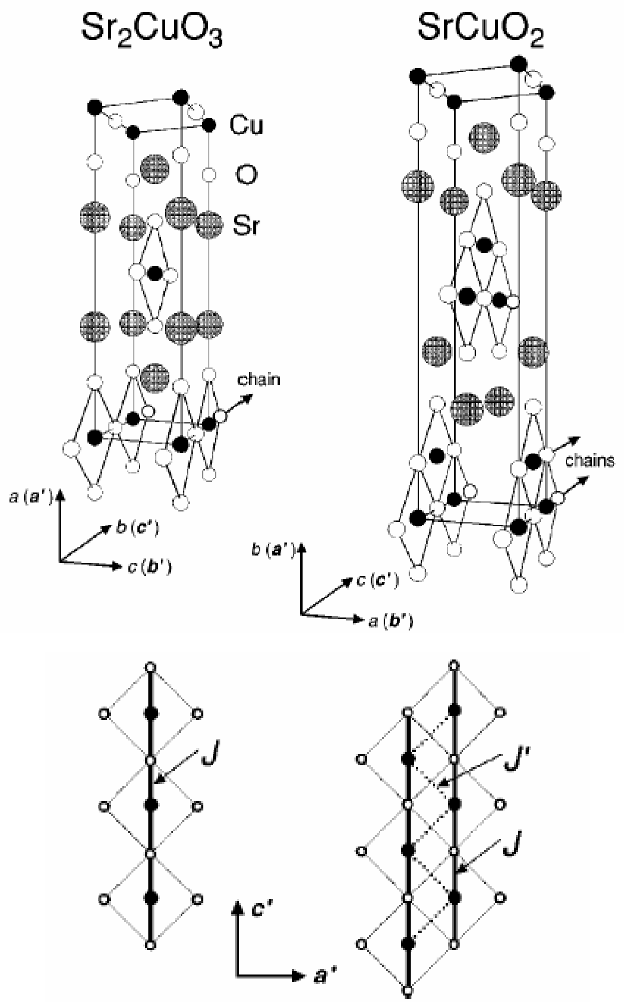
cuprate high temperature superconductors

