Emergence of quantum phases in novel materials

Magnetism

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Magnetism is a collective phenomenon

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Microscopic description

Magnetic moments

Interactions

Environment

Macroscopic description

Phases

Dimensionality

Symmetry

Universality

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Outline

- Classical Phase Transitions
- Free magnetic ions
- Environment
- Magnetic order and susceptibility
- Interactions
  - Exchange between localized moments
  - Indirect exchange through itinerant electrons
  - Magnetism in metals
- Excitations

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Outline

- Classical Phase Transitions
  - Symmetry
  - Landau theory
    - Order of phase transitions
  - Goldstone theorem
  - Mermin-Wagner Theorem
  - Kosterlitz-Thouless transition

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Symmetry

- Invariance of a physical law under transformations: translation symmetry, time reversal, rotation, reflection…

- Symmetries form groups: O(3), U(1)…
  - Contains the identity
  - The combination of any pair of elements is also an element of the group.
  - Each element must have an inverse

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Kinds of symmetries

- External (space time) symmetries (Galilean symmetry, rotational symmetry, Lorentz symmetry…)
- Internal symmetries (Gauge symmetries…)

- Global symmetries: act simultaneous in all variables x_i
- Local symmetries: depend on x_i

- Continuous symmetry: rotations O(n)
- Discrete symmetry: spin group Z_2

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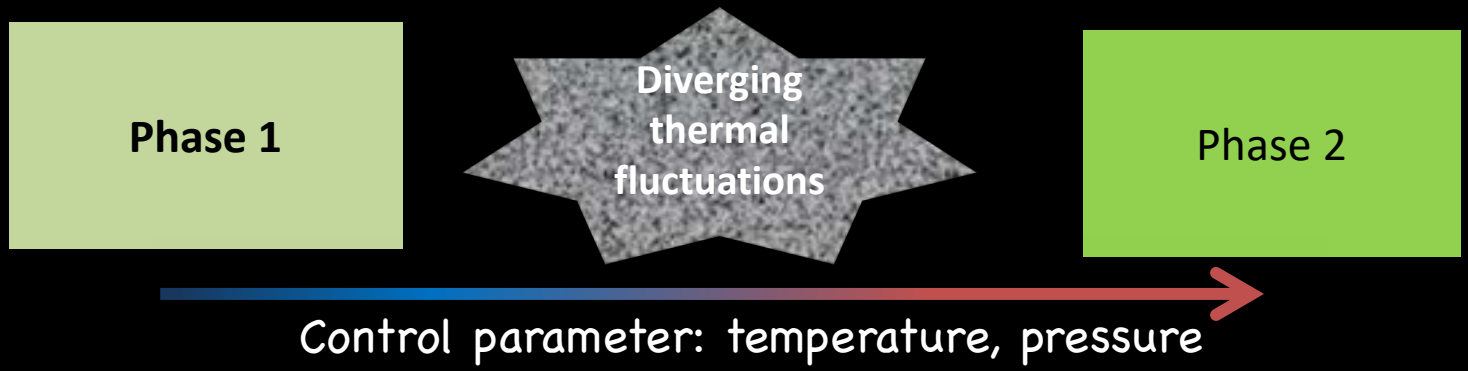
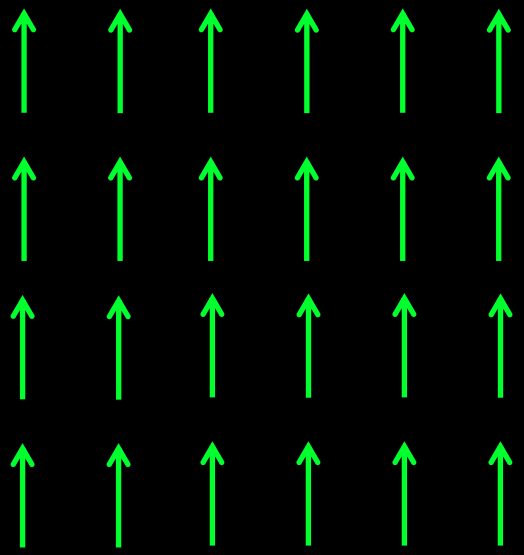
Classical phase transitions

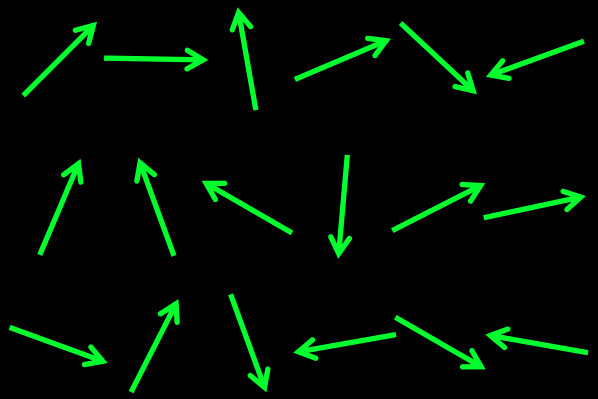


Lower symmetry
Lower energy



At T_c : symmetry breaking

Uncorrelated, isotropic, homogeneous, high symmetry higher entropy



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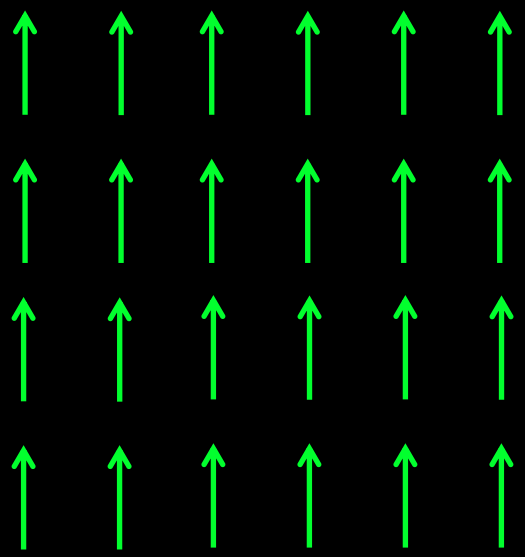
Classical phase transitions

$$H = -J \sum_{ij} S_i S_j$$

The hamiltonian has O(3) symmetry but this symmetry is broken in the ordered phase.

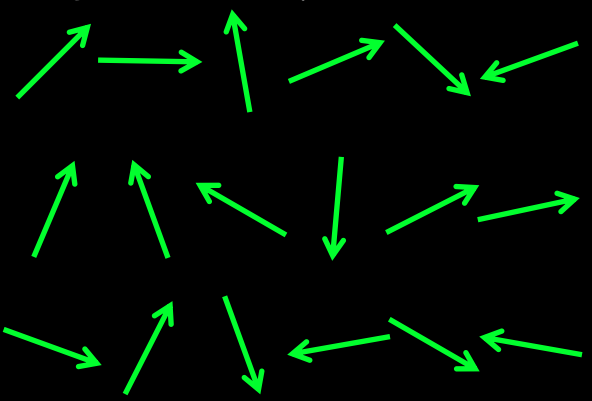
Lower symmetry
Lower energy



At T_c
spontaneous
symmetry
breaking

(rotation)

Uncorrelated, isotropic,
homogeneous, high symmetry
higher entropy



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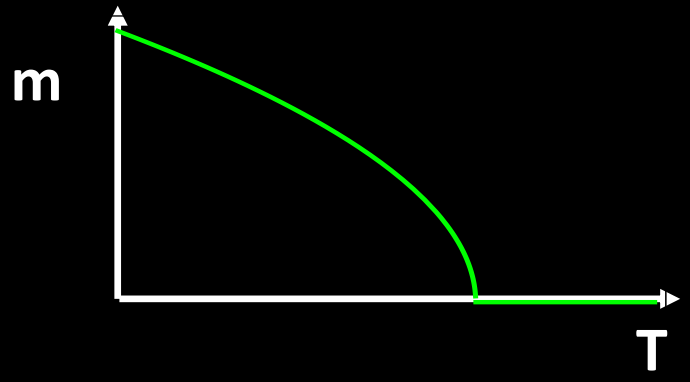
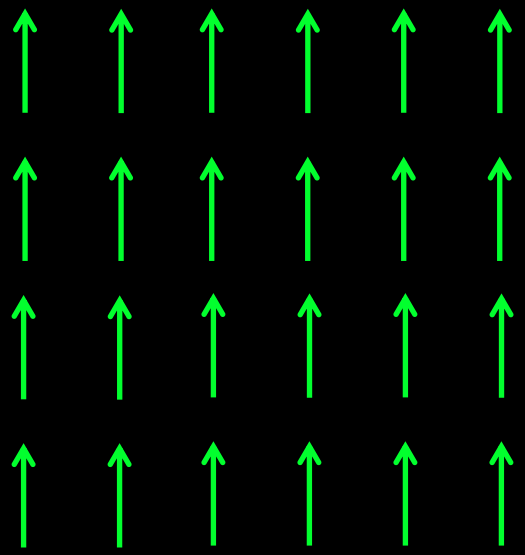
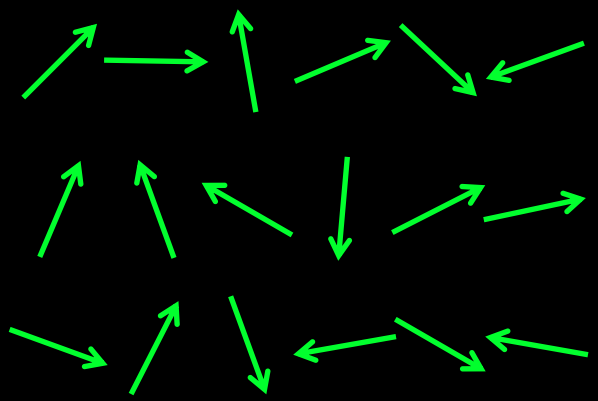
Classical phase transitions



Order parameter m≠0



Order parameter m=0



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Classical phase transitions

Landau mean-field theory (formal connection with the microscopic model through a Hubbard Stratonovic transformation). Express the free energy as a power series expansion in terms of the order parameter.

Example: Ising model (Z_2 symmetry)

$$H = -J \sum_{i,j} \sigma_i \sigma_j \quad \sigma_i = \pm 1$$

The free energy has the symmetries of the hamiltonian (in this case: no odd terms in the expansion)

Simplest expansion (assuming B>0)

$$f(m,h) = Am^2 + Bm^4 - hm$$

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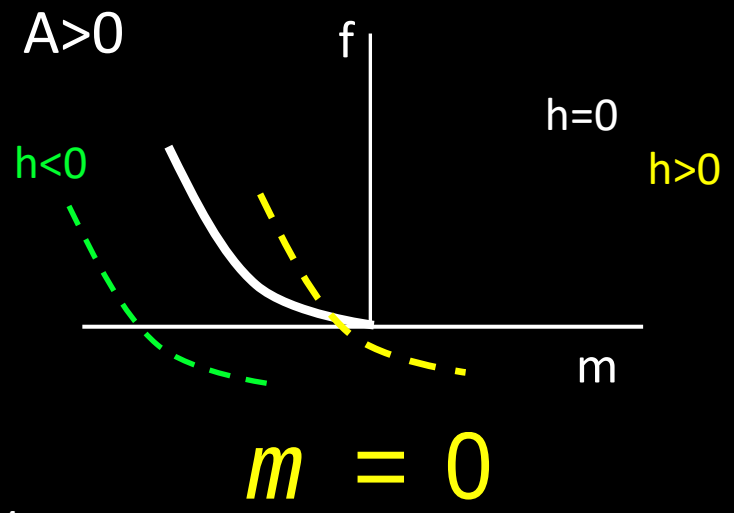
Classical phase transitions

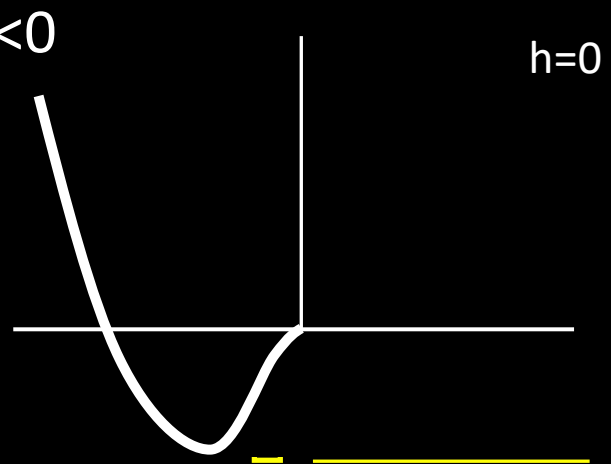
Landau mean-field theory

$$f(m,h) = Am^2 + Bm^4 - hm$$

$$\frac{\partial f(m,h)}{\partial m} = 0 \qquad 2Am + 4Bm^3 - h = 0$$



$$m = 0$$



$$m = \pm\sqrt{-A/2B}$$

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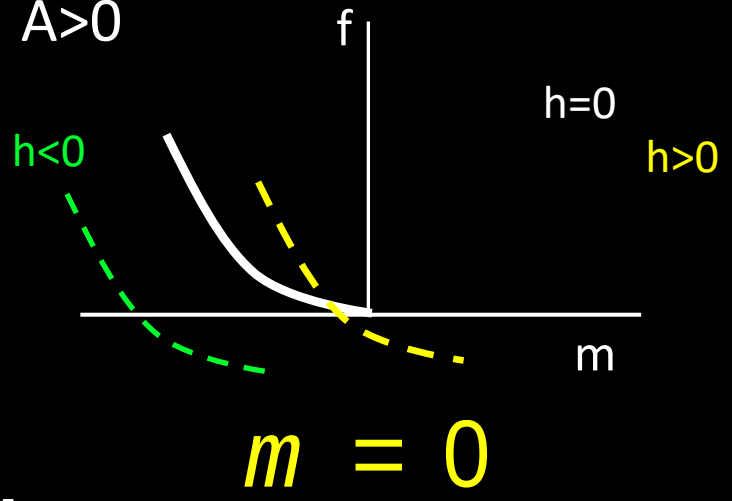
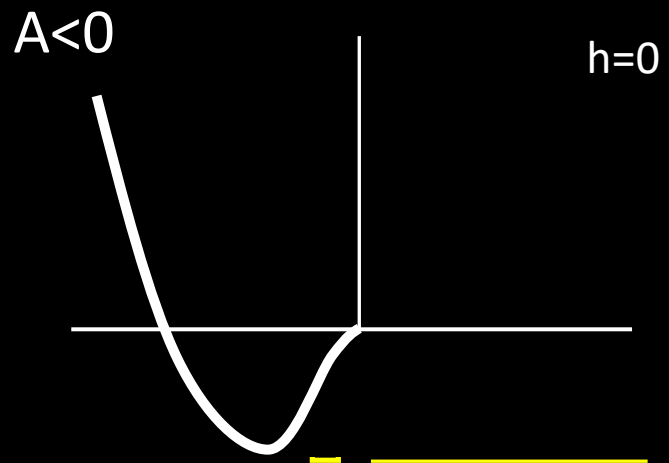
Classical phase transitions

$$A = (T - T_C)/2T_C$$

$$m(h=0) = \begin{cases} 0, & T > T_C \\ -\dfrac{T_C - T}{4T_C B(T)}, & T < T_C \end{cases}$$



$$m = 0$$



$$m = -\sqrt{-A/2B}$$

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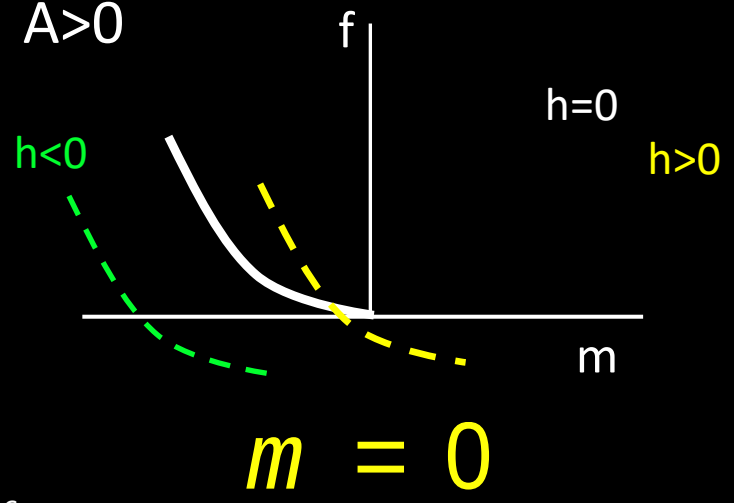
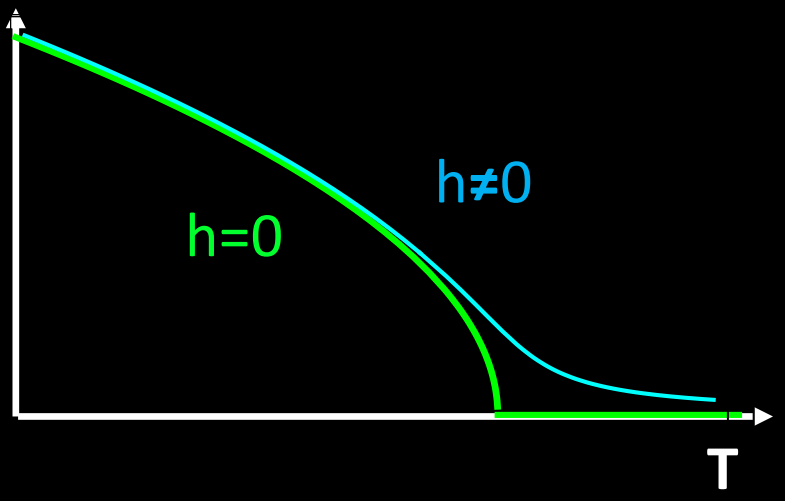


$$m = 0$$



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Susceptibility

$$\chi = \frac{\partial m}{\partial h} \rightarrow \chi^{-1} = \frac{\partial h}{\partial m}$$

$$f(m,h) = \frac{(T-T_c)}{2T_c}m^2 + Bm^4 - hm$$

$$\frac{(T-T_c)}{T_c}m + 4Bm^3 = h$$

$$\frac{\partial h}{\partial m} = \frac{(T-T_c)}{T_c} + 12Bm^2$$

$$\chi^{-1} = \begin{cases} \dfrac{(T-T_c)}{T_c}, & T > T_c \\ 2\dfrac{(T_c-T)}{T_c}, & T < T_c \end{cases}$$

The susceptibility diverges at the transition

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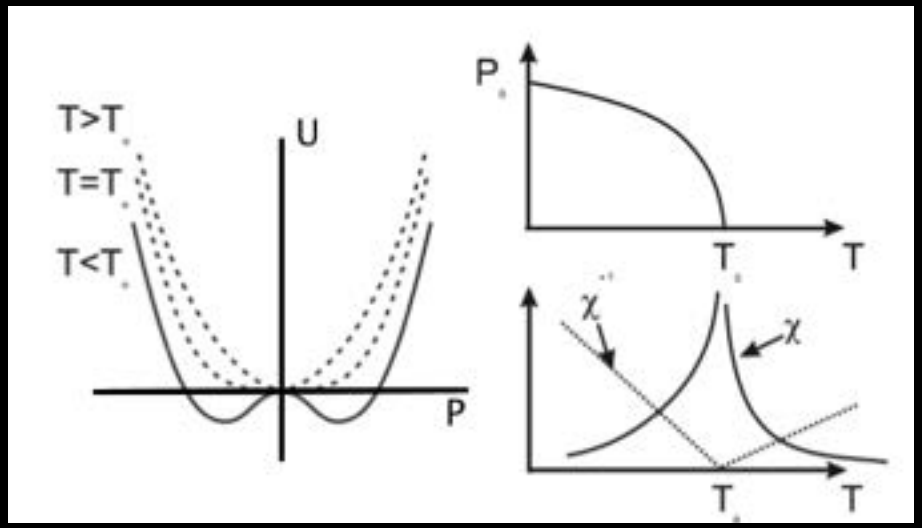
Continuous phase transitions (2^{nd} order)

- Order parameter goes continuously to zero

$$m \sim (T_c - T)^{1/2}$$

- Susceptibility diverges

$$\chi \sim |T - T_c|^{-1}$$



$$f(m,h) = Am^2 + Bm^4 - hm$$

B>0

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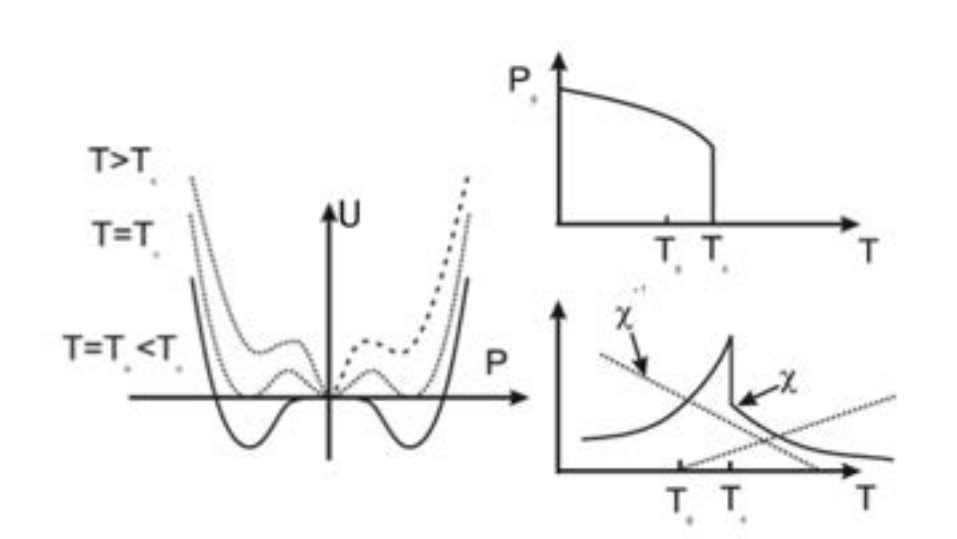
1st order phase transitions

Both the order parameter and the susceptibility have a jump at T_c



- ✓ Phase separation
- ✓ Hysteresis
- ✓ Latent heat

$$f(m,h) = Am^2 + Bm^4 + Cm^6 - mh$$

B<0

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Ginzburg Landau

Long-wavelengths fluctuations can be added in Landau theory. $\phi(x)$ is slowly varying. The simplest functional is:

$$f_{GL}[T,\Phi] = \frac{c}{2}(\nabla\Phi)^2 + \frac{r}{2}\Phi^2 + g(T)\Phi^4 - h\Phi$$

A new scale is introduced: Correlation length ξ
(the scale at which the fluctuations of the microscopic degrees of freedom are correlated).
It diverges at T_c in second order transitions.

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Correlation and susceptibility

Connected by the fluctuation-dissipation theorem

Correlation function: measure how correlated is the system over a certain range of space

$$G_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \frac{1}{(\beta\mu)^2} \frac{\partial^2 \ln Z}{\partial B_i \partial B_j}\bigg|_{B=0}$$

Z is the partition function
B is the magnetic field

Susceptibility

$$\chi = \frac{\partial m}{\partial B} = \frac{1}{\beta} \sum_{ij} \frac{\partial^2 \ln Z}{\partial B_j \partial B_i} = \beta\mu^2 \sum_{ij} \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$$

- ✓ Correlations can be measured!
- ✓ At a phase transition χ diverges → infinite fluctuations

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Universality

The singular behaviour close to the critical point is characterized by critical exponents:

$$\xi \propto (T - T_c)^{-\nu}$$

$$\chi \propto (T - T_c)^{-\gamma}$$

$$C \propto (T - T_c)^{-\alpha}$$

The critical exponents depend on:

- Dimensionality of the space
- Dimensionality of the order parameter
- Symmetries of the local couplings

but not on the details of the interaction (universality).

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Universality

The singular behaviour close to the critical point is characterized by critical exponents:

Table 1 | Critical behaviour from 2D to 3D Nature Nanotechnology 14, 408 (2019)

Model	β	γ	ν	δ
	$M(T<T_c) \propto \lvert t\rvert^{\beta}$	$\chi \propto \lvert t\rvert^{-\gamma}$	$\xi \propto \lvert t\rvert^{-\nu}$	$M(T_c) \propto \lvert B\rvert^{1/\delta}$
2D Ising	1/8	7/4	1	15
3D Ising	0.3265	1.237	0.630	4.789
3D XY	0.348	1.318	0.672	4.787
3D Heisenberg	0.369	1.396	0.711	4.783
Mean field	0.5	1	0.5	3

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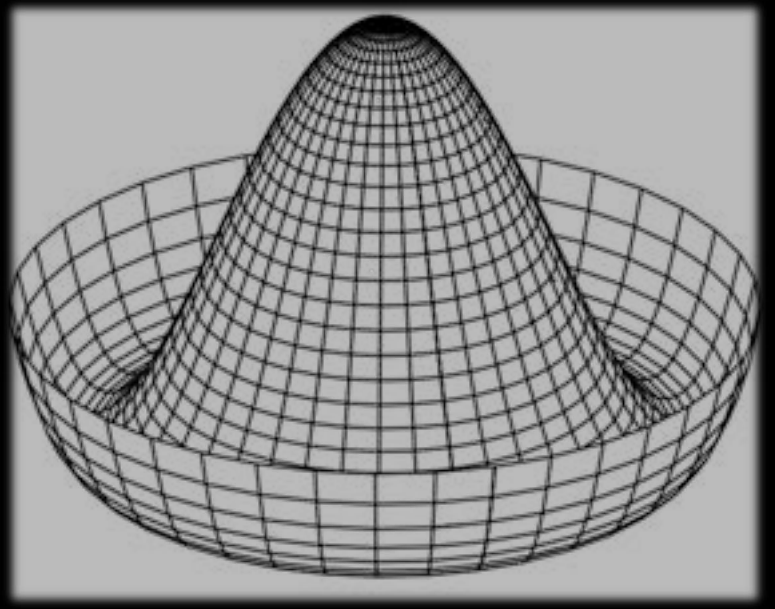
Goldstone theorem

Low energy excitations are possible in systems with continuous symmetry.

Example: Heisenberg model [invariant under O(3)]

$$H = -J \sum_{i,j} \vec{S}_i \vec{S}_j = -J \sum_{i,j} \cos(\theta_{i,j})$$



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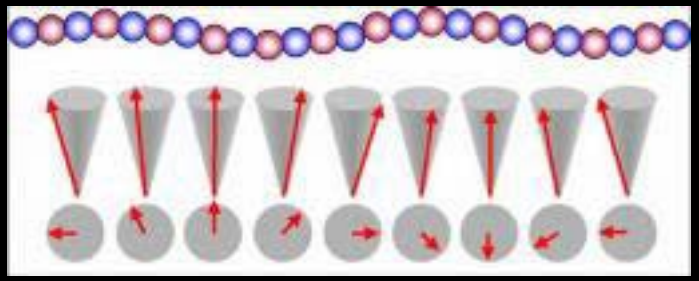
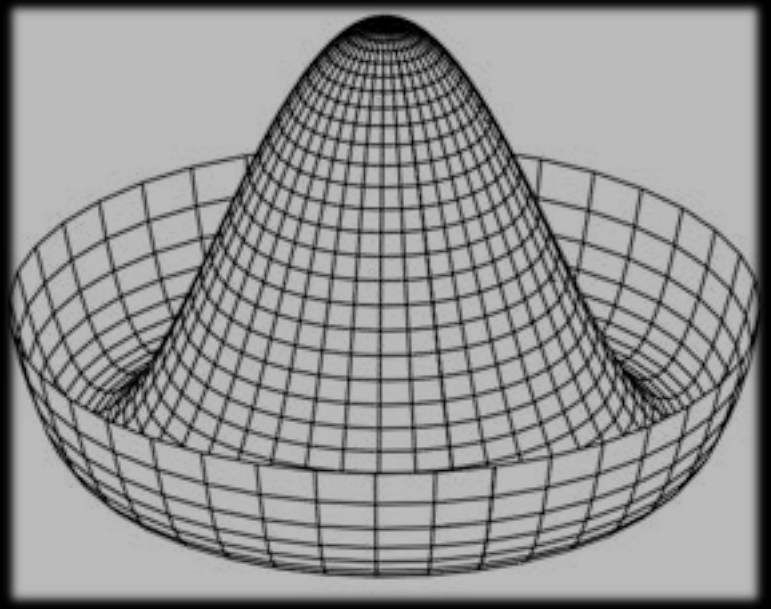
Excitations:
infinitesimal rotation of a single spin





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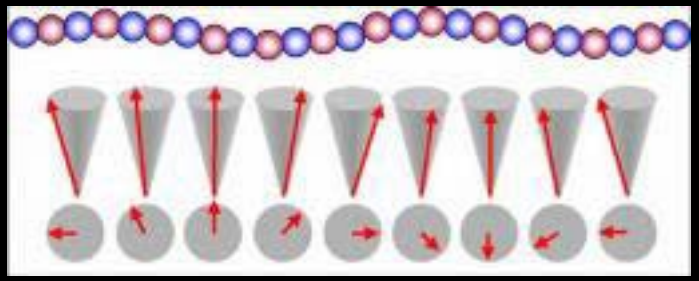

Gapless excitation spectrum: Goldstone modes Magnons

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Goldstone theorem

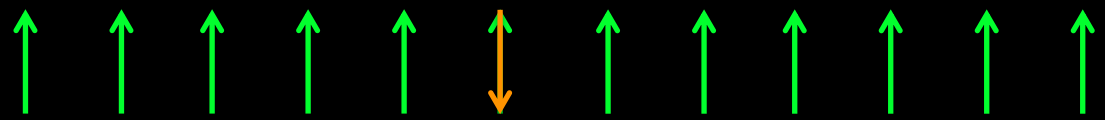
Low energy excitations are possible in systems with continuous symmetry.

Example: Heisenberg model [invariant under O(3)]

On the other hand:

Ising model (Z_2 symmetry) $H = -J \sum_{i,j} \sigma_i \sigma_j \quad \sigma_i = \pm 1$

An excitation involves flipping a single spin (finite energy ~ J).



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Mermin-Wagner

Goldstone modes gives rise to large fluctuation effects in low dimensions such that the ordered phase is destroyed.

The number of magnons diverges in 1D and 2D Heisenberg models for any T>0.

In general, there is no phase transition for dimension d≤2 (for T > 0) if we have:

- Spontaneous symmetry of a continuous group
- Short range forces

Mermin, N. D. & Wagner, H. *Phys. Rev. Lett.* **17**, 1133–1136 (1966).

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2D magnetic materials

Nature Nanotechnology 14, 408 (2019)

FM in a 2D systems first measured in 2017 on monolayer CrI_3

Mermin-Wagner doesn't apply because of interaction anisotropies.

$$H = -\frac{1}{2}\sum_{i,j}\left(J\,\mathbf{S}_i\cdot\mathbf{S}_j + \Lambda\,S_i^z S_j^z\right) - \sum_i A\,(S_i^z)^2$$

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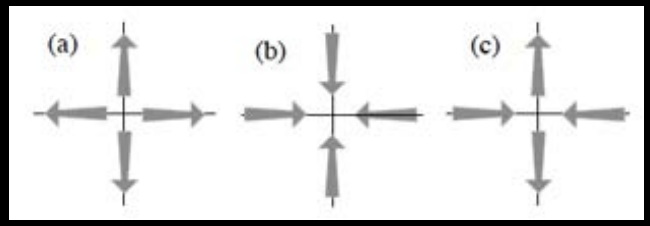
2D XY model : Berezinskii -Kosterlitz-Thouless transition

The XY model (2D) has continuous symmetry U(1)/O(2).

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

Vortices (topological defects)



BKT Transition:

Low T	High T
Vortex-antivortex binding	Free vortices
Correlations show an algebraic decay (quasi long range order)	Exponential correlation decay (disorder)

No long range order but a diverging correlation length.

