Recap

- Effective spin Hamiltonian:

$$H = \frac{p_1^2}{2m} + \frac{e^2}{\left|\vec{r}_1 - \vec{R}_a\right|} + \frac{p_2^2}{2m} + \frac{e^2}{\left|\vec{r}_2 - \vec{R}_b\right|} + \frac{e}{\left|\vec{r}_1 - \vec{r}_2\right|}$$

$$H_{eff} = \frac{1}{4}(E_S + 3E_T) - (E_S - E_T)\mathbf{S}_1 \cdot \mathbf{S}_2 \Rightarrow -2J\mathbf{S}_1 \cdot \mathbf{S}_2$$

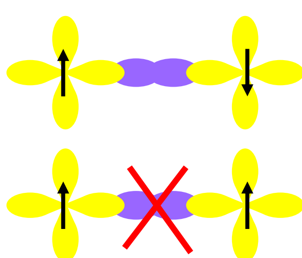
- Nearest-neighbor Heisenberg model: $H = J\sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$
  - N.B: Change of sign (historical reason)
- Exchange interaction:

$$J = \int d\vec{r}_1 d\vec{r}_2 \phi_a^*(\vec{r}_1)\phi_b^*(\vec{r}_2) V(\vec{r}_1, \vec{r}_2)\phi_a(\vec{r}_2)\phi_b(\vec{r}_1)$$

- Direct exchange interaction is usually small
- Indirect exchange
  - Superexchange (kinetic exchange)
  - Itinerant exchange (RKKY interaction)
  - Double exchange

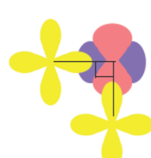
Superexchange

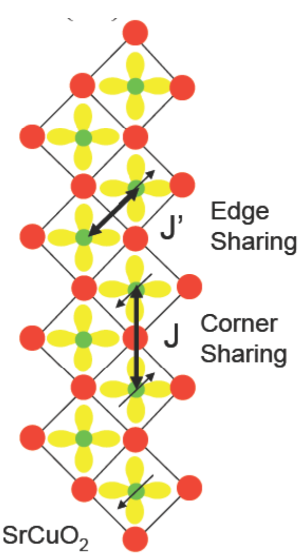
- Kinetic exchange



- Goodenough-Kanamori-Anderson rule

90 degree bond:
ferromagnetic and
weak superexchange





Hubbard model

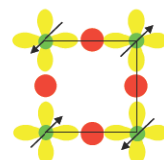
- t: Hopping matrix element
- U: on-site Coulomb energy

$$H = -t \sum_{<i,j>\sigma} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c. \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

- For strong coupling (U>>t): 2nd order perturbation theory in t gives:

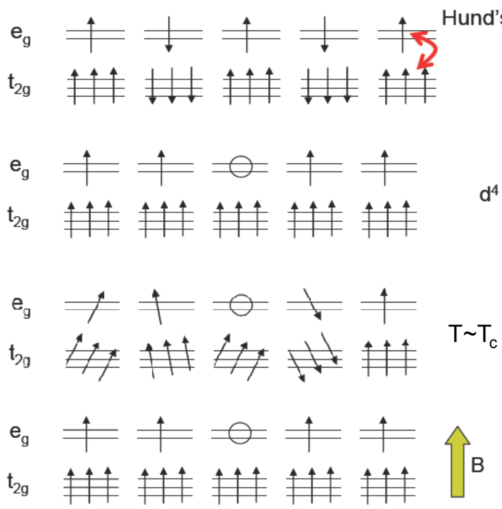
$$J = \frac{4t^2}{U}$$

- For three band model in cuprates:



$$J = \frac{4t_{pd}^{\;4}}{(\Delta + U_{pd})^2} \left(\frac{1}{U_d} + \frac{2}{\Delta + U_p} \right)$$

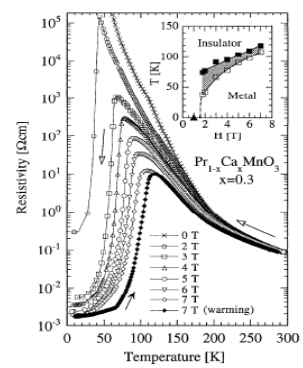
Double exchange



Hund's rule coupling J_H

d^4: $LaMnO_3$

d^4 and d^3 $La_{1-x}Sr_xMnO_3$



Colossal Magnetoresistance (CMR)

How do we calc/measure J?

