Main Collaborators

G. Alvarez (FSU) J. Burgy (FSU)

T. Hotta (Tokai) M. Mayr (Max Planck)

A. Moreo (FSU) S. Yunoki (Trieste)

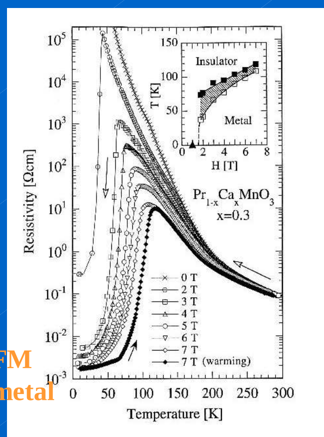
Other collaborators: Aliaga, Arispe, Capponi, Feiguin, Furukawa, Hallberg, Hu, Koizumi, Malvezzi, Martin-Mayor, Moraghebi, Poilblanc, Riera, Takada, Xavier, Verges

Huge worldwide effort in manganites!

Hundreds of references in: E. Dagotto, ``Nanoscale Phase Separation and Colossal Magnetoresistance'' Springer-Verlag, Berlin, Oct. 2002

ITP, Nov. 2002

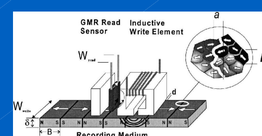
Motivation I: Colossal Magnetoresistance (CMR)



FM metal

- Drastic reduction of resistivity with small magnetic fields.
- Potential application in "read sensors"?

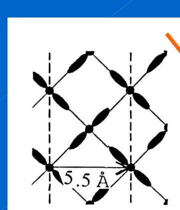
Tomioka and Tokura, (1999).



ITP, Nov. 2002

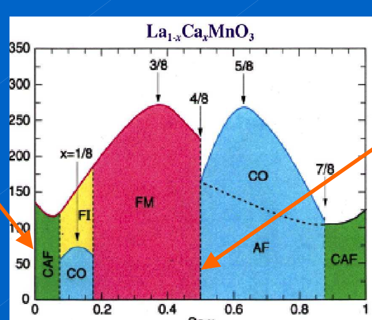
Motivation II:

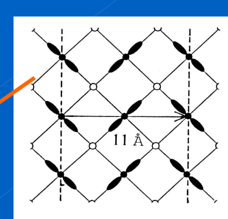
- Understand the complex phase diagram that experiments are unveiling.



A-type AF
Orbital order

T



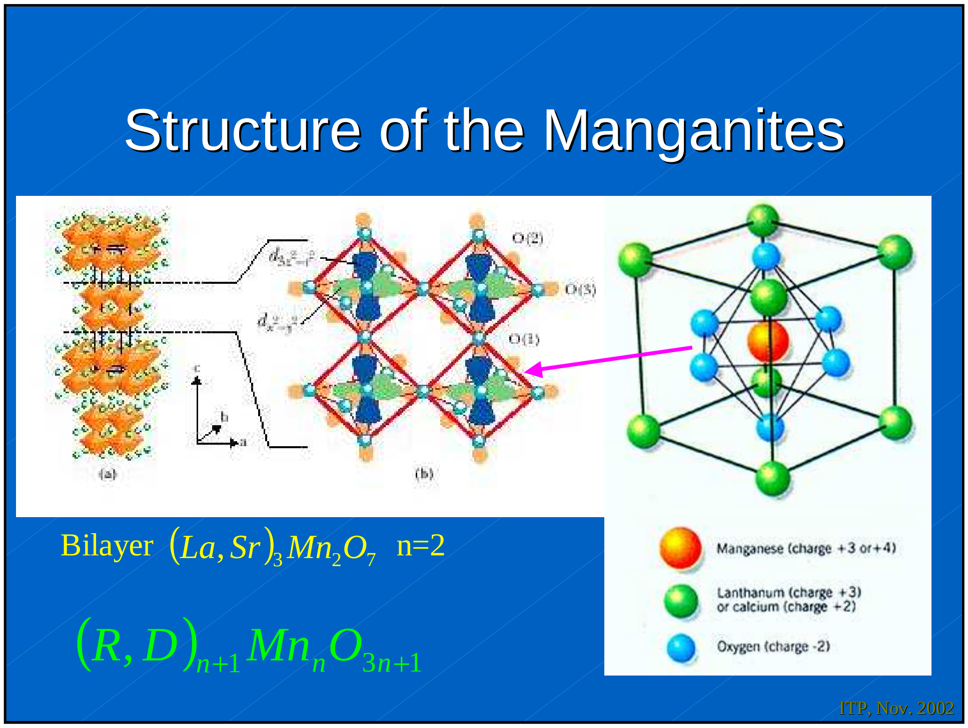


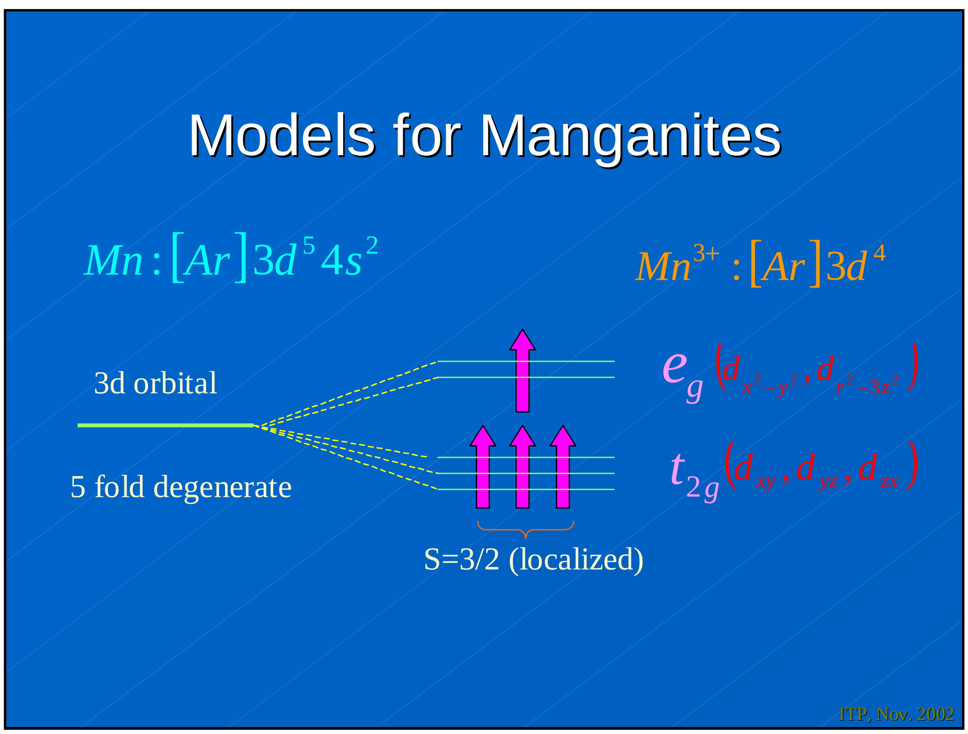
CE-type
Spin/charge/orbital order

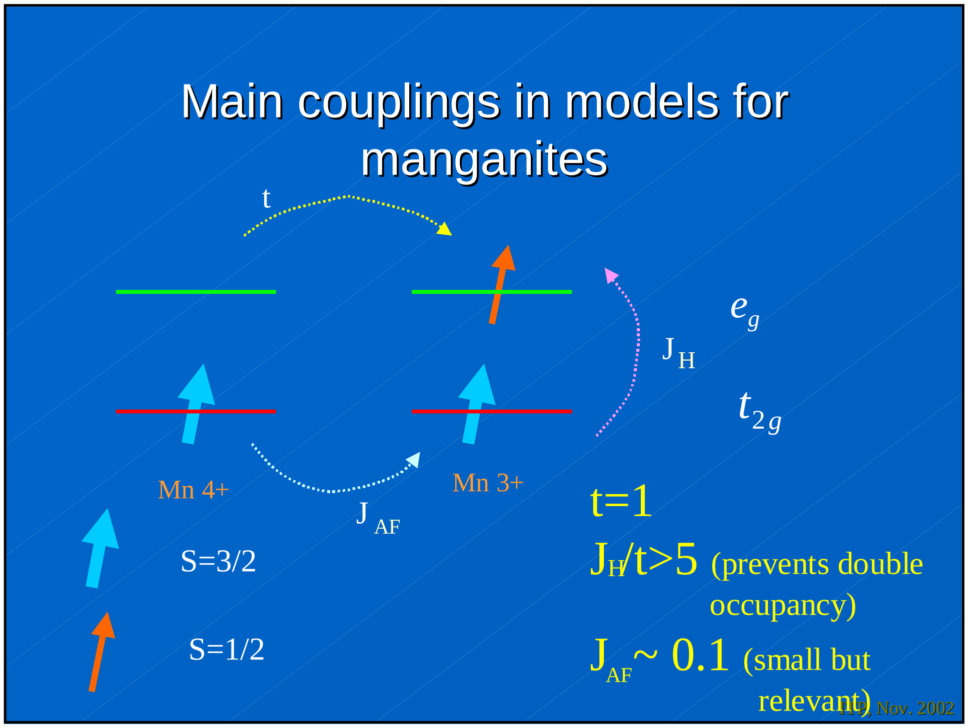
Cheong et al., Schiffer et al.

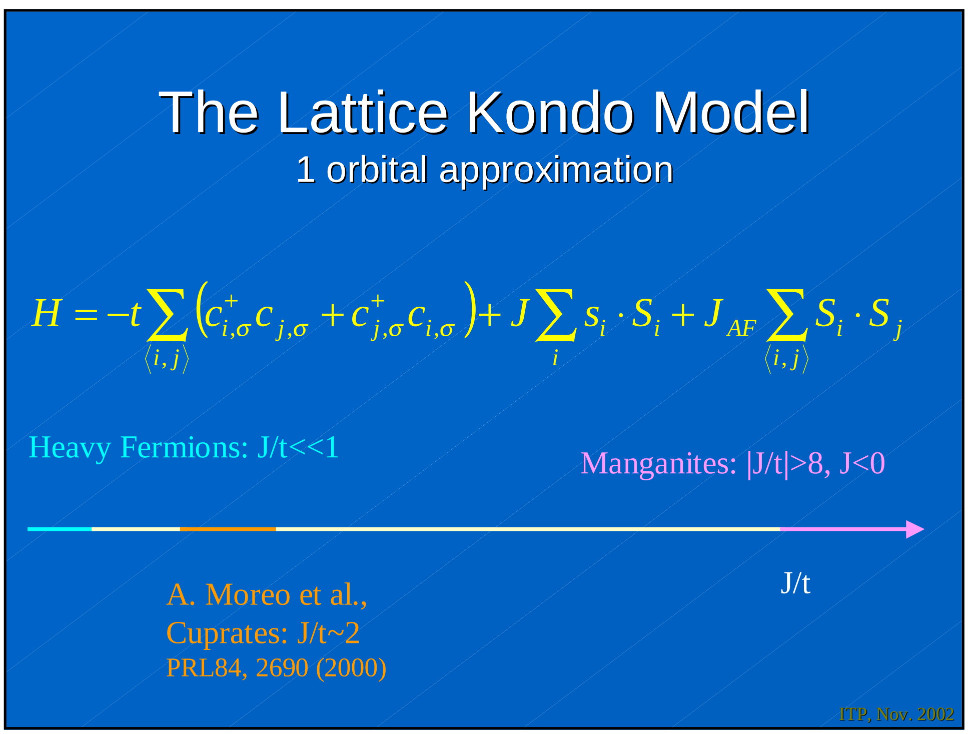
Fraction of holes

ITP, Nov. 2002


Structure of the Manganites
O(2)
O(3)
O(1)
(a)
(b)
Bilayer $(La,Sr)_3Mn_2O_7$ n=2
$(R,D)_{n+1}Mn_nO_{3n+1}$
Manganese (charge +3 or+4)
Lanthanum (charge +3) or calcium (charge +2)
Oxygen (charge -2)
ITP, Nov. 2002

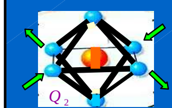

Models for Manganites
$Mn:[Ar]3d^5 4s^2$
$Mn^{3+}:[Ar]3d^4$
3d orbital
5 fold degenerate
$e_g\left(d_{x^2-y^2}, d_{r^2-3z^2}\right)$
$t_{2g}\left(d_{xy}, d_{yz}, d_{zx}\right)$
S=3/2 (localized)
ITP, Nov. 2002


Main couplings in models for manganites
t
e_g
J_H
t_{2g}
Mn 4+
Mn 3+
J_{AF}
S=3/2
S=1/2
t=1
$J_H/t>5$ (prevents double occupancy)
$J_{AF}\sim 0.1$ (small but relevant)
ITP, Nov. 2002

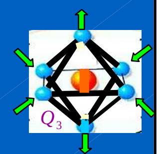

The Lattice Kondo Model
1 orbital approximation
$H = -t\sum_{\langle i,j\rangle}\left(c^{+}_{i,\sigma}c_{j,\sigma} + c^{+}_{j,\sigma}c_{i,\sigma}\right) + J\sum_{i