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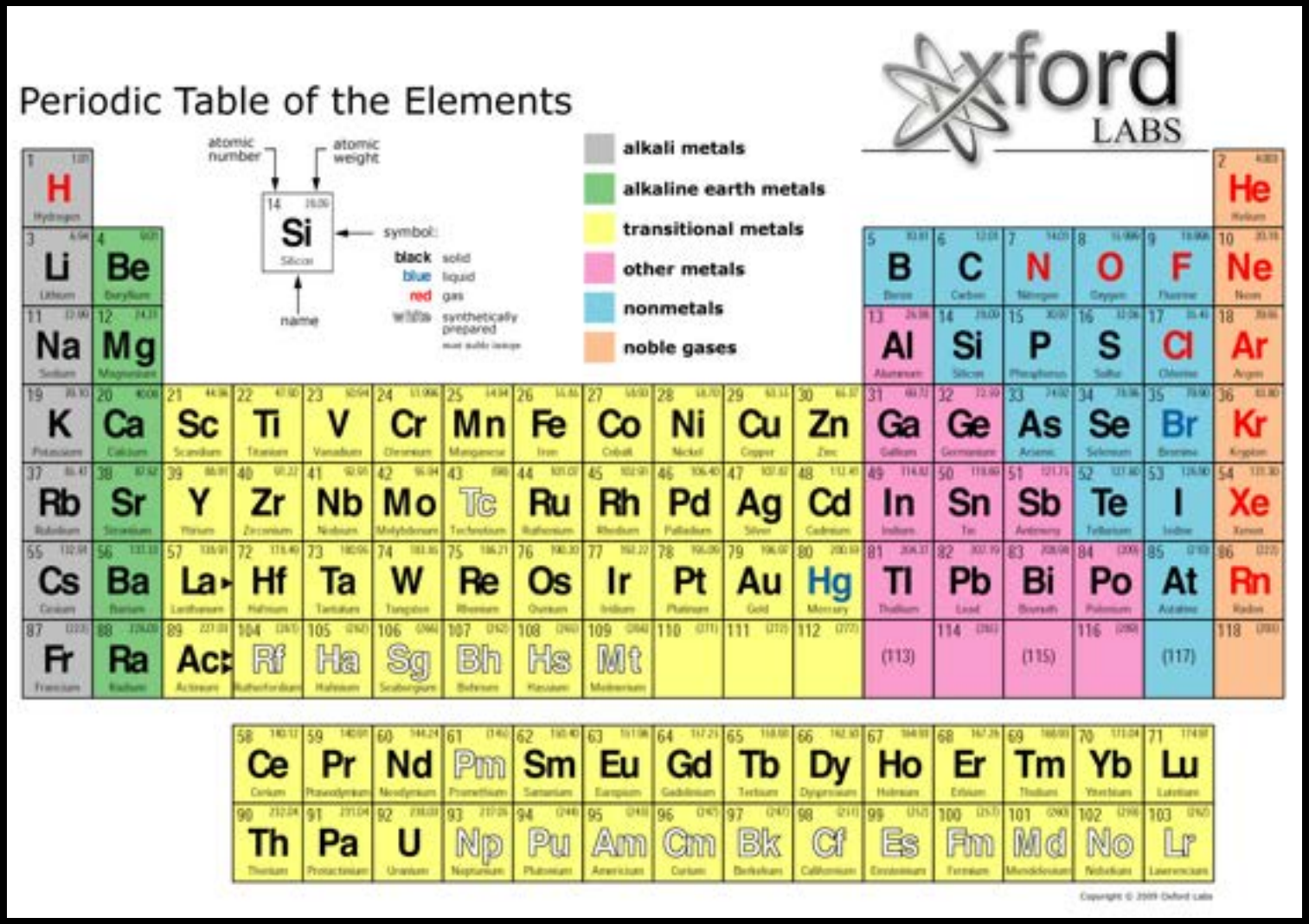
Free magnetic ions
electrons in incomplete shells (d or f orbitals)



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Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Spin angular momentum operator $\hat{\mathbf{S}} = \frac{1}{2}\sigma$

Eigenvalues of S_z: $m_s = \pm 1/2$

Eigenvectors:

$$|\uparrow_z\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |\downarrow_z\rangle = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Spinor representation

$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |\downarrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$|\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \quad |\downarrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

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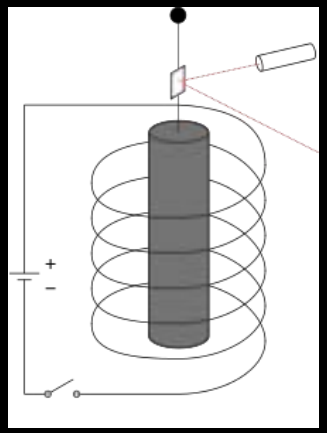
Free magnetic ions

Magnetism originates from the magnetic moment of electrons (angular momentum: Einstein-de Hass effect)



Intrinsic angular momentum m_s

(spin quantum number s)

$$\mu_s = -g\mu_B m_s$$

$m_s = \pm 1/2$

$g = 2.0023$

Orbital angular momentum m_l

(angular momentum quantum number l)

$$\mu_O = -\frac{e}{2c}(r \times v) = -\frac{e}{2mc}(r \times p) = -\mu_B m_l$$

Note that for atomic nuclei

$\mu_N << \mu_B$ (due to the much larger mass of the proton)

$$\mu_B = \frac{e\hbar}{2mc}$$

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Free magnetic ions
electrons in incomplete shells (d or f orbitals)

Electrons move in the effective potential created by the nucleus plus an average potential from the other electrons (Hartree approx)

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)Y_l^m(\theta,\phi)$$

An ion has a net magnetic moment if it has an incomplete atomic shell (characterized by the atomic numbers n and l). L and S are zero for complete shells.

$$L = \sum_i m_{l_i} \quad S = \sum_i m_{s_i}$$

(2S+1)(2L+1) possible multiplets. L and S are constants of motion in the absence of spin-orbit coupling. The degeneracy is lifted by the correlation energy (deviation of the electron-electron interaction with respect to Hartree): maximize S and maximize L (Hund's rules).

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Spin orbit coupling

Interaction between the electron and the magnetic field created by the orbiting nucleus (in the electron frame)

$$\vec{B} = \frac{\vec{E} \times \vec{v}}{c^2} \qquad \vec{E} = -\nabla V(r) = -\frac{\vec{r}}{r}\frac{dV(r)}{dr}$$

$$H_{so} = -\frac{1}{2}\vec{m} \cdot \vec{B} = \frac{e\hbar^2}{2m_e c^2 r}\frac{dV(r)}{dr}\vec{S} \cdot \vec{L} = \lambda \vec{S} \cdot \vec{L}$$

For a hydrogen like atom

$$\frac{1}{r}\frac{dV(r)}{dr} = \frac{Z_{\text{eff}}\, e}{4\pi\epsilon r^3}$$

$$H_{so} \sim Z_{\text{eff}} \langle r^{-3} \rangle \vec{S} \cdot \vec{L}$$

Spin orbit is more important for small r (f-electrons)
For a Hydrogen like atom, $\langle r^{-3} \rangle \sim Z^3$

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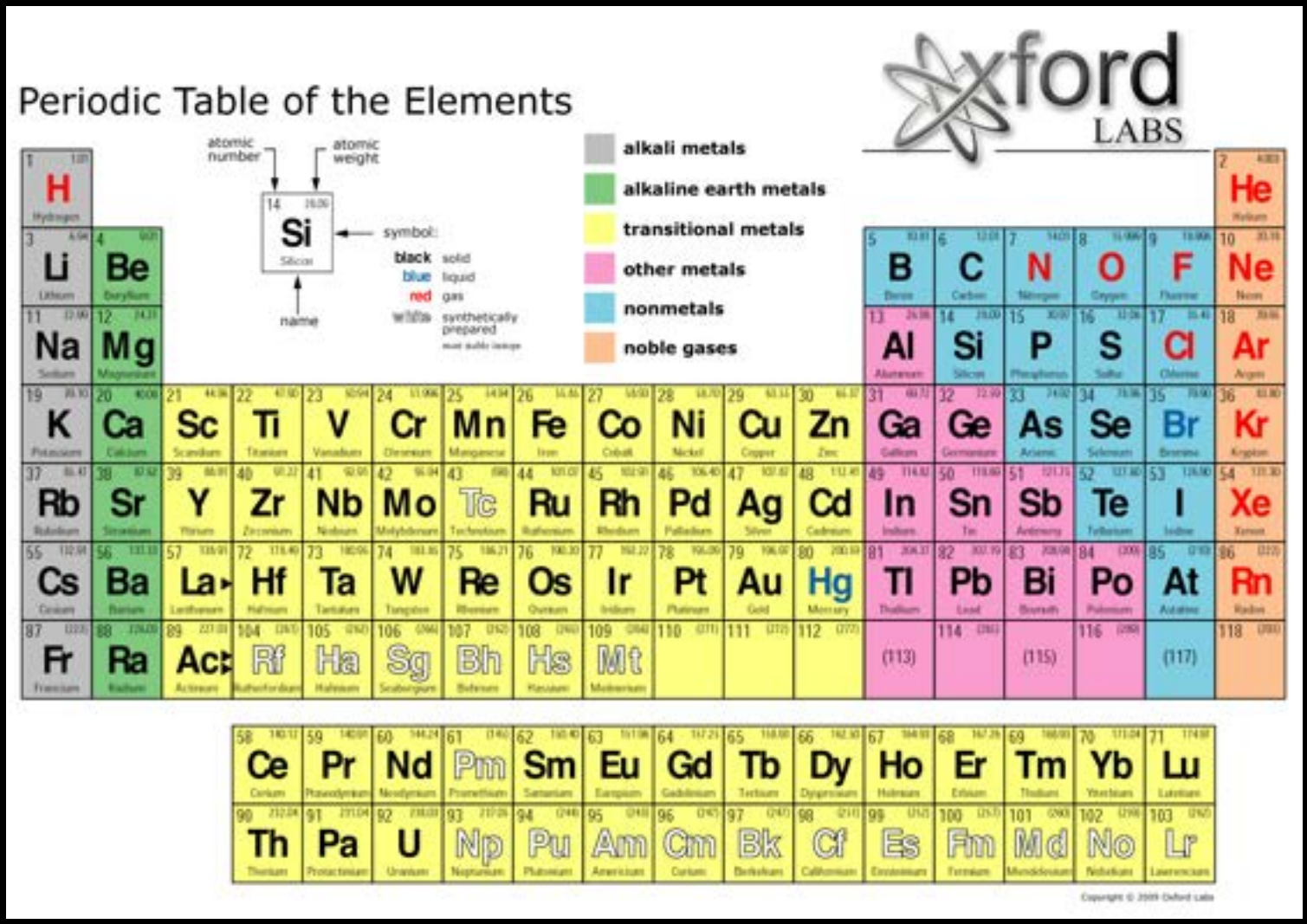
Free magnetic ions
electrons in incomplete shells (d or f orbitals)

Increasing SO



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Free magnetic ions

Total angular momentum: **J=L+S**

$|L-S| \leq J \leq L+S$

$$\sum_{J=|L-S|}^{L+S} 2J+1 = (2L+1)(2S+1)$$

With spin-orbit coupling (λLS),
L and S are not constants of motion but J is.

For Russel-Saunders coupling (SO as a weak perturbation):

The (2S+1)(2L+1)-fold degenerate level splits into (2J+1) degenerate (2S+1) [for L>S] or (2L+1) [for L<S] levels.

The lowest energy state is J=L+S if the shell is more than half filled or J=|L-S| otherwise (3rd Hund's rule)

$$\mu_{eff} = g_J \mu_B \sqrt{J(J+1)} \qquad g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

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Example d^1 : *L=2, S=1/2*

L>S → 2S+1=2 states with degeneracy 2J+1

deg:(2J+1)=6 J=L+S=5/2

deg:(2L+1)(2S+1)=10

deg:(2J+1)=4 J=|L-S|=3/2

fine structure

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Free magnetic ions

Ground state (GS) selection: Hund's rules

1. Maximize S
2. Maximize L
3. Minimize spin-orbit energy:
   - J=|L-S| if shell is less than half-full
   - J=L+S if shell is more than half full

$^{2S+1}L_J$

L	0	1	2	3	4	5	6
	S	P	D	F	G	H	I

$$\mu_{eff} = g_J \mu_B \sqrt{J(J+1)} \qquad g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

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Free magnetic ions

Ground state (GS) selection: Hund's rules

$$\mu_{eff} = g_J \mu_B \sqrt{J(J+1)}$$

1. Maximize S
2. Maximize L
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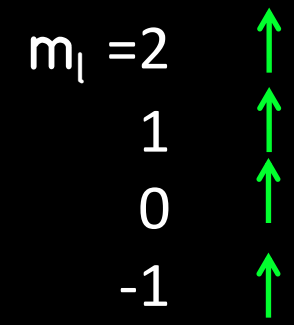
   J=|L-S| if shell is less than half-full
   J=L+S if shell is more than half full

$^{2S+1}L_J$

Mn^{3+} $(3d)^4$



S=2

L=2

J=|L-S|=0

$^3D_0$

$\mu_{eff}=0$

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Free magnetic ions

Ground state (GS) selection: Hund's rules

1. Maximize S
2. Maximize L
3. Minimize spin-orbit energy:
   J=|L-S| if shell is less than half-full
   J=L+S if shell is more than half full

$$\mu_{eff} = g_J \mu_B \sqrt{J(J+1)}$$

$^{2S+1}L_J$

Dy^{3+} $(4f)^9$

S=5/2

L=5

J=5+5/2=15/2

$^6H_{15/2}$

$\mu_{eff}=10.63\mu_B$

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Free magnetic ions

Ground state (GS) selection: Hund's rules

1. Maximize S
2. Maximize L
3. Minimize spin-orbit energy:
   J=|L-S| if shell is less than half-full
   J=L+S if shell is more than half full

Note

For $(3d)^4$, we got $\mu_{eff}=0$.
But experimentally (in a solid) $\mu_{exp}=4.82\mu_B$

In contrast, for $(4f)^9$, $\mu_{eff} \approx \mu_{exp}$

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Free magnetic ions

Ground state (GS) selection: Hund's rules

1. Maximize S
2. Maximize L
3. Minimize spin-orbit energy:
   J=|L-S| if shell is less than half-full
   J=L+S if shell is more than half full

Why $\mu_{eff} \neq \mu_{exp}$ for $(3d)^4$ in a solid?

Environment: crystal field

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Environment (breaking orbital degeneracy)

- Crystal field (CF):
  - Electrostatic interaction with electrons in surrounding ions. The medium is not isotropic: it has the symmetry of the crystal.
  - More important for d-electrons than for f-electrons because the former are less confined.

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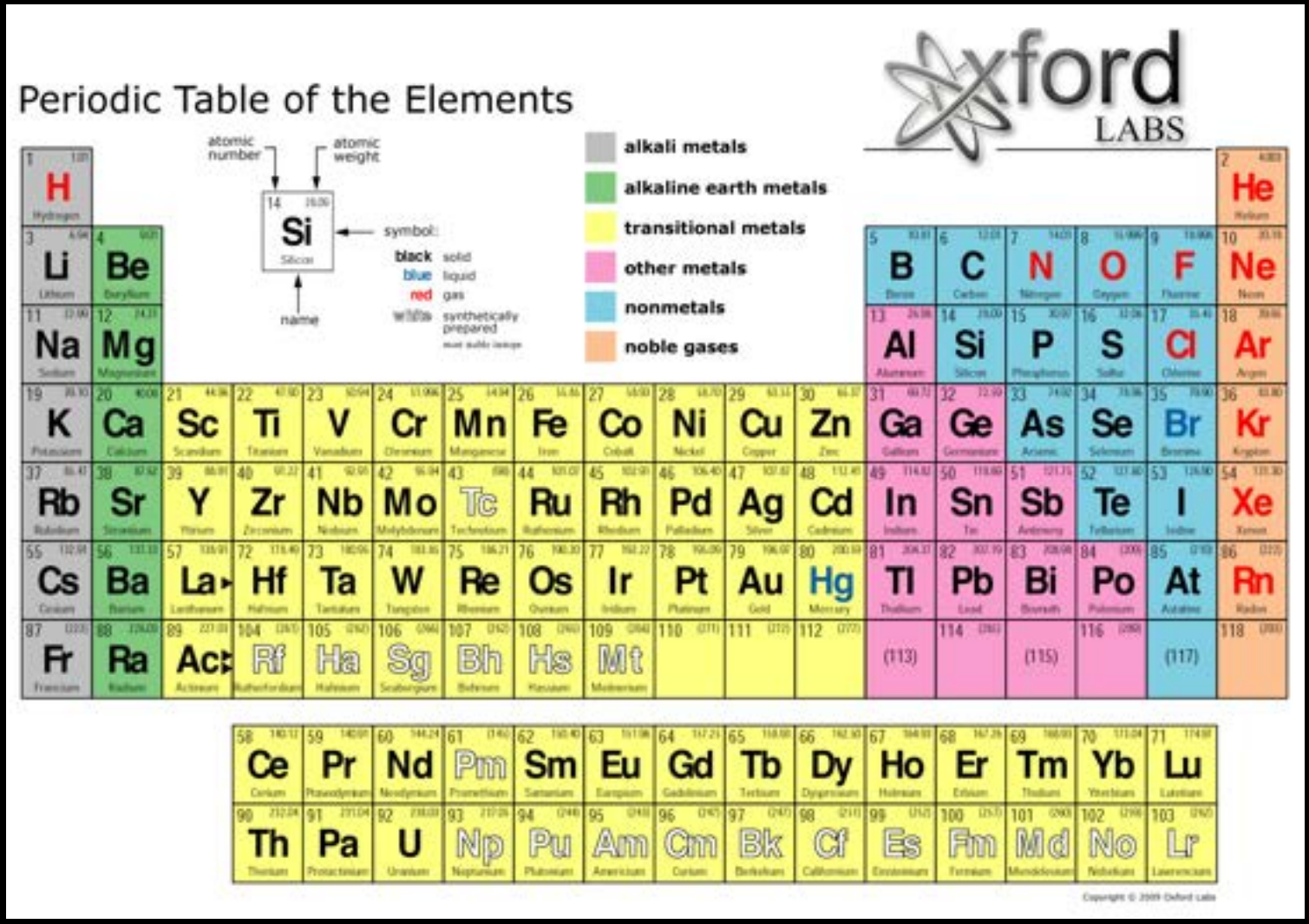
Free magnetic ions
electrons in incomplete shells (d or f orbitals)

Large CF
Small SO



Small CF
Large SO

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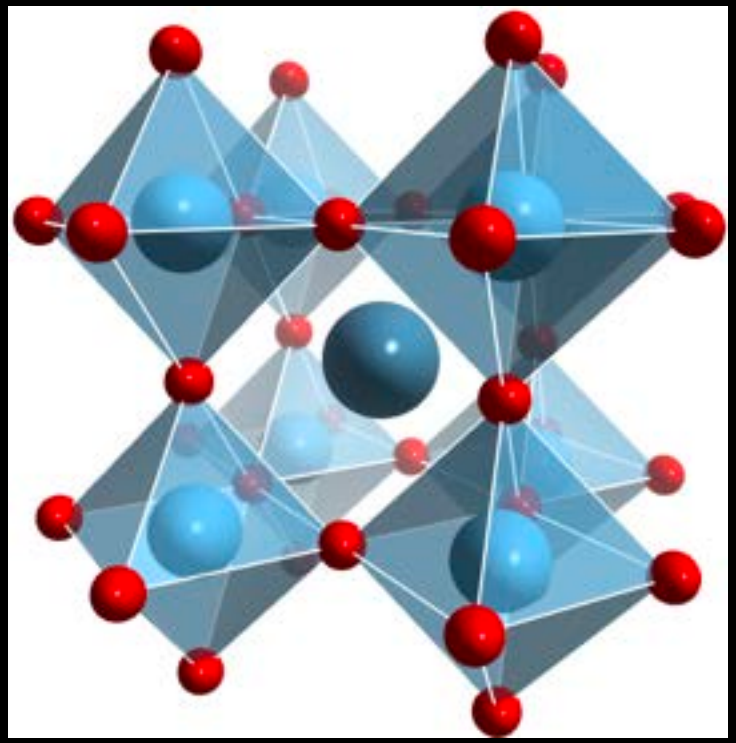
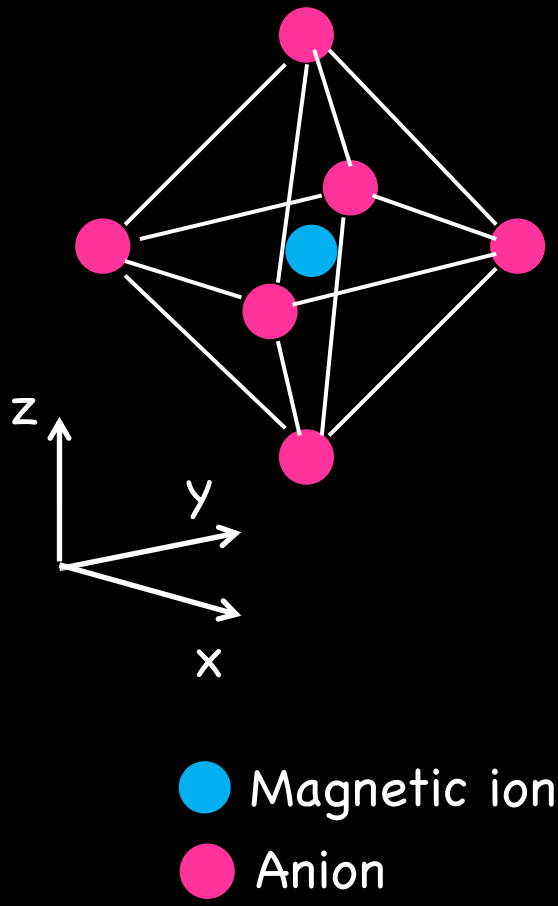
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in cubic symmetry (perovskite structure)



ABO_3



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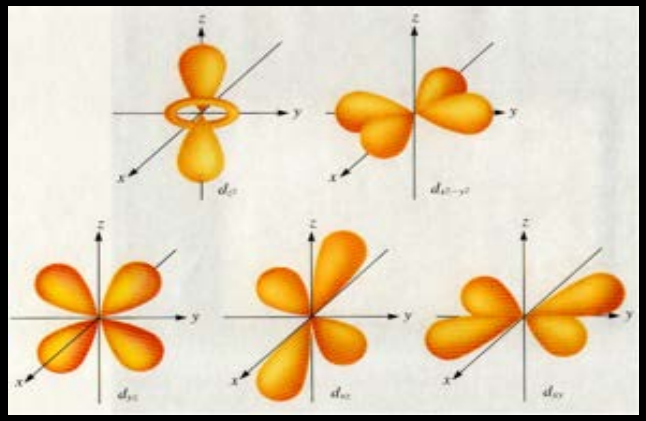
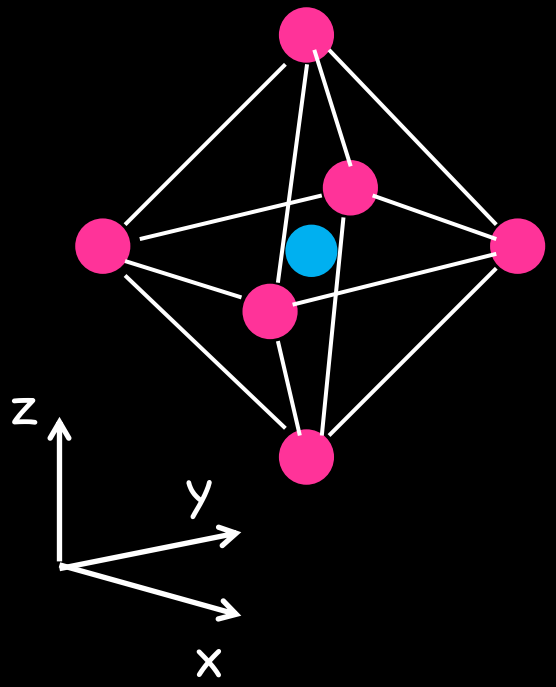
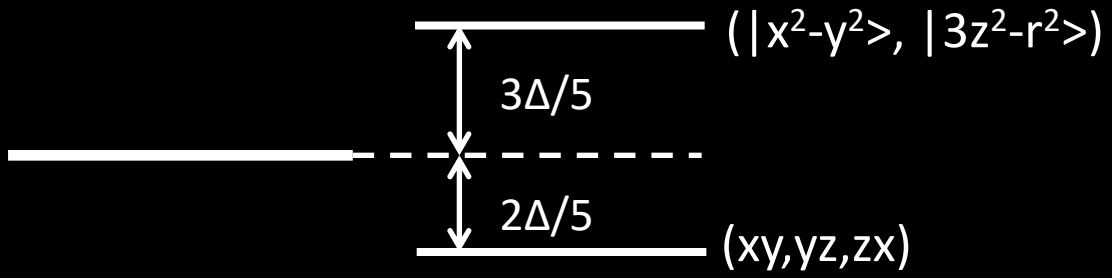
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in cubic symmetry (perovskite structure)







Magnetic ion

Anion

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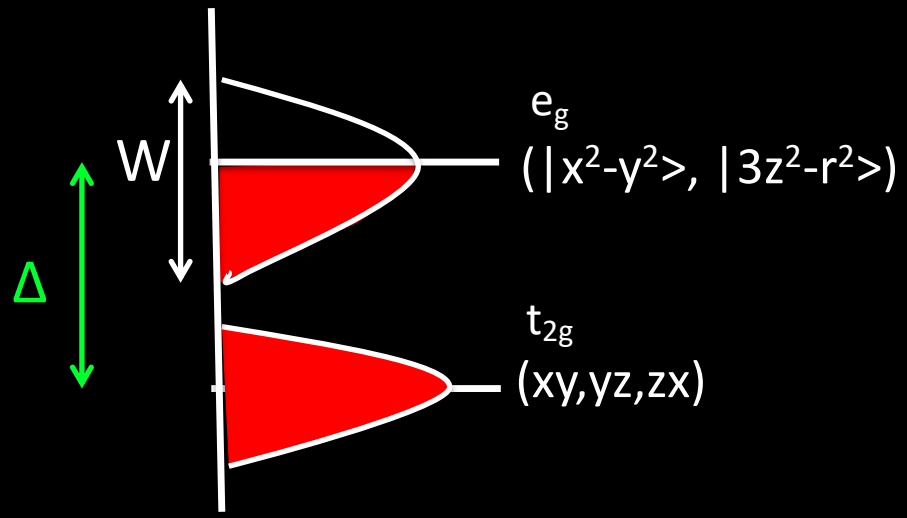
Environment (breaking orbital degeneracy)

- Crystal field (splitting Δ)

  d-electrons in cubic symmetry (perovskite structure)

In many cases (manganites, titanates) the splitting Δ is large compared to the bandwidth W.



Manganites $La_xSr_{1-x}MnO_3$
e_g orbitals at E_F
(t_{2g} localized)

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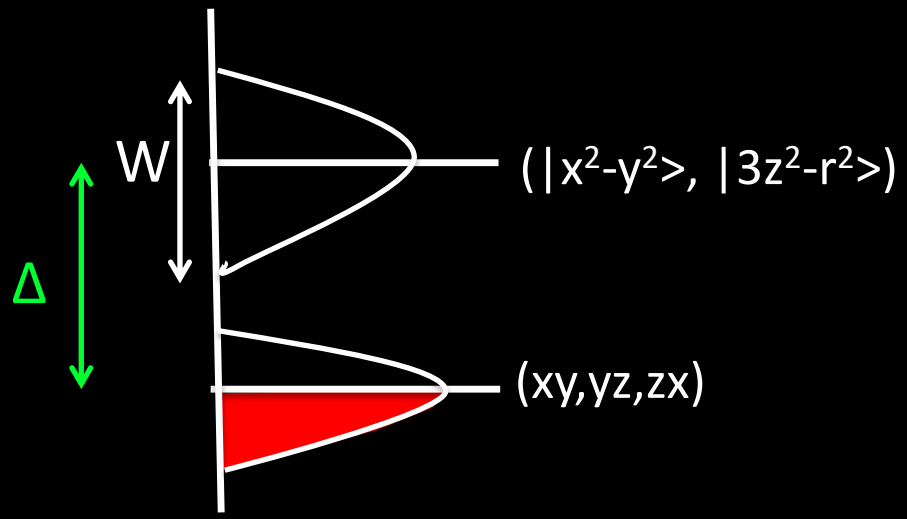
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in cubic symmetry (perovskite structure)

In many cases (manganites, titanates) the splitting Δ is large compared to the bandwidth W.



Doped $SrTiO_3$
t_{2g} orbitals at E_F

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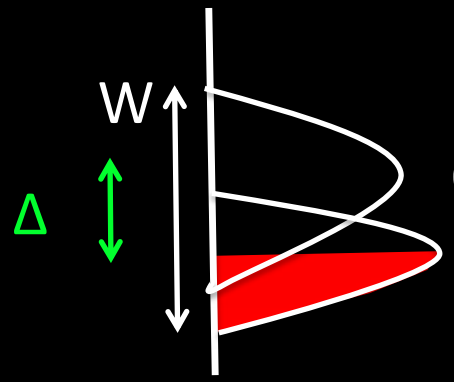
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in cubic symmetry
  (perovskite structure)

If the splitting Δ is small compared to the bandwidth W.