Typical Antiferromagnetic Susceptibility

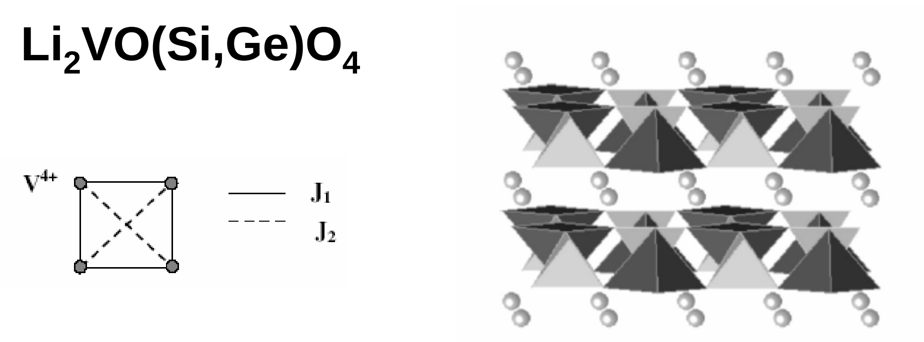




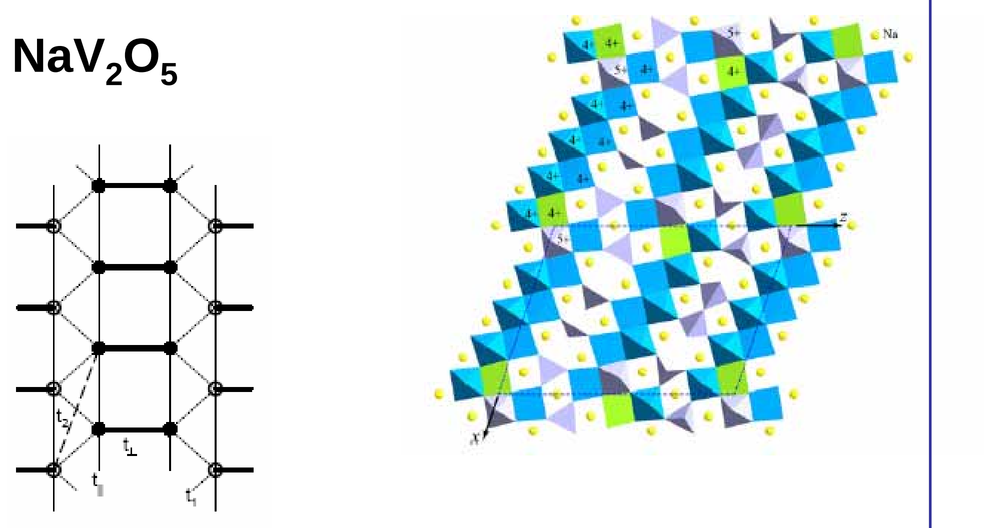
Low Dimensional Magnetic Materials



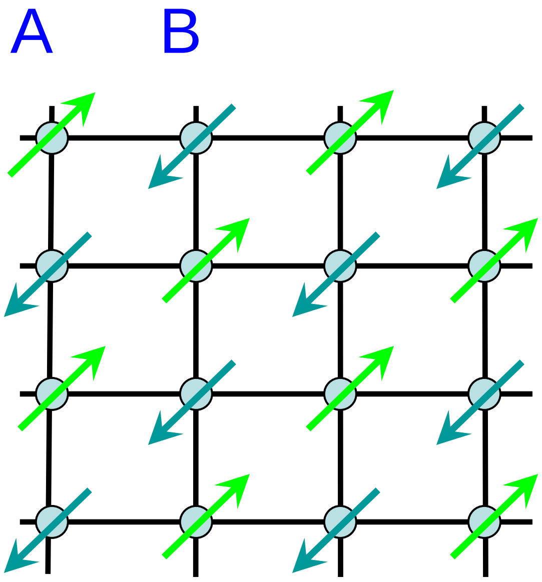
$Li_2VO(Si,Ge)O_4$



NaV_2O_5



Two Sublattices HP Transformation



A sublattice

$$S_i^+ = \sqrt{2S}\, b_i^+$$

$$S_i^- = \sqrt{2S}\, b_i$$

$$S_{iz} = b_i^+ b_i - S$$

B sublattice

$$S_j^- = \sqrt{2S}\, b_j^+$$

$$S_j^+ = \sqrt{2S}\, b_j$$

$$S_{jz} = S - b_j^+ b_j$$

Antiferromagnetic Spin Wave

$$H = J\sum_{\langle ij\rangle}\left[\frac{1}{2}\left(S_i^+S_j^- + S_i^-S_j^+\right) + S_{iz}S_{jz}\right]$$