- In principle, ab initio calculation
  - But often incorrect/difficult (correlation)
- Experimentally
  - T_C or T_N
  - Spectroscopy
  - Rough estimate (CW law)

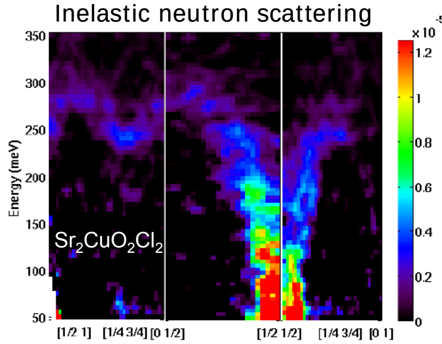
Magnon dispersion

- Diagonalize the spin Hamiltonian:

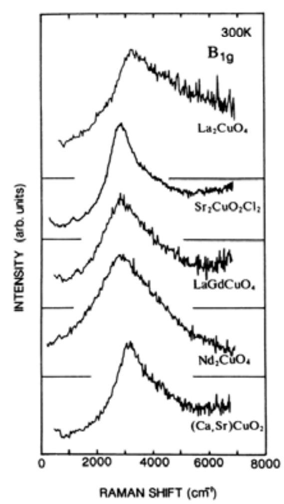
$$H = -JzS^2N + \sum_{\mathbf{k}} \omega_k a_k^+ a_k$$

$$\omega_k = 2JzS(1-\gamma_{\mathbf{k}}) \qquad \gamma_{\mathbf{k}} \equiv \frac{1}{z}\sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}$$

Inelastic neutron scattering

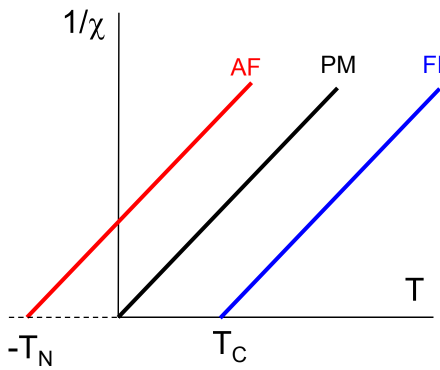


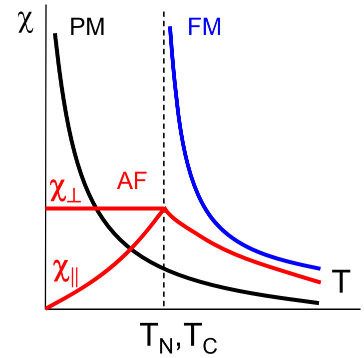
2-magnon Raman



Magnetic susceptibility

- Curie's law $\chi = \dfrac{C}{T}$
- Curie-Weiss law $\chi = \dfrac{C}{T-\Theta}$ Θ : Weiss Temperature





$$p_{theory} = g_J\sqrt{J(J+1)}$$

$$g_J = \frac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)}$$

But what about S_i?

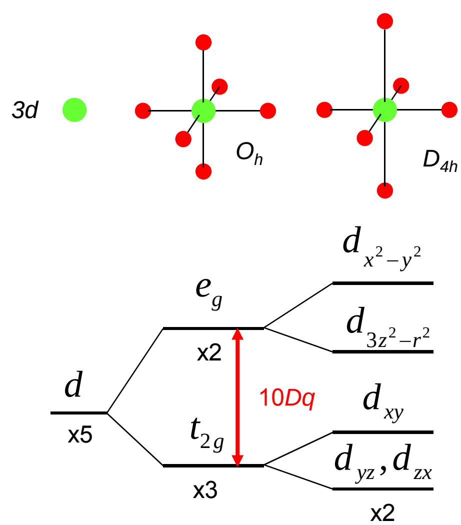
Calculated and Measured Magneton Numbers of Rare Earth Ions

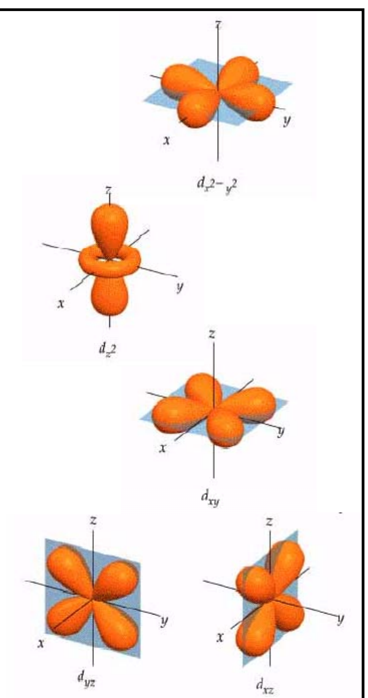
Ion	Electronic Configuration	Ground State Term $^{(2S+1)}L_J$	magneton p_{theory}	magneton p_{expt}
La^{3+}	[Xe] $4f^0$	$^1S_0$	0.00	< 0
Ce^{3+}	[Xe] $4f^1$	$^2F_{5/2}$	2.54	2.4
Pr^{3+}	[Xe] $4f^2$	$^3H_4$	3.58	3.5
Nd^{3+}	[Xe] $4f^3$	$^4I_{9/2}$	3.62	3.5
Pm^{3+}	[Xe] $4f^4$	$^5I_4$	2.68	–
Sm^{3+}	[Xe] $4f^5$	$^6H_{5/2}$	0.84	1.5
Eu^{3+}	[Xe] $4f^6$	$^7F_0$	0.00	3.4
Gd^{3+}	[Xe] $4f^7$	$^8S_{7/2}$	7.94	8.0
Tb^{3+}	[Xe] $4f^8$	$^7F_6$	9.72	9.5
Dy^{3+}	[Xe] $4f^9$	$^6H_{15/2}$	10.63	10.6
Ho^{3+}	[Xe] $4f^{10}$	$^5I_8$	10.60	10.4
Er^{3+}	[Xe] $4f^{11}$	$^4I_{15/2}$	9.59	9.5
Tm^{3+}	[Xe] $4f^{12}$	$^3H_6$	7.57	7.3
Yb^{3+}	[Xe] $4f^{13}$	$^2F_{7/2}$	4.54	4.5
Lu^{3+}	[Xe] $4f^{14}$	$^1S_0$	0.00	< 0

Calculated and Measured Magneton Numbers of Transition Metal Ions					
Ion	Electronic Configuration	Ground State Term $^{(2S+1)}L_J$	magneton $p_{\text{theory}}^{J=\vert L\pm S\vert}$	magneton $p_{\text{theory}}^{J=S}$	magneton p_{expt}
Ti^{3+}	[Ar] $3d^1$	$^2D_{3/2}$	1.55	1.73	–
V^{4+}	[Ar] $3d^1$	$^2D_{3/2}$	1.55	1.73	1.8
V^{3+}	[Ar] $3d^2$	$^3F_2$	1.63	2.83	2.8
V^{2+}	[Ar] $3d^3$	$^4F_{3/2}$	0.77	3.87	3.8
Cr^{3+}	[Ar] $3d^3$	$^4F_{3/2}$	0.77	3.87	3.7
Mn^{4+}	[Ar] $3d^3$	$^4F_{3/2}$	0.77	3.87	4.0
Cr^{2+}	[Ar] $3d^4$	$^5D_0$	0.00	4.90	4.8
Mn^{3+}	[Ar] $3d^4$	$^5D_0$	0.00	4.90	5.0
Mn^{2+}	[Ar] $3d^5$	$^6S_{5/2}$	5.92	5.92	5.9
Fe^{3+}	[Ar] $3d^5$	$^6S_{5/2}$	5.92	5.92	5.9
Fe^{2+}	[Ar] $3d^6$	$^5D_4$	6.70	4.90	5.4
Co^{2+}	[Ar] $3d^7$	$^4F_{9/2}$	6.54	3.87	4.8
Ni^{2+}	[Ar] $3d^8$	$^3F_4$	5.59	2.83	3.2
Cu^{2+}	[Ar] $3d^9$	$^2D_{5/2}$	3.55	1.73	1.9

- Orbital momentum quenching

Crystal field splitting





Orbital angular momentum quenching

- When the ground state is non-degenerate and real (both due to the real crystal field): $\left\langle 0 \middle| \vec{\mathbf{L}} \middle| 0 \right\rangle = 0$
- N.B. ***L*** is pure imaginary and hermitian: $\vec{\mathbf{L}} = -i\vec{\mathbf{r}} \times \nabla$
- Result: For transition metal (3d) ions J=S
  - Not quite...
  - due to SO coupling

Crystal field > Spin orbit: 3d
Crystal field ≈ Spin orbit: 4d and 5d
Crystal field < Spin orbit: 4f (rare earth)