($|x^2-y^2>$, $|3z^2-r^2>$)
(xy,yz,zx)

All d-orbitals at E_F

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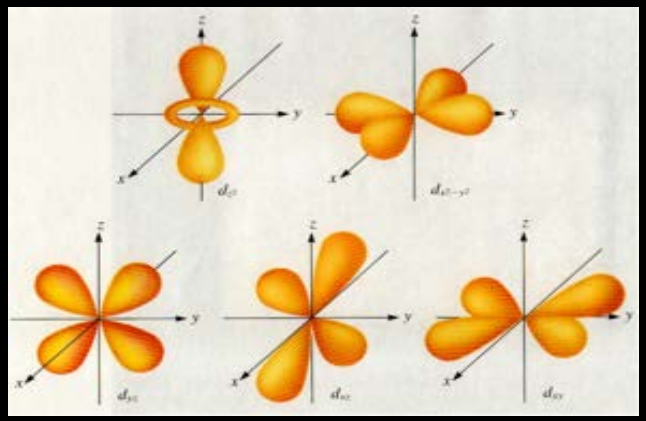
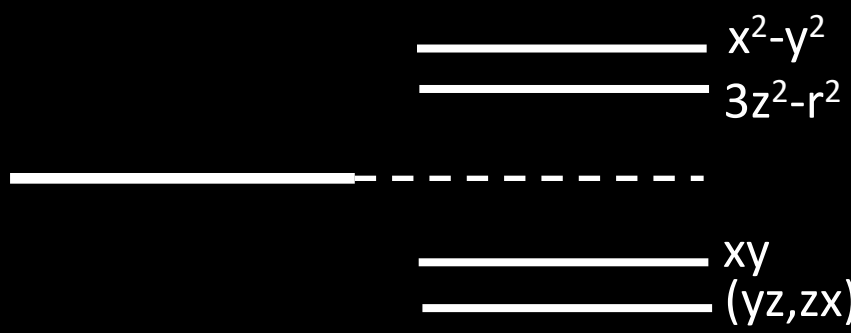
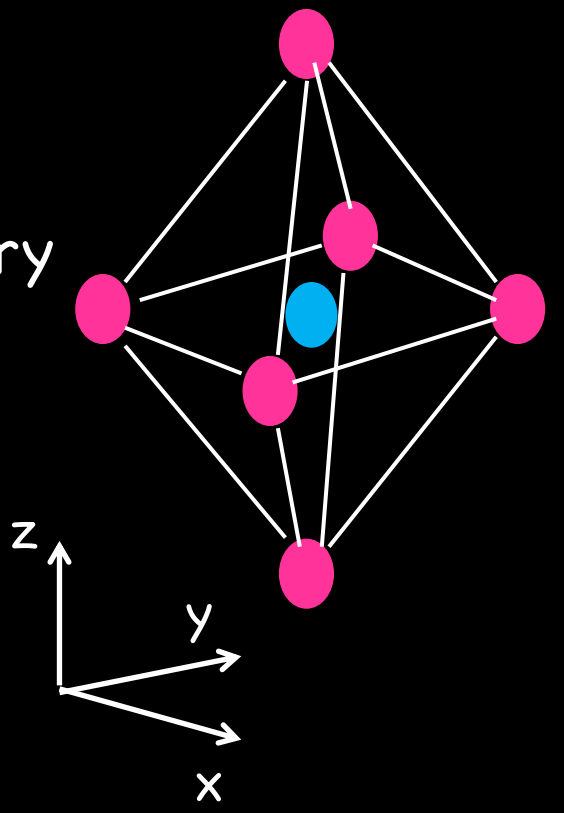
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in tetragonal symmetry (perovskite structure)







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Which orbitals are at E_F is important to determine the bands in the model. (Mott physics in multiorbital systems by Leni Bascones)

Hoppings are determined by
the symmetry of the orbitals and the lattice

$E_{xy,\,xy}$	$3l^2m^2(dd\sigma)+(l^2+m^2-4l^2m^2)(dd\pi)+(n^2+l^2m^2)(dd\delta)$
$E_{xy,\,yz}$	$3lm^2n(dd\sigma)+ln(1-4m^2)(dd\pi)+ln(m^2-1)(dd\delta)$
$E_{xy,\,zx}$	$3l^2mn(dd\sigma)+mn(1-4l^2)(dd\pi)+mn(l^2-1)(dd\delta)$
$E_{xy,\,x^2-y^2}$	$\frac{3}{2}lm(l^2-m^2)(dd\sigma)+2lm(m^2-l^2)(dd\pi)+\frac{1}{2}lm(l^2-m^2)(dd\delta)$
$E_{yz,\,x^2-y^2}$	$\frac{3}{2}mn(l^2-m^2)(dd\sigma)-mn[1+2(l^2-m^2)](dd\pi)+mn[1+\frac{1}{2}(l^2-m^2)](dd\delta)$
$E_{zx,\,x^2-y^2}$	$\frac{3}{2}nl(l^2-m^2)(dd\sigma)+nl[1-2(l^2-m^2)](dd\pi)-nl[1-\frac{1}{2}(l^2-m^2)](dd\delta)$
$E_{xy,\,3z^2-r^2}$	$\sqrt{3}lm[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)-2\sqrt{3}lmn^2(dd\pi)+\frac{1}{2}\sqrt{3}lm(1+n^2)(dd\delta)$
$E_{yz,\,3z^2-r^2}$	$\sqrt{3}mn[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}mn(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}mn(l^2+m^2)(dd\delta)$
$E_{zx,\,3z^2-r^2}$	$\sqrt{3}ln[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}ln(l^2+m^2-n^2)(dd\pi)-\frac{1}{2}\sqrt{3}ln(l^2+m^2)(dd\delta)$
$E_{x^2-y^2,\,x^2-y^2}$	$\frac{3}{4}(l^2-m^2)^2(dd\sigma)+[l^2+m^2-(l^2-m^2)^2](dd\pi)+[n^2+\frac{1}{4}(l^2-m^2)^2](dd\delta)$
$E_{x^2-y^2,\,3z^2-r^2}$	$\frac{1}{2}\sqrt{3}(l^2-m^2)[n^2-\frac{1}{2}(l^2+m^2)](dd\sigma)+\sqrt{3}n^2(m^2-l^2)(dd\pi)+\frac{1}{4}\sqrt{3}(1+n^2)(l^2-m^2)(dd\delta)$
$E_{3z^2-r^2,\,3z^2-r^2}$	$[n^2-\frac{1}{2}(l^2+m^2)]^2(dd\sigma)+3n^2(l^2+m^2)(dd\pi)+\frac{3}{4}(l^2+m^2)^2(dd\delta)$

Slater and Koster, Phys. Rev. 94, 1498 (1954)

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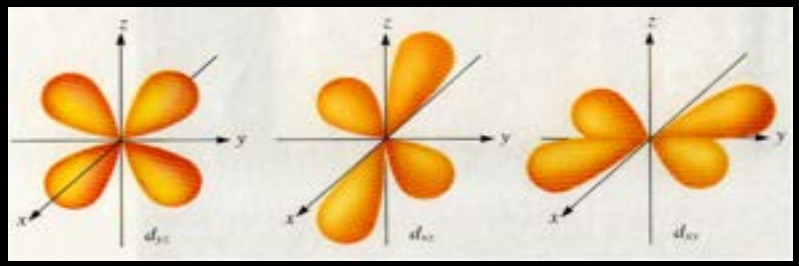
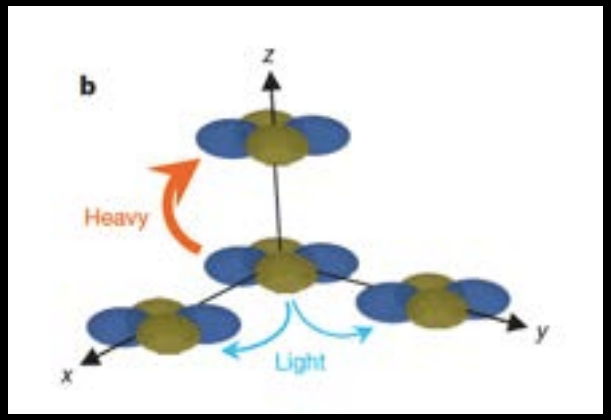
For instance, t_{2g} orbitals:



In a cubic lattice (l,m,n): (1,0,0), (0,1,0), (0,0,1)



Nature 469, 189 (2011)

$$t^x_{xy,xy} = t^y_{xy,xy} = t^y_{yz,yz} = t^z_{yz,yz} = t^z_{zx,zx} = t^x_{zx,zx}$$

$$t_{\alpha,\beta} = 0$$

t_{2g} orbitals don't mix: three 2dim bands

If only one t_{2g} orbital (as for a low crystal symmetry): 2dim model

Slater and Koster, Phys. Rev. 94, 1498 (1954)

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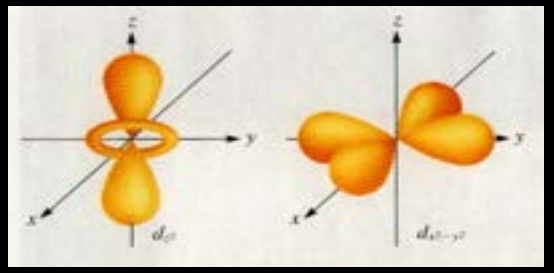
For e_g orbitals



In a cubic lattice (l,m,n): (1,0,0), (0,1,0), (0,0,1)

$$t^{x,y}_{3z^2-r^2,3z^2-r^2} = 1/4t \qquad t^{x,y}_{x^2-y^2,x^2-y^2} = 3/4t \qquad t^{x,y}_{x^2-y^2,3z^2-r^2} = \pm\sqrt{3}/4t$$

$$t^{z}_{3z^2-r^2,3z^2-r^2} = t \qquad t^{z}_{x^2-y^2,x^2-y^2} = 0 \qquad t^{z}_{x^2-y^2,3z^2-r^2} = 0$$

e_g orbitals mix.

For Cuprates, further splitting (tetragonal) Cu (9±x) electrons.

Carriers on x^2-y^2: 2dim band

Slater and Koster, Phys. Rev. 94, 1498 (1954)

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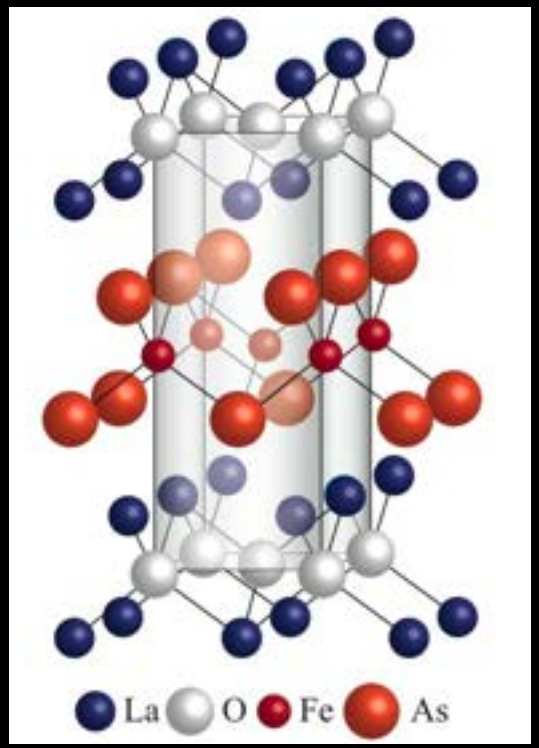
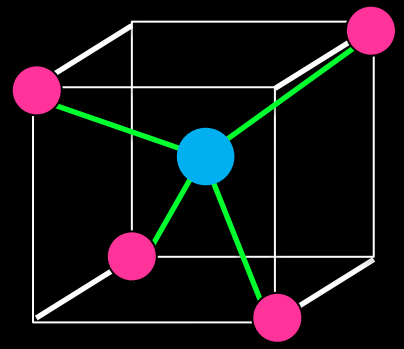
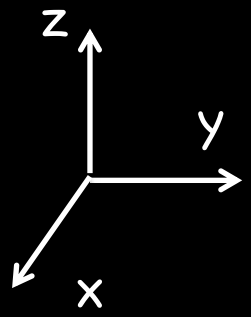
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in a tetrahedral symmetry







Magnetic ion

Anion

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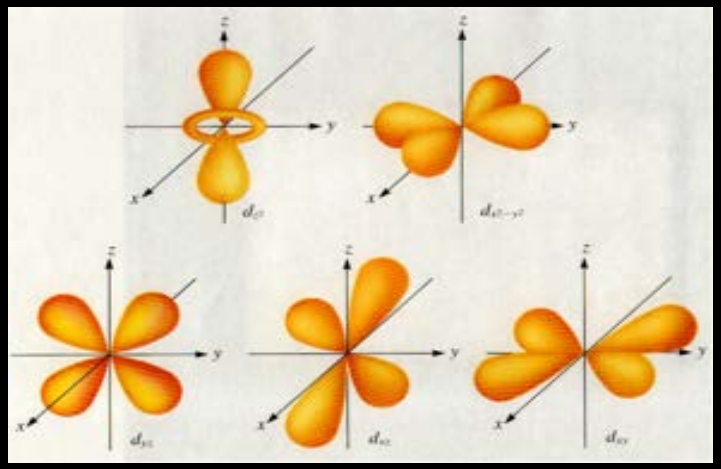
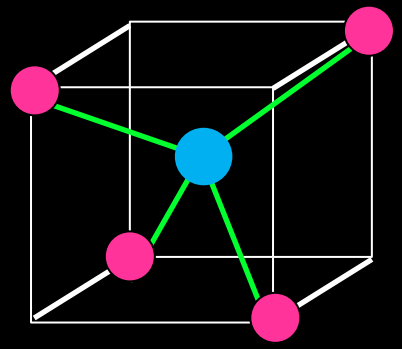
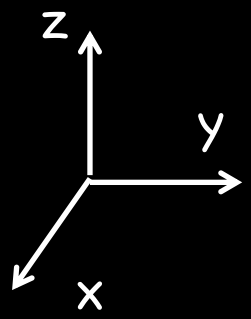
Environment (breaking orbital degeneracy)

- Crystal field

  d-electrons in a tetrahedral symmetry

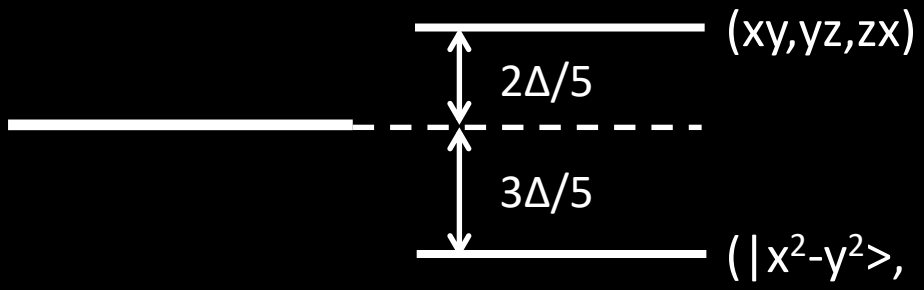






Magnetic ion

Anion



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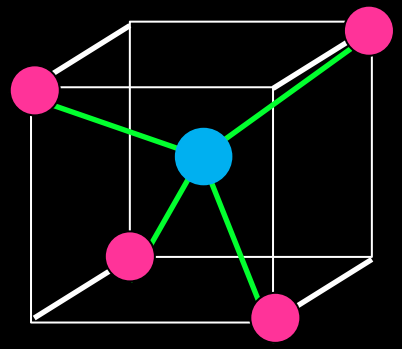
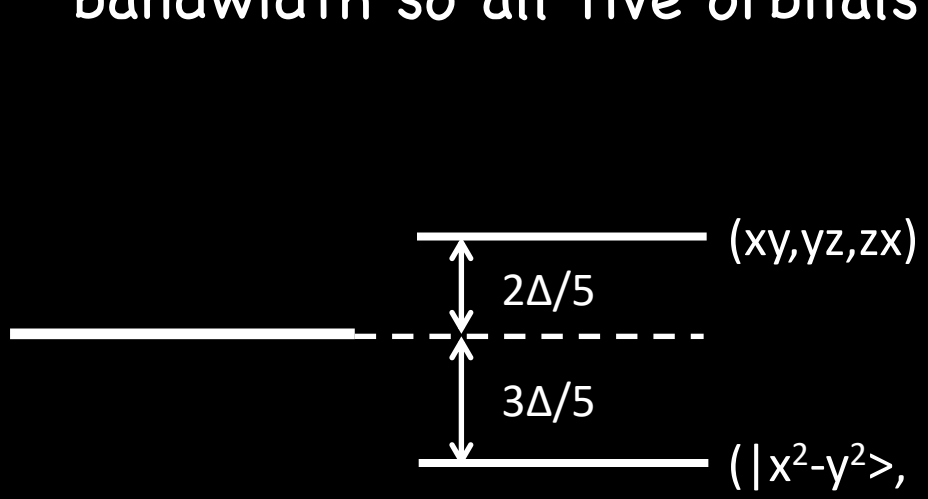
Environment (breaking orbital degeneracy)

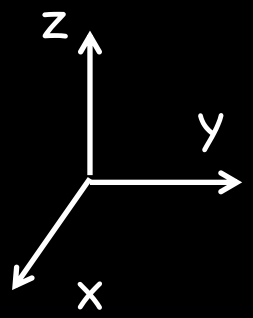
- Crystal field

  d-electrons in a tetrahedral symmetry

In iron superconductors, the splitting Δ is small compared to the bandwidth so all five orbitals at E_F







Magnetic ion

Anion

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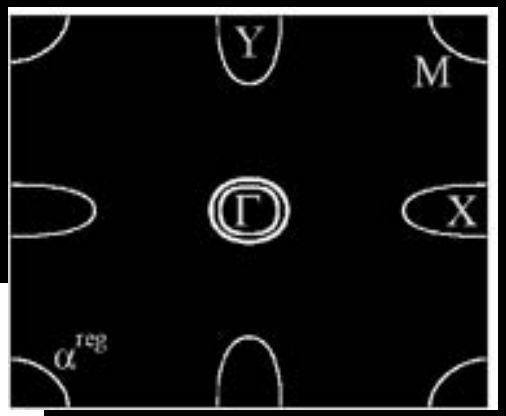
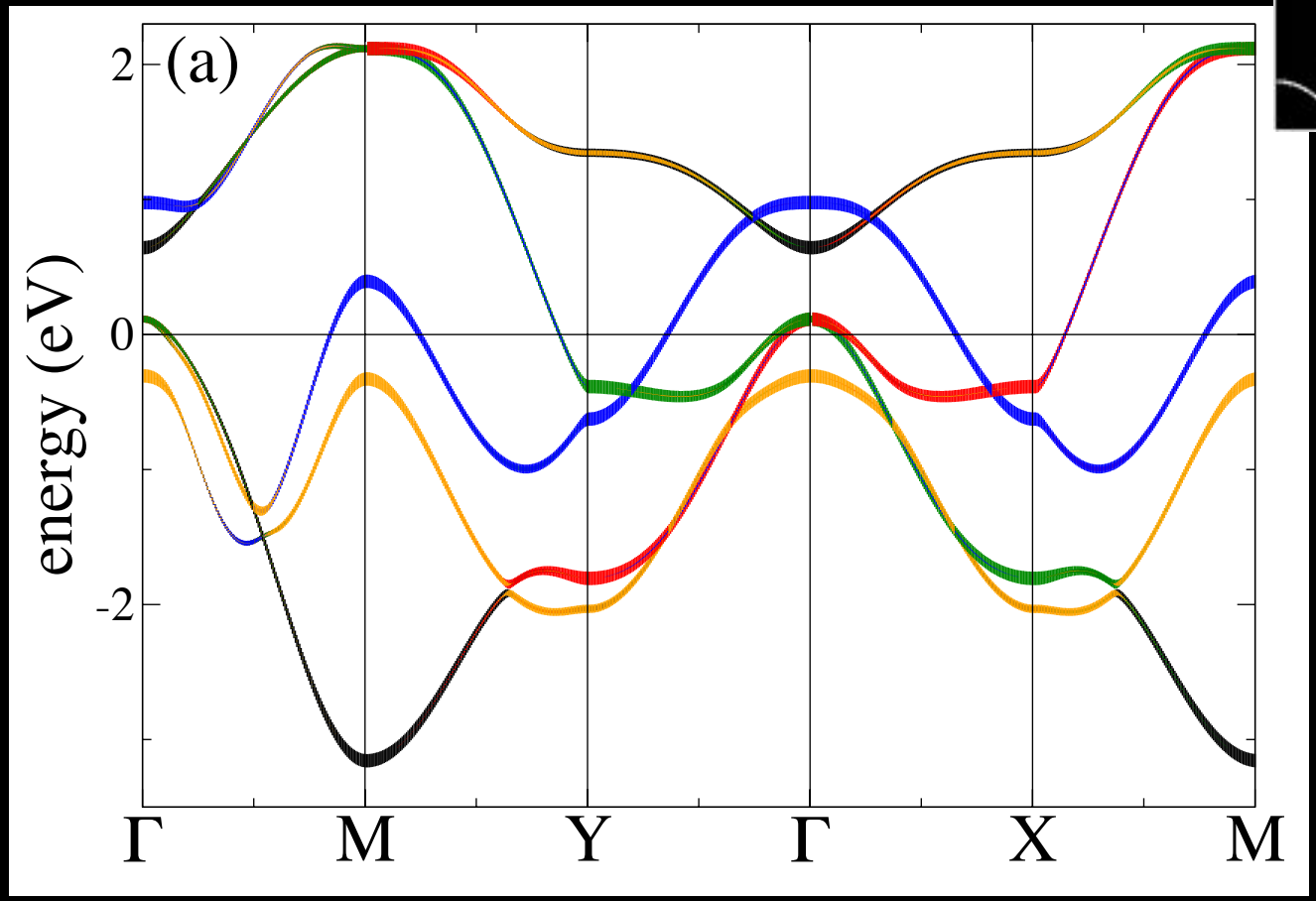
d-bands for iron superconductors





PRB 87, 075136

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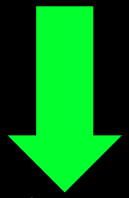
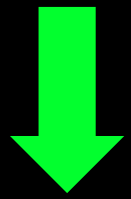
Crystal field



Orbital "selection"



anisotropies

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Environment (breaking orbital degeneracy)

- Crystal field. Calculation (sketch)

Treat surrounding ions as point charges

$$V_{cryst} = \sum_i \frac{q_i}{|\mathbf{r} - \mathbf{R}_i|}$$

...expand for r<R

$$V_{cryst} = \sum_l \sum_{m=-l}^{l} K_{lm} r^l P_l^{|m|}(\cos\theta) e^{im\varphi}$$

$$K_{lm} = \frac{(l-|m|)!}{(l+|m|)!} \sum_i \frac{q_i}{R_i^{l+1}} P_l^{|m|}(\cos\theta_i) e^{im\varphi_i}$$

R_i has the information of the crystal symmetry

And rewrite as a function of spherical harmonics.

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Environment (breaking orbital degeneracy)

- Crystal field. Calculation (sketch)

Treat surrounding ions as point charges

$$V_{cryst} = \sum_i \frac{q_i}{|\mathbf{r} - \mathbf{R}_i|}$$

Calculate expected values of atomic orbitals (also expressed in spherical harmonics)

$$\langle \Psi_{lm}(r) | H_{cryst}(r_i) | \Psi_{lm'}(r) \rangle$$

The calculations involve averages over radial wave-functions $\langle r^n \rangle$

The results depend on the number of electrons

Yosida, Chapter 3.

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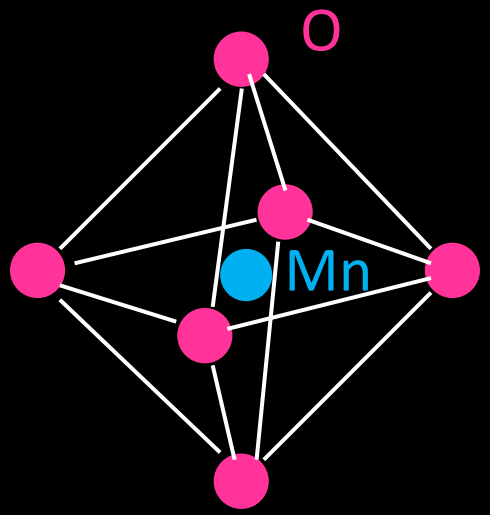
Environment (breaking orbital degeneracy)

- Jahn-Teller: when the orbital ground state is degenerate, a distortion in the lattice splits orbitals to minimize energy.

For a cubic perovskite lattice:

$(x^2-y^2,$
$3z^2-r^2)$

(xy,yz,zx)



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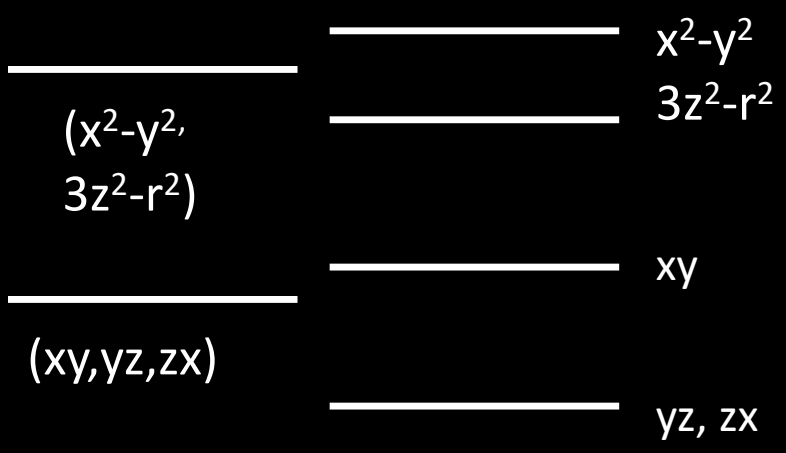
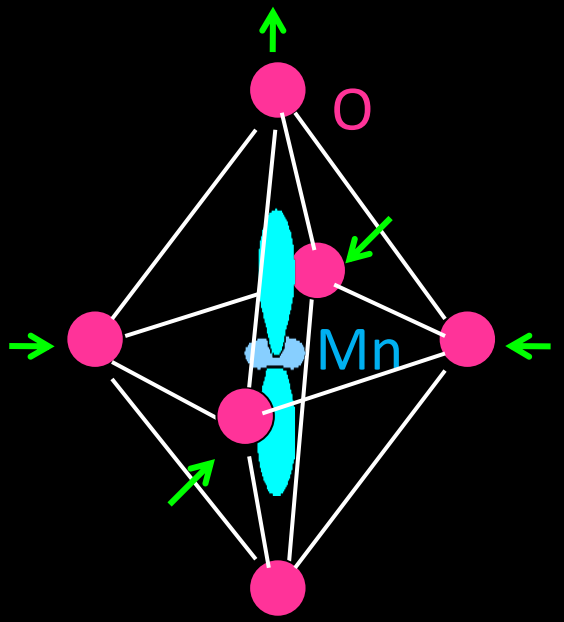
For a cubic perovskite lattice:





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Environment (breaking orbital degeneracy)

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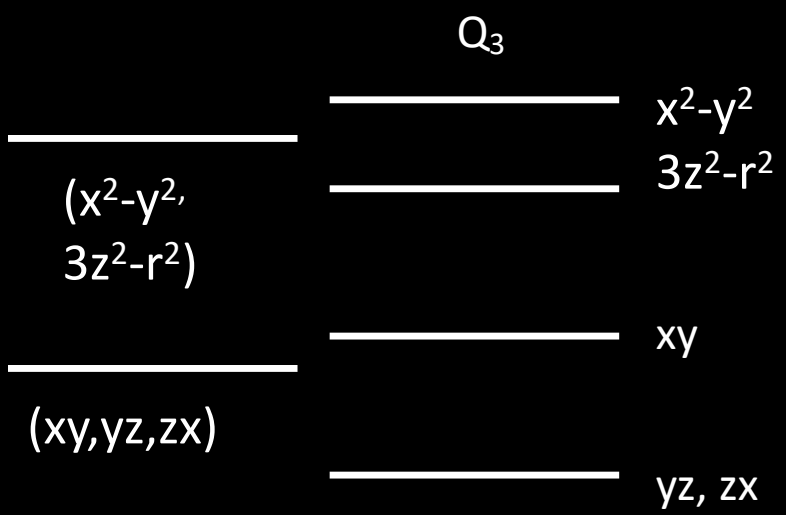

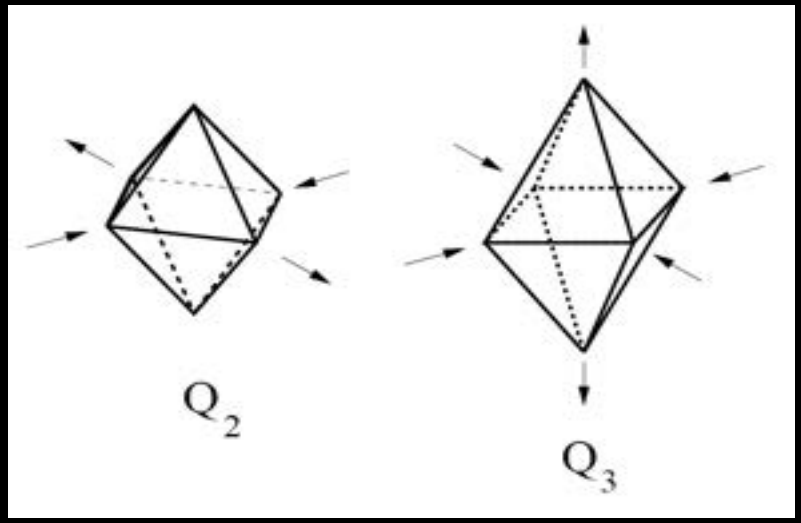

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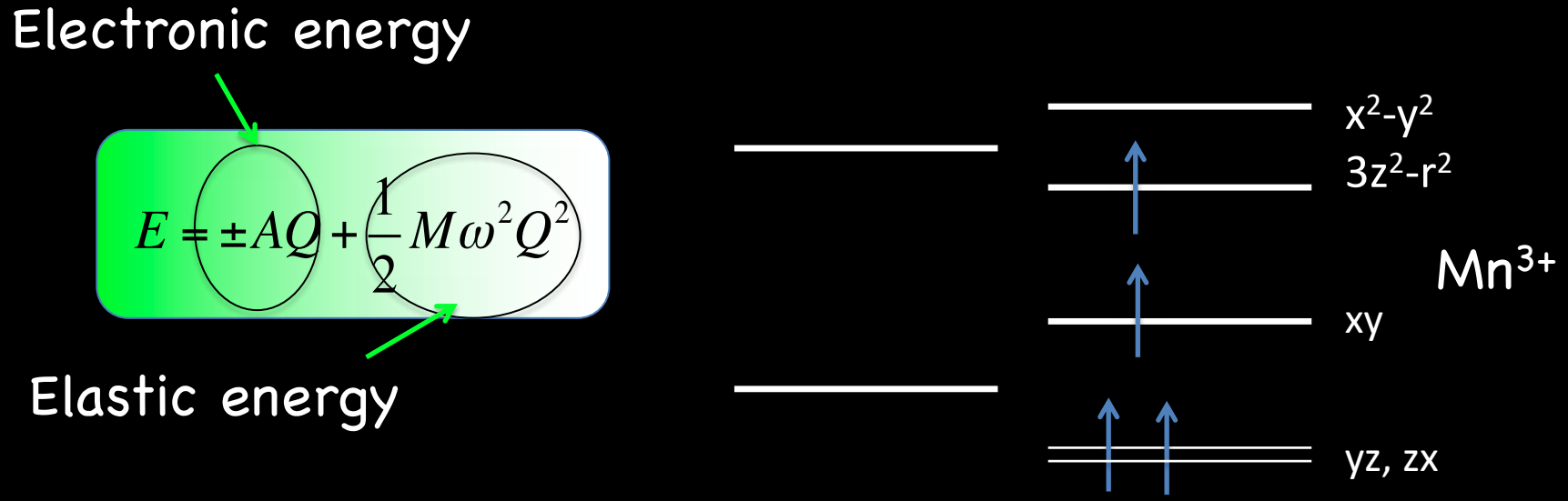
Environment (breaking orbital degeneracy)

- Jahn-Teller: when the orbital ground state is degenerate, a distortion in the lattice splits orbitals to minimize energy.



Note: if you remove (Mn4+) or remove (Mn4+) one electron there is no energy gain by the splitting, hence there is no distortion.

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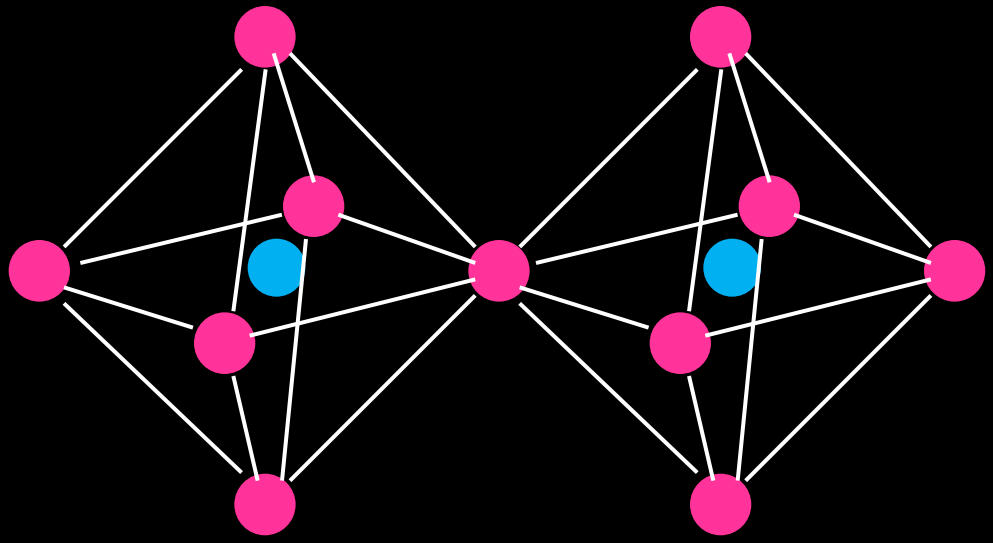
Environment (breaking orbital degeneracy)

Jahn-Teller distortions are cooperative.
They may lead to structural phase transitions



Cubic to tetragonal transitions:
$LaMnO_3$ (T_s=800K). Perovskite.
$CuFe_2O_4$ (T_s=713K). Spinel.
Mn_3O_4 (T_s=1443K). Spinel.