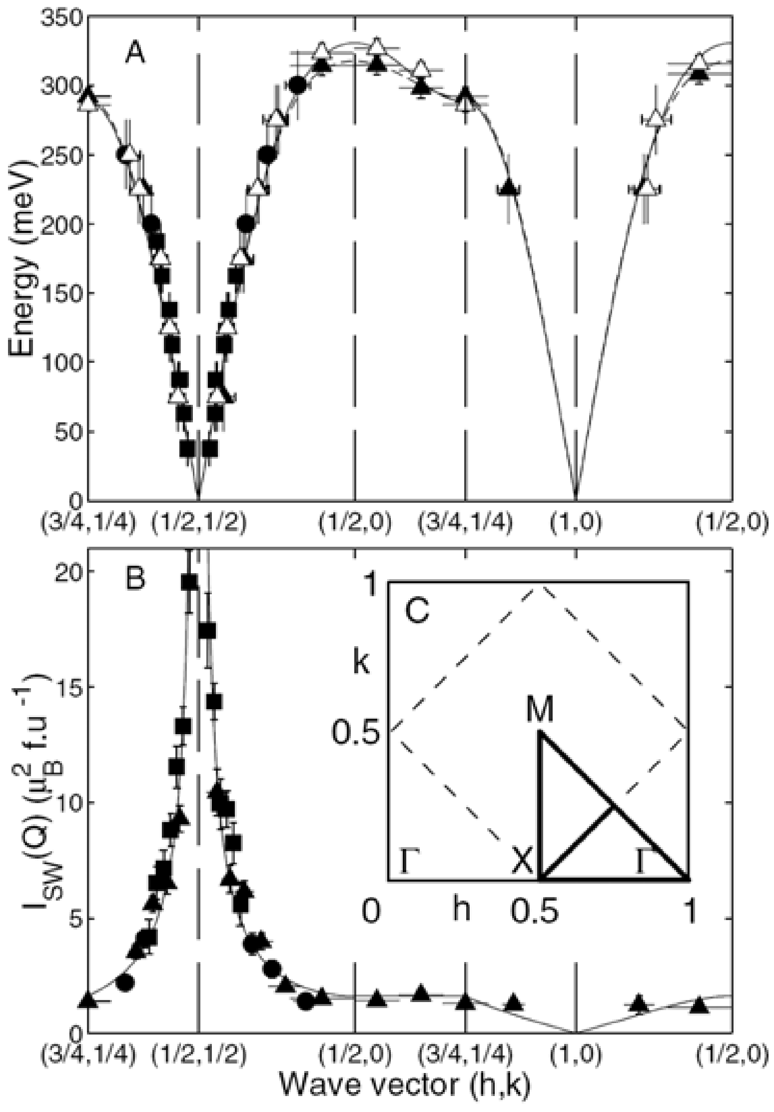
$$\approx J\sum_{\langle ij\rangle}\left[S\left(b_i^+b_j^+ + b_jb_i\right) - 2Sb_i^+b_i - S^2\right]$$

Bogoliubov transformation

$$= \sum_{\langle ij\rangle}\omega_k\left(\alpha_k^+\alpha_k + \frac{1}{2}\right) - JNdS(S+1)$$

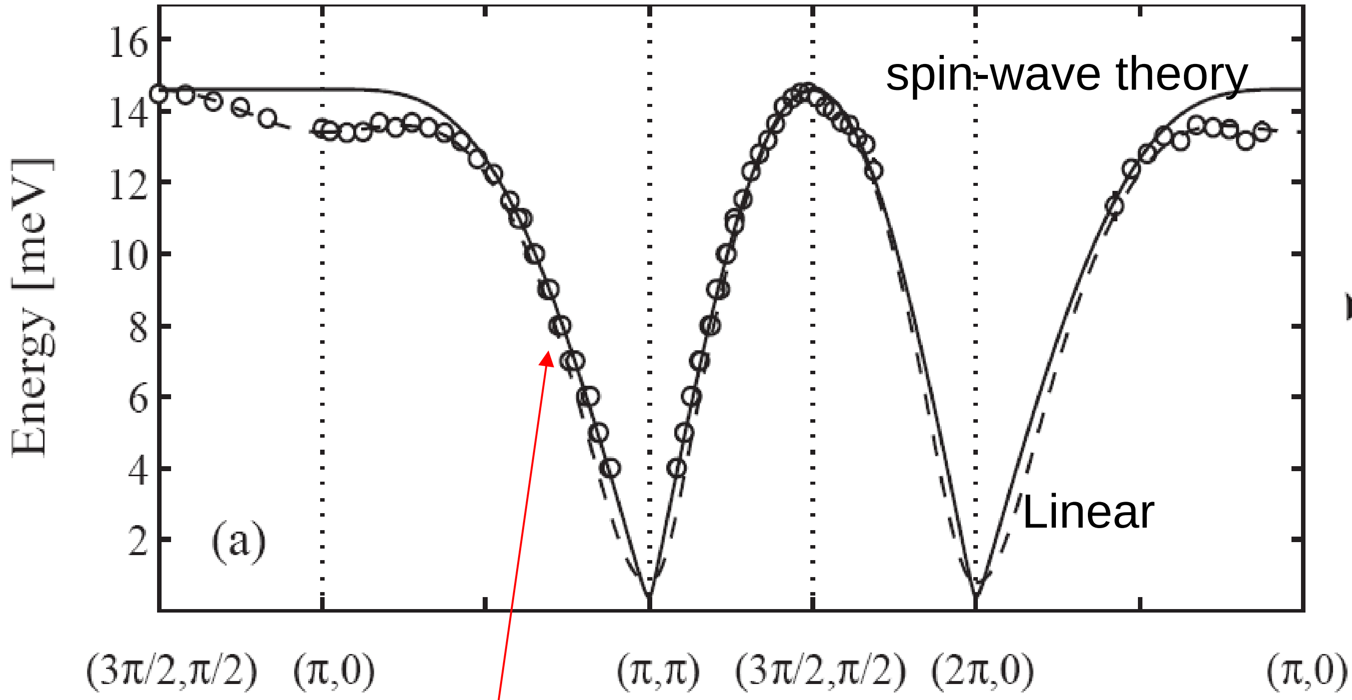
$$\omega_k = SdJ\sqrt{1-\left(\frac{1}{d}\sum_{\alpha=1}^{d}\cos k_\alpha\right)^2} \sim v|k|$$

