Magnetic Interactions and Order-out-of-disorder in Insulating Oxides

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Les Houches summer school on Quantum Magnetism, June 2006

Lecture 1:

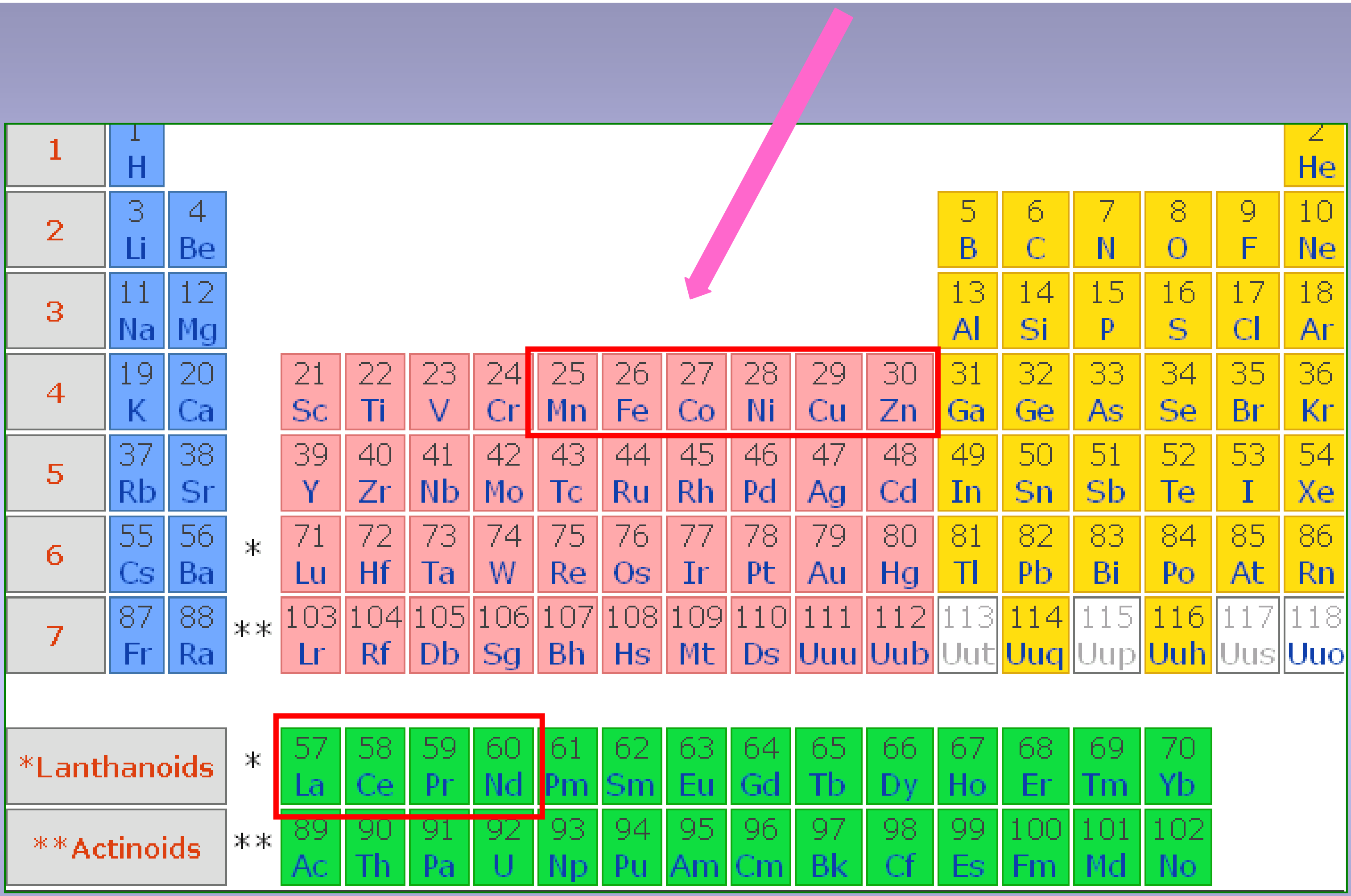
Introduction to perovskites and other transition metal – rare earth oxides.

Introduction to superexchange theory.

Posing the question: How does a particular system choose its magnetic structure?

Cuprates

transition-metal oxides—RMO_3 ; R_2MO_4



1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca		21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr		39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	*	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	**	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Uuu	112 Uub	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

*Lanthanoids	*	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb
**Actinoids	**	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No

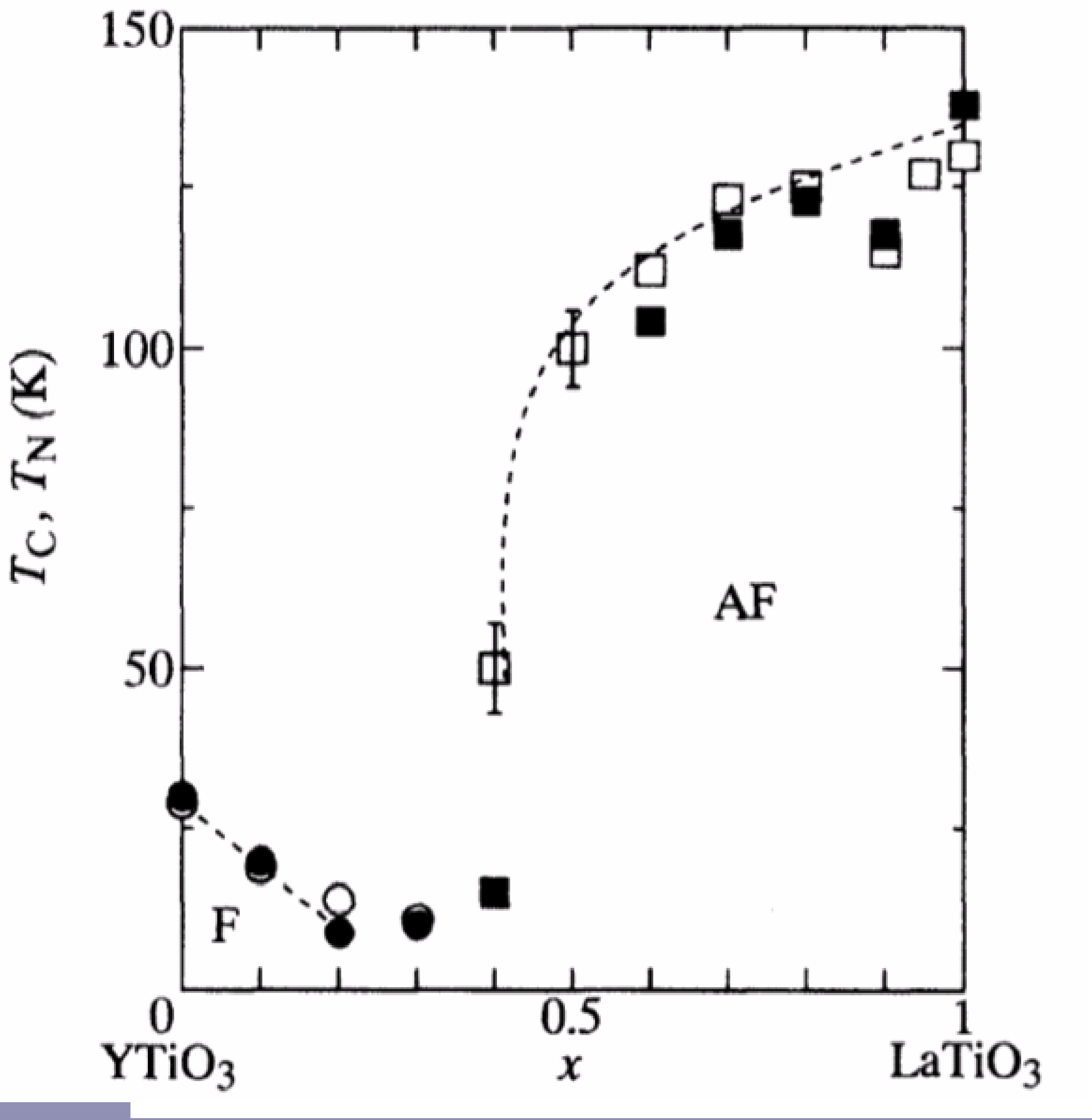
transition-metal oxides—RMO_3 ; R_2MO_4

High-T_c cuprates, e.g., La_2CuO_4;

Colossal magnetoresistance manganites;

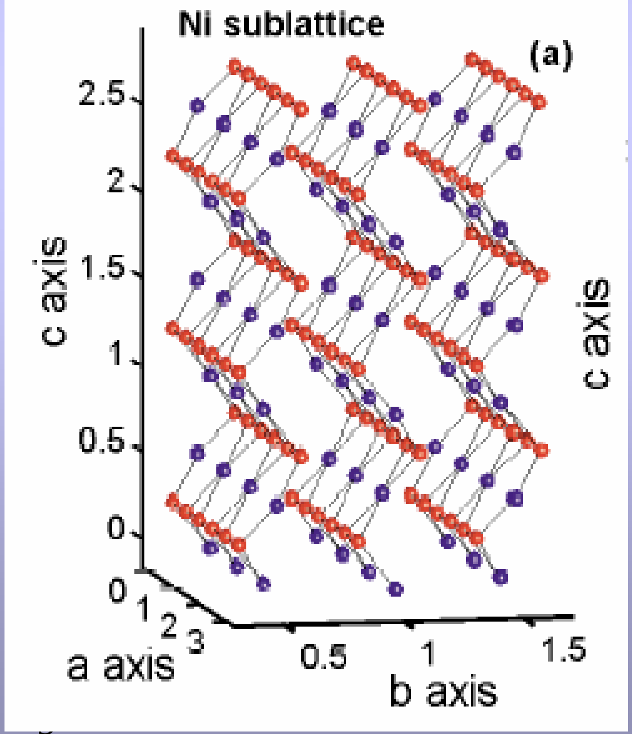
Mott-Hubbard insulator titanates (close to MIT)