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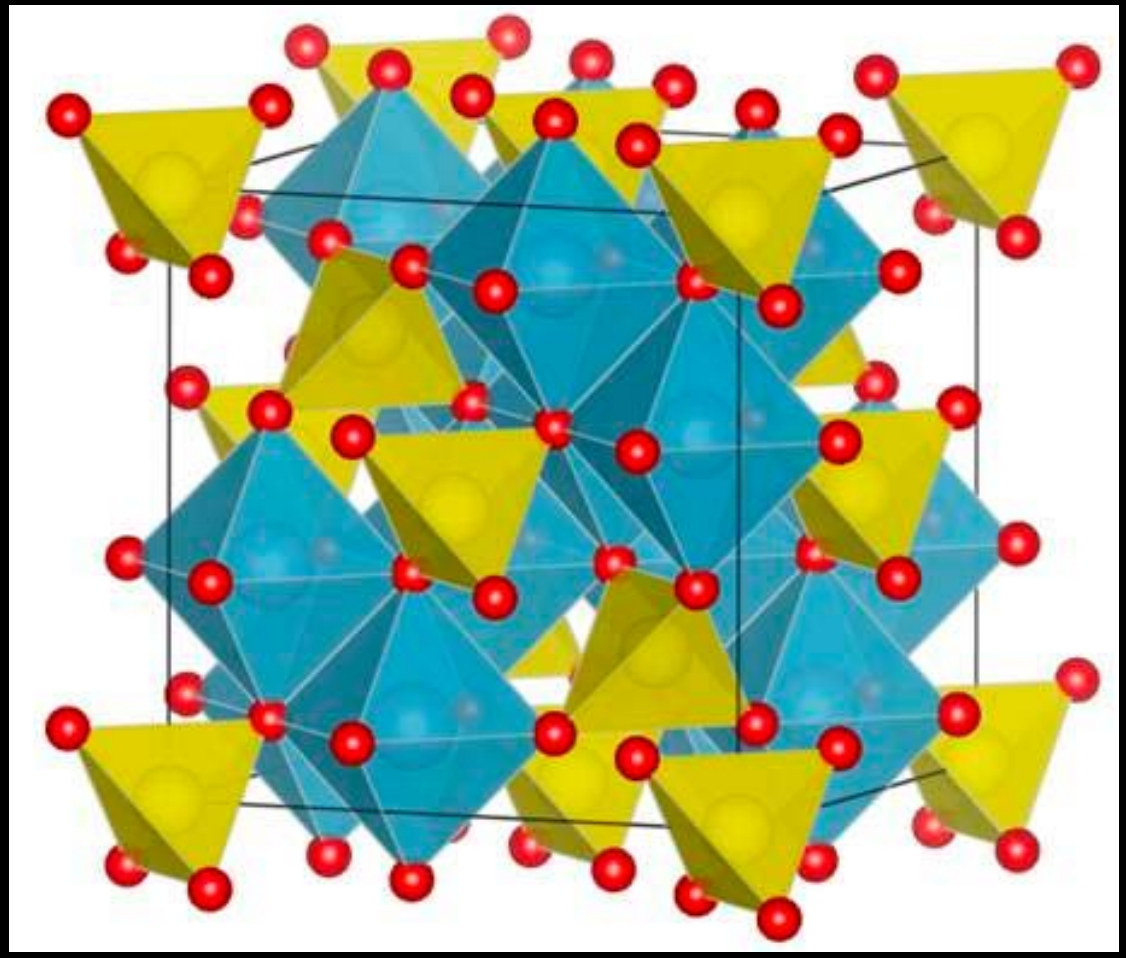
Spinel structure



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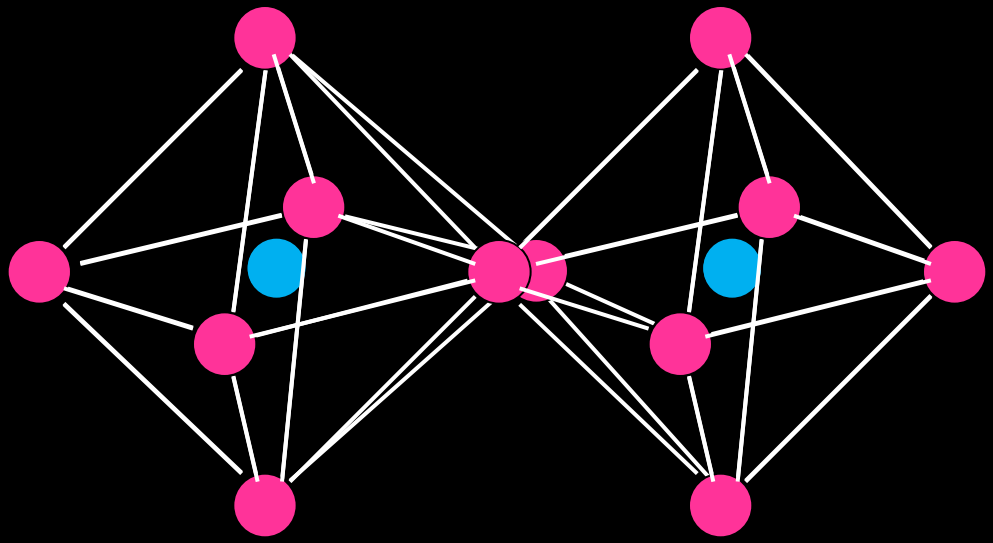
Environment (breaking orbital degeneracy)

Jahn-Teller distortions are cooperative.
They may lead to structural phase transitions
…and orbital ordering



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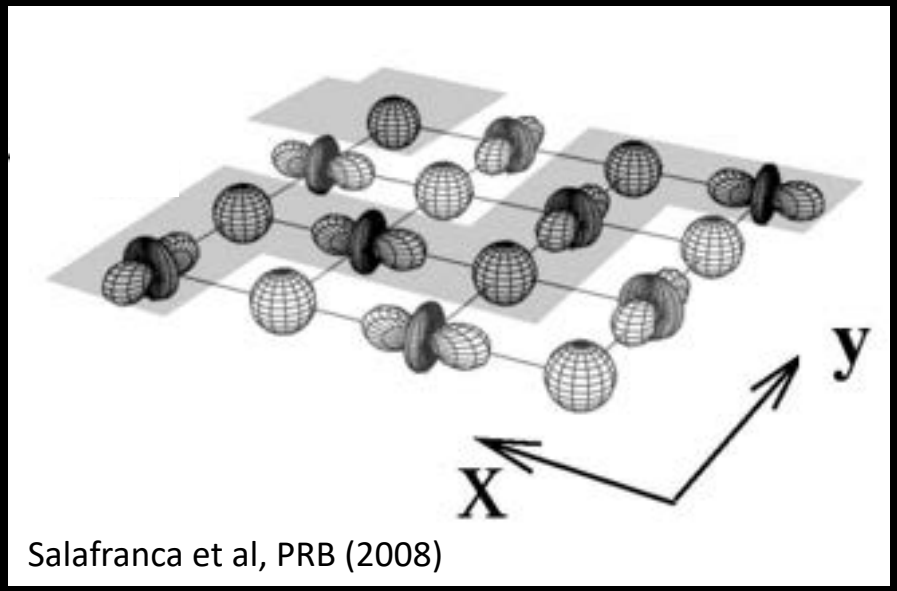
Environment (breaking orbital degeneracy)

Jahn-Teller distortions are cooperative.
They may lead to structural phase transitions and orbital ordering

Orbital order in manganites
(0.5 e- per Mn)



Salafranca et al, PRB (2008)

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Environment (breaking orbital degeneracy)

Jahn-Teller distortions are cooperative.
They may lead to structural phase transitions and orbital ordering

At high temperatures:
dynamic Jahn-Teller effect

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Why $\mu_{eff} \neq \mu_{exp}$ for $(3d)^4$ in a solid?

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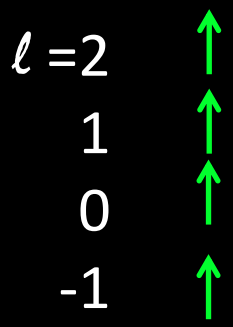
Free magnetic ions

Ground state (GS) selection: Hund's rules

1. Maximize S
2. Maximize L
3. Minimize spin-orbit energy:
   J=|L-S| if shell is less than half-full
   J=L+S if shell is more than half full

Mn^{3+} $(3d)^4$



S=2

L=2

J=0

$^3D_0$

$\mu_{eff}=0$

But experimentally $\mu_{exp}=4.82\mu_B$

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Orbital quenching

- If we considered L=0 for (3d) ions

$$\mu_{eff} = g_J \mu_B \sqrt{J(J+1)} \qquad g_J = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)}$$

$$\mu_{eff} = g_J \mu_B \sqrt{S(S+1)} \qquad g_J = 2$$

With L=0, for $(3d)^4$ we would get μ_{eff}=4.89 μ_B
(experimentally μ_{exp}=4.82 μ_B)

(diff between μ_{eff} and μ_{exp} due to finite orbital angular momentum)

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Orbital quenching

Experimental observation: When crystal field effects are larger than spin-orbit coupling (as for 3d ions), the ground state is such that L=0. Why?

<GS|L|GS> must be real

L is purely imaginary

Non-degenerate

GS is real

(is an eigenfunction of the crystal field)

<GS|L|GS> =0

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Orbital quenching

NOTE:

For degenerate levels, you can define the d-levels in different basis involving any combination of the angular momenta involved.

When the e_g and t_{2g} levels are split by crystal field, you can only make combinatios within the restricted set of degenerate levels. In the e_g sector, any combination leads to L=0. In the t_{2g} sector, you can choose a combination with L^z=1. Therefore, 1 electron in a t_{2g} level has a partially quenched orbital.

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Spin-orbit coupling for d-atoms

- Partially restores the quenched orbital momentum
- Induces magnetic anisotropy (the spin feels, through the orbital, the orientation of the crystal axes).

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Spin-orbit coupling for d-atoms

Start from a quenched orbital (L=0) and introduce LS and magnetic field within second order perturbation theory

$$V = \lambda \mathbf{L}\cdot\mathbf{S} + \mu_B \mathbf{H}\cdot(2\mathbf{S}+\mathbf{L})$$

$$H_S = \sum_{\mu\nu} 2\mu_B H_\mu (\delta_{\mu\nu} - \lambda\Lambda_{\mu\nu}) S_\nu - \lambda^2 S_\mu \Lambda_{\mu\nu} S_\nu - \mu_B^2 H_\mu \Lambda_{\mu\nu} H_\nu$$

$g_{\mu\nu}/2$

Induced orbital moment

$$\Lambda_{\mu\nu} = \sum_n \frac{\langle 0|L_\mu|n\rangle\langle n|L_\nu|0\rangle}{E_n - E_0}$$

Anisotropy spin Hamiltonian

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Spin-orbit coupling for d-atoms

The anisotropy spin Hamiltonian can be written:

$$H = DS_z^2 + E(S_x^2 - S_y^2)$$

- H lifts the (2S+1) degeneracy.
- The first term:
  - For integer S, splitting into doubly degenerate $S_z=\pm S$, $\pm(S-1)$... ± 1, and non-degenerate 0.
  - For half-integer S, splitting into doubly degenerate $S_z=\pm S$, $\pm(S-1)$... $\pm 1/2$.
- S_x^2 and S_y^2 produce transitions $\Delta S_z=\pm 2$. Therefore the second term further splits the levels for integer S.
- For half integers ($\Delta S_z=\pm 2$ not possible): Kramers doublet.
- Kramers degeneracy holds as long as the Hamiltonian is invariant under time reversal (and lifted by, for instance, Zeeman energy)

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Crystal field for f-atoms

- Crystal field is weak so you have to start from the total angular momentum predicted by third Hund's rule: (2J+1) degeneracy. This degeneracy is usually lifted by the weak crystal field as a (2J+1) degeneracy is too large.
- We have to work with total angular momentum J rather than L. In principle J could be quenched but in practice the crystal field is so small that an external magnetic field or an exchange field can change the relative position of the levels.

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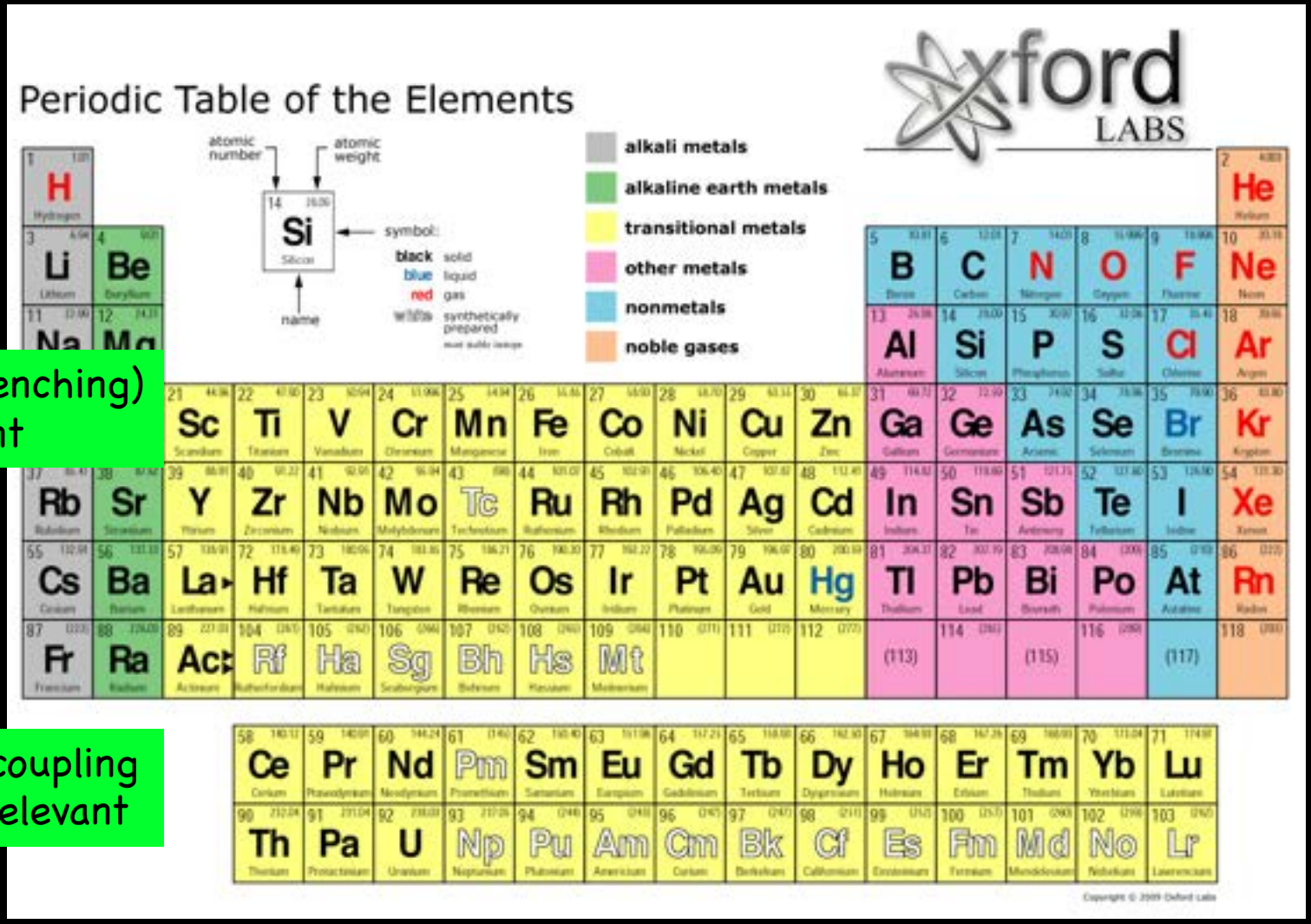
L=0 (orbital quenching)
S relevant

SO coupling
J relevant



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Three energy scales to determine local moments in a solid

- Hund's coupling (local exchange)
- Crystal field (environment)
- Spin-orbit coupling

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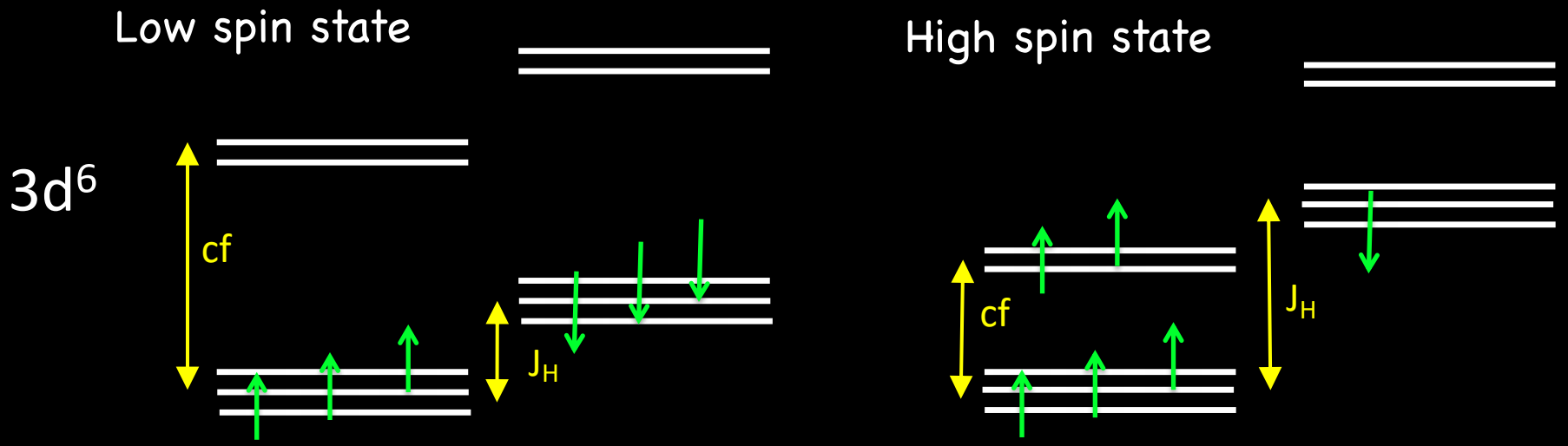
Crystal field vs Hund's coupling



Crystal field > J_H

S=0

Crystal field < J_H

S=2

Crystal fields may be changed with pressure

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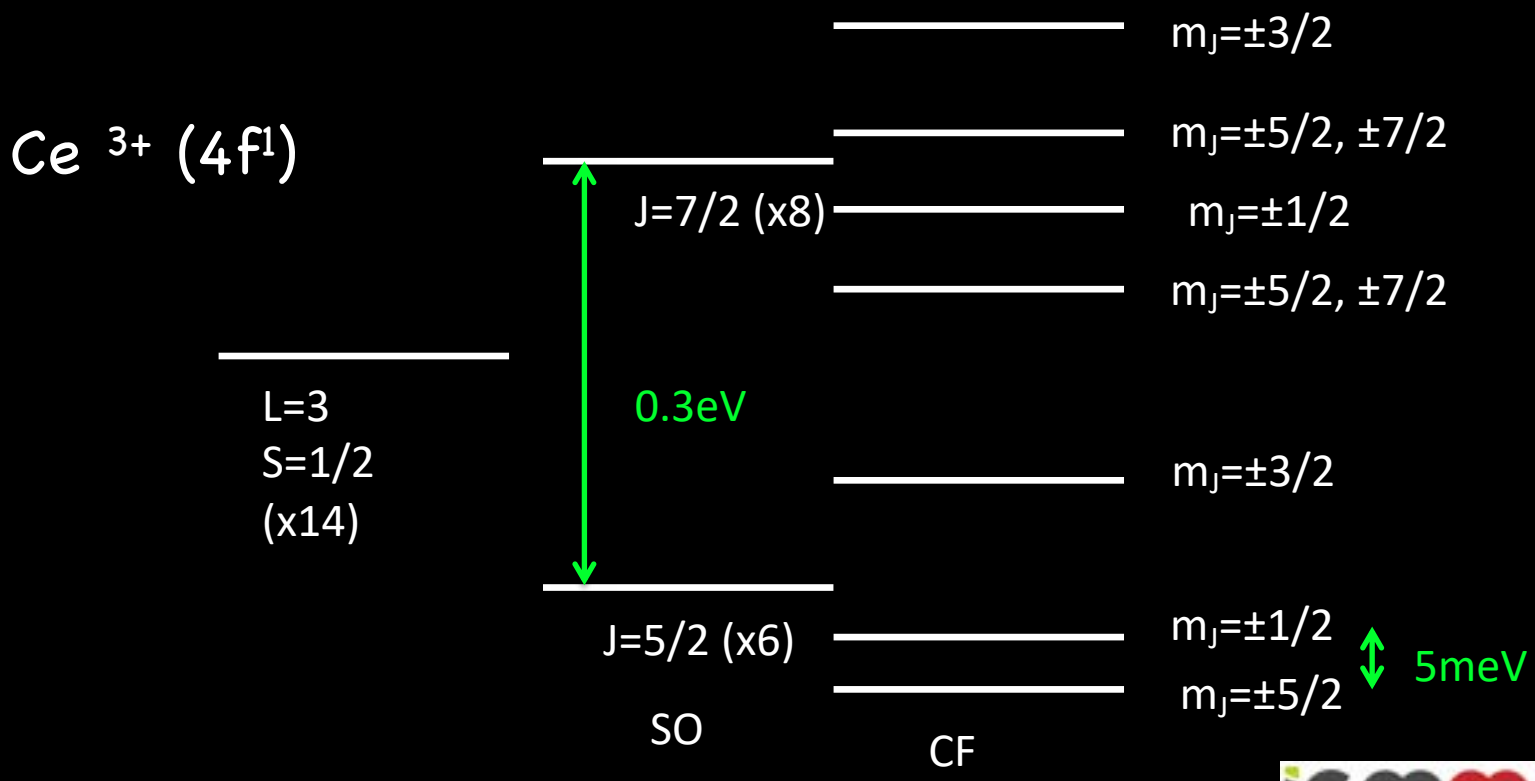
Crystal field vs spin-orbit coupling

3d ions: crystal-field >> spin-orbit coupling
4f and 5f ions: crystal-field << spin-orbit coupling



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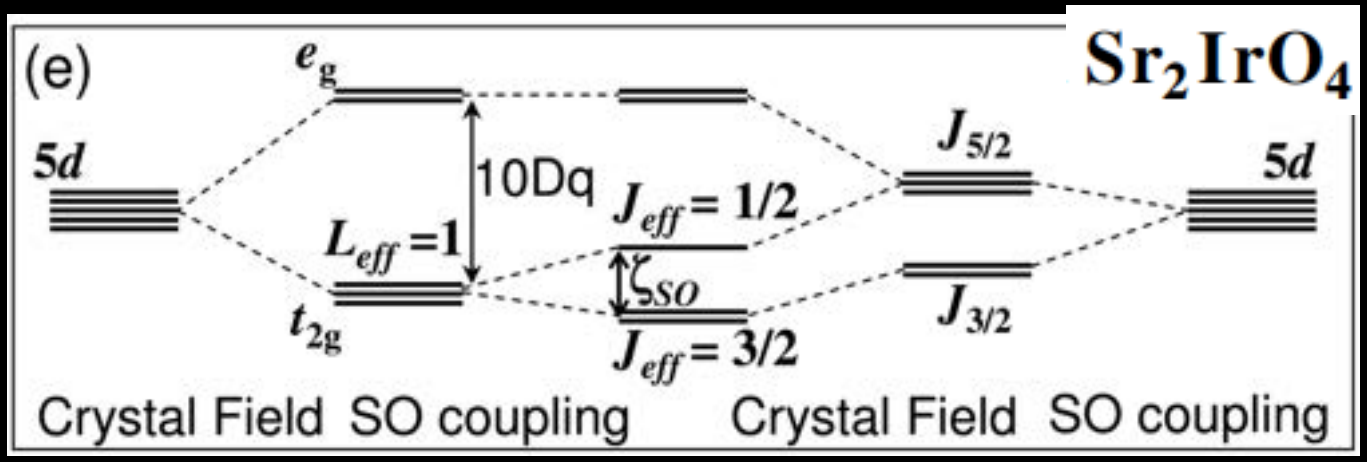
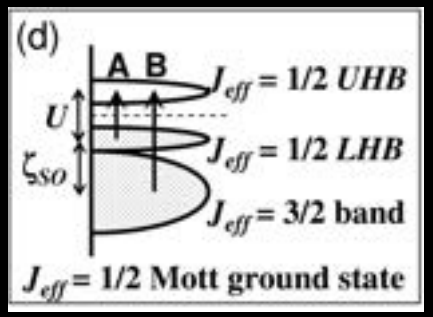
Crystal field vs spin-orbit coupling

3d ions: crystal-field >> spin-orbit coupling
4f and 5f ions: crystal-field << spin-orbit coupling
4d-5d: crystal-field ≈ spin-orbit coupling



Kim et al, PRL 101, 076402

$5d^5$



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Three energy scales to determine local moments

- Hund's coupling (local exchange)
- Crystal field (environment)
- Spin-orbit coupling

3d ions:

- Crystal field >> spin-orbit coupling
  - orbital quenching (L=0)
- Crystal field vs Hund's coupling: low spin-high spin

4f-5f:

- Crystal field << spin-orbit coupling
- Large total magnetic moments J

4d-5d: All scales relevant. U competes with LS

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Outline

- Free magnetic ions
- Environment
- Magnetic order and phase transitions
- Interactions
  - Exchange between localized moments
  - Indirect exchange through itinerant electrons
  - Magnetism in metals
- Excitations

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Susceptibility

Response to a perturbation (e.g. external field).

In general $\chi(r,t)$ [or $\chi(q,\omega)$]

Here: magnetic susceptibility

$$\chi = \frac{\partial M}{\partial H}$$

A measure of correlations

$$\chi_{ij} = \frac{(g\mu_B)^2}{kT}\left(\langle S_i S_j\rangle - \langle S_i\rangle\langle S_j\rangle\right)$$

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An atom in a magnetic field (non-interacting moments)

$$H = \sum_{i=1}^{Z} \left(\frac{[\vec{p}_i + e\vec{A}(\vec{r}_i)]^2}{2m_e} + V_i \right) + g\mu_B \vec{B} \cdot \vec{S} =$$

$$\sum_i \left(\frac{p_i^2}{2m_e} + V_i \right) + \mu_B (\vec{L} + g\vec{S}) \cdot \vec{B} + \frac{e^2}{8m_e} \sum_i (\vec{B} \times \vec{r}_i)^2$$

Paramagnetic term. $\chi > 0$

A magnetic field aligns local magnetic moments J

$$\mathbf{A}(\mathbf{r}) = \frac{\mathbf{B} \times \mathbf{r}}{2} \qquad \hbar\mathbf{L} = \sum_i \mathbf{r}_i \times \mathbf{p}_i$$

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Paramagnetic susceptibility

$$\sum_i \left(\frac{p_i^2}{2m_e} + V_i \right) + \mu_B(\vec{L} + g\vec{S}) \cdot \vec{B} + \frac{e^2}{8m_e} \sum_i (\vec{B} \times \vec{r}_i)^2$$

Partition function

Free energy

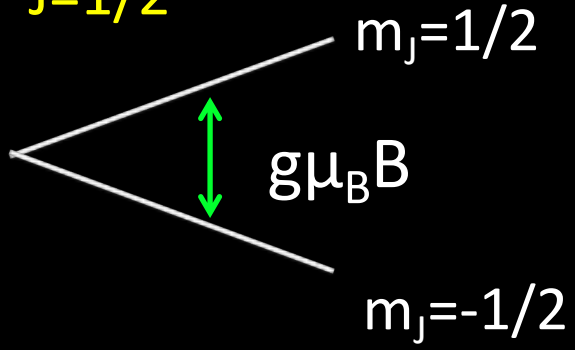
Magnetization

$$Z = e^{\mu_B B/k_B T} + e^{-\mu_B B/k_B T}$$

$$F = -k_B T \ln Z$$

$$M = -\left(\frac{\partial F}{\partial B} \right)_T$$

J=1/2



Magnetic susceptibility

Curie's Law

$$\chi = \frac{\partial M}{\partial H} \propto \frac{1}{T}$$

In 2nd order perturbation theory there is another contribution to the paramagnetic susceptibility (van Vleck). Relevant when J=0. Small and independent of T.

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An atom in a magnetic field (non-interacting moments)

$$H = \sum_{i=1}^{Z} \left(\frac{[\vec{p}_i + e\vec{A}(\vec{r}_i)]^2}{2m_e} + V_i \right) + g\mu_B \vec{B} \cdot \vec{S} =$$

$$\sum_i \left(\frac{p_i^2}{2m_e} + V_i \right) + \mu_B (\vec{L} + g\vec{S}) \cdot \vec{B} + \frac{e^2}{8m_e} \sum_i (\vec{B} \times \vec{r}_i)^2$$

Diamagnetic term. $\chi < 0$

- Orbital effect
- Usually weak: relevant when there are no unpaired electrons.

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Diamagnetic susceptibility

$$\sum_i \left(\frac{p_i^2}{2m_e} + V_i \right) + \mu_B(\vec{L} + g\vec{S}) \cdot \vec{B} + \frac{e^2}{8m_e} \sum_i (\vec{B} \times \vec{r}_i)^2$$

Apply B_z. For a spherically symmetric atom

$$\Delta E_0 = \frac{e^2 B^2}{8m_e} \sum_{i=1}^{Z} \langle 0|(x_i^2 + y_i^2)|0\rangle = \frac{e^2 B^2}{12m_e} \sum_{i=1}^{Z} \langle 0|r_i^2|0\rangle$$

$$M = -\frac{\partial F}{\partial B} = -\frac{N}{V}\frac{\partial \Delta E_0}{\partial B} = -\frac{Ne^2 B}{6m_e V} \sum_{i=1}^{Z} \langle r_i^2 \rangle$$

$$\chi \propto -Z_{\text{eff}} r^2$$

- r is the ionic radius
- Independent of T

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Magnetic order

Now let the magnetic moments interact…

Broken symmetry: rotational symmetry

But note: there can be a magnetocrystalline anisotropy (easy axes/hard axes), originated by spin-orbit coupling, that would reduce the rotational symmetry.

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Magnetic order

Now let the magnetic moments interact…

Given a pair of magnetic moments, they can interact ferromagnetically (FM) or antiferromagnetically (AF).

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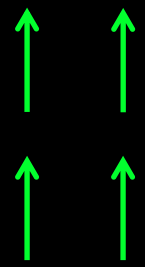
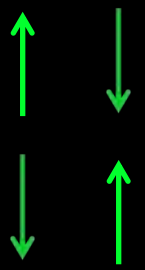
Magnetic order

Different orders

Ferromagnetism FM

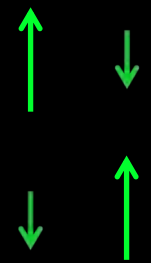


Antiferromagnetism AF

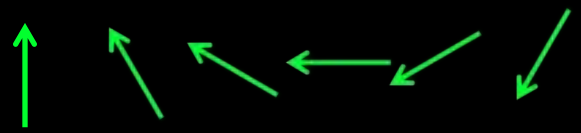


Néel order

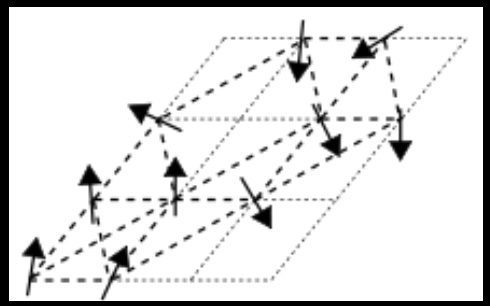
Ferrimagnetism



Helical (J_1, J_2)

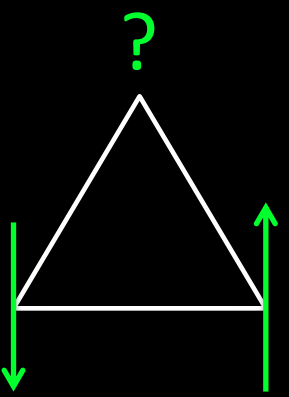


Spin glass



Frustration

(non-bipartite lattice)



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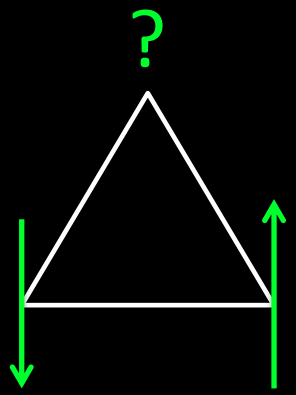
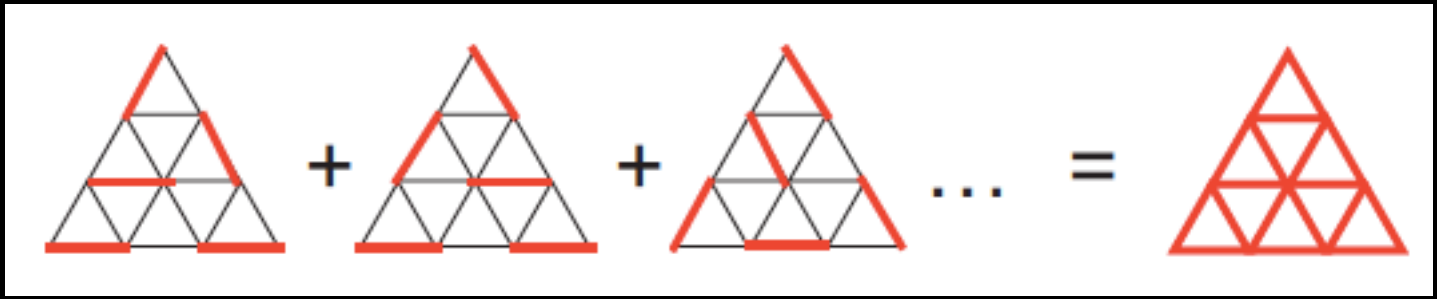
Frustration



Anderson proposed quantum spin-liquid (resonating valence bond)

Pairs of spins correlated in singlets with no long range magnetic order and no spontaneously broken symmetry.



Materials Research Bulleting 8, 153 (1973)

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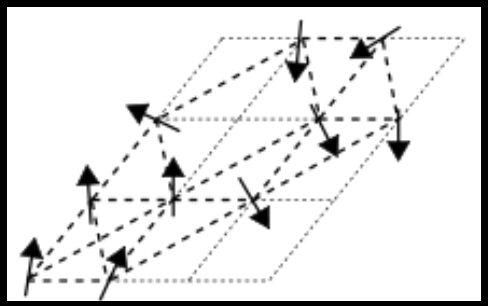
Spin glasses

Due to randomness:

- Site randomness
- Bond randomness (between 2 different magnetic ions which are distributed randomly)
- Random magnetic anisotropies in amorphous materials.