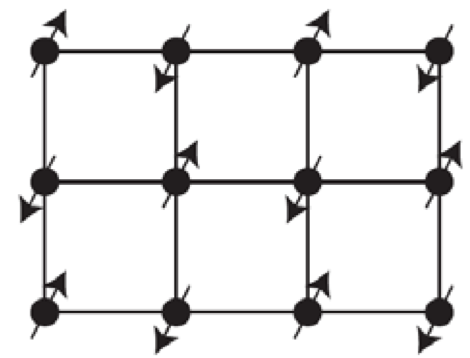
Spin Wave in La_2CuO_4



S=1/2 Heisenberg antiferromagnet on square lattice

Magnon excitations





Data points for
Cu(DCOO)$_2$ 4D$_2$0

Schwinger Boson Representation

$$\vec{S}_i = \begin{pmatrix} b_{i\uparrow}^+ & b_{i\downarrow}^+ \end{pmatrix} \frac{\vec{\sigma}}{2} \begin{pmatrix} b_{i\uparrow} \\ b_{i\downarrow} \end{pmatrix}$$

$$b_{i\uparrow}^+ b_{i\uparrow} + b_{i\downarrow}^+ b_{i\downarrow} = 2S$$

- SU(2) symmetric
- Commonly used in the mean-field treatment
- Magnetic long range order corresponding to the condensation of bosons