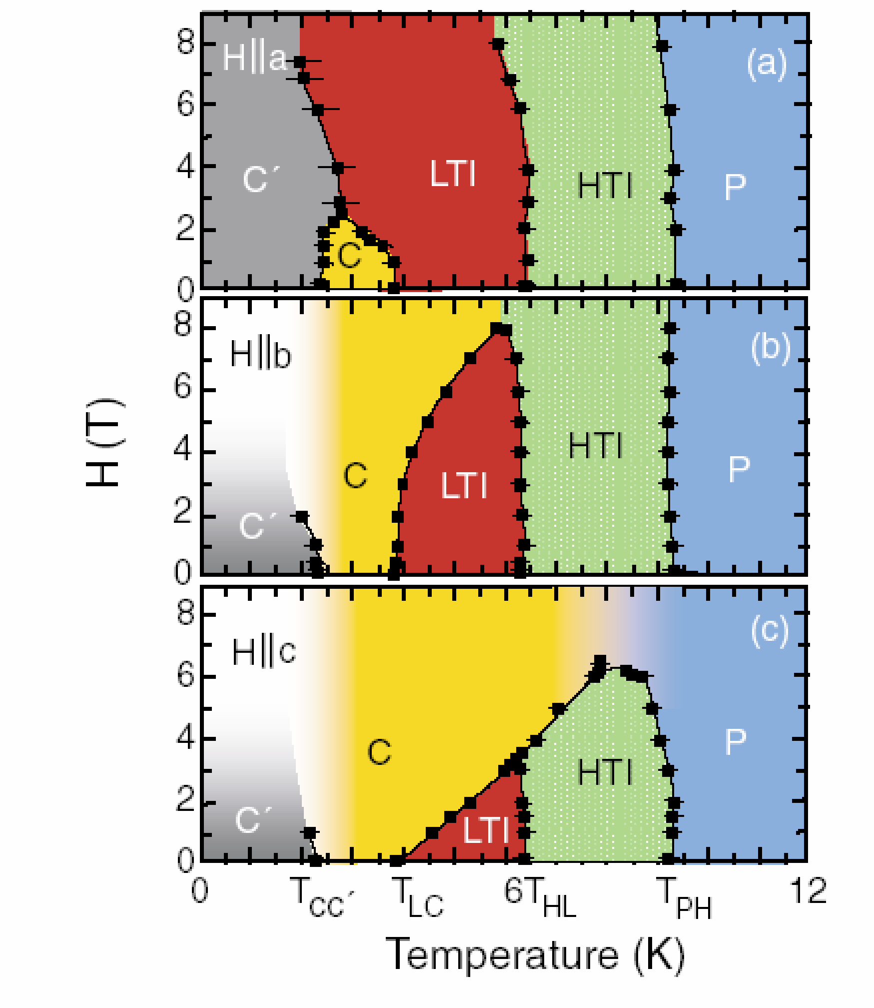
e.g., $LaTiO_3$ or $BaTiO_3$;



transition-metal oxides — $Ni_3V_2O_8$ $Co_3V_2O_8$

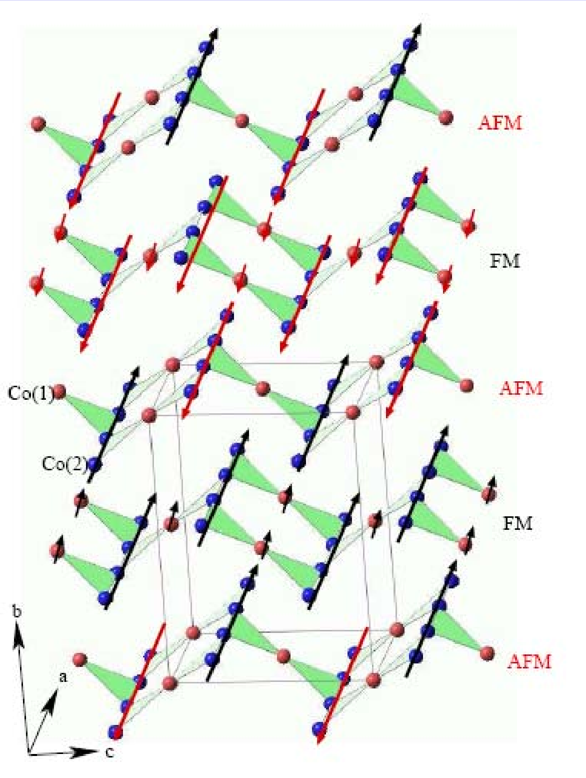
$Ni_3V_2O_8$ (NVO)

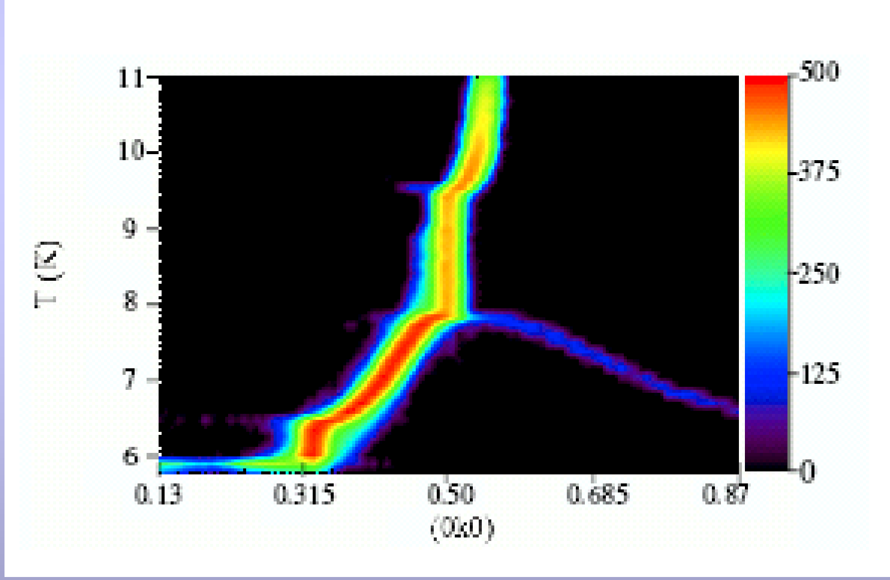




transition-metal oxides — $Ni_3V_2O_8$ $Co_3V_2O_8$

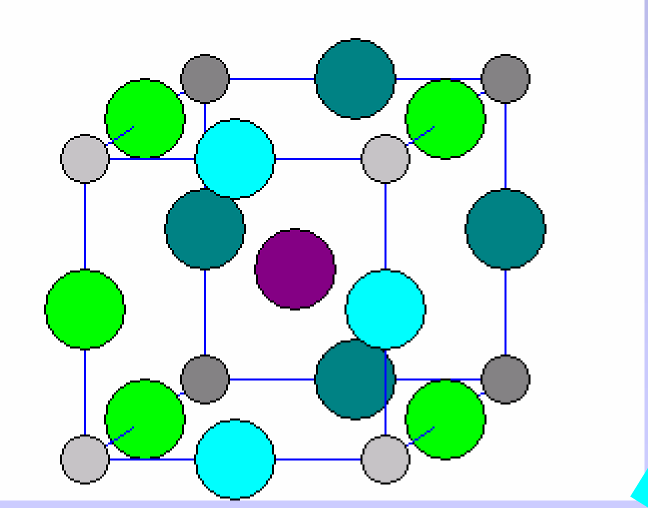
$Co_3V_2O_8$

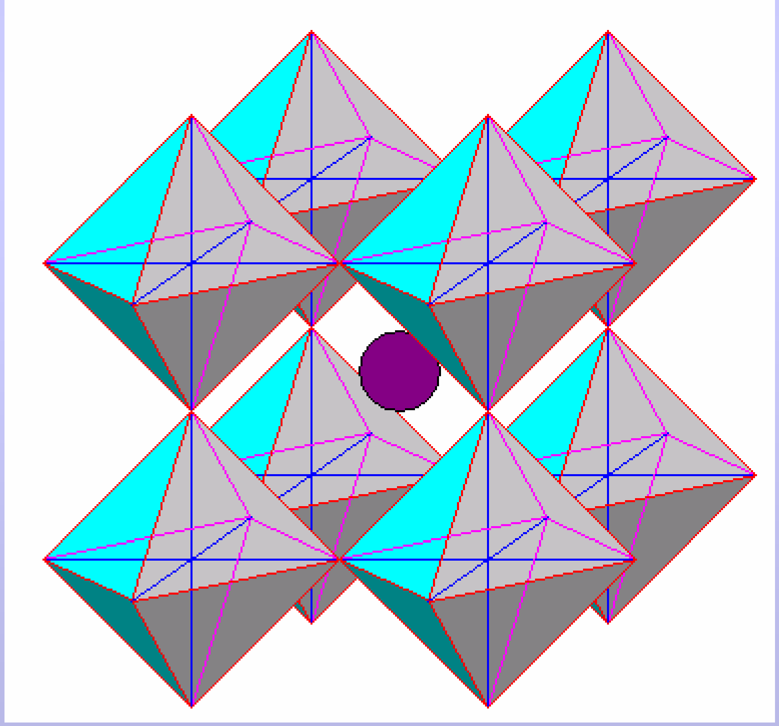




Sequence of incommensurate structures

perovskite structure



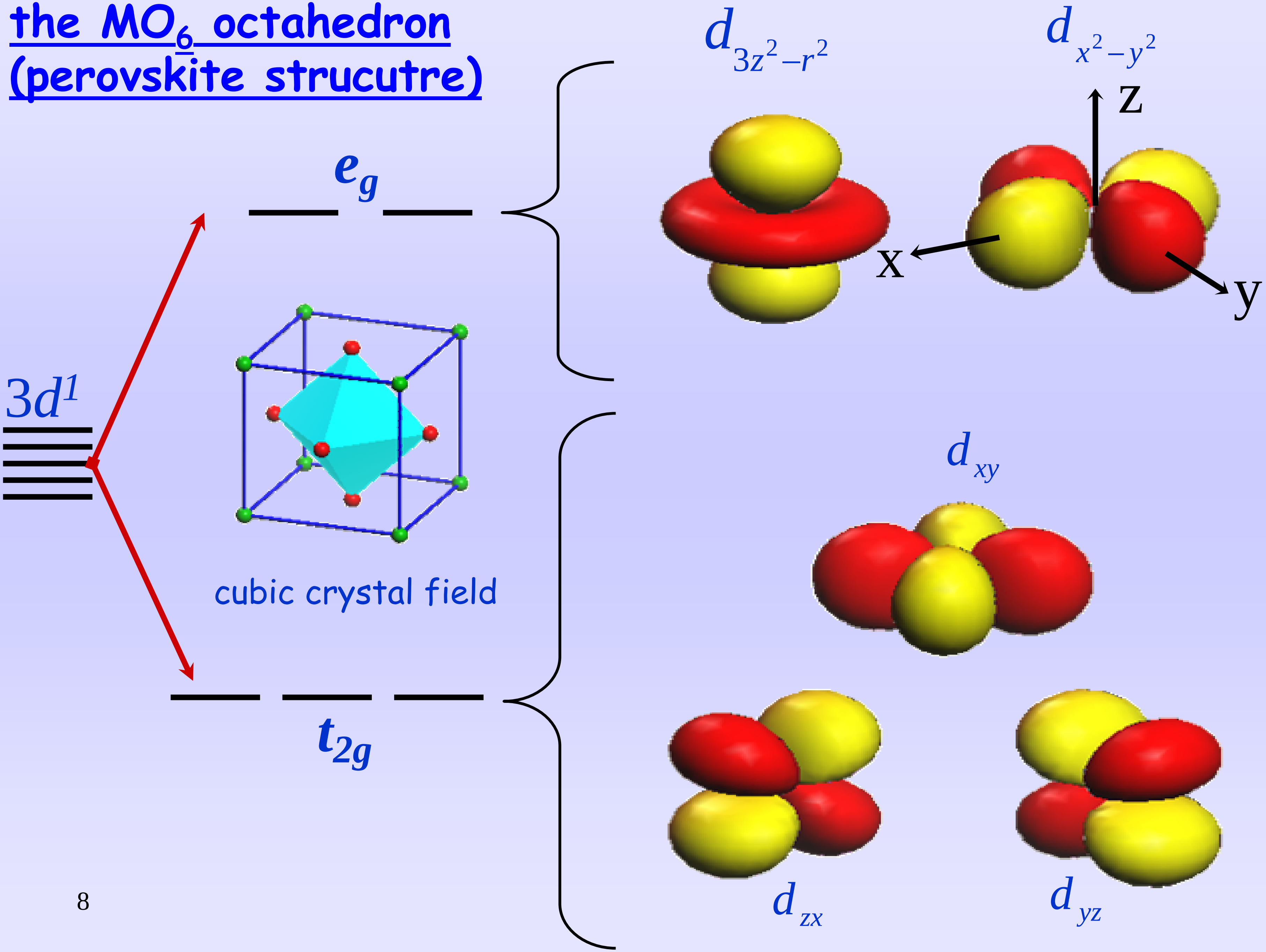


● oxygen

● rare earth

● transition metal

the MO_6 octahedron (perovskite strucutre)



$3d^1$

e_g

t_{2g}

cubic crystal field

$d_{3z^2-r^2}$

$d_{x^2-y^2}$

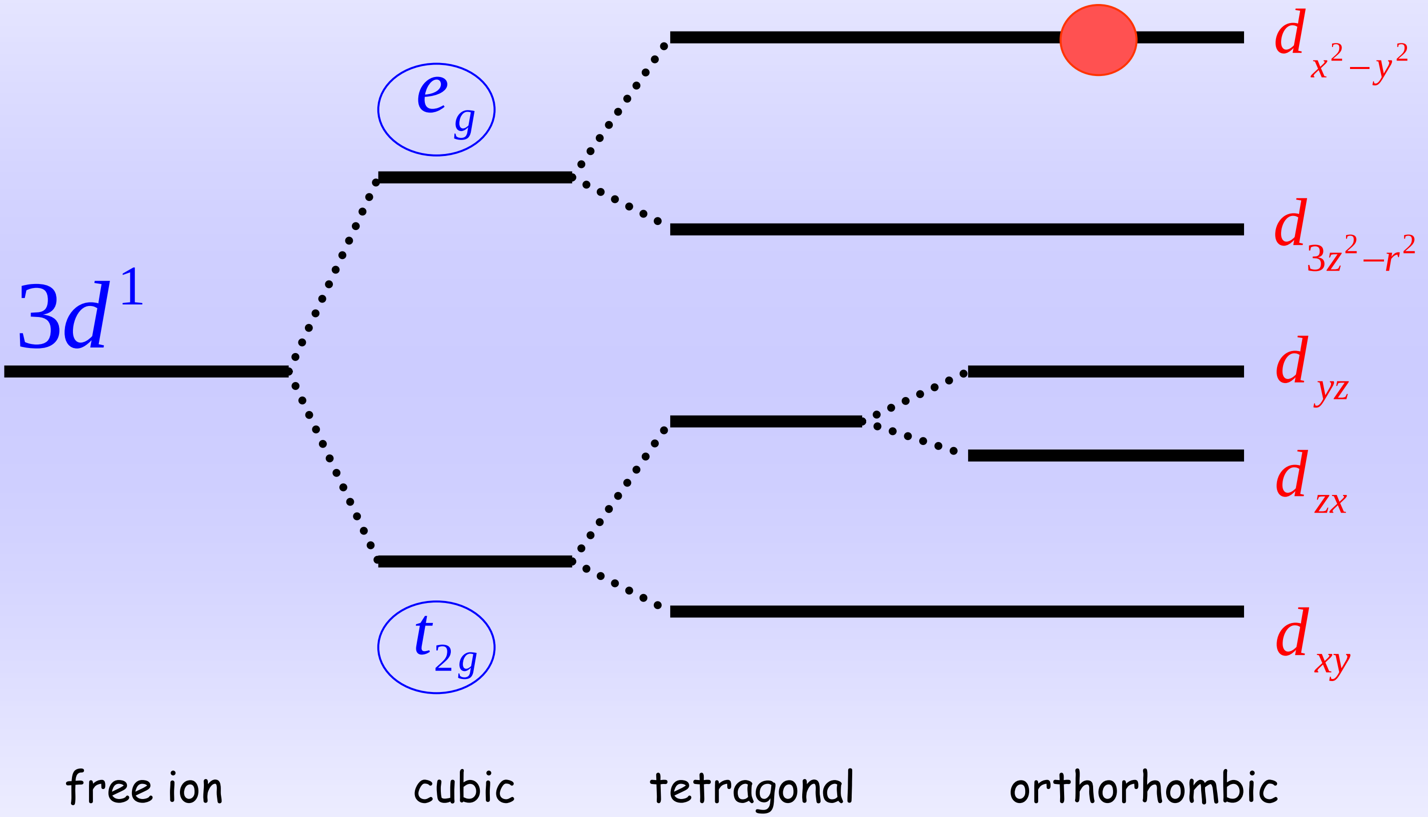
d_{xy}

d_{zx}

d_{yz}

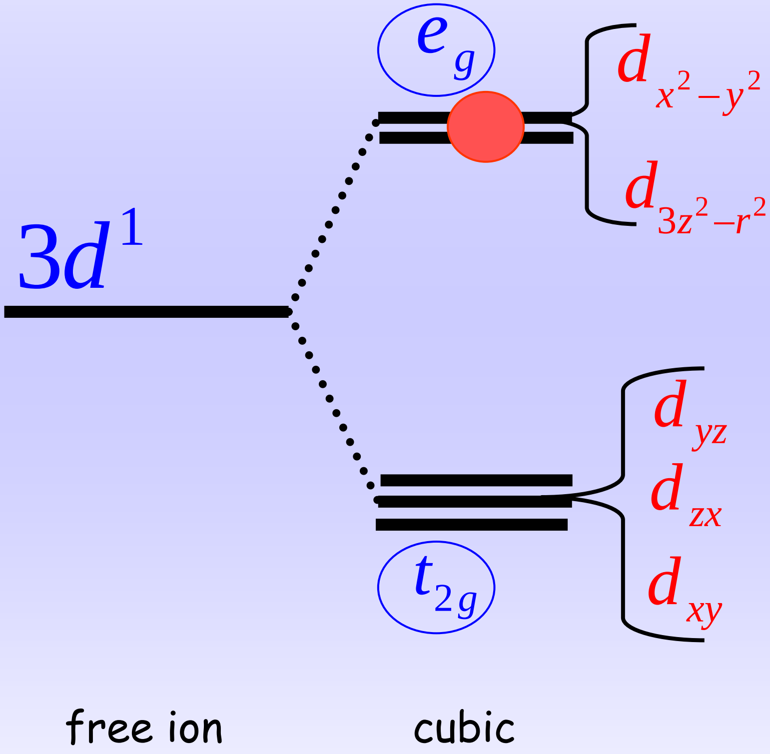
cuprates

crystal-field splitting of 3d orbitals—lifting of orbital degeneracy



9 d--electrons → **effective spin-only Hamiltonian, s=1/2**

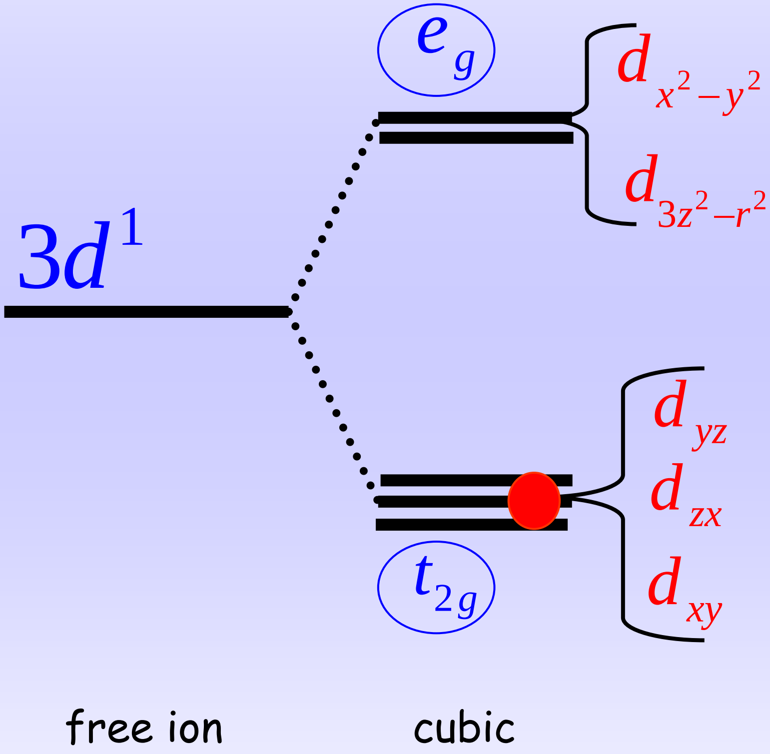
manganites



2 degenerate states

spin and orbital degrees of freedom

titanates



$LaTiO_3$:a single d electron, s=1/2

↓

spin and orbital degrees of freedom

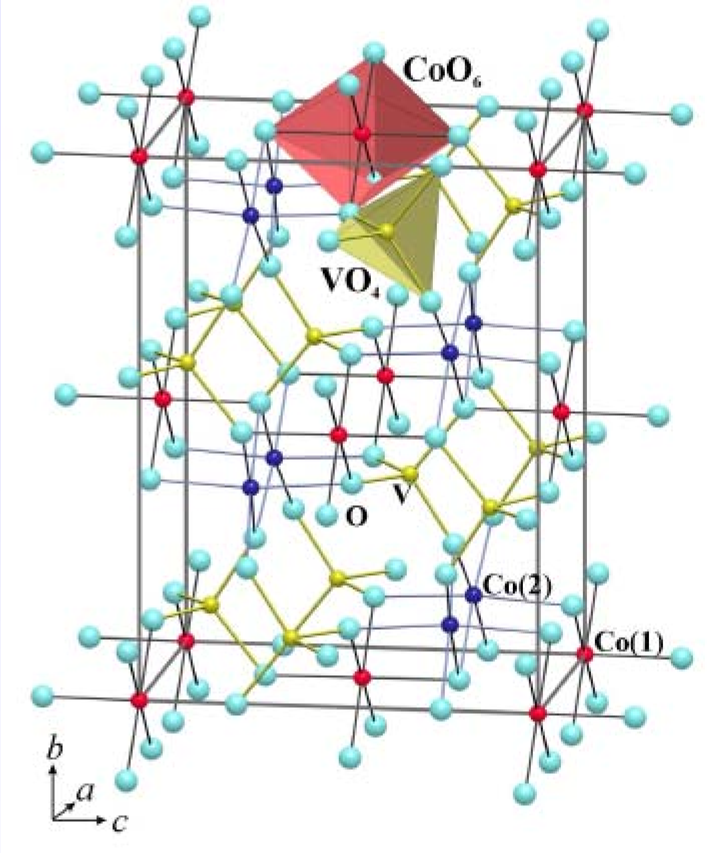
Also:

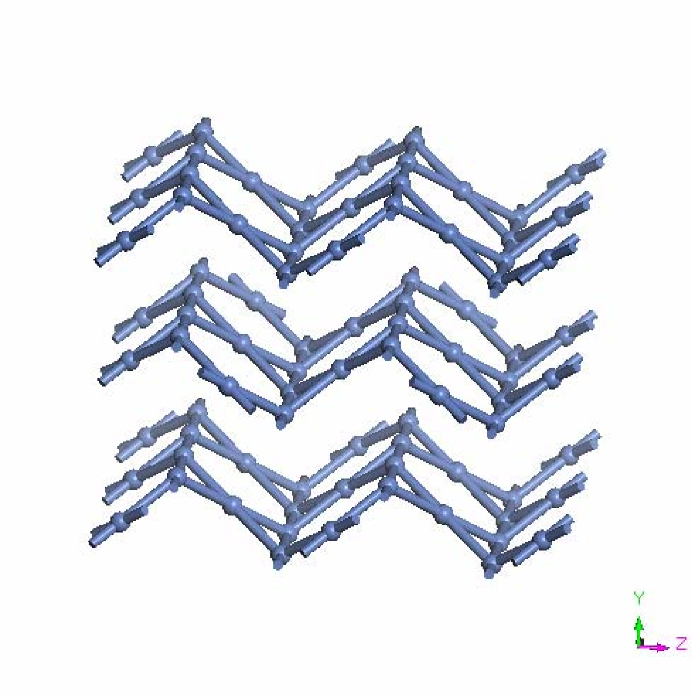
Buckled Kagome

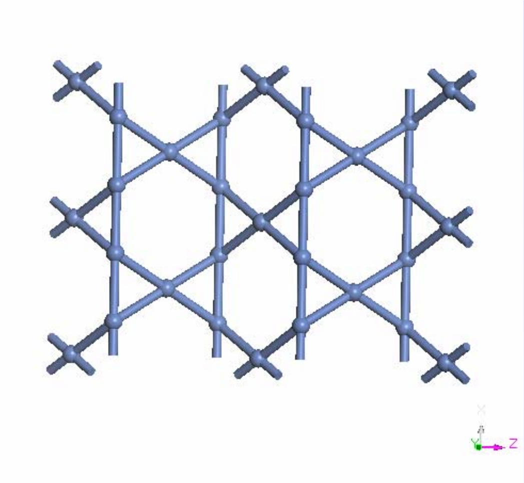
$Ni_3V_2O_8$ $Co_3V_2O_8$

S=1

S=3/2







General outline:

→ **Cuprates**

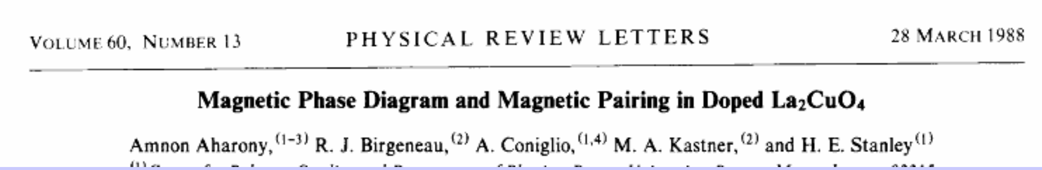
Vanadates

Titanates

References can be found at http://www.tau.ac.il/~aharony

CUPRATES

High-Tc materials exhibit interesting **phase diagrams**, with many potential **multicritical points**



VOLUME 60, NUMBER 13 PHYSICAL REVIEW LETTERS 28 MARCH 1988

Magnetic Phase Diagram and Magnetic Pairing in Doped La_2CuO_4

Amnon Aharony,(1-3) R. J. Birgeneau,(2) A. Coniglio,(1,4) M. A. Kastner,(2) and H. E. Stanley(1)

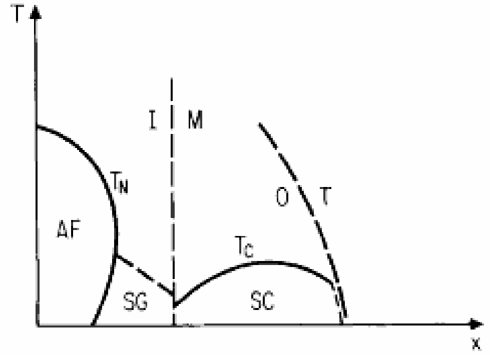


FIG. 1. Schematic phase diagram, as a function of hole concentration x. AF=antiferromagnetic; SG=spin-glass; I=insulator; M=metal; SC=superconductor; O=orthorhombic; T=tetragonal.

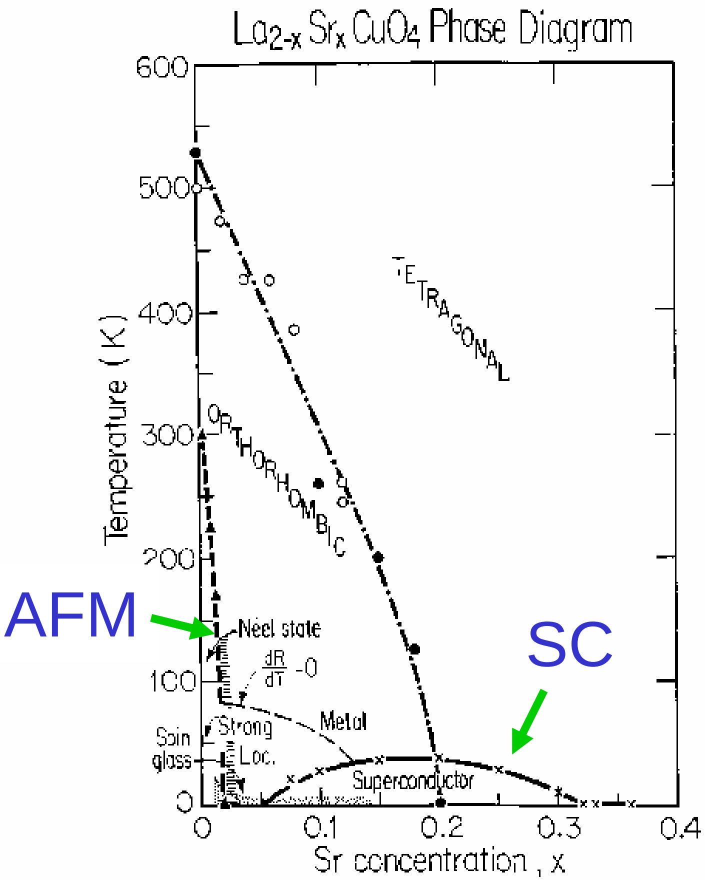
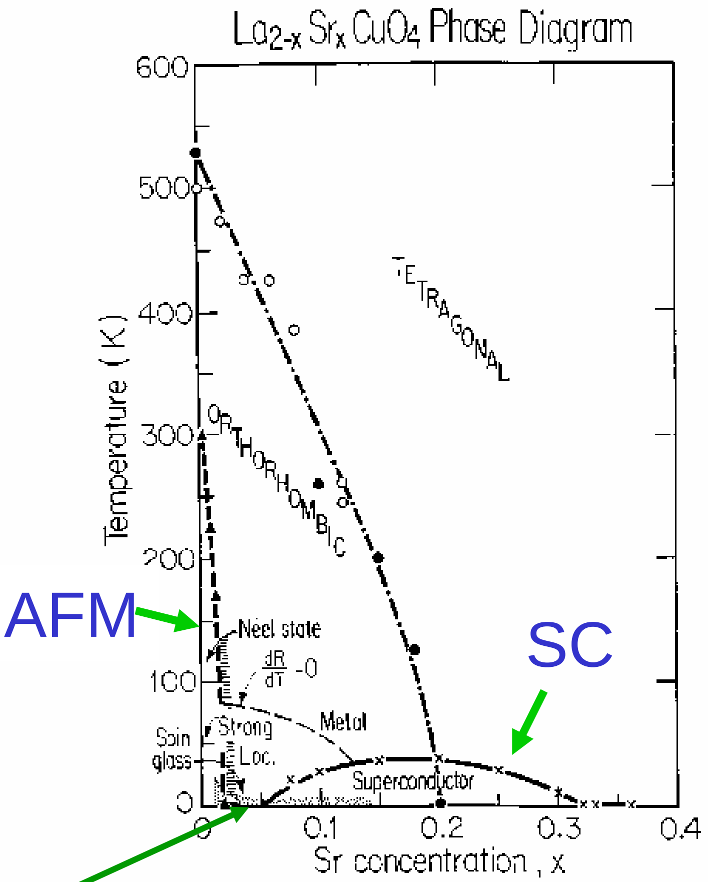


FIG. 1. Phase diagram for $La_{2-x}Sr_xCuO_4$ summarizing structural, magnetic, and transport properties. The narrow dashed line ($dR/dT = 0$) separates the region of metallic linear resistance from that of logarithmically increasing resistance. The conductance in the Néel state is strongly localized. From Keimer, Belk *et al.*, 1992.

High-Tc materials exhibit interesting **phase diagrams**, with many potential **multicritical points**

High temperature superconductivity
Srtuctural phase transitions
Low dimensionality: 2D to 3D xover
Quantum magnetism
Metal-Insulator transition
Spin glasses
Frustrated magnetism



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Incommensurate magnetism? Stripes?

Cuprates

Magnetic structure of cuprates (214, 2122): La_2CuO_4, $Sr_2CuCl_2O_2$, Pr_2CuO_4, Nd_2CuO_4

Frustrated sublattices (2342): $Sr_2Cu_3O_4Cl_2$

Theory: Superexchange ➡ Heisenberg model + anisotropies

Quantum fluctuations: Order out of disorder

Explain magnetic structures

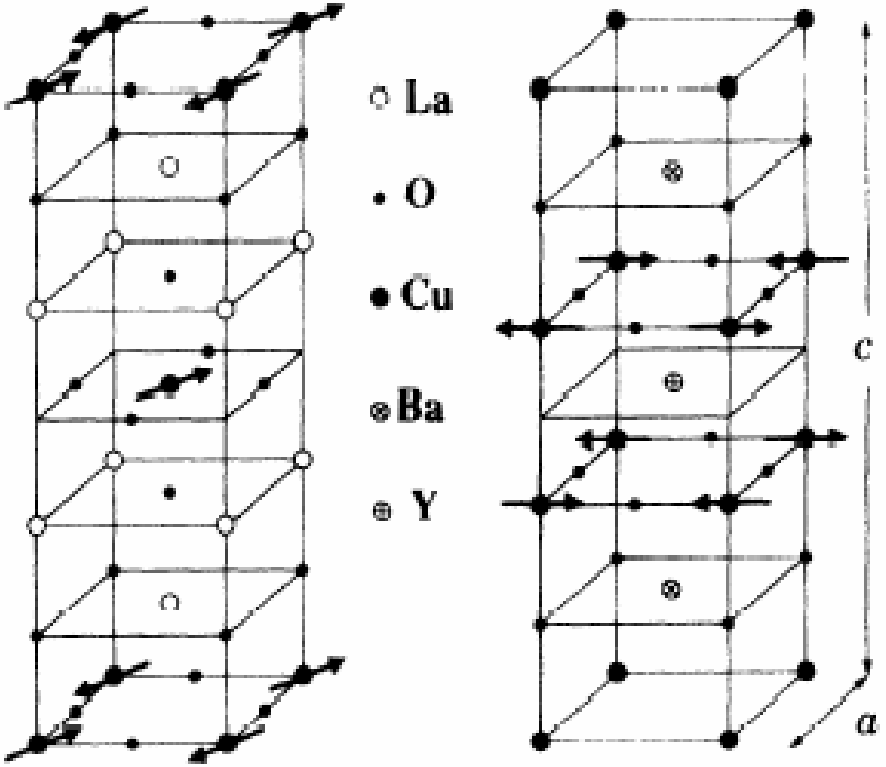
Explain magnetism in 2342

Relevance to ladders, chains?

References can be found at http://www.tau.ac.il/~aharony

LCO, 214

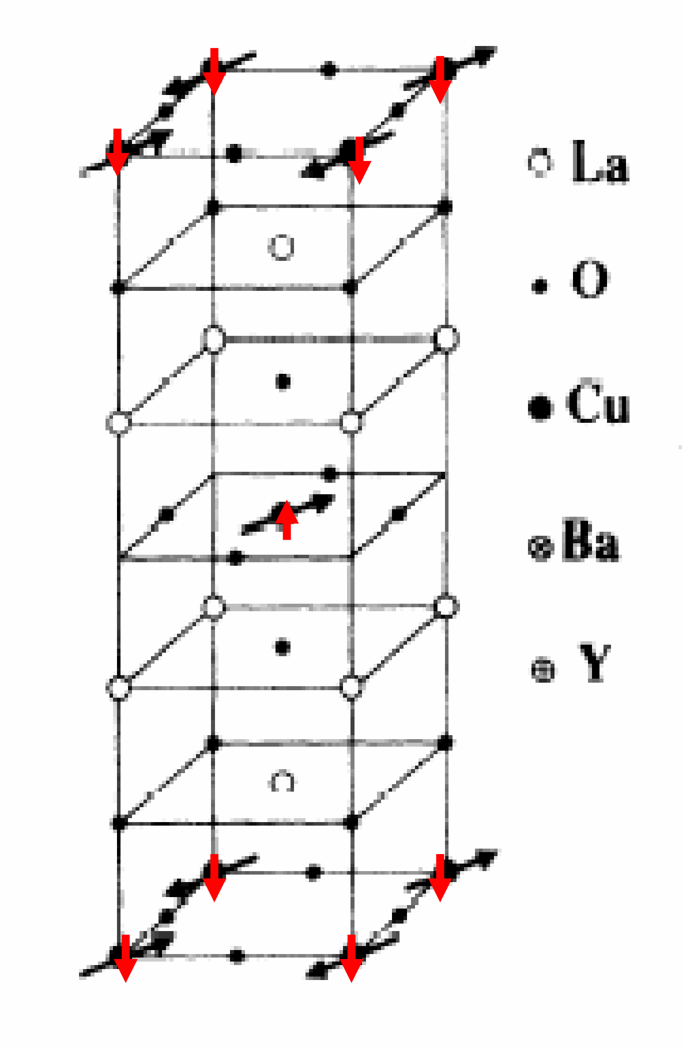
La_2CuO_4, $Sr_2CuCl_2O_2$:



YBCO, 123

What determines the easy axes for the spins (in plane and between planes)?

La_2CuO_4,



214: orthorhombic, **Weak ferromagnetism** in layers: flop with magnetic field

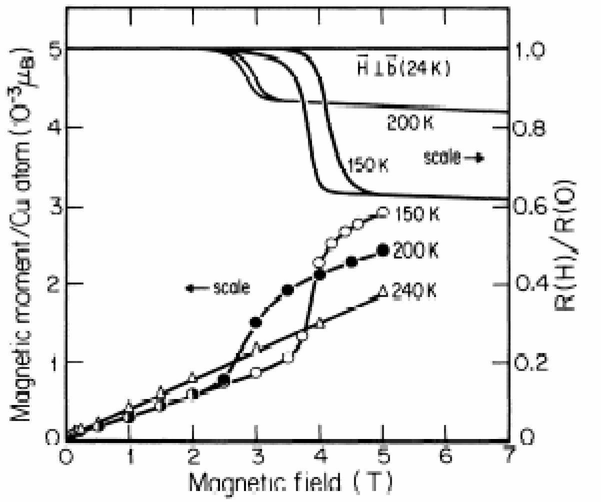
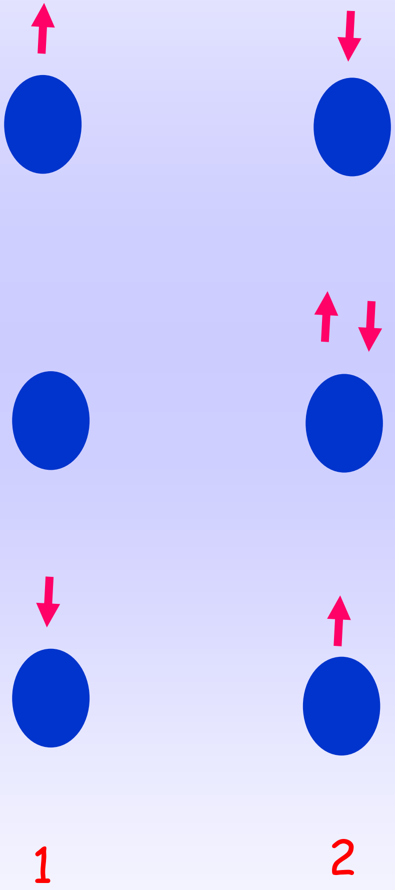


FIG. 1. Resistance and magnetic moment vs magnetic field in the *b* direction (except as noted).

FM moment proportional to staggered moment; spin flop

Simple theory: Super-exchange



Hubbard Hamiltonian:

$$H=\sum_{<ij>}\sum_{\sigma}t_{ij}c_{i\sigma}^{+}c_{j\sigma}+U\sum_{i}n_{i\uparrow}n_{i\downarrow}$$

$t<<U$ Perturb in *t*, keep low energy states

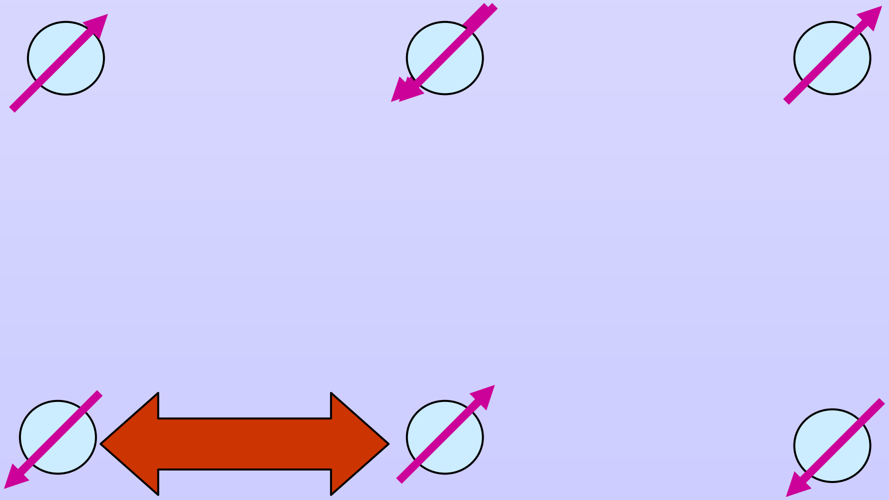
Heisenberg Hamiltonian:

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

$$J\approx\frac{t^2}{U}$$

ordered moment: $\leq\mu_B$

(the $U\to\infty$ manifold, each site has only a single electron)



Superexchange:

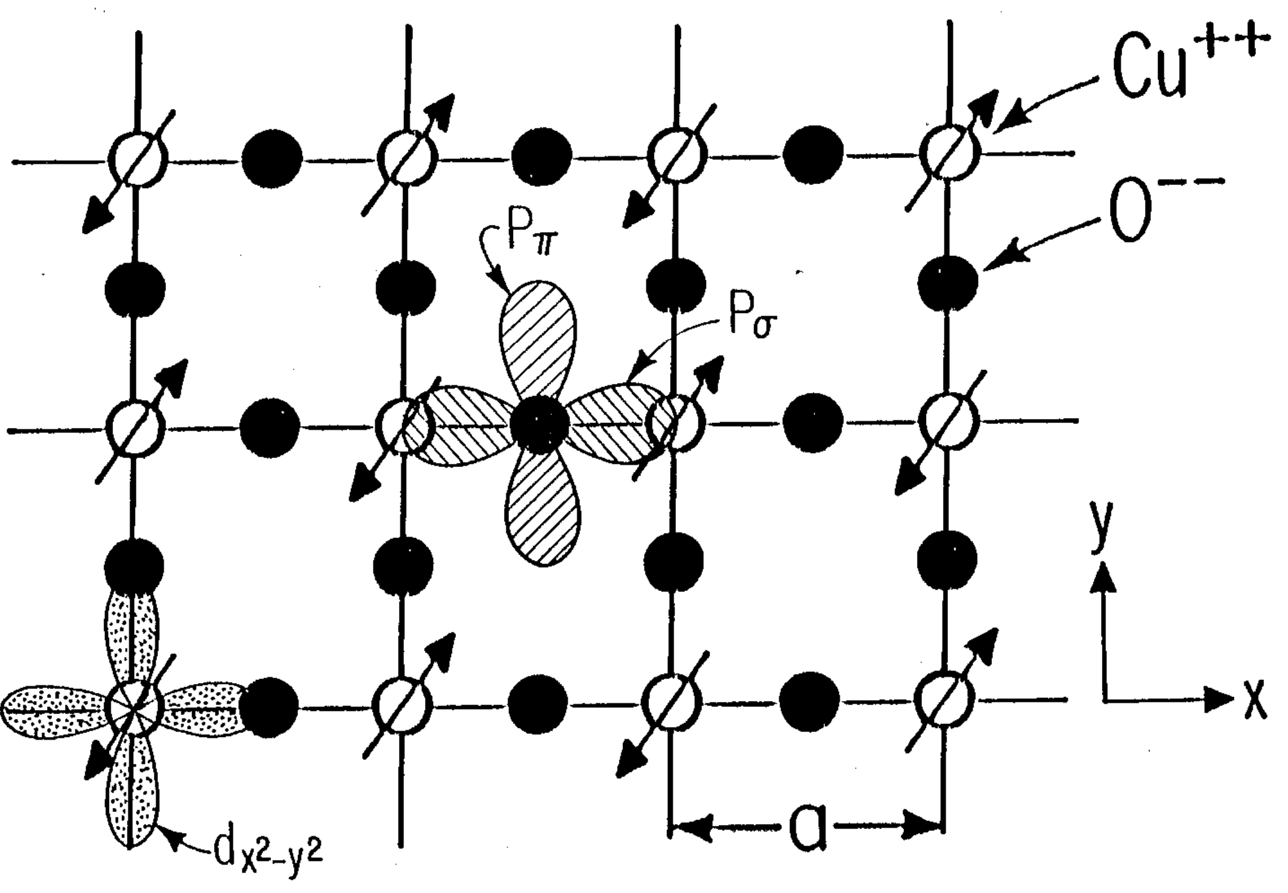
$$\mathcal{H} = J\mathbf{S}_1 \cdot \mathbf{S}_2$$

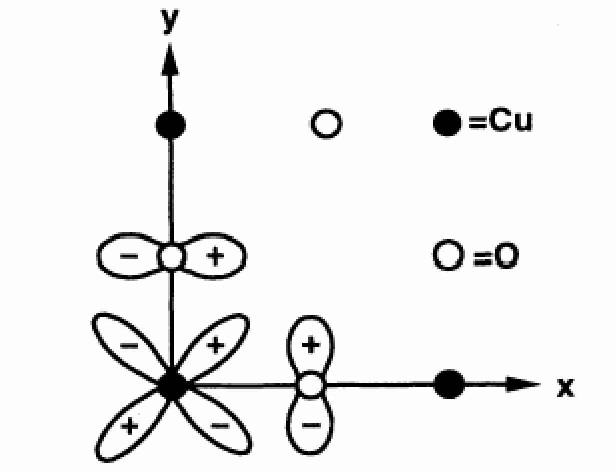
$$J = t^2 / U$$

No phase transition in the **2D isotropic** Heisenberg model??

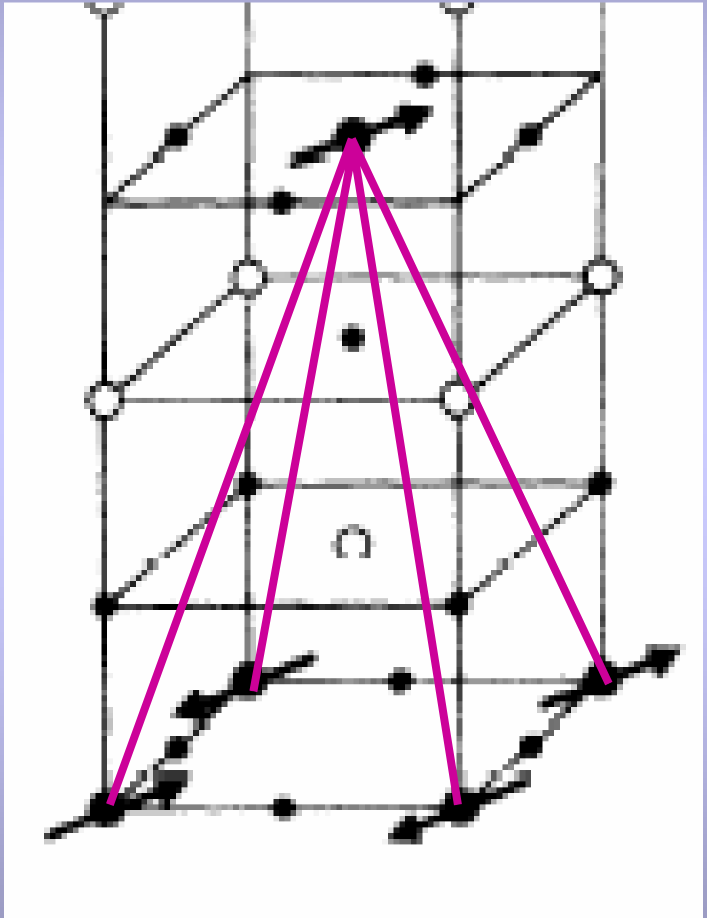
⇒

Order arises due to **small anisotropies** plus weak **interplane coupling**
Plus **quantum fluctuations!**


Cu++
O--
Pπ
Pσ
dx2-y2
y
x
a


y
=Cu
=O
−
+
−
+
+
−
+
−
x

Interplane **frustration** in **tetragonal** 2122



$Sr_2CuCl_2O_2$.

Pr_2CuO_4, Nd_2CuO_4

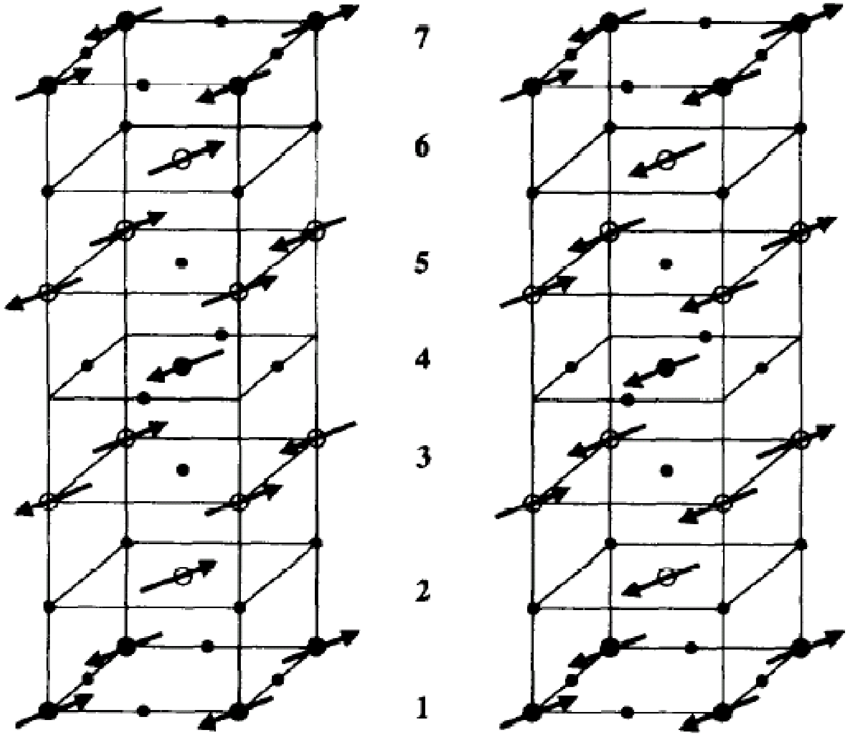
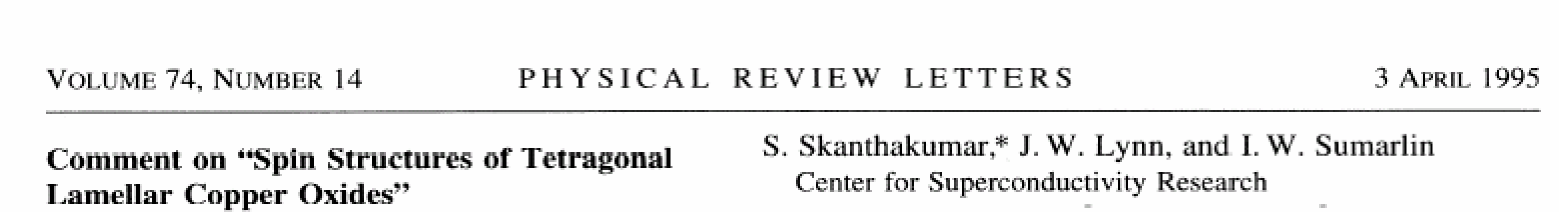


FIG. 2. Magnetic structure of Pr_2CuO_4 (left) and Nd_2CuO_4 (right) as for “214” in Fig. 1, except that open circles represent the rare earth ions.



VOLUME 74, NUMBER 14 PHYSICAL REVIEW LETTERS 3 APRIL 1995

Comment on "Spin Structures of Tetragonal Lamellar Copper Oxides"

S. Skanthakumar,* J. W. Lynn, and I. W. Sumarlin
Center for Superconductivity Research

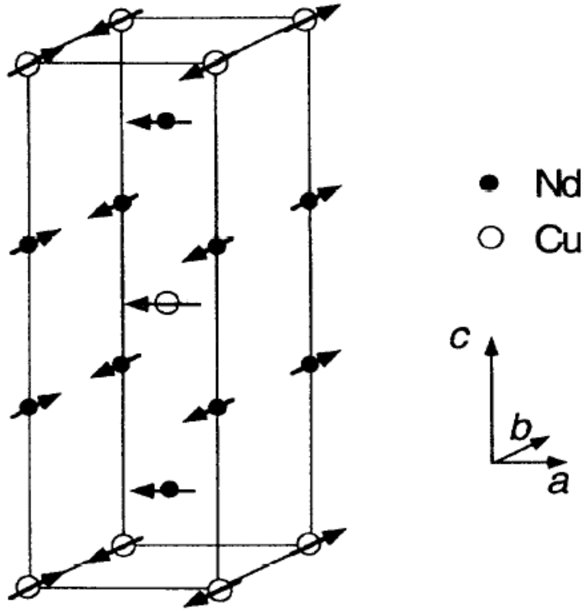
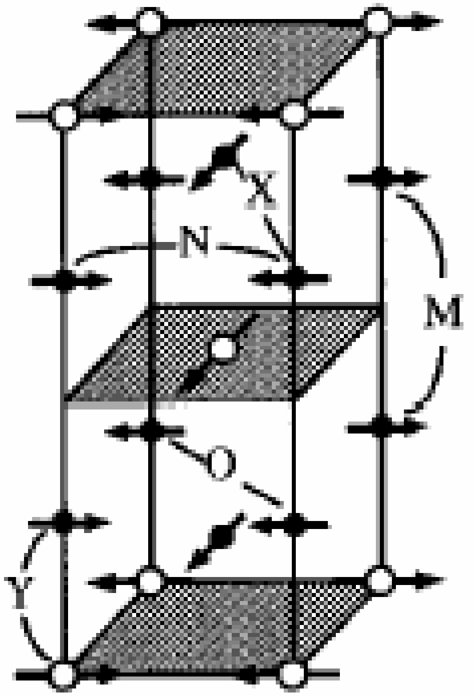
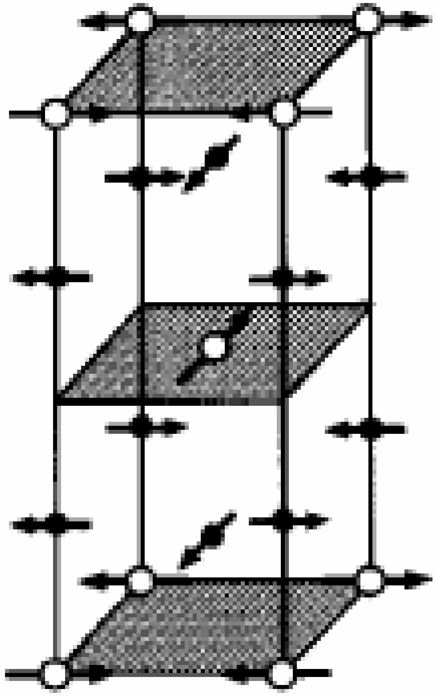


FIG. 1. The Cu spins occupy a bct lattice, and form a noncollinear magnetic structure in which the spin direction alternates between (100) and (010) as one proceeds along the *c* axis. The Nd magnetic structure observed at low temperature is also noncollinear, and is shown for completeness.

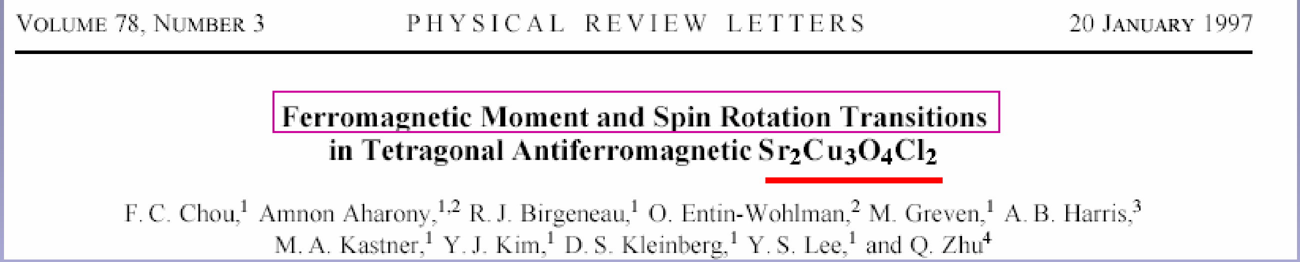
Pr_2CuO_4, Nd_2CuO_4



(a) Noncollinear Phase I&III



(b) Noncollinear Phase II

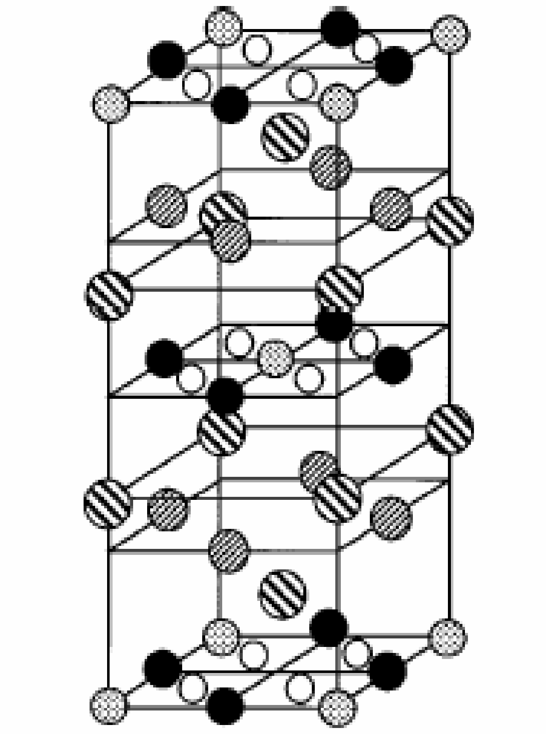


VOLUME 78, NUMBER 3 PHYSICAL REVIEW LETTERS 20 JANUARY 1997

Ferromagnetic Moment and Spin Rotation Transitions in Tetragonal Antiferromagnetic $Sr_2Cu_3O_4Cl_2$

F. C. Chou,[1] Amnon Aharony,[1,2] R. J. Birgeneau,[1] O. Entin-Wohlman,[2] M. Greven,[1] A. B. Harris,[3]
M. A. Kastner,[1] Y. J. Kim,[1] D. S. Kleinberg,[1] Y. S. Lee,[1] and Q. Zhu[4]

2342



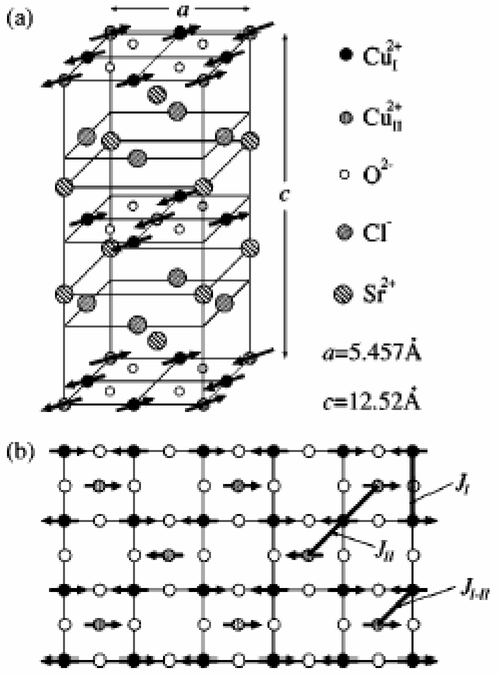
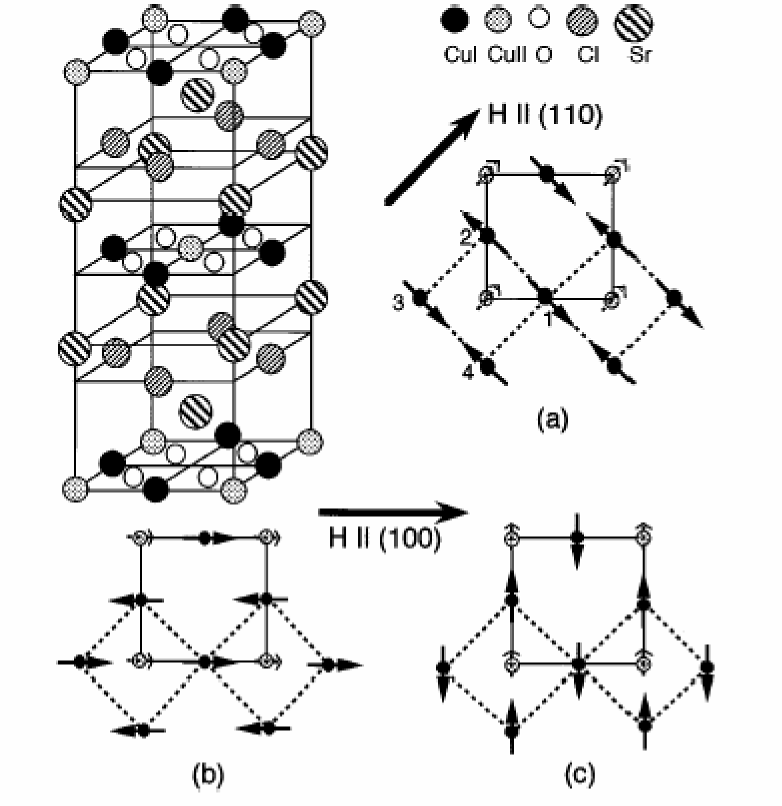


FIG. 1. (a) Crystal and magnetic structure of $Sr_2Cu_3O_4Cl_2$. Ordered spin directions for copper spins are shown as arrows. (b) Cu_3O_4 plane and various exchange interactions between spins.

2 decoupled AFM sublattices: **frustration**



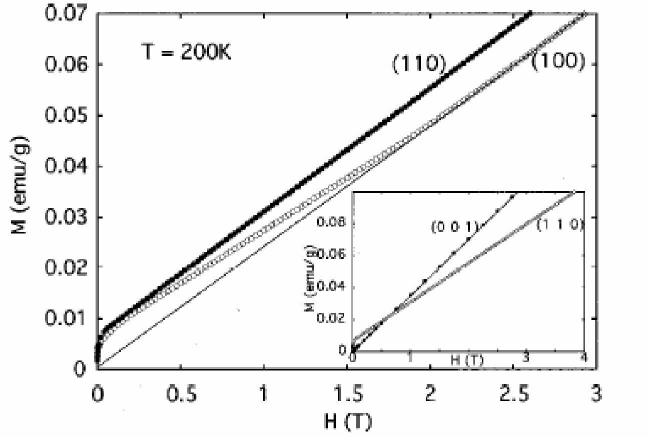


FIG. 3. Magnetic moment M vs H for $\mathbf{H}\|(110)$ and (100) at 200 K. The inset compares M for $\mathbf{H}\|(110)$ and $\mathbf{H}\|(001)$.

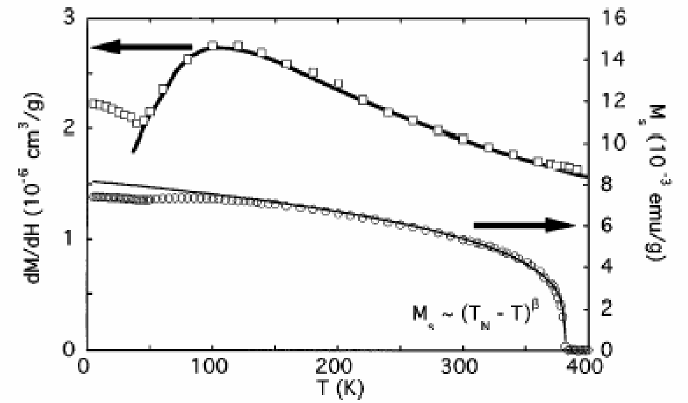
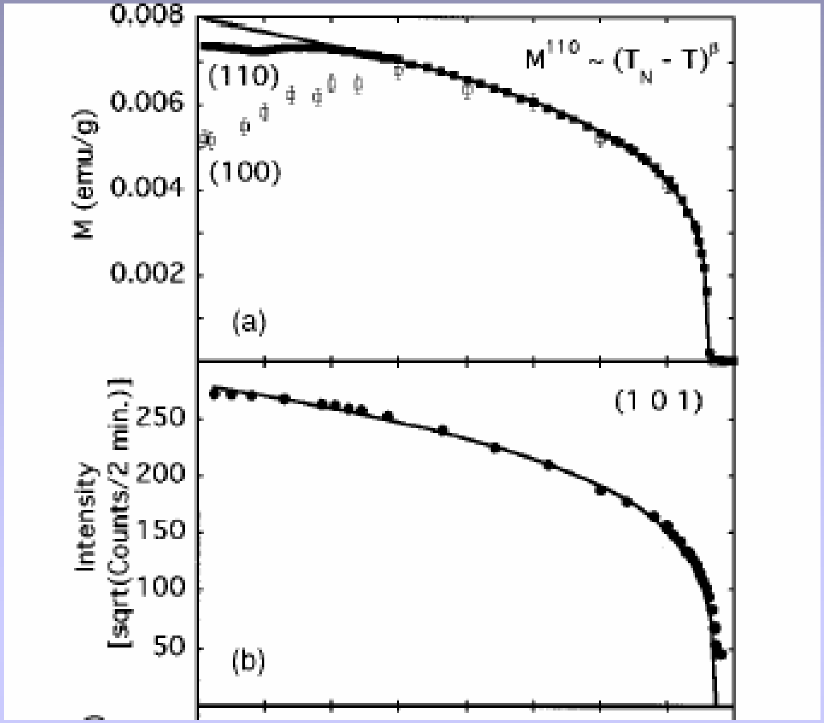


FIG. 2. Saturated FM moment $M_S^{(110)}$ and susceptibility $\chi^{(110)}$. The full lines represent $M_S \sim (T_{N,\mathrm{I}} - T)^\beta$ and a simulation of χ_{II} for the $S = 1/2$ SLQHA (see text).



Weak **FM moment** proportional to **staggered AFM moment!**

VOLUME 83, NUMBER 4 PHYSICAL REVIEW LETTERS 26 JULY 1999

Ordering due to Quantum Fluctuations in $Sr_2Cu_3O_4Cl_2$

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A. B. Harris,[5] M. A. Kastner,[1] I. Ya. Korenblit,[3] Y. S. Lee,[1] and G. Shirane[6]

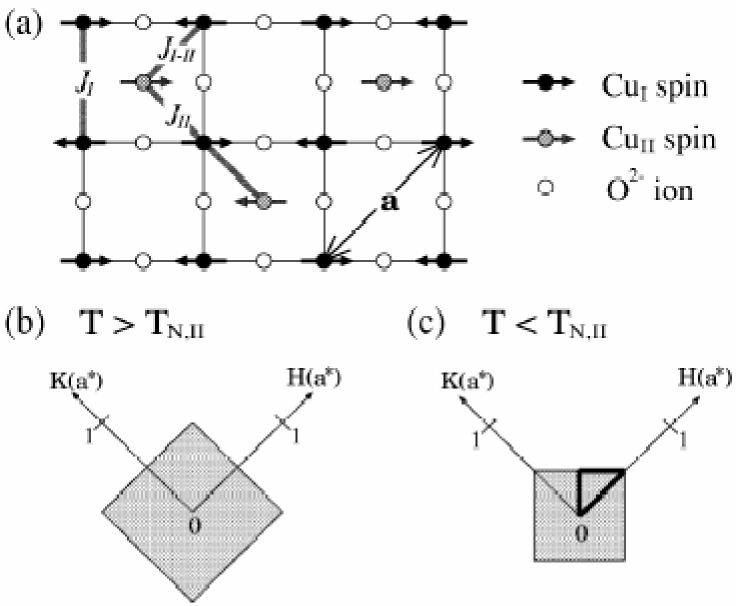

FIG. 1. (a) Magnetic structure of the Cu_3O_4 plane in 2342 at $T < T_{N,II}$. The corresponding 2D reciprocal lattices are shown in (b) for $T > T_{N,II}$, and in (c) for $T < T_{N,II}$. The shaded area is the 2D Brillouin zone.

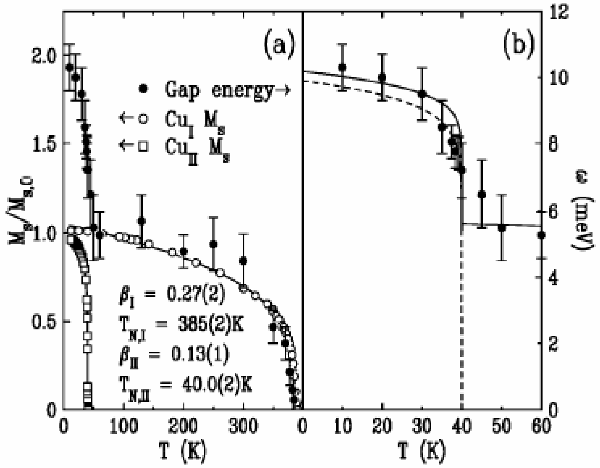

FIG. 2. (a) Temperature dependence of the Cu_I out-of-plane gap energy and of the staggered magnetizations M_s of Cu_I and

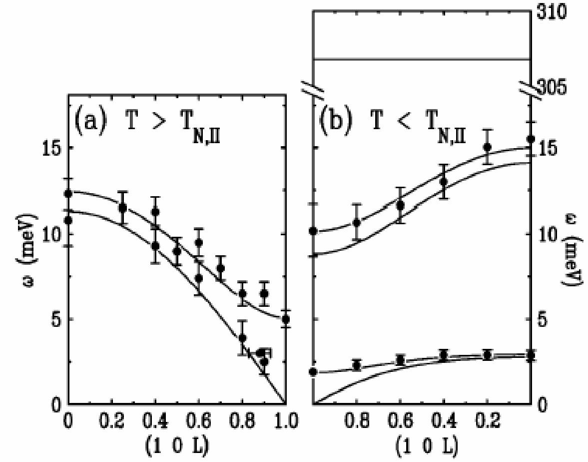

FIG. 3. (a) Magnon dispersion along the L direction at the 2D zone center for $T = 200$ K (solid circles). (b) Same for $T = 10$ K. The solid lines show Eq. (2).

THE END

(More tomorrow)