Cooperative freezing transition:
the system freezes in one of its many possible ground states



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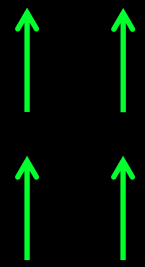
Magnetic order

Order parameter

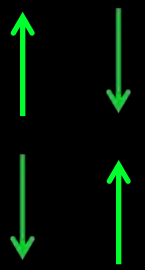
Ferromagnetism FM



Magnetization

$M^z = \lim_{H\to 0}\langle S^z\rangle$

Antiferromagnetism AF



Staggered magnetization

$M_{st}=\langle\Sigma_A S^z\rangle-\langle\Sigma_B S^z\rangle$

Sublattices A,B

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Magnetic order

Order parameter

Ferromagnetism FM

Magnetization

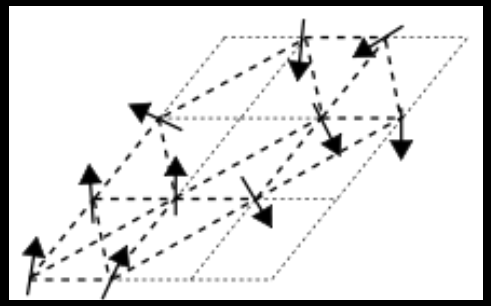
$M^z = \lim_{H\to 0} \langle S^z \rangle$

Antiferromagnetism AF

Staggered magnetization

$M_{st} = \langle \Sigma_A S^z \rangle - \langle \Sigma_B S^z \rangle$

Spin glass



$$q = \lim_{t\to\infty} \left\langle \left\langle S_i(0) S_i(t) \right\rangle_T \right\rangle_C$$

(freezing)

Order parameter → 0 at phase transitions

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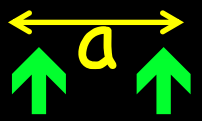
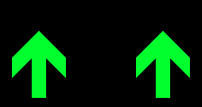
The different orders can be characterized by a wave-vector

FM Q=(0,0)





AF Q=(π/a,π/a)

Q=π/2a

Q=π/4a

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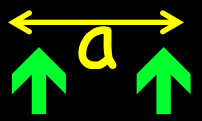
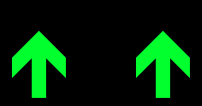
The different orders can be characterized by a wave-vector

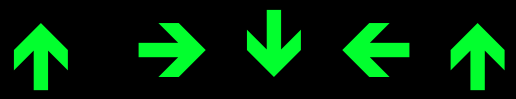
FM Q=(0,0)



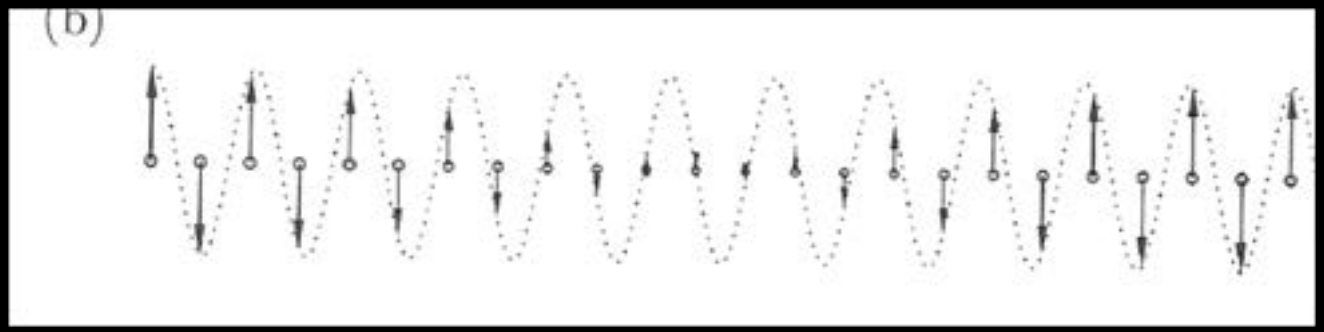
AF Q=(π/a,π/a)



Q=π/2a



Q can be incommensurate with the lattice



Blundell's book

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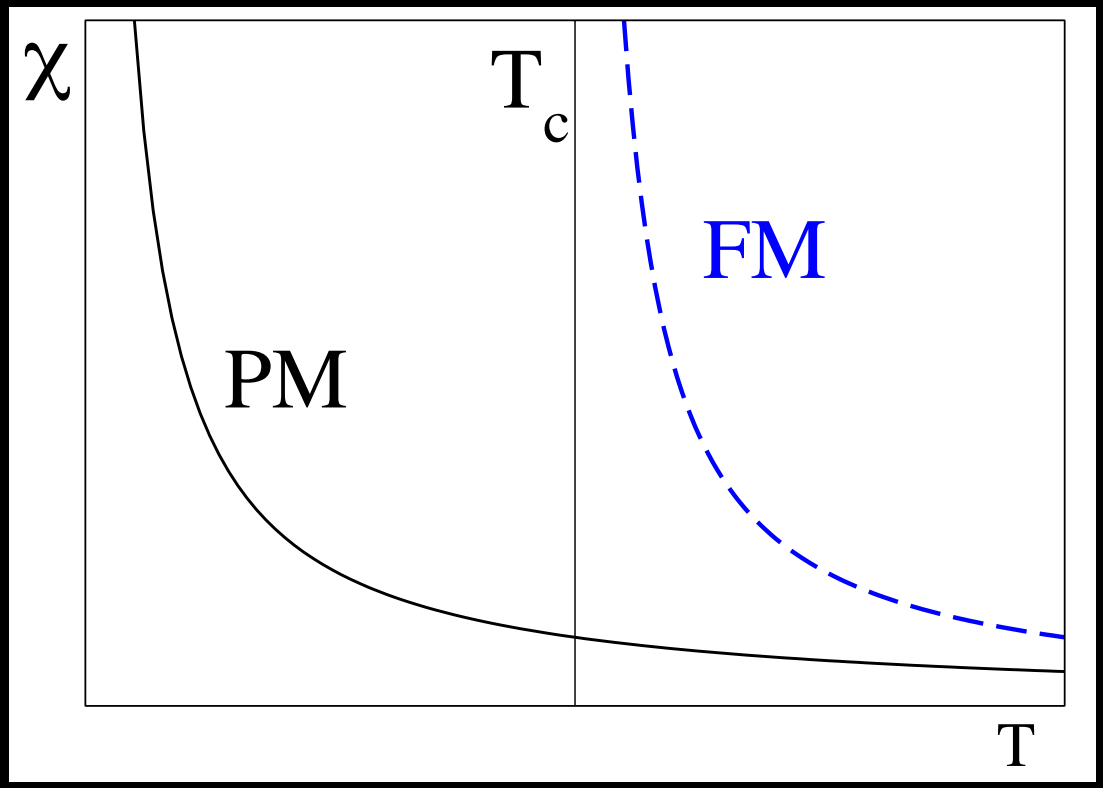
Susceptibility: FM

In mean field, the magnetization of a FM system produces an effective molecular field $B_{mf}=\lambda M$ (typically much larger than any applied field)

For T>Tc

$$\chi \propto \frac{1}{T} \rightarrow \frac{1}{T - T_c}$$

Curie-Weiss law



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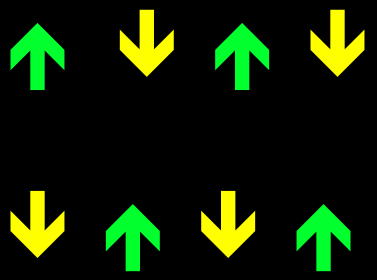
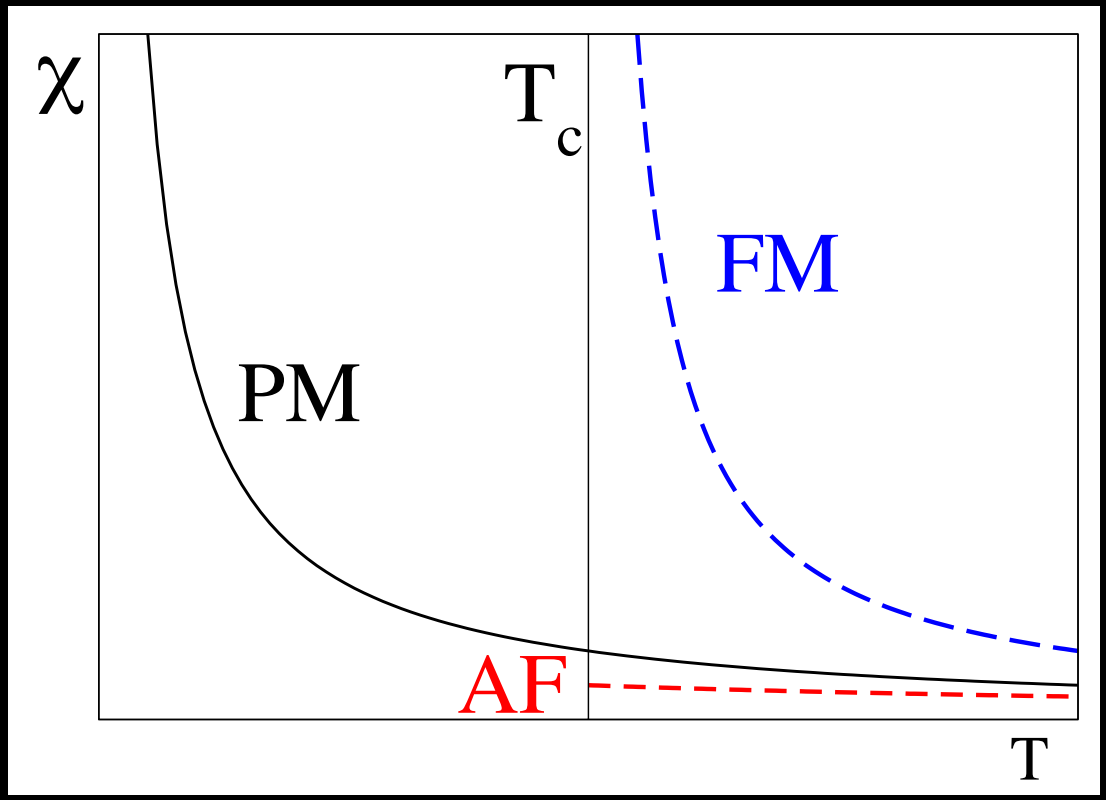
Susceptibility: AF

For an AF there is a different molecular field for each sublattice, B_+ and B_-

For $T>T_N$

$$\chi \propto \frac{1}{T+T_N}$$





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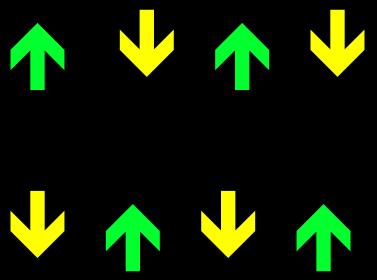
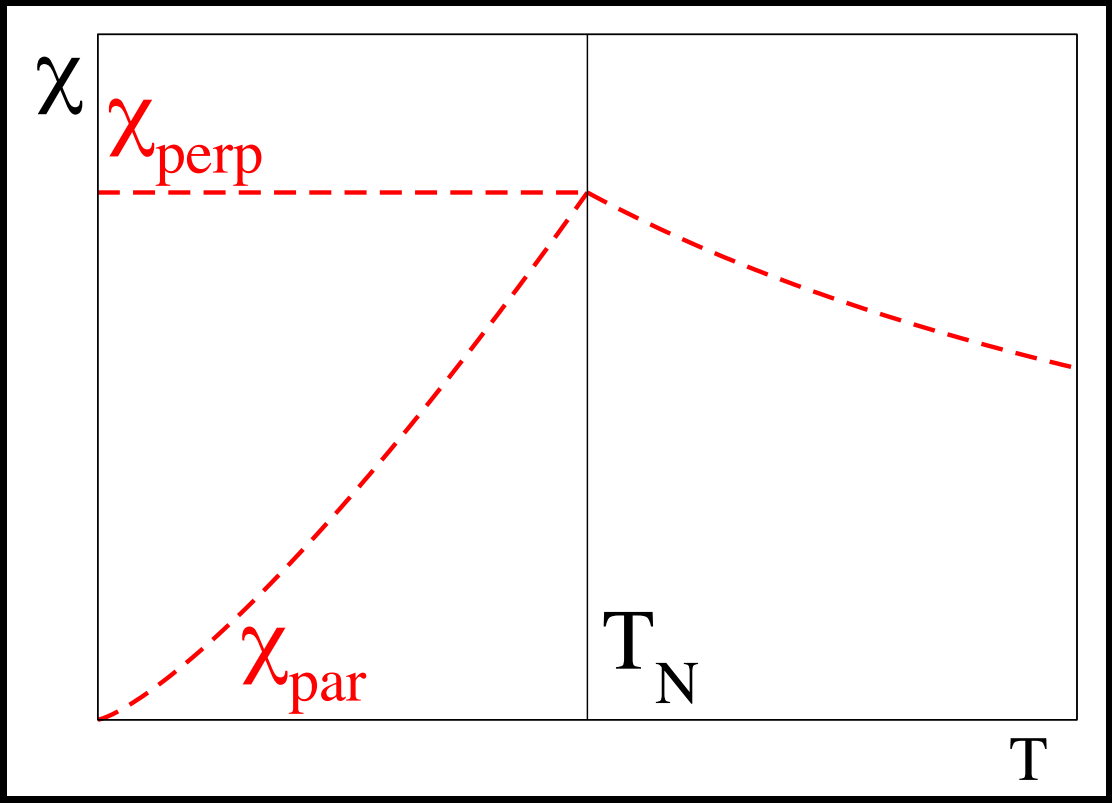
Susceptibility: AF

For an AF there is a different molecular field for each sublattice, B_+ and B_-

For $T<T_N$
χ depends on the direction of the applied field.





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Outline

- Free magnetic ions
- Environment
- Magnetic order and susceptibility
- Interactions
  - Exchange between localized moments
  - Indirect exchange through itinerant electrons
  - Magnetism in metals
- Excitations

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Interactions

Different mechanisms

1. Localized moments. Heisenberg model.
2. Localized moments + itinerant electrons.
3. Itinerant electrons. Fermi surface instability.

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Interaction between localized moments

Magnetic dipolar interactions too weak to explain typical magnetic critical temperatures

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Interaction between localized moments

EXCHANGE

Heisenberg model $\Sigma_{ij}\ J\ \mathbf{S}_i\ \mathbf{S}_j$

- J is the exchange parameter.
- J>0, AF. J<0, FM.
- Strong interaction: it arises from Coulomb interactions between electrons.
- Intra-atomic exchange: Hund's coupling J_H

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Interaction between localized moments

Hamiltonian: electrons in a lattice (bands)

+ electron-electron interaction

$$H = T + V(r) + \frac{e^2}{r_{12}}$$

Heisenberg model

$$H = J \sum_{i,j} \mathbf{S}_i \mathbf{S}_j$$

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Direct exchange (or potential exchange)

- Basic idea: electron-electron repulsion energy is minimized when two electrons have the same spin (due to Pauli exclusion principle the electrons are as further away as possible).
- Therefore, direct exchange is ferromagnetic.
- Between orthogonal orbitals.
- Hund's coupling is an onsite direct exchange.
- Heisenberg 1928.

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Direct exchange

$$\iint \Psi^*(r_1)\Psi^*(r_2)\frac{e^2}{r_{12}}\Psi(r_2)\Psi(r_1)\,d\tau_1 d\tau_2$$

Expand $\Psi(r)$ in terms of orthogonal wave functions localized at the magnetic ions $\phi_n(r)$. No double occupancy is allowed.

Two kinds of terms arise:

$C_{n,n'}$ Coulomb int. between electrons at n and n′ ions

$$\iint \phi_n^*(r_1)\phi_{n'}^*(r_2)\frac{e^2}{r_{12}}\phi_{n'}(r_2)\phi_n(r_1)\,d\tau_1 d\tau_2$$

$J_{n,n'}$ Exchange int. Due to Fermi statistics

$$-\iint \phi_n^*(r_1)\phi_{n'}^*(r_2)\frac{e^2}{r_{12}}\phi_n(r_2)\phi_{n'}(r_1)\,d\tau_1 d\tau_2$$

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Direct exchange

In second quantization $J_{n,n'}$

$$\sum_{s,s'} a^{+}_{ns} a_{ns'} a^{+}_{n's'} a_{n's}$$

$$s_z = \frac{1}{2}(a^{+}_{\uparrow} a_{\uparrow} - a^{+}_{\downarrow} a_{\downarrow})$$

$$s_x + i s_y = a^{+}_{\uparrow} a_{\downarrow} \; ; \; s_x - i s_y = a^{+}_{\downarrow} a_{\uparrow}$$

Heisenberg:

$$-J_{n,n'}\left(\frac{1}{2} + 2 s_n \cdot s_{n'}\right)$$

$J_{n,n'}$ is always +ve: Ferromagnetism

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Direct exchange

- But note: The same mechanism gives antiferromagnetism if the orbitals involved are non-orthogonal !
- The simplest example: The H_2 molecule ground state is a spin-singlet (Wigner's theorem for the 2-electron problem: the ground state does not have a node)

$$H = T_1 - \frac{e^2}{r_{a1}} + T_2 - \frac{e^2}{r_{b2}} - \frac{e^2}{r_{a2}} - \frac{e^2}{r_{b1}} + \frac{e^2}{r_{12}} + \frac{e^2}{r_{ab}}$$

The exchange is the difference between the energy of the spin-singlet and the spin-triplet

$$\text{Exchange} = 2\frac{S^2 C_{ab} - J_{ab}}{1 - S^4}$$

S here is the overlap!
S=0 for orthogonal orbitals

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Direct exchange

- But note: The same mechanism gives antiferromagnetism if the orbitals involved are non-orthogonal !
- The simplest example: The H_2 molecule ground state is a spin-singlet (Wigner's theorem for the 2-electron problem: the ground state does not have a node)
- Wigner's theorem does not apply to our magnetic ions because a shell in a $3d^2$ configuration is not a 2-electron problem!

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Kinetic exchange

- Basic idea: due to virtual electron transfers. Consider hopping as a perturbation and go to second order perturbation theory.
- Kramers 1934. Formalized by Anderson 1950.
- Kinetic exchange is antiferromagnetic.
- Start from single band Hubbard Hamiltonian (on-site interactions) with U>>t. (The strong interacting limit of the Hubbard model is an AF Heisenberg model)

$$H = -\sum_{ij\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) + U\sum_{j} n_{j\uparrow}n_{j\downarrow}$$

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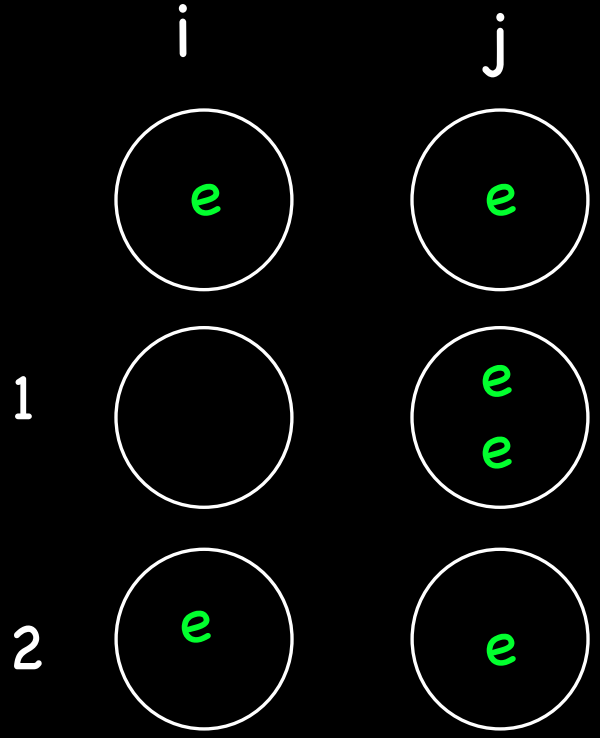
Kinetic exchange

- Treat kinetic energy in second-order perturbation (one band model)



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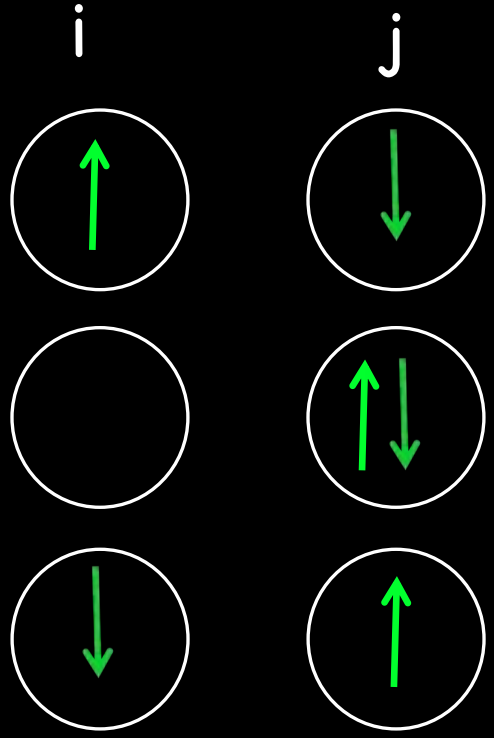
Kinetic exchange

- Treat kinetic energy in second-order perturbation (one band model)



For this process to take place you need antiparallel moments (Pauli principle)

$$\Delta E_2 = -\sum_{\substack{i,j \\ \sigma,\sigma'}} \frac{|t_{ij}|^2}{U} a^+_{i\sigma} a_{j\sigma} a^+_{j\sigma'} a_{i\sigma'}$$

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Kinetic exchange

$$\Delta E_2 = -\sum_{\substack{i,j \\ \sigma,\sigma'}} \frac{|t_{ij}|^2}{U} a^+_{i\sigma} a_{j\sigma} a^+_{j\sigma'} a_{i\sigma'}$$

$$s_z = \frac{1}{2}(a^+_\uparrow a_\uparrow - a^+_\downarrow a_\downarrow)$$

$$s_x + i s_y = a^+_\uparrow a_\downarrow \; ; \; s_x - i s_y = a^+_\downarrow a_\uparrow$$

Heisenberg:

$$\Delta E_2 = \sum_{\substack{i,j \\ \sigma,\sigma'}} \frac{|t_{ij}|^2}{U} \left(-\frac{1}{2} + 2 s_i \cdot s_j \right)$$

Antiferromagnetic

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Hubbard model

$$H = -\sum_{ij\sigma} t_{ij}(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}) + U\sum_{j} n_{j\uparrow}n_{j\downarrow}$$

U>>t

$$J = 4|t|^2/U$$

Heisenberg model

At half-filling
(1 electron per site)

$$J\sum_{i,j}\vec{S}_i\vec{S}_j$$

t-J model

Away from
half-filling

$$-\sum_{ij\sigma} t_{ij}(b^{+}_{i\sigma}b_{j\sigma} + b^{+}_{j\sigma}b_{i\sigma}) + J\sum_{ij}\vec{S}_i\vec{S}_j$$

Hopping only between an empty and a filled site.

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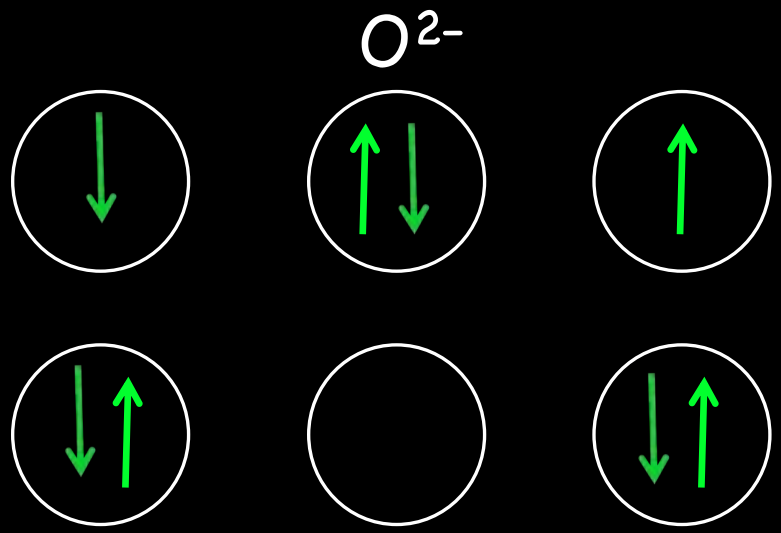
Superexchange

Exchange mediated by an anion: $E_{direct}+E_{kin}$.



Note that we are assuming half-filling (1 electron per site)

From this, SE is antiferromagnetic but…

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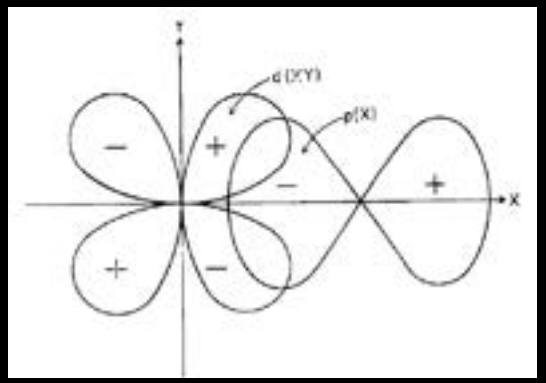
Goodenough-Kanamori rule

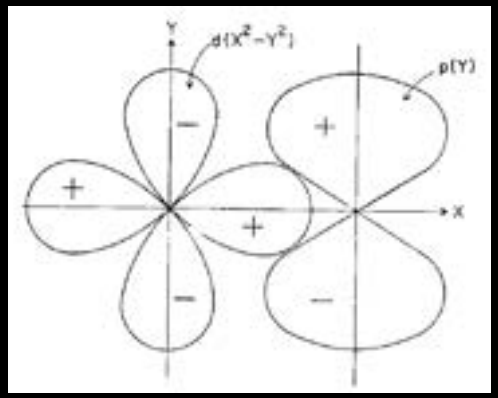
Superexchange is AF when the virtual hopping involves overlapping half-filled orbitals while it can be FM when:

- overlap is zero: $t_{ij}=0$

(note that t_{ij} depends on the orientation of the M-O-M bonds)

$$E_{kin} = -\sum_{\substack{i,j \\ \sigma,\sigma'}} \frac{|t_{ij}|^2}{U} a^+_{i\sigma} a_{j\sigma} a^+_{j\sigma'} a_{i\sigma'}$$





Kanamori,
J. Phys. Chem. Solids 10, 87 (1959)
Goodenough, PR 100, 564 (1955)

http://www.scholarpedia.org/article/Goodenough-Kanamori_rule

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Goodenough-Kanamori rule

Superexchange is AF when the virtual hopping involves overlapping half-filled orbitals while it can be FM when:

- overlap is zero: $t_{ij}=0$
- it involves transfers between a half-filled and an empty orbital. Kinetic exchange can be FM because it is not restricted by Pauli principle. (Related to double exchange – see later)

http://www.scholarpedia.org/article/Goodenough-Kanamori_rule

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Goodenough-Kanamori rule

Superexchange is AF when the virtual hopping involves overlapping half-filled orbitals while it can be FM when:

- overlap is zero: $t_{ij}=0$
- it involves transfers between a half-filled and an empty orbital.
- **in multiorbital systems:*

* Generalization

http://www.scholarpedia.org/article/Goodenough-Kanamori_rule

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For multiorbital systems

$$H = H_0 + \bar{U} \sum_{i,\ell} n_{i\ell\uparrow} n_{i\ell\downarrow} + \bar{U}' \sum_{i,\ell'<\ell} n_{i\ell} n_{i\ell'}$$
$$+ \bar{J} \sum_{i,\ell'<\ell} \sum_{\sigma,\sigma'} c^{\dagger}_{i\ell\sigma} c^{\dagger}_{i\ell'\sigma'} c_{i\ell\sigma'} c_{i\ell'\sigma}$$
$$+ \bar{J}' \sum_{i,\ell'\neq\ell} c^{\dagger}_{i\ell\uparrow} c^{\dagger}_{i\ell\downarrow} c_{i\ell'\downarrow} c_{i\ell'\uparrow}$$

Spin rotational invariance:

$U' = U - 2J_H$ *$J' = J_H$*

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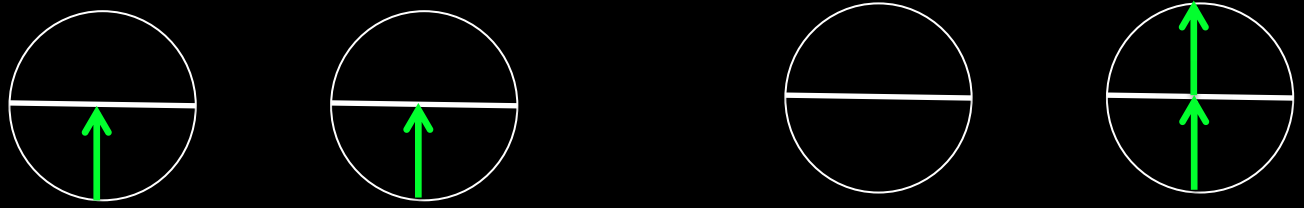
Goodenough-Kanamori rule

Superexchange is AF when the virtual hopping involves overlapping half-filled orbitals while it can be FM when:

- overlap is zero: $t_{ij}=0$
- it involves transfers between a half-filled and an empty orbital.
- **in multiorbital systems: the onsite interaction for electrons in different orbitals is $U' - J_H$ (and $U'=U-2J_H$),* $J_{kin} = -t^2/(U-3J_H)$



* Generalization

http://www.scholarpedia.org/article/Goodenough-Kanamori_rule

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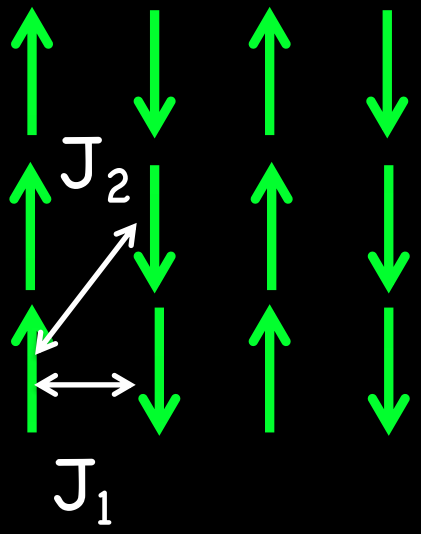
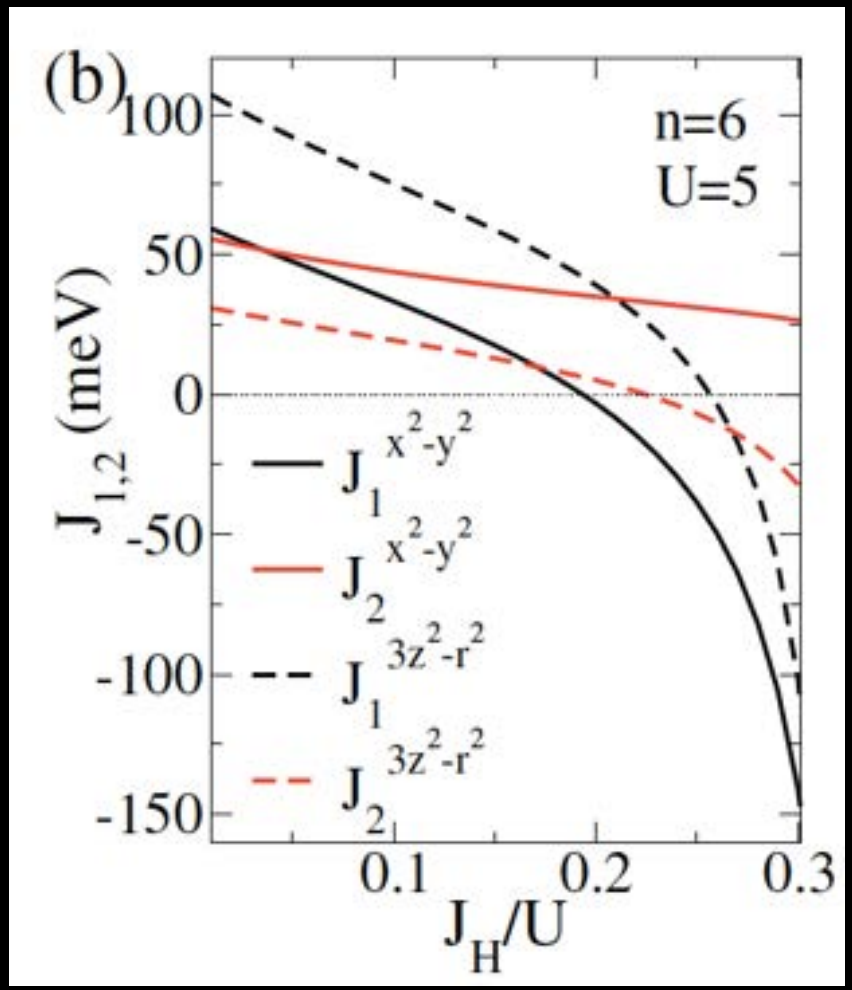
For multiorbital iron superconductors, the sign of exchange depends on the parameters (J_H, U, crystal field. The anisotropies in the hoppings are included).

$J_2 > J_1/2$





Physical Review B 86, 104514 (2012).

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Goodenough-Kanamori rule: consequences

- Superexchange can be of different strengths and signs in the different directions of the crystal. The crystal symmetry and the orbitals symmetry has to be taken into account (Slater-Koster).

- Associated to orbital order (competing sometimes with Jahn-Teller distortions)

Millis, PRB 55, 6405 (1997).

Slater and Koster, Phys. Rev. 94, 1498 (1954)

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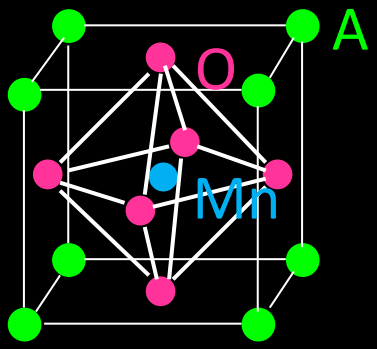
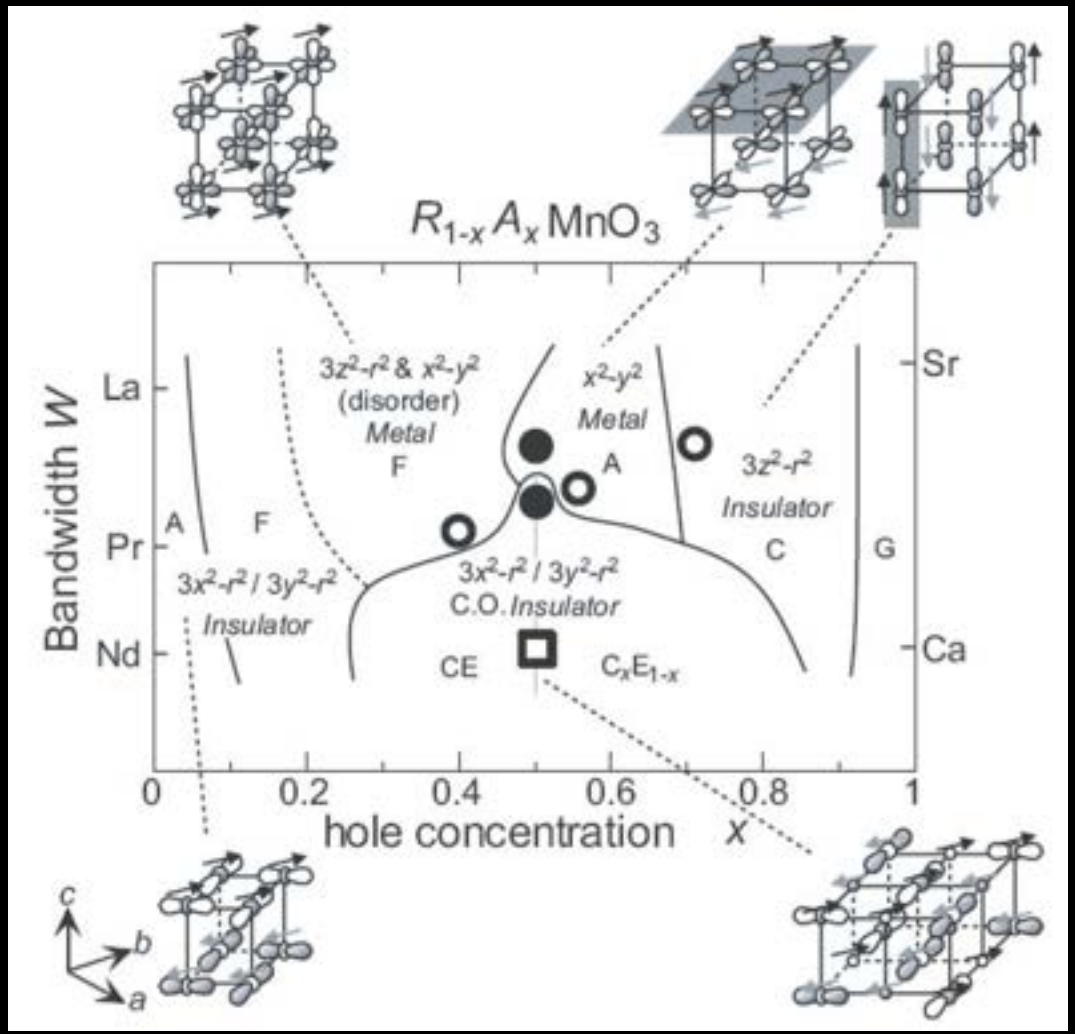
Example: Manganites

Interplay of spin, orbital and lattice

Kanamori, J. Phys. Chem. Solids 10, 87 (1959)
Goodenough, PR 100, 564 (1955)





Tokura, Rep. Prog. Phys. 69, 797 (2006)

Millis, PRB 55, 6405 (1997).

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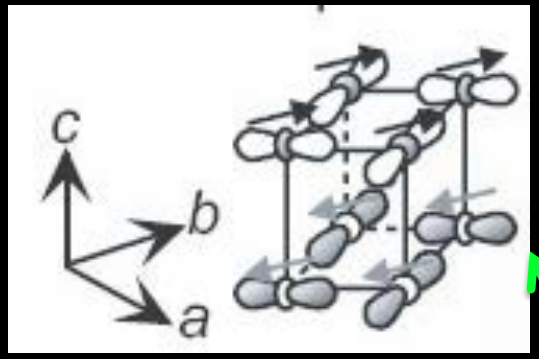
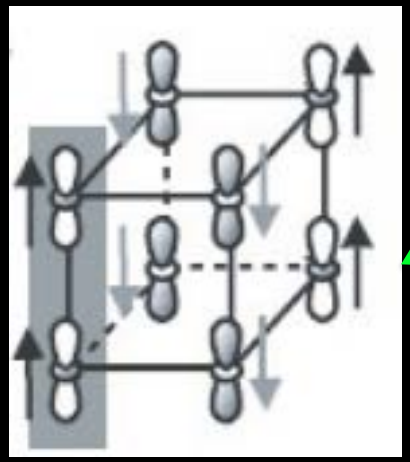
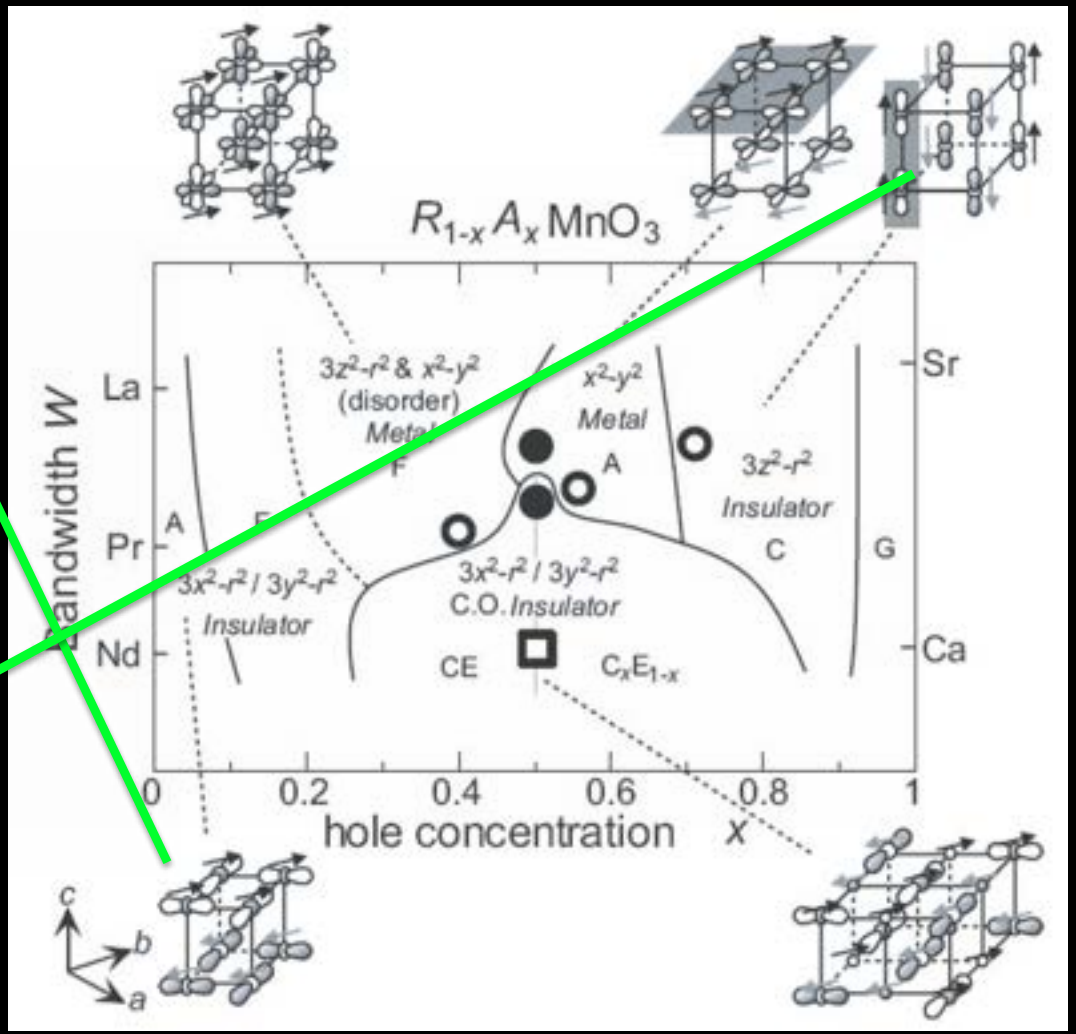


Type A: Q=(0,0,π)



Type C: Q=(π, π,0)



Tokura, Rep. Prog. Phys. 69, 797 (2006)

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Anisotropic exchange
(for d-orbitals)

It's a kind of superexchange in which the excited intermediate state is not due to an interceding anion but to an excited state produced by spin-orbit interaction in one of the magnetic ions.

$$H' = \lambda(\mathbf{L}_1 \cdot \mathbf{S}_1) + \lambda(\mathbf{L}_2 \cdot \mathbf{S}_2) + V_{exch}$$

Dzyaloshinskii-Moriya $H_{DM} = \mathbf{D} \cdot (\mathbf{S}_1 \times \mathbf{S}_2)$

D=0 with inversion symmetry between the 2 ions

D direction depends on symmetry

Causes AF spins to cant by a small angle: weak ferromagnetism. Examples: α-Fe_2O_3, $MnCoO_3$, $RFeO_3$ (R: rare-earth).

K. Yosida's book.

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Interactions

Different mechanisms

1. Localized moments. Heisenberg model.
2. Localized moments + itinerant electrons.
3. Itinerant electrons. Fermi surface instability.

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Itinerant electrons coupled to localized moments

- Kondo model (coupling to magnetic impurities)

$$H = -\sum_{i,j,\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) - J_{local}\mathbf{S}\cdot\mathbf{s}$$

- Kondo Lattice

$$H = -\sum_{i,j,\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) - J_{local}\sum_{i}\mathbf{S}_i\cdot\mathbf{s}_i$$

For f-electrons S→J

See Kondo regime in Ramon Aguado's lectures

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Itinerant electrons coupled to localized moments

- Kondo model (coupling to magnetic impurities)

$$H = -\sum_{i,j,\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) - J_{local}\mathbf{S}\cdot\mathbf{s}$$

Basic idea: the local exchange with an impurity polarizes the surrounding Fermi sea which carries this information to other magnetic impurities.

How effective is this process of the magnetic polarization of the Fermi sea? → susceptibility

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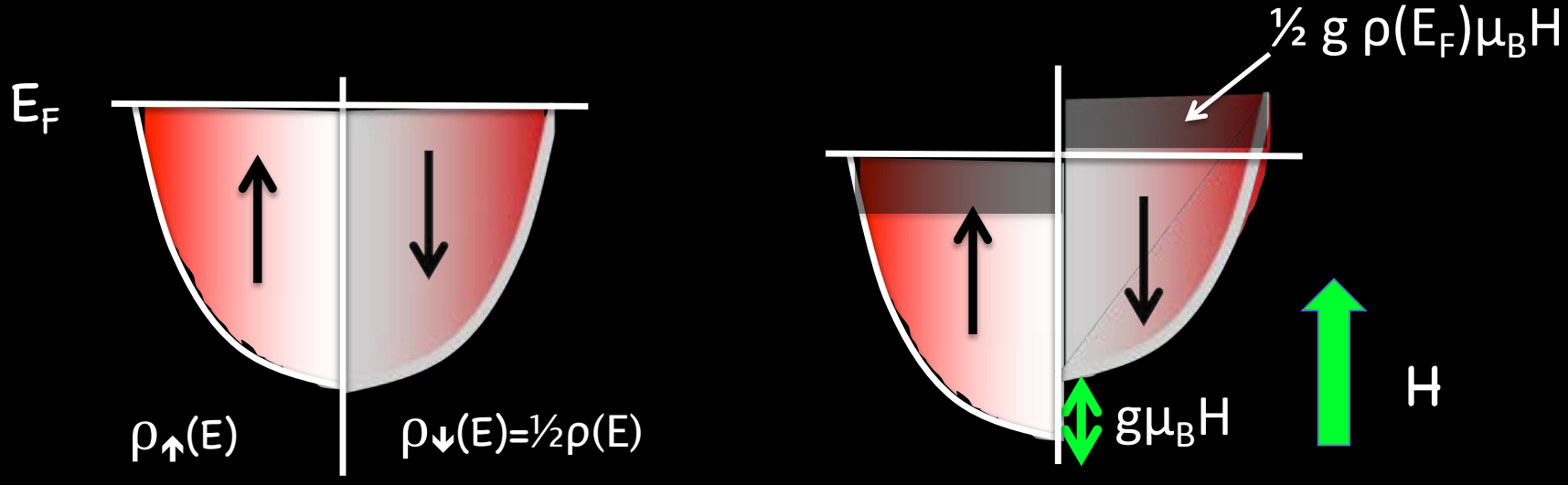
Paramagnetic susceptibility of conduction electrons

In a uniform magnetic field



$M=\mu_B(n_\uparrow - n_\downarrow)$

$$\chi_{\text{Pauli}} = \frac{1}{2} g^2 \mu_B^2 \rho(E_F)$$

Pauli PM only affects electrons close to E_F. Constant with T.

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PM susceptibility in a non-uniform magnetic field

$$H(\mathbf{r}) = \sum_q H_q e^{-i\mathbf{q}\cdot\mathbf{r}}$$

Consider the perturbative effect of H_q on the electron spin

Within first order perturbation theory on a plane wave state

$$\psi_{\mathbf{k}\pm}(\mathbf{r}) = \frac{1}{\sqrt{V}}\left(e^{i\mathbf{k}\cdot\mathbf{r}} \pm \frac{g\mu_0\mu_B\mathbf{H}_\mathbf{q}}{4}\left[\frac{e^{i(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}}{E_{\mathbf{k}+\mathbf{q}} - E_\mathbf{k}} + \frac{e^{i(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}}{E_{\mathbf{k}-\mathbf{q}} - E_\mathbf{k}}\right]\right)|\pm\rangle$$

$M(r)=\mu_B(|\Psi_{k+}(r)|^2-|\Psi_{k-}(r)|^2)$

↓

M_q

$$\chi_q = \chi_{\text{Pauli}} f\left(\frac{q}{2k_F}\right)$$

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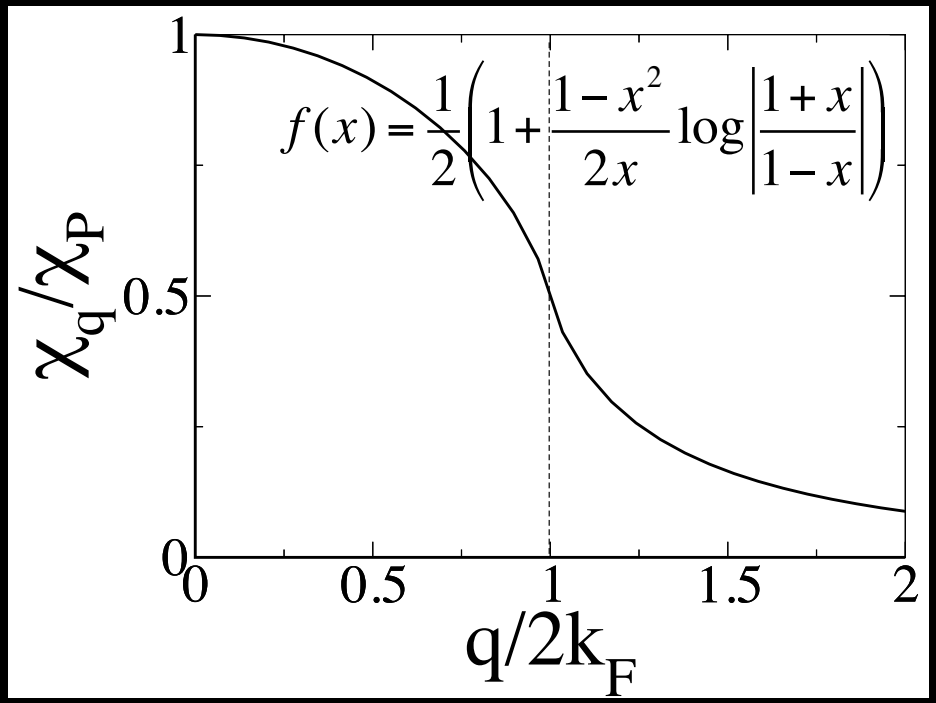
PM susceptibility in a non-uniform magnetic field

$$H(\mathbf{r}) = \sum_q H_q e^{-i\mathbf{q}\cdot\mathbf{r}}$$

Consider the perturbative effect of H_q on the electron spin



(3dim)
Linhard function

(in momentum space)

$$\chi_q = \chi_{\text{Pauli}} f\left(\frac{q}{2k_F}\right)$$

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Itinerant electrons coupled to localized moments

- Kondo model (coupling to magnetic impurities)

$$H = -\sum_{i,j,\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) - J_{local}\mathbf{S}\cdot\mathbf{s}$$

Basic idea: the local exchange with an impurity polarizes the surrounding Fermi sea which carries this information to other magnetic impurities.

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RKKY exchange
Rudderman-Kittel-Kasuya-Yosida

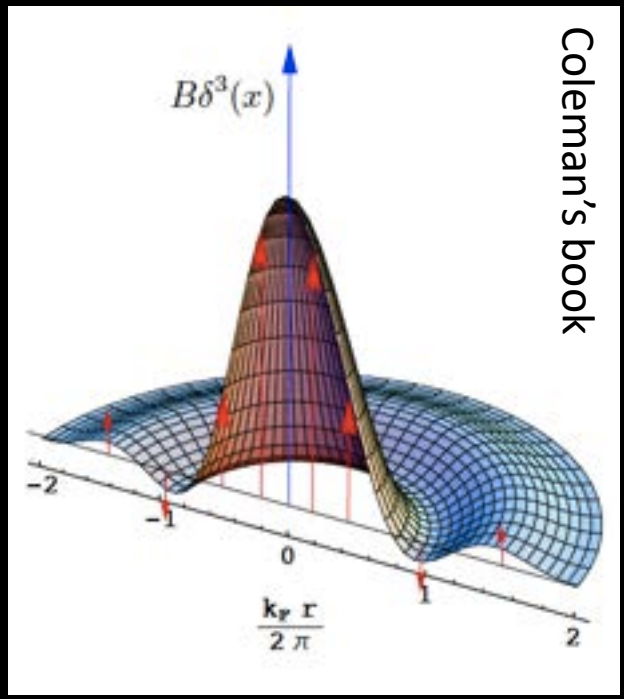
A magnetic impurity with local exchange amounts to having a local external field: H(r) ~ δ(r)
J_{local} can be J_H or s-d or s-f exchange.

$$H_q = \frac{2J_{local}}{Ng\mu_B} S_z$$

$$\chi_q = \chi_{\text{Pauli}} f\left(\frac{q}{2k_F}\right)$$

Real space susceptibility:
Friedel oscillations $\lambda = 2\pi/k_F$

$$\chi(\mathbf{r}) = \frac{1}{(2\pi)^3}\int d^3\mathbf{q}\,\chi_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} = \frac{2k_F^3\chi_P}{\pi} F(2k_F r)$$



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RKKY exchange

The conduction electron interacting with the single magnetic impurity suffer a spin polarization that depends on distance

$$|\psi_\uparrow|^2 - |\psi_\downarrow|^2 \propto J_{local} F(2k_F r)$$

Now this polarized cloud interacts with another magnetic impurity

$$J_{RKKY} \propto J_{local}^2 F(2k_F r)$$

(The sign of J_{local} does not matter)

J_{RKKY} oscillates with distance: A local magnetic moment produces a wave-like local perturbation.

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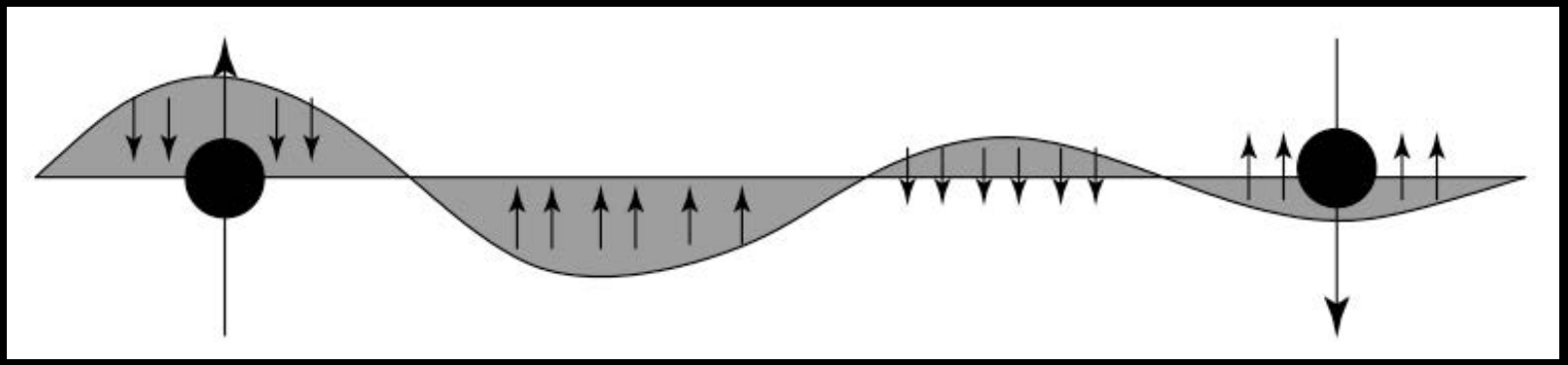
RKKY exchange



$$J_{RKKY} \propto J_{local}^2 F(2k_F r)$$

(The sign of J_{local} does not matter)

J_{RKKY} oscillates with distance: A local magnetic moment produces a wave-like local perturbation.

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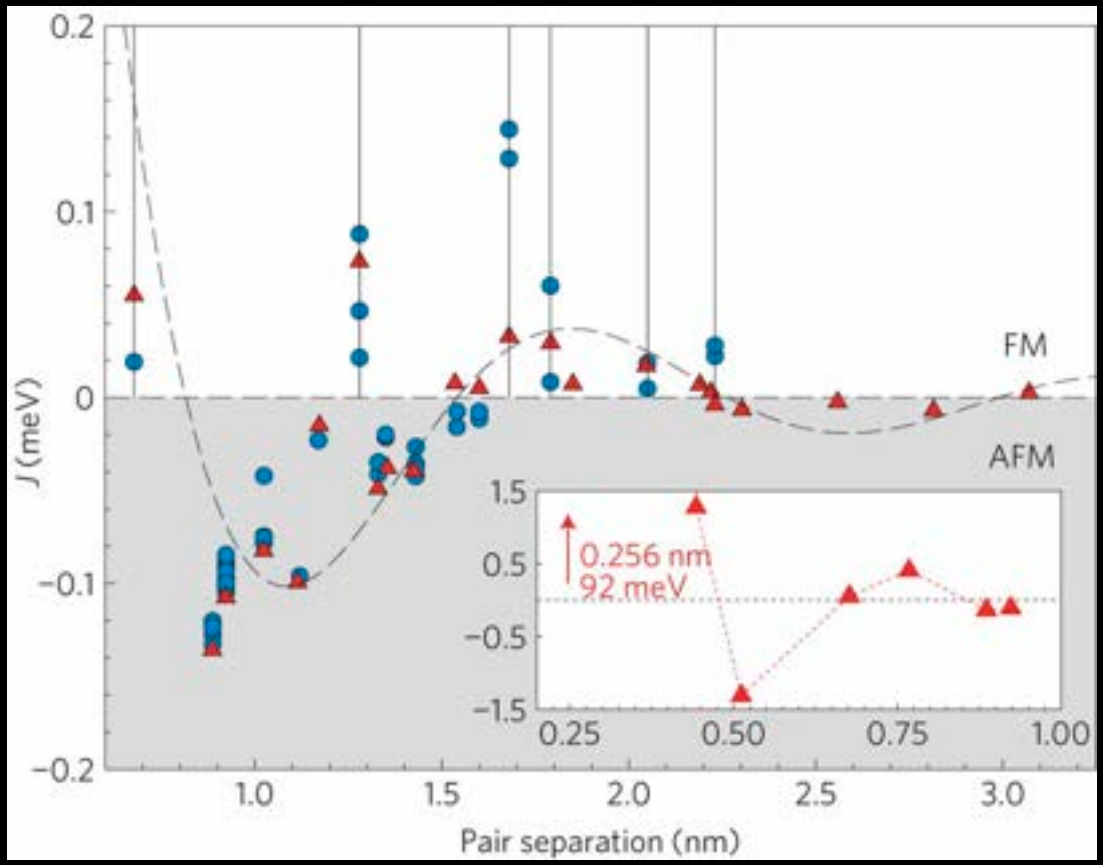
RKKY exchange

Fe atoms on Cu(111)



Nature Physics 8, 497–503 (2012)

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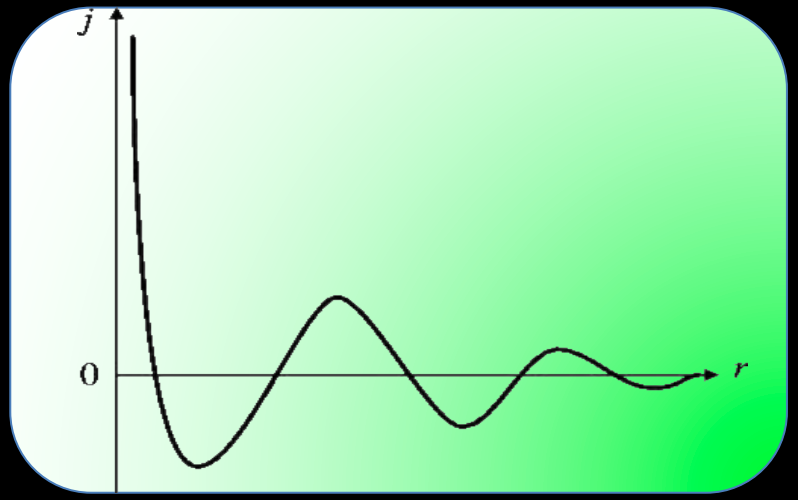
RKKY exchange

Note that if $k_F r$ is small, J_{RKKY} is FM.



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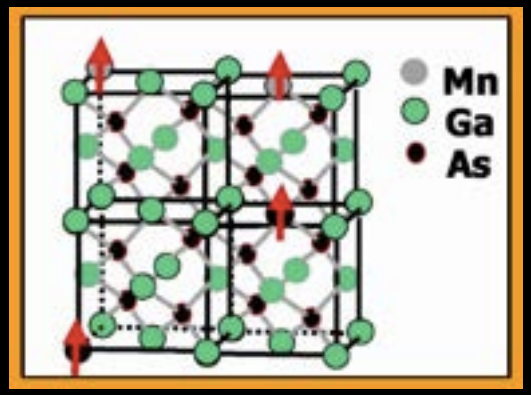
RKKY exchange

- Spin glass in CuMn (Mn is random in Cu lattice).
- FM in diluted magnetic semiconductors, like (Ga,Mn)As or diluted magnetic oxides as $(Ti,Co)O_2$

(Important for spintronics, where you need carriers to be spin polarized).



RKKY competes with Kondo effect (R. Aguado's Lectures)

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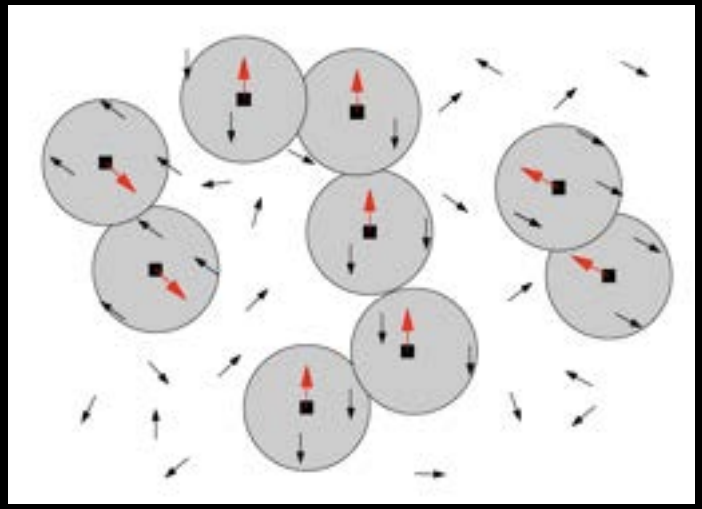
Other effects of local exchange: Bound magnetic polarons

Carriers are bound (not-itinerant!) electrostatically by the Coulomb potential and the spin-polarization is a secondary phenomenon. Polaron: FM cloud.

Proposed for diluted magnetic semiconductors. Percolation → Tc

Due to the local exchange, the size of the bound electron wave-function R_p depends on T as

$$k_B T = |J|(a_0/a_B)^3 Ss \exp(-2R_p/a_B)$$



Annals of Physics 322, 2618 (2007)

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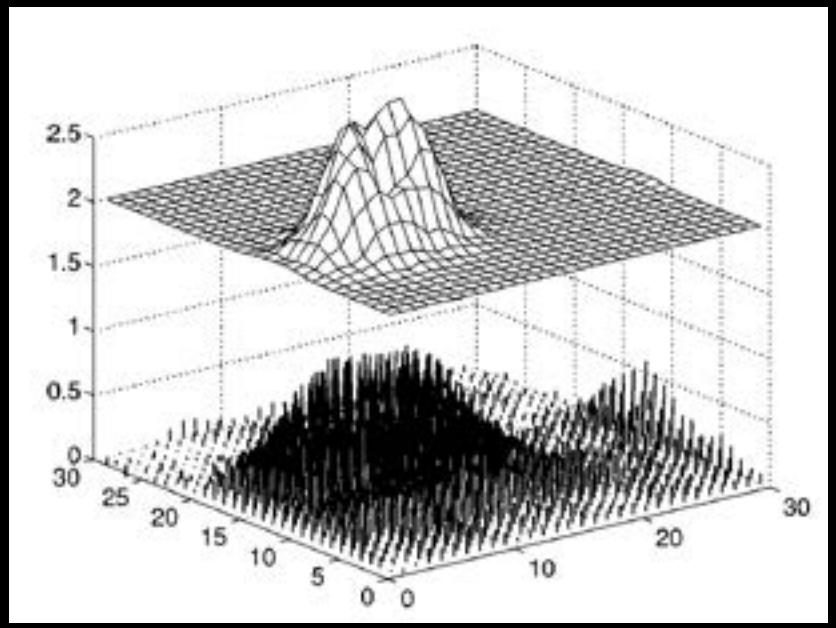
Other effects of local exchange: Free magnetic polarons

Carriers are self-trapped by a FM cloud they have formed themselves in a background of disordered spins (above the FM T_c). Low carrier density is required. Can also form in an AF background

Some pyrochlores

EuB_6



PRB 62, 3368 (2000)

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Double exchange ($J_{local} \rightarrow \infty$ limit of Kondo lattice)

$$\sum_{\alpha,\beta} t^{\alpha\beta} \sum_{i,j,\sigma} c^{\dagger}_{i,\alpha,\sigma} c_{j,\beta,\sigma} + J_H \sum_i S_i s_i \xrightarrow[J_H \rightarrow \infty]{} \sum_{i,j} \sum_{\alpha,\beta} t^{\alpha\beta}_{ij} d^{\dagger}_{i\alpha} d_{j\beta}$$

$J_H \rightarrow \infty$ implies the spin of the conduction electrons is always parallel to the localized spin

This model was proposed for manganites

$A_{1-x}A'_xMn^{3+}_{1-x}Mn^{4+}_xO_3$

C. Zener, Phys. Rev. **82**, 403, (1951)
P. W. Anderson y A. Hasegawa , Phys Rev **100**, 675 (1955)

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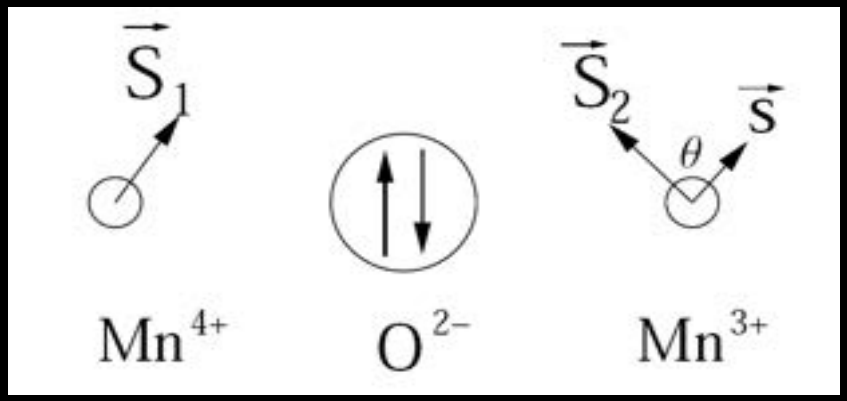
Double exchange

$$\sum_{\alpha,\beta} t^{\alpha\beta} \sum_{i,j,\sigma} c^{\dagger}_{i,\alpha,\sigma} c_{j,\beta,\sigma} + J_H \sum_i S_i s_i \xrightarrow[J_H \to \infty]{} \sum_{i,j} \sum_{\alpha,\beta} t^{\alpha\beta}_{ij} d^{\dagger}_{i\alpha} d_{j\beta}$$

$$t^{\alpha\beta}_{ij} = t^{\alpha\beta} \cos\left(\frac{\theta_{ij}}{2}\right)$$

Note: spinless Hamiltonian



Kinetic exchange with real (not virtual) electron hopping

Promotes FM with metallicity (as observed in manganites)

C. Zener, Phys. Rev. **82**, 403, (1951)
P. W. Anderson y A. Hasegawa , Phys Rev **100**, 675 (1955)

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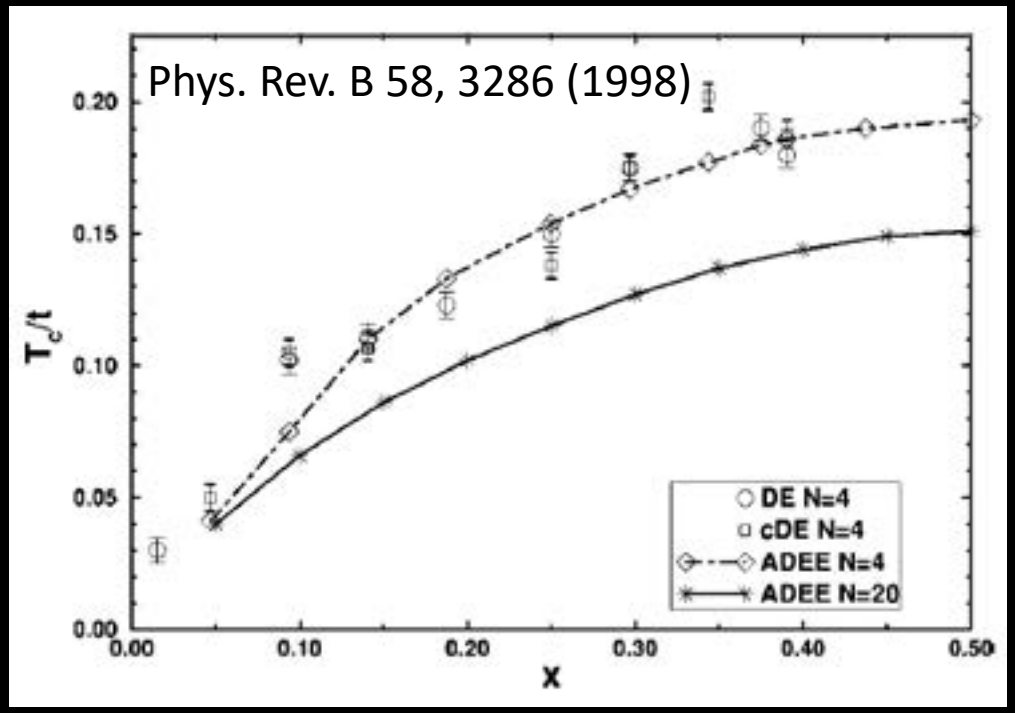
Double exchange

$A_{1-x}A'_xMn^{3+}_{1-x}Mn^{4+}_xO_3$ (x≠0 or 1 → mixed valency)



T_c proportional to number of carriers

(actually, manganites are governed by a much more complex Hamiltonian and DE competes with AF superexchange)

C. Zener, Phys. Rev. **82**, 403, (1951)
P. W. Anderson y A. Hasegawa , Phys Rev **100**, 675 (1955)

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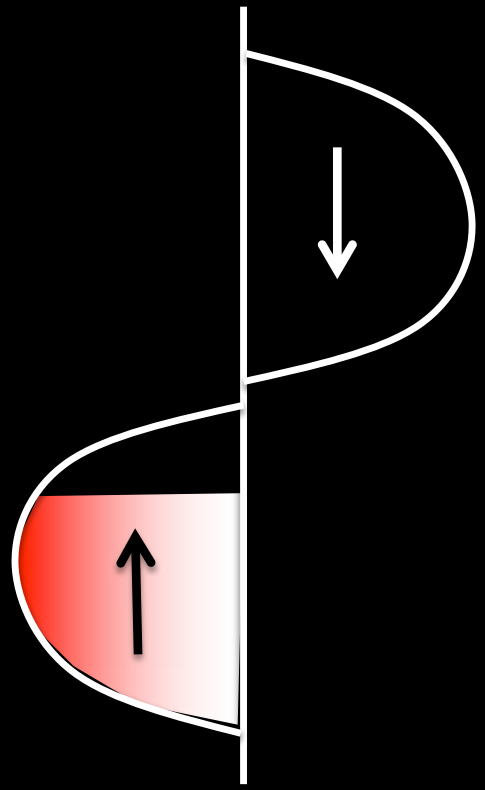
Double exchange

Half-metal: metallic conduction for one spin electrons but insulator for the other spin electrons.

Useful for spintronics.



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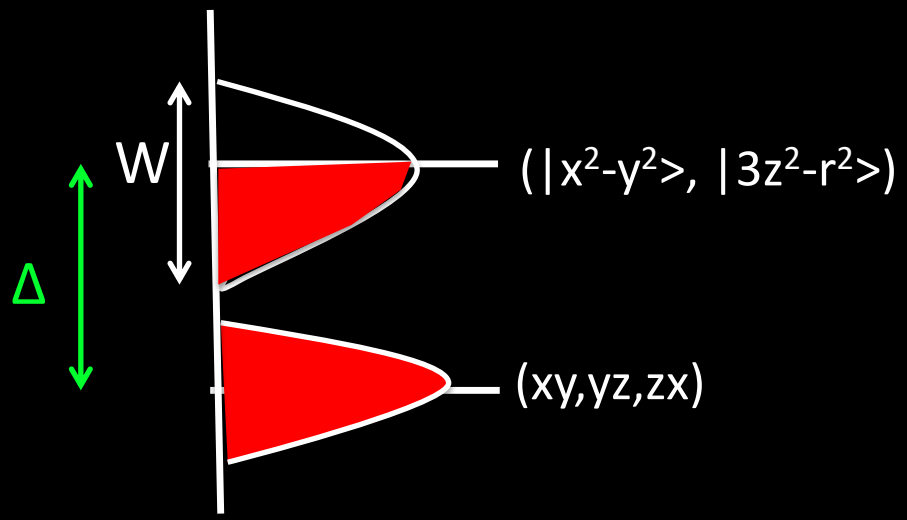
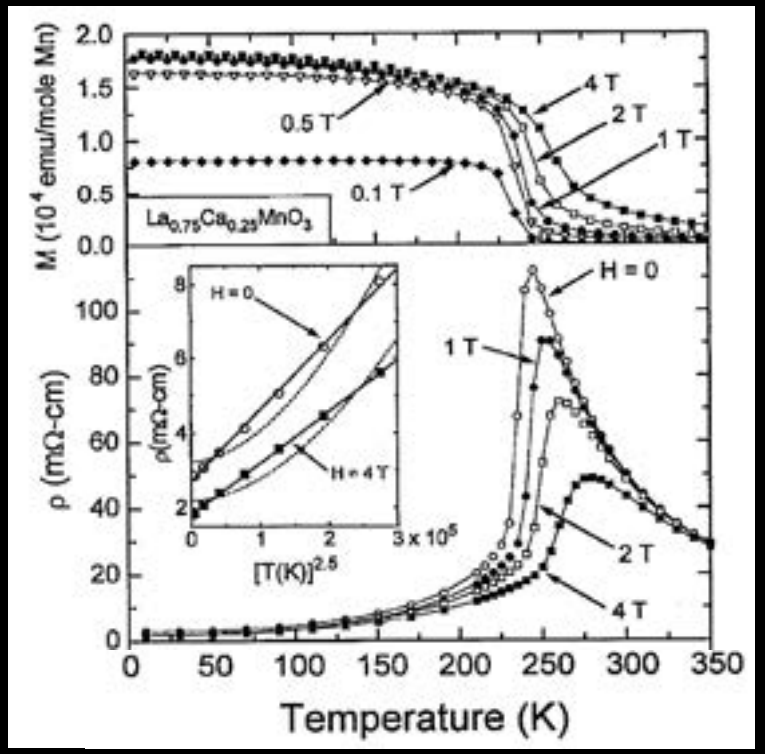
Manganites





PRL 75, 3336 (1995)

- Double exchange among the e_g electrons.
- AF superexchange among the t_{2g} electrons.
- Jahn-Teller interactions.

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Interactions

Different mechanisms

1. Localized moments. Heisenberg model.
2. Localized moments + itinerant electrons.
3. Itinerant electrons. Fermi surface instability.

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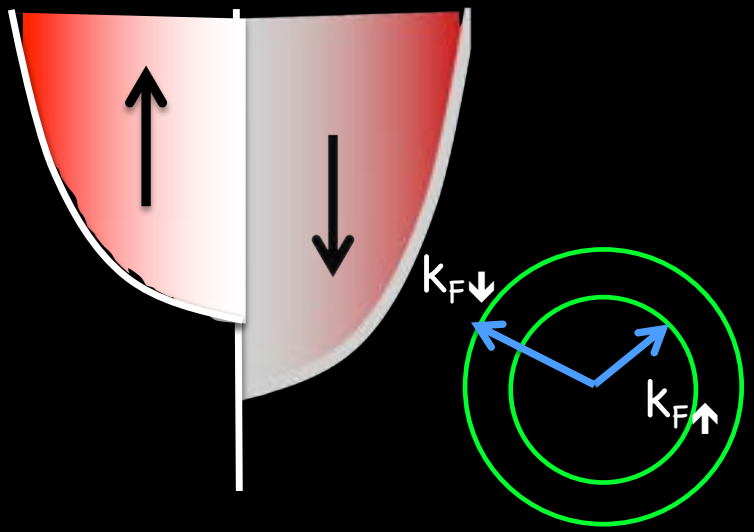
Itinerant ferromagnetism: spontaneouly spin-split bands

Question: Is it energetically favourable to have a spin imbalance for the itinerant electrons?

In mean-field, a polarized electron gas produces a molecular field (similar to an external field) which magnetizes the electron gas - Pauli PM).



Spin imbalance is

- non favoured in terms of kinetic energy
- favoured by the interaction with the molecular field.

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Itinerant magnetism

Hubbard model in a magnetic field

$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} - \frac{g\mu_B H}{2} \sum_j (n_{j\uparrow} - n_{j\downarrow})$$

$$\langle n_{j\uparrow,\downarrow} \rangle = \frac{n}{2} \pm m$$

$$n_{j\uparrow} n_{j\downarrow} \rightarrow n_{j\uparrow} \langle n_{j\downarrow} \rangle + n_{j\downarrow} \langle n_{j\uparrow} \rangle - \langle n_{j\uparrow} \rangle \langle n_{j\downarrow} \rangle$$

Energy density

$$\mathrm{E}(m) = \int^{\mu\uparrow} \varepsilon \rho(\varepsilon) d\varepsilon + \int^{\mu\downarrow} \varepsilon \rho(\varepsilon) d\varepsilon + U\left(\frac{n^2}{4} - m^2\right) - g\mu_B H m$$

Fazekas's book

At some value of U, $-m^2U$ will favour a finite magnetization m (polarizing the spins makes them less likely to meet)

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Itinerant magnetism

Hubbard model in a magnetic field

$$H = \sum_{k\sigma} \varepsilon_k n_{k\sigma} + U \sum_j n_{j\uparrow} n_{j\downarrow} - \frac{g\mu_B H}{2} \sum_j (n_{j\uparrow} - n_{j\downarrow})$$

Calculate susceptibility

$$\chi = \frac{\chi_{\text{Pauli}}}{1 - U\rho(E_F)}$$

Stoner enhancement

(Pauli susceptibility is enhanced by electron-electron interaction)

U $\rho(E_F)$ = 1 (Stoner criterium for itinerant FM)

Band narrowing and peaks in $\rho(E_F)$ promote FM

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Itinerant magnetism

Itinerant FM: Fe, Co, Ni, and alloys YCo_5, $La_2Fe_{14}B$

If Stoner criterium is marginally satisfied:

- Nearly FM metals (very large susceptibility)
  Example: Pd
  U $\rho(E_F)$ ~0.9.
  Alloying with 0.1% Fe or Co, turns Pd FM

- Weak (m<<n) itinerant ferromagnetism
  Example: $ZrZn_2$ (neither Zr nor Zn is magnetic)

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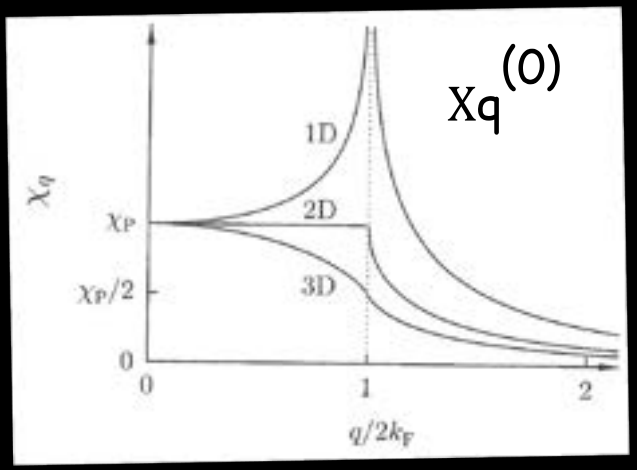
Instabilities with wave-vector q≠0. Spin density waves. Nesting

Generalized susceptibility: Stoner criterium for finite q. For a non-uniform magnetic field we calculated a q dependent susceptibility

$$\chi_q^{(0)} = \chi_{\text{Pauli}} f\left(\frac{q}{2k_F}\right)$$

In the presence of Coulomb interactions

$$\chi_q = \frac{\chi_q^{(0)}}{1-\alpha\chi_q^{(0)}} = \frac{\chi_{\text{Pauli}} f\left(\frac{q}{2k_F}\right)}{1-U\rho(E_F) f\left(\frac{q}{2k_F}\right)}$$



S. Blundell, OUP

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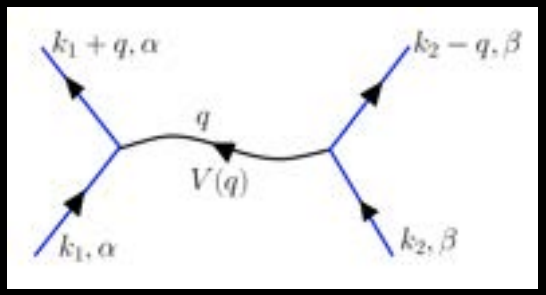
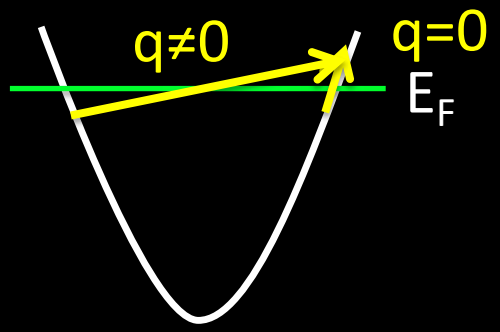
Instabilities with wave-vector q≠0. Spin density waves. Nesting

If $\chi_q^{(0)}$ diverges, you can have a collective mode even for very weak electron-electron interaction U. The instability that sets in is the one corresponding to the lowest U.



Coleman's book

$$V(r) = \sum_q V(q) e^{iqr}$$



Reminder: a metal is in the degenerate limit $T \ll E_F$
Excitations around E_F

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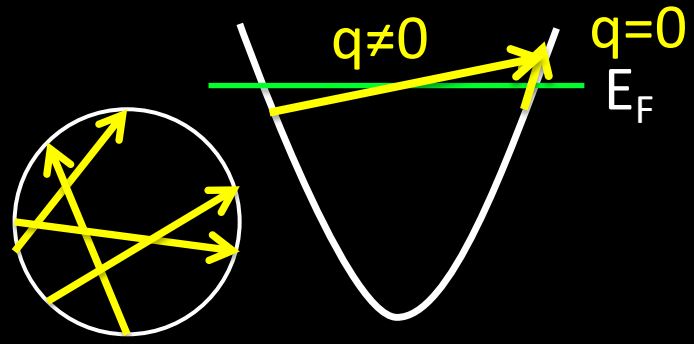
Instabilities with wave-vector q≠0. Spin density waves. Nesting

For a parabolic band you can have excitations at all possible q. q=0 is going to dominate (max χ at q=0)



However, if there are sectors of the Fermi surface that are connected by the same q, the maximum of the susceptibility can be at that particular q: nesting.

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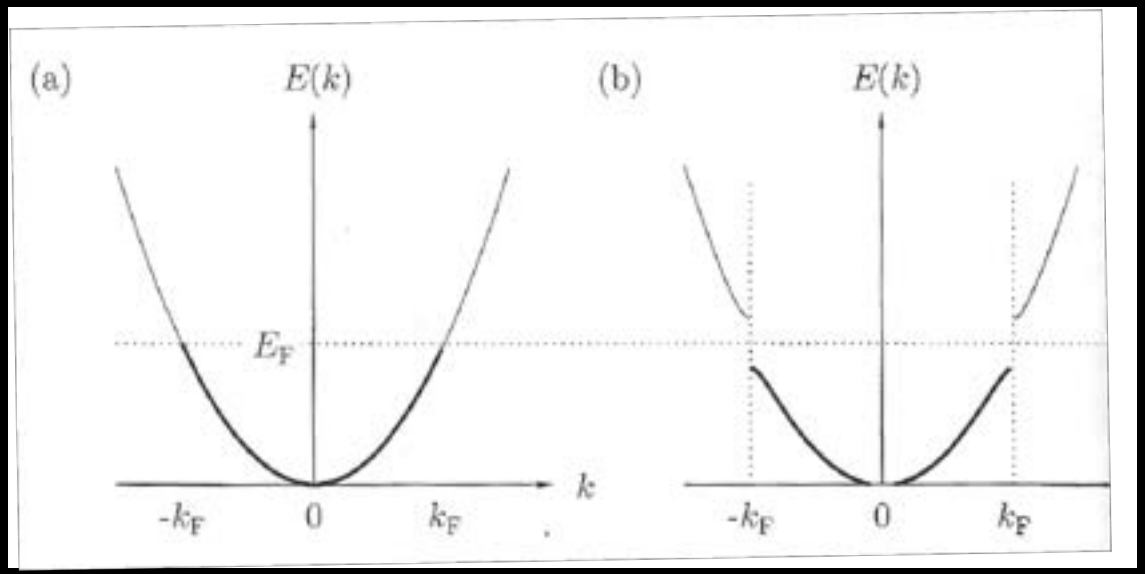
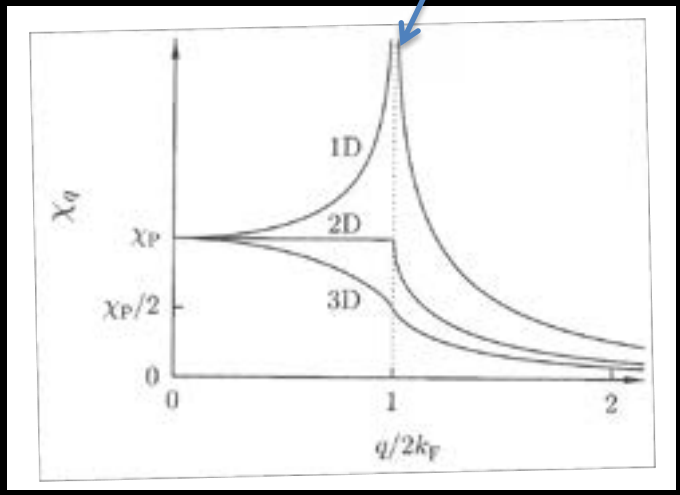
Nesting in 1d

In 1d there is always nesting at $q=2k_F$

Peierls instability: dimerization and charge density wave.



Kohn anomaly



S. Blundell, OUP

For d>1, the nesting condition is more restrictive

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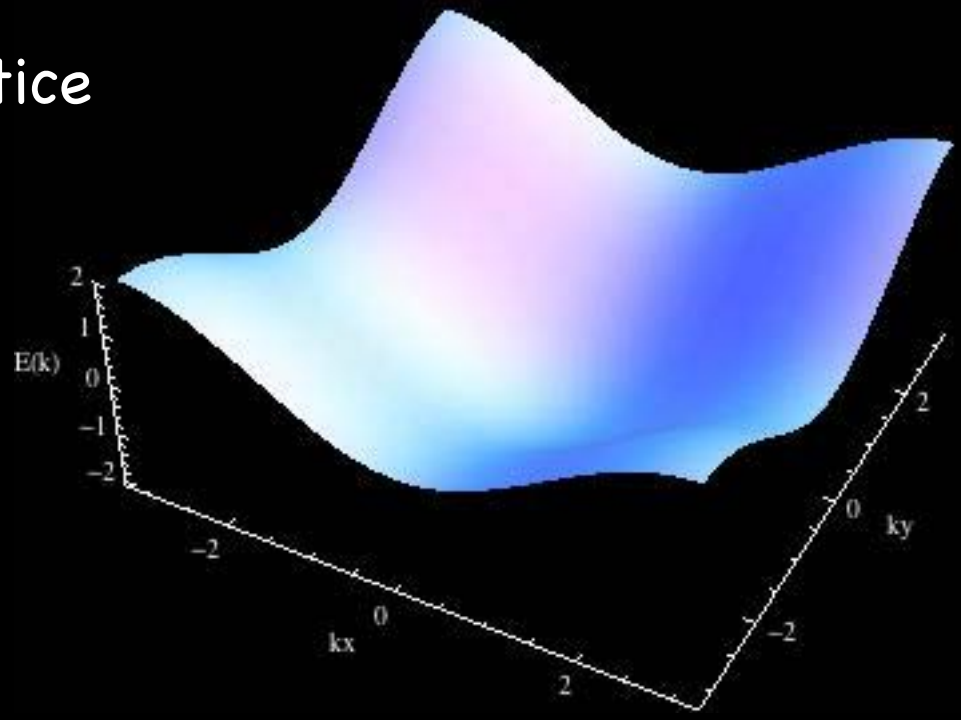
Instabilities with wave-vector q≠0. Spin density waves. Nesting

Special case: Square lattice

$\varepsilon(k)=-2t(\cos k_x+\cos k_y)$



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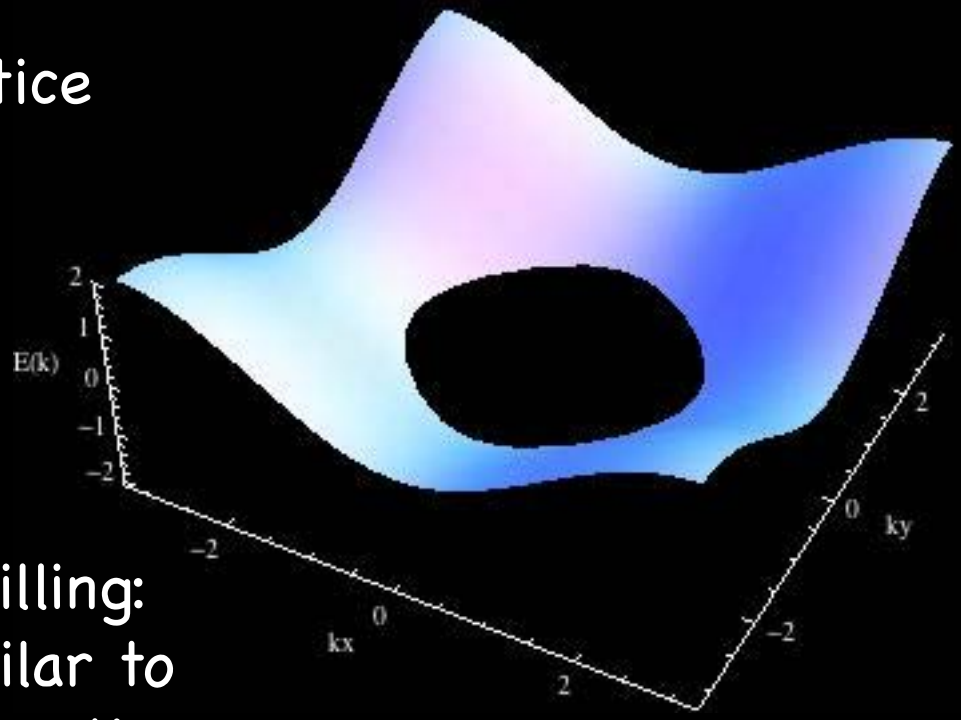
Instabilities with wave-vector q≠0. Spin density waves. Nesting

Special case: Square lattice

$\varepsilon(k)=-2t(\cos k_x+\cos k_y)$



For an incommensurate filling:
The Fermi surface is similar to the parabolic bands: no nesting

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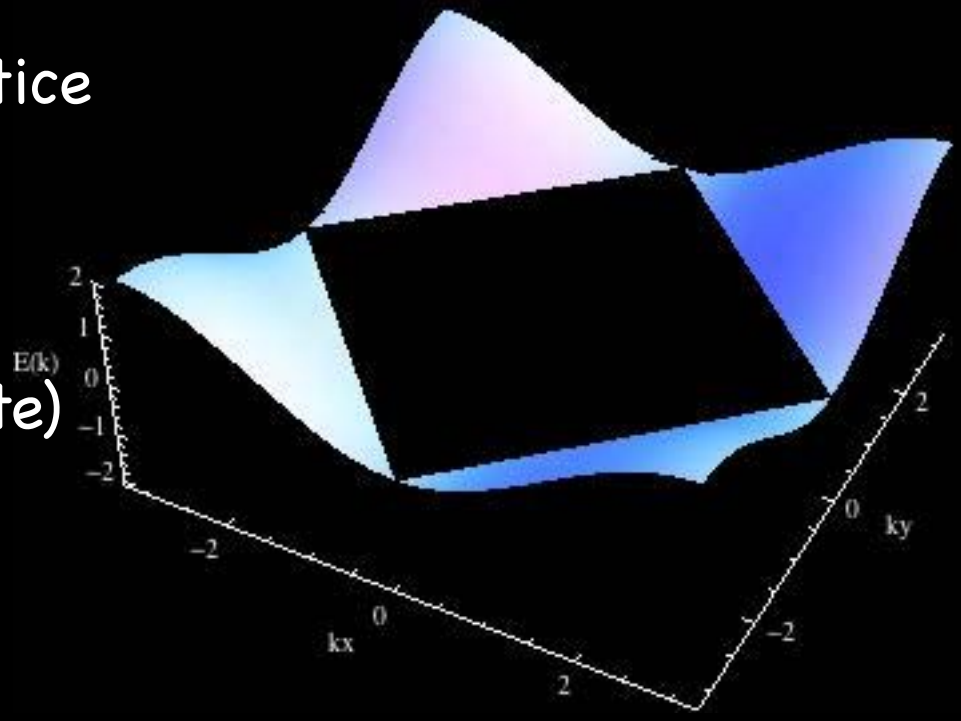
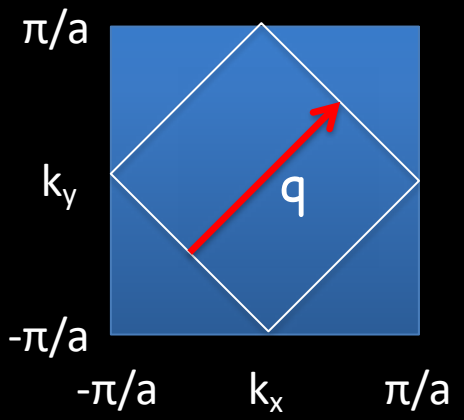
Instabilities with wave-vector q≠0. Spin density waves. Nesting

Special case: Square lattice

$\varepsilon(k)=-2t(\cos k_x+\cos k_y)$

For half filling (1 e- per site)





There is perfect nesting with q=(π/a,π/a)

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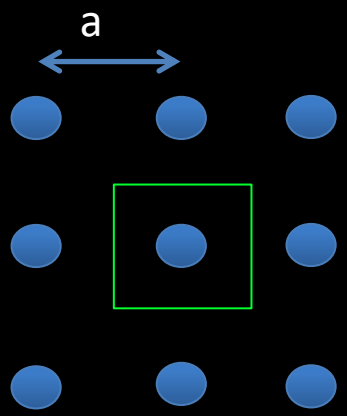
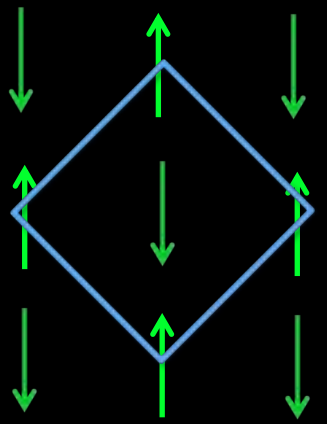
Instabilities with wave-vector q≠0. Spin density waves. Nesting

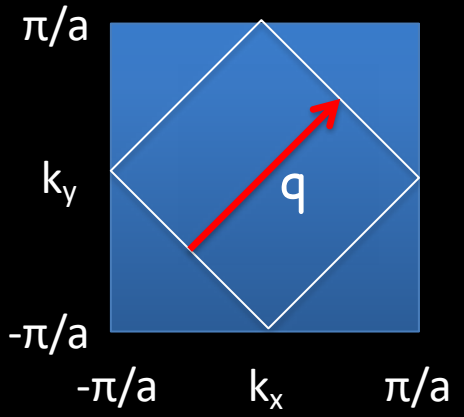


AF: Doubling of unit cell

⬇

Folding of Brillouin zone





A gap opens at the zone boundary: the system is insulating at half-filling even in the weak coupling regime if there is perfect nesting.

(Slater insulator)

Note that we have used U=0!!

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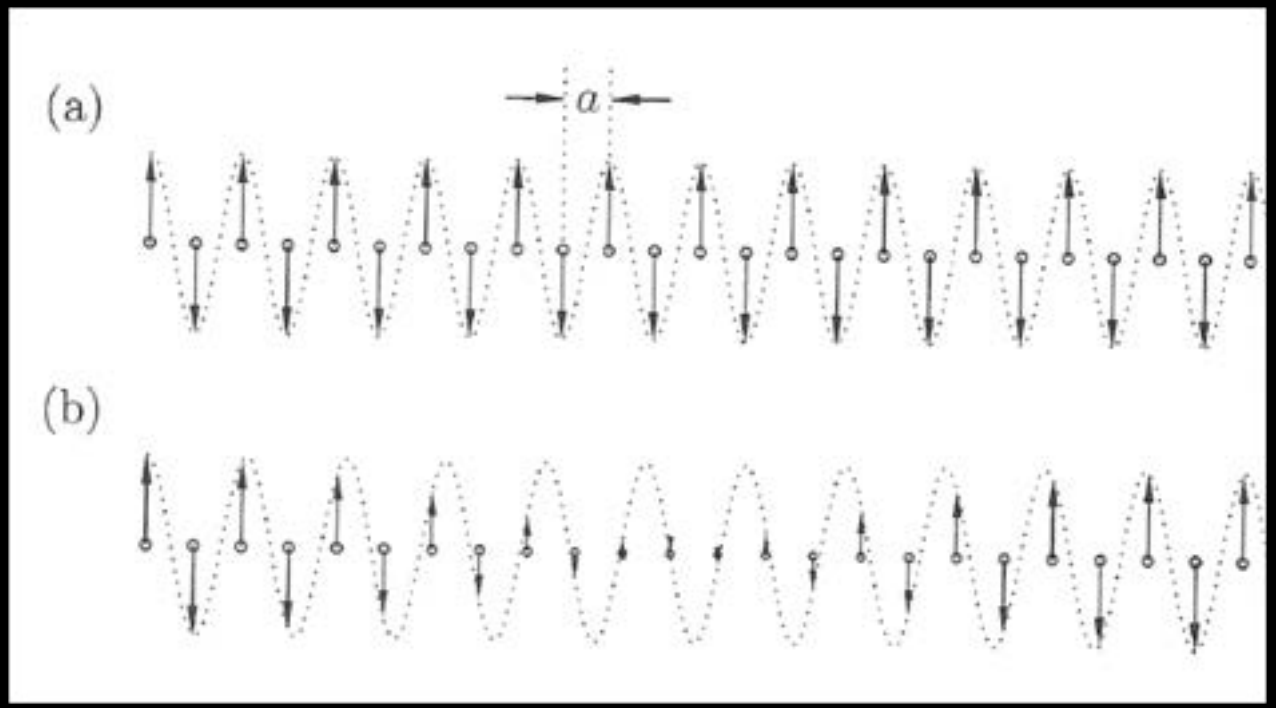
Instabilities with wave-vector q≠0. Spin density waves. Nesting

In general, **q** can be an incommensurate vector



S. Blundell's book

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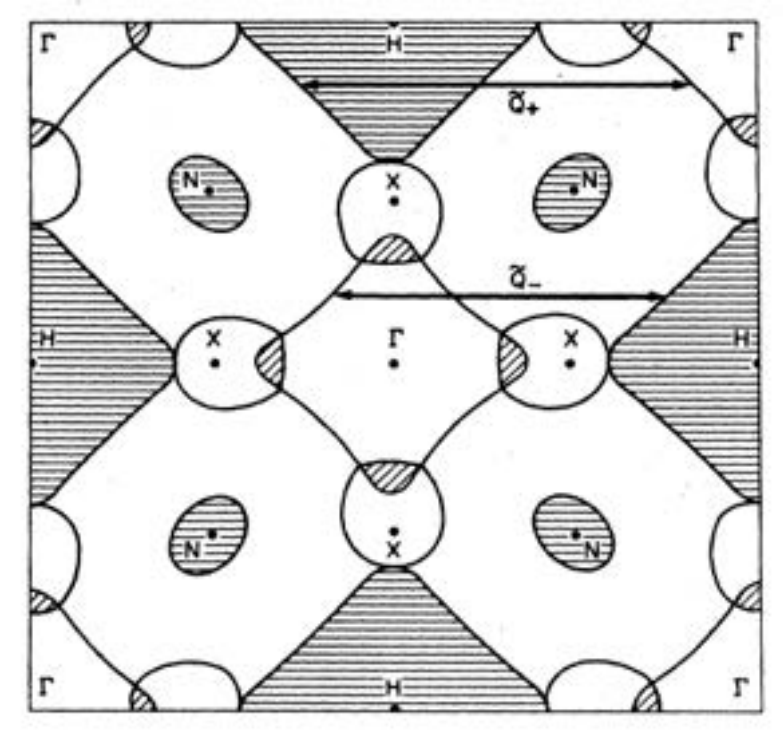
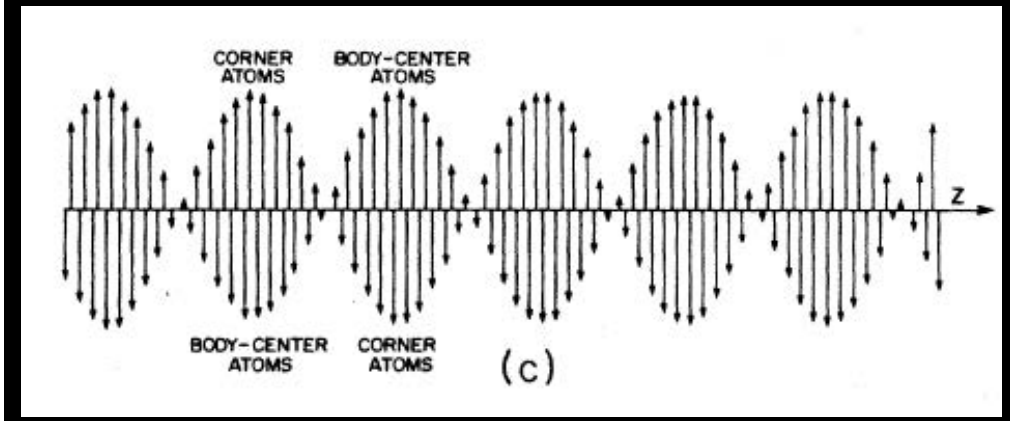
Instabilities with wave-vector q≠0. Spin density waves. Nesting

Example: SDW in Cr



Q=(0,0,1-δ) 2π/a (0.037 < δ < 0.048)



RMP 60, 209 (1988)

The SDW does not open a gap over the entire Fermi surface: the system is metallic

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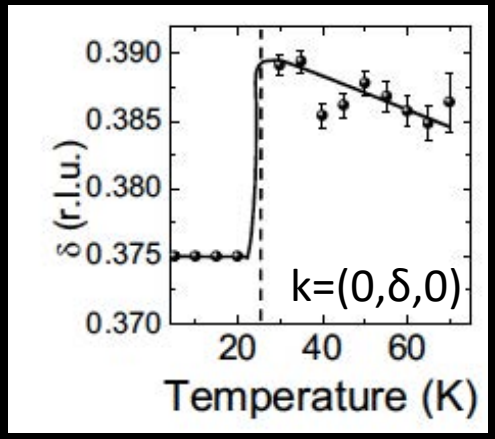
- Nesting can lead to different Fermi surface instabilities (charge density wave, superconducting pairing) that would compete with the spin-density wave.

  The one with the largest Tc would set in.

- Incommensurate instabilities sometimes suffer "lock-in" transitions becoming commensurate at low temperatures.

Example: $CaFe_4As_3$



PRB 81, 184402 (2010)

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Lock in transitions

Ginzburg-Landau formalism

Complex order parameter

$$\psi(r) = \rho(r) e^{i(\mathbf{Q_c}.\mathbf{r}+\phi(r))}$$

Free energy

$$\mathcal{F}_\psi = \tfrac{1}{2}\, a_\rho (T - T_{CO}) |\psi|^2 + \tfrac{1}{4}\, b_\rho |\psi|^4 + \tfrac{1}{2}\, \xi_\rho^2 \left|(\nabla - i\, \vec{q_o})\, \psi\right|^2 + \tfrac{1}{n}\, \eta\, \Re\left[\psi^n e^{-i\vec{G}.\vec{r}}\right]$$

Elastic term

Umklapp term

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Lock in transitions

$$\begin{aligned}\mathcal{F}_\psi &= \tfrac{1}{2}\,a_\rho(T-T_{CO})\rho^2+\tfrac{1}{4}\,b_\rho\rho^4 \\ &+ \tfrac{1}{2}\,\xi_\rho^2(\nabla\rho)^2+\tfrac{1}{2}\,\xi_\rho^2\rho^2\,(\nabla\phi-\vec{q}_o)^2+\tfrac{1}{n}\,\eta\,\rho^n\cos[n\phi]\end{aligned}$$

q_0 is the incommensurate nesting vector.

n is the period of the lattice

Elastic term favours $\nabla\phi = q_0$ INCOMMENSURABILITY

Umklapp term favours COMMENSURABILITY

$$\phi = \left(\frac{\pi}{n}+\frac{2\pi j}{n}\right) \quad \forall j \in \mathbf{Z}$$

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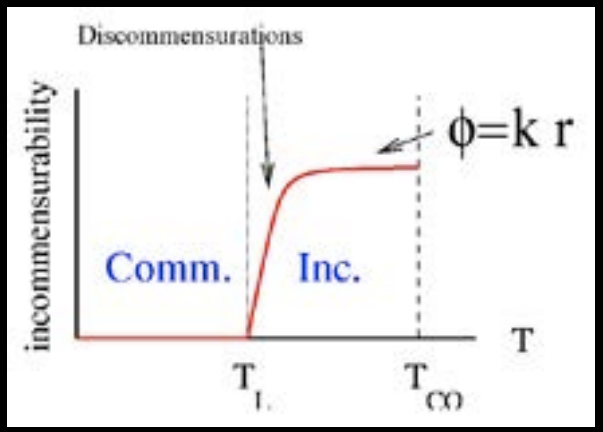
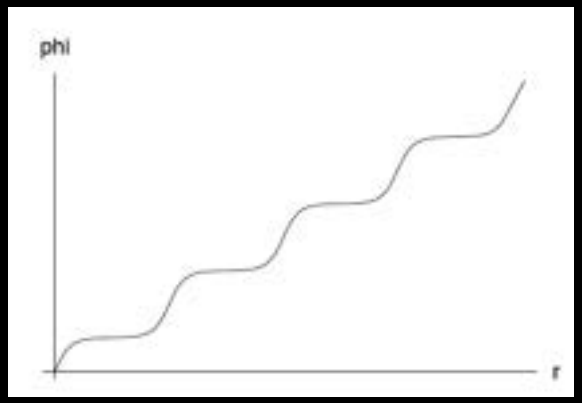
Lock in transitions

$$\begin{aligned}\mathcal{F}_\psi &= \tfrac{1}{2}\,a_\rho(T-T_{CO})\rho^2+\tfrac{1}{4}\,b_\rho\rho^4 \\ &+ \tfrac{1}{2}\,\xi_\rho^2(\nabla\rho)^2+\tfrac{1}{2}\,\xi_\rho^2\rho^2\,(\nabla\phi-\vec{q}_o)^2+\tfrac{1}{n}\,\eta\,\rho^n\cos[n\phi]\end{aligned}$$

For n>2, at high T, ρ is small and the elastic term wins. At lower T, ρ is large and the Umklapp term wins.





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Outline

- Free magnetic ions
- Environment
- Interactions
  - Exchange between localized moments
  - Indirect exchange through itinerant electrons
  - Magnetism in metals
- Excitations

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Excitations: spin waves

Low T excitations of a Heisenberg model (localised moments)

Breaking a global continuous symmetry. (Goldstone theorem): it is possible to produce long-wavelength excitations in the order parameter with a vanishingly small energy cost. Excitations are (massless) Goldstone bosons.

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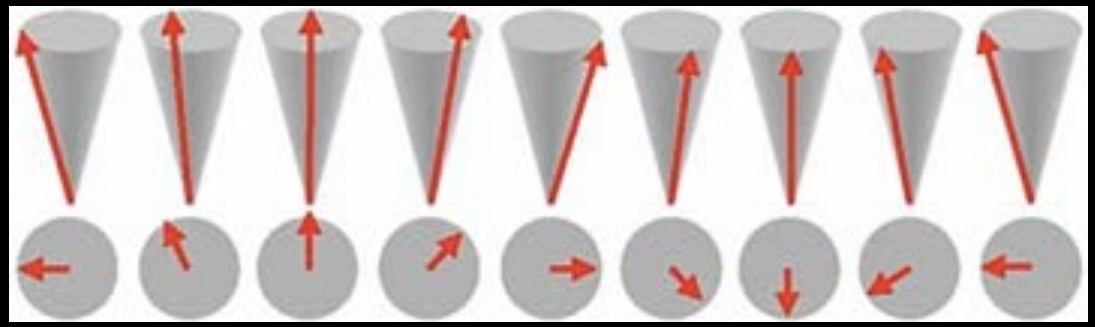
Excitations: spin waves

Low T excitations of a Heisenberg model (localised moments)

In a FM: flip a single spin. The new eigenstate is a state with a wave of spins.



http://www.uni-muenster.de/

This excitation can be described as the formation of a bosonic quasiparticle called magnon

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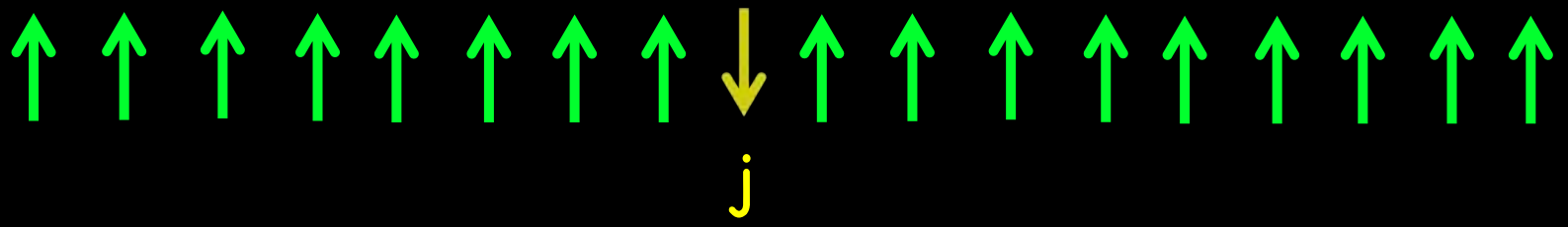
Excitations: spin waves

For a ferromagnetic Heisenberg model

$$H = -2J\sum_i \mathbf{S}_i\mathbf{S}_{i+1} = -2J\sum_i\left[S_i^zS_{i+1}^z + \frac{1}{2}\left(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+\right)\right] \qquad S^{\pm} = S_x \pm iS_y$$

To create an excitation: flip spin j

$$|j\rangle = S_j^-|\phi\rangle$$



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Excitations: spin waves

For a ferromagnetic Heisenberg model

$$H = -2J\sum_i \mathbf{S}_i\mathbf{S}_{i+1} = -2J\sum_i\left[S_i^zS_{i+1}^z + \frac{1}{2}\left(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+\right)\right] \qquad S^{\pm} = S_x \pm iS_y$$

To create an excitation: flip spin j

$$|j\rangle = S_j^-|\phi\rangle$$

|j> is not an eigenstate of H: diagonalize the Hamiltonian by looking for plane-wave solutions

$$|q\rangle = \frac{1}{\sqrt{N}}\sum_j e^{iqR_j}|j\rangle$$

$$E(q) = -2NJS^2 + 4JS(1-\cos qa)$$

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Excitations: spin waves

$$E(q) = -2NJS^2 + 4JS(1-\cos qa)$$

small q

$$\hbar\omega \approx 2JSq^2a^2$$

Gapless
Goldstone modes

Goldstone theorem: if a continuous symmetry is spontaneously broken and the forces are sufficiently short ranged, there must be a branch of excitations with the property that the energy vanishes for q→0.

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Excitations: spin waves

$$E(q) = -2NJS^2 + 4JS(1-\cos qa)$$

small q

$$\hbar\omega \approx 2JSq^2a^2$$

Gapless
Goldstone modes

In 3dim the density of states is

$$\rho(q)dq \propto q^2 dq$$

$$n_{magnon} = \int_0^\infty \frac{\rho(\omega)d\omega}{\exp(\hbar\omega / k_B T) - 1} \propto T^{3/2}$$

At low T: $M(T) \approx 1 - aT^{3/2}$

Bloch $T^{3/2}$ law

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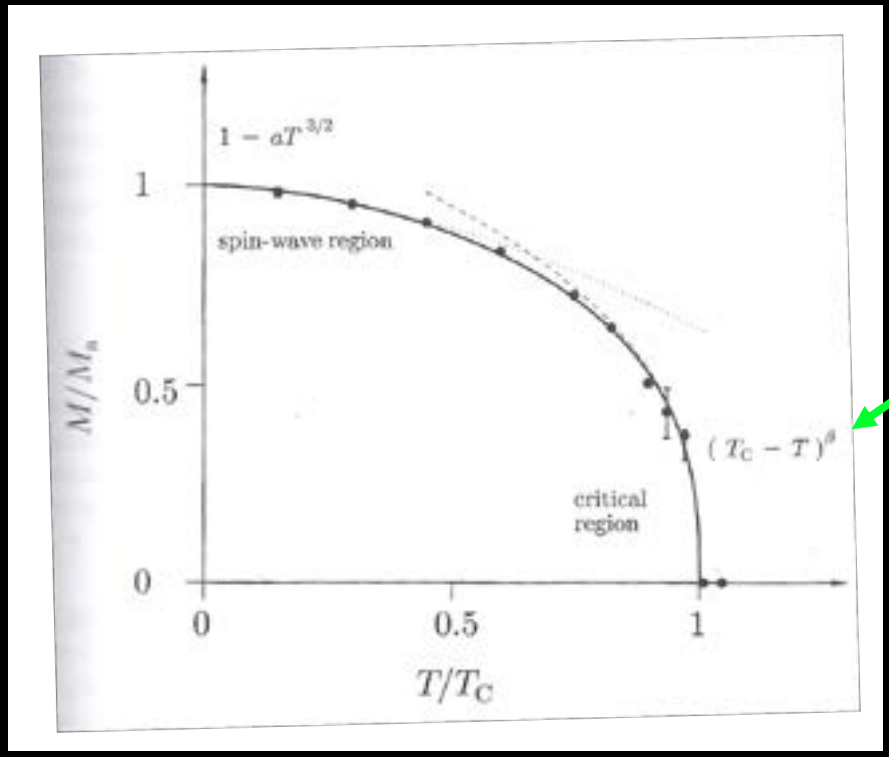
Excitations: spin waves



Blundell's book

Close to T_c, critical exponent 1/2

At low T: $M(T) \approx 1-aT^{3/2}$

Bloch $T^{3/2}$ law

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Excitations: spin waves

$$E(q) = -2NJS^2 + 4JS(1-\cos qa)$$

small q

$$\hbar\omega \approx 2JSq^2a^2$$

$$n_{\text{magnon}} = \int_0^\infty \frac{g(\omega)d\omega}{exp(\hbar\omega/k_BT) - 1}$$

In 2dim and 1dim n_{magnon} diverges → spontaneous FM is not possible for isotropic 1dim and 2dim Heisenberg models (Mermin-Wagner-Berezinskii theorem)

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Excitations: spin waves

But note: Anisotropies stabilize FM in low dimensional systems and the spin-wave spectrum acquires a gap

$$H = J \sum_{i,j} (S_i^x S_j^x + S_i^y S_j^y + A S_i^z S_j^z)$$

A>1 (easy axes)

$$\Delta E = 4JS(1 - \cos qa) \sim q^2 a^2 \quad \text{(isotropic)}$$

$$\Delta E = 4JS(A - \cos qa) \sim (A - 1 + q^2 a^2)$$

GAP

There can also be a gap due to dipole-dipole interactions (which can be important for f-systems)

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Excitations: spin waves

Ground state of the antiferromagnetic Heisenberg model

$$H_{AF} = 2J\sum_i \mathbf{S}_i\mathbf{S}_{i+1} = 2J\sum_i\left[S_i^zS_{i+1}^z + \frac{1}{2}\left(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+\right)\right]$$

$|\phi_0\rangle = |\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\ldots\rangle$ (classical Néel state)

Φ_0 is not an eigenstate of H_{AF}. From this molecular field approximation, you can decrease the energy by letting S^z fluctuate. These quantum fluctuations lower the energy with respect to the Néel state.

$$-NzJS^2\left(1+\frac{1}{zS}\right) < E_g < -NzJS^2$$

z: number of neighbors

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Excitations: spin waves

$$H_{AF} = 2J\sum_i \mathbf{S}_i\mathbf{S}_{i+1} = 2J\sum_i\left[S_i^zS_{i+1}^z + \frac{1}{2}\left(S_i^+S_{i+1}^- + S_i^-S_{i+1}^+\right)\right]$$

Spin waves have to be defined in the two sublattices. These spin waves are interdependent. The spin wave spectrum is twofold degenerate (±1 excitations are degenerate)

$$\hbar\omega \approx JzS\,|\,q\,|\,a$$

Antiferromagnons
(gapless Goldstone mode)

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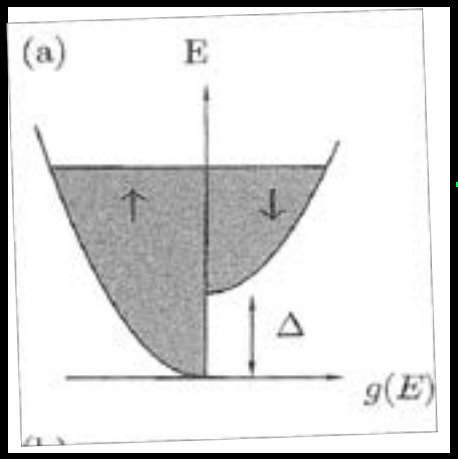
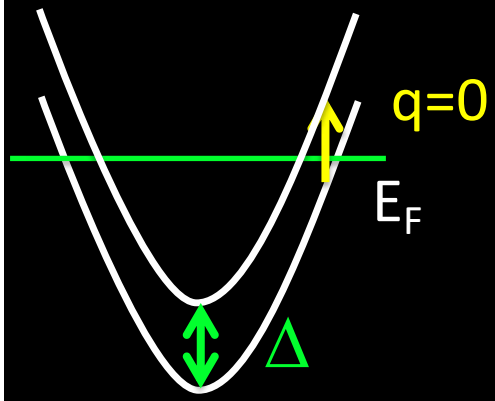
Excitations in the electron gas

- Also spin waves
- Stoner excitations

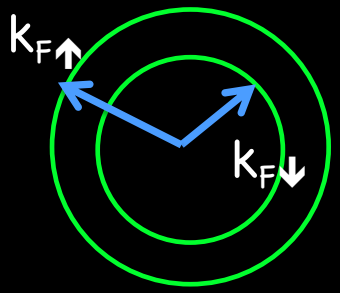
$$\hbar\omega = E_{k+q} - E_k + \Delta$$

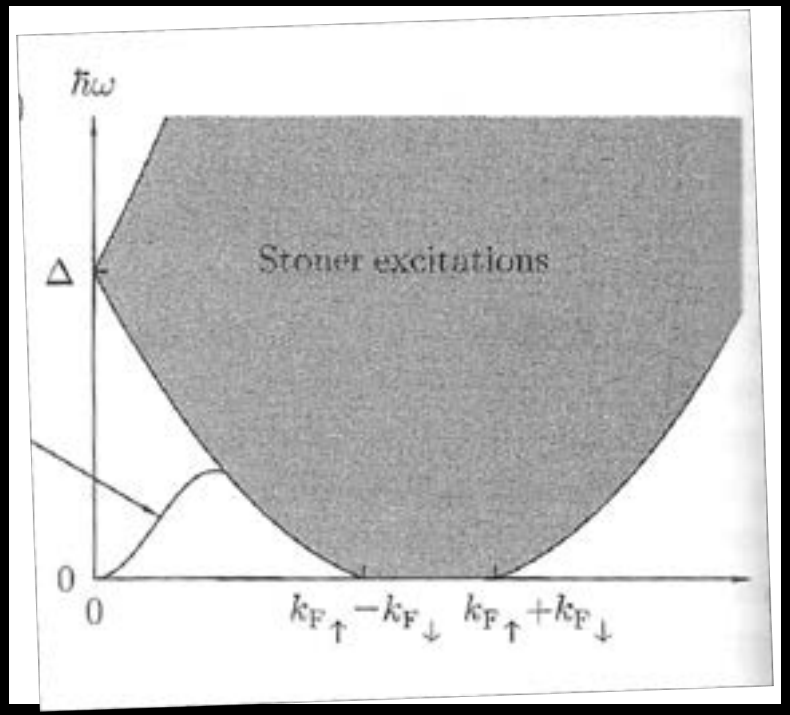
Δ: exchange splitting





Spin wave





Blundell's book

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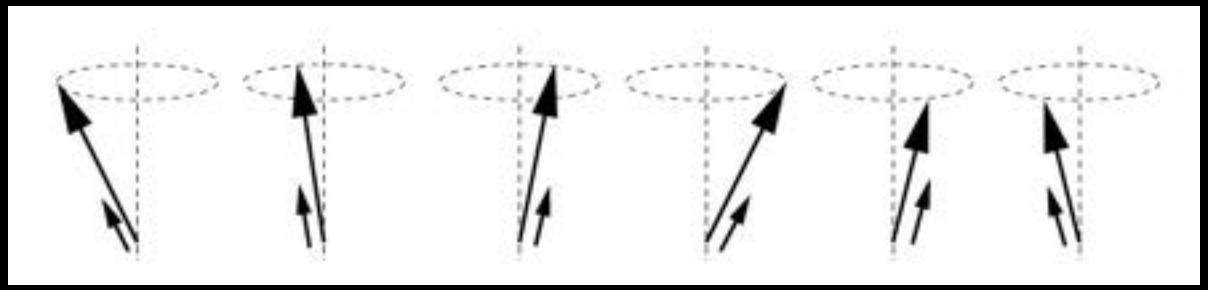
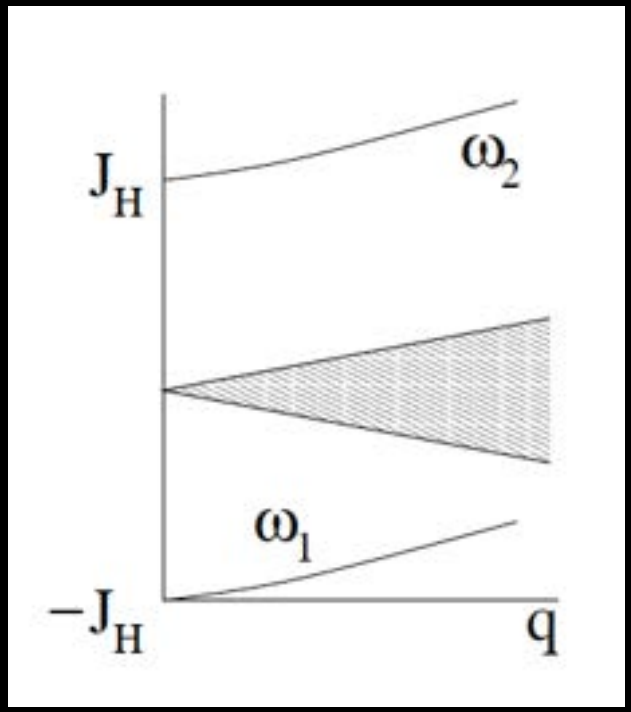
Spin waves in a double exchange system: localized +itinerant

Composite spin waves





PRB 64, 140403

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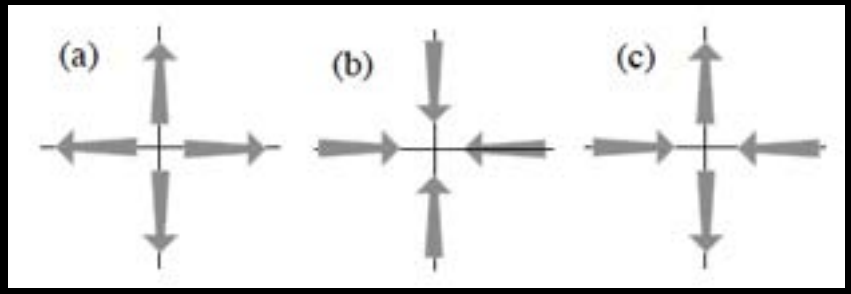
Topological defects

Distortions which cannot be restored into ordering by continuous deformations.

↓

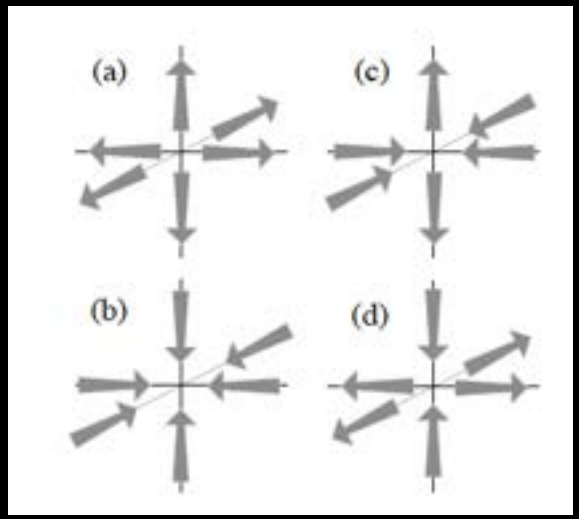
Vortices

XY model in 2dim



Vortices have a topological charge.

Heisenberg model in 3dim



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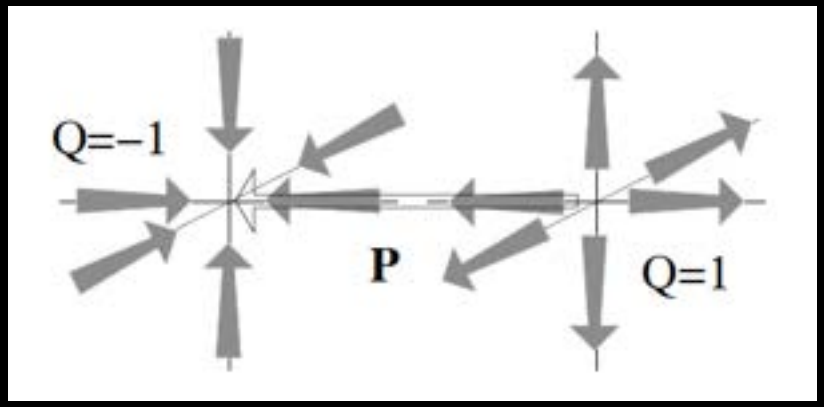
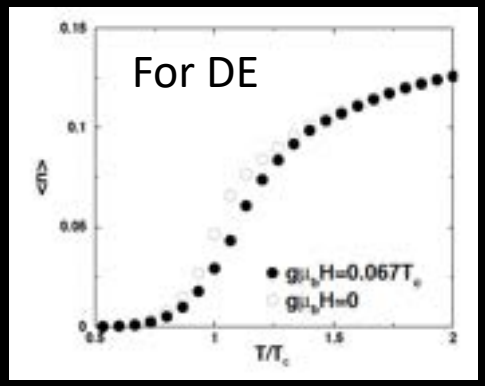
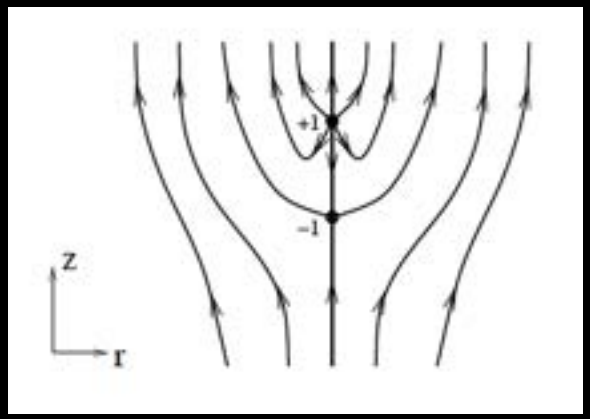
Topological defects

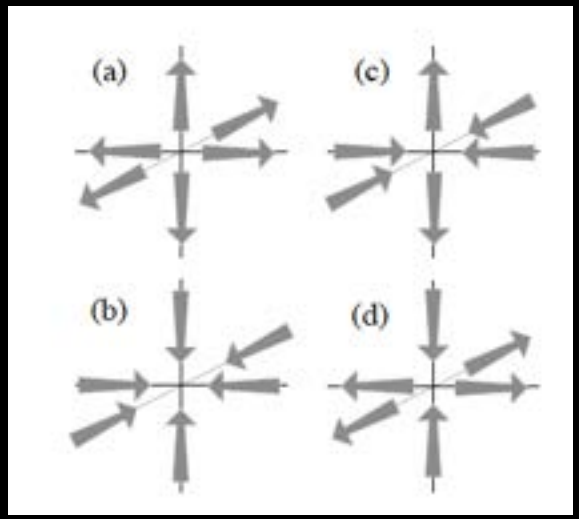






$$\langle n \rangle = \alpha e^{-\beta E_c}$$

Heisenberg model in 3dim



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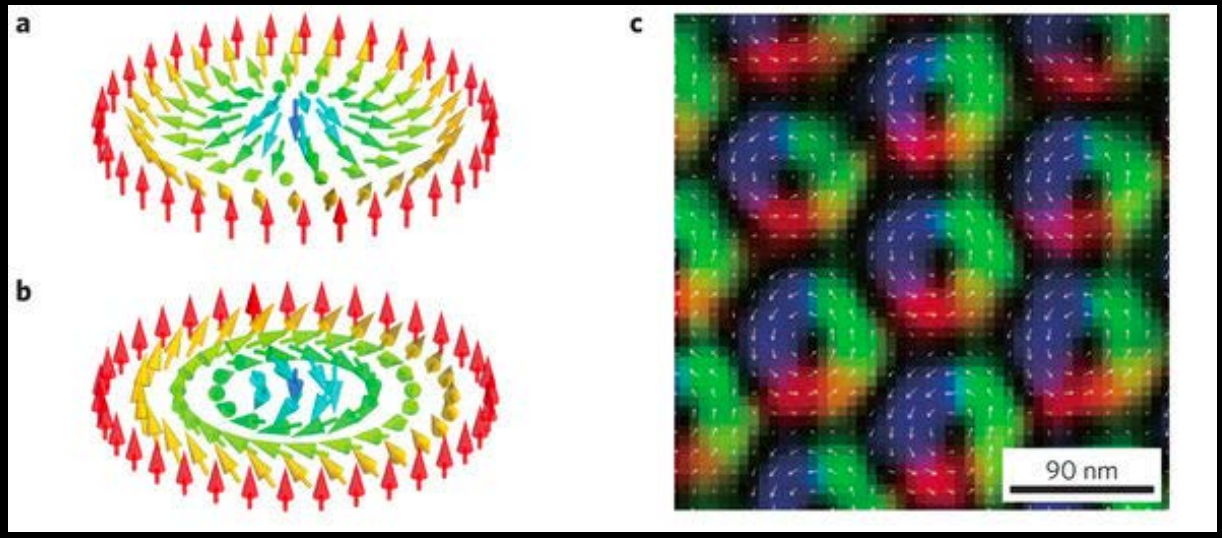
Observation of magnetic skyrmions



✓ Induced by Dzyaloshinskii-Moriya interaction (consequence of spin-orbit interaction). Requires no inversion symmetry.

✓ Spintronic storage.

$$H_{DM} = \mathbf{D} \cdot (\mathbf{S}_1 \times \mathbf{S}_2)$$

Science **323**, 915–919 (2009).

A. Fert, et al Nature Nanotechnology 8, 152–156 (2013)

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Summary

- Classical phase transitions
- Free magnetic ions
- Environment
- Magnetic order and susceptibility
- Interactions
  - Exchange between localized moments
  - Indirect exchange through itinerant electrons
  - Magnetism in metals
- Excitations

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