Jordan-Wigner Transformation

S=1/2 spin operators in 1D can be represented using purely Fermion operators

$$S_i^+ = a_i^+ \exp\left(i\pi \sum\nolimits_{j<i} a_j^+ a_j \right)$$

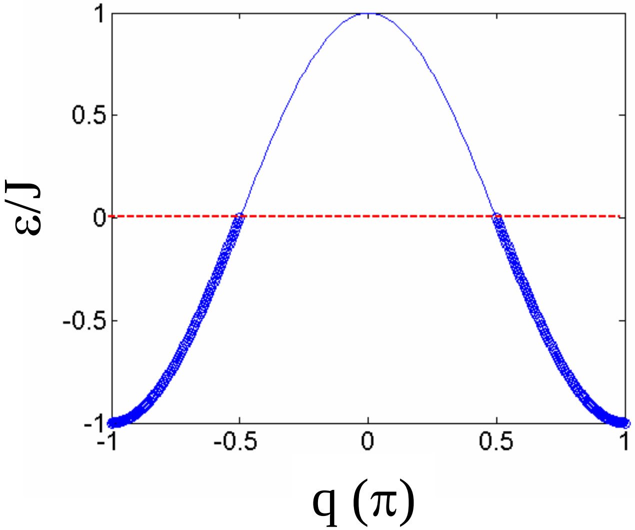
$$S_i^z = a_i^+ a_i - \tfrac{1}{2}$$

$$\left\{ a_i , a_j^+ \right\} = \delta_{ij}$$

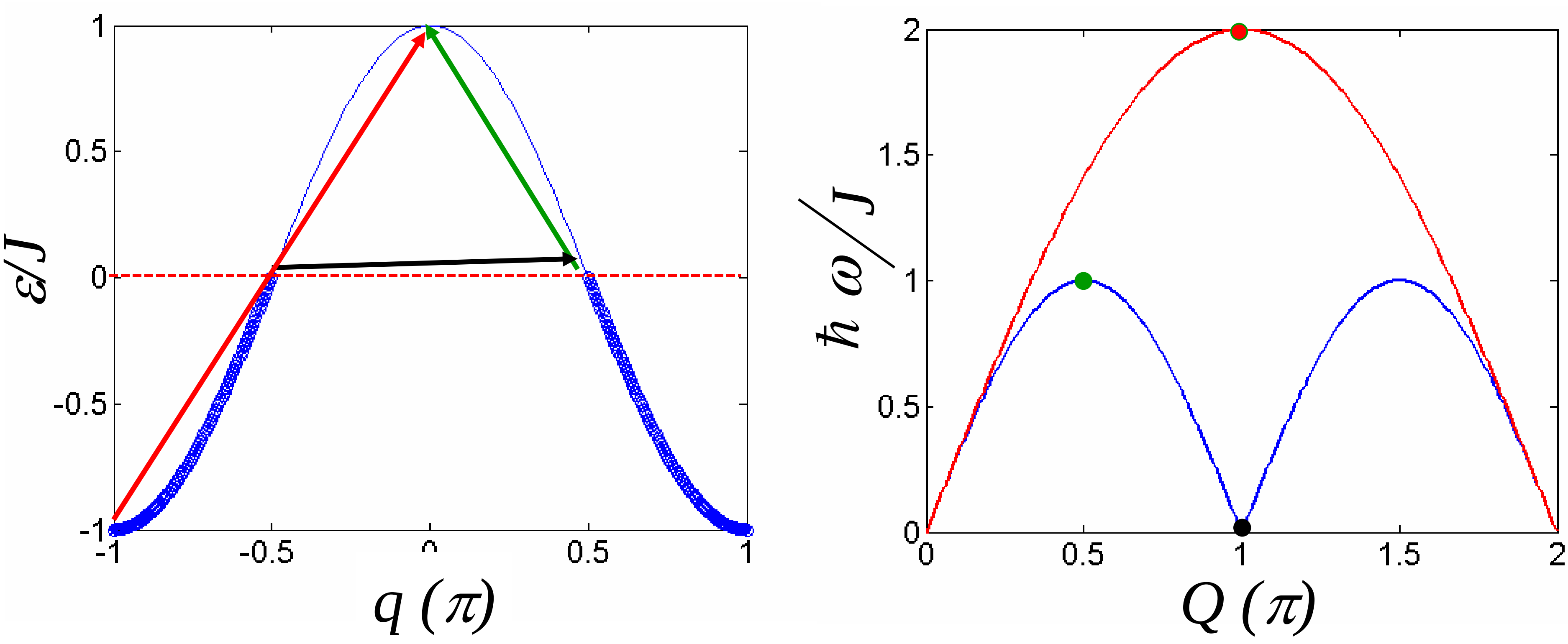
1D X-Y model can be readily diagonalized with this transformation

$$H = \tfrac{1}{2} \sum\nolimits_i \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right)$$

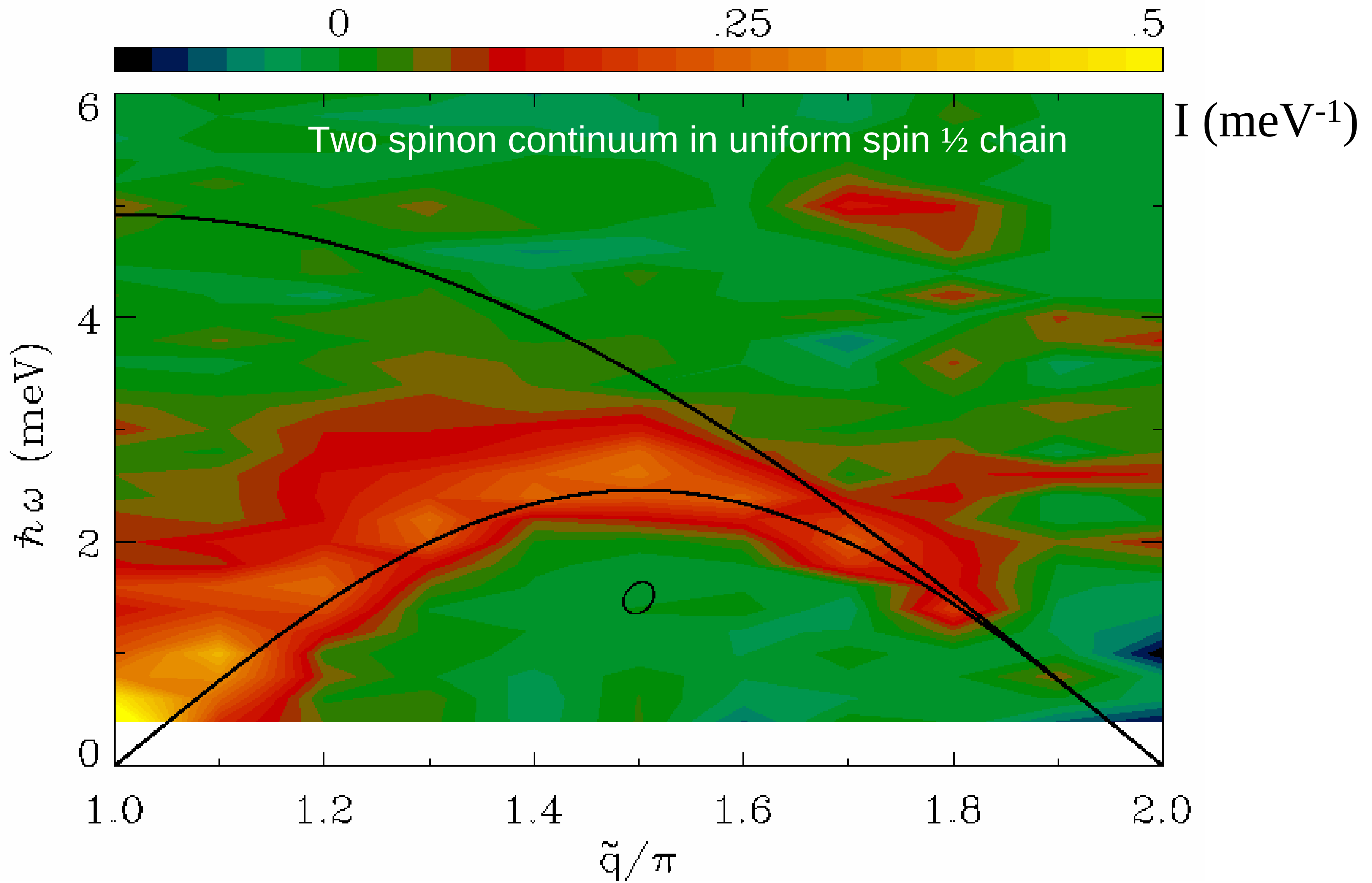
$$H = \sum_k \cos k \, a_k^+ a_k$$



Two Spinon contribution to S(Q,w)



Two Spinon Excitation in S=1/2 Spin Chain



Paradigm of Quantum Magnetism

Phenomena

↓

Theory

↓

Crisis

↓

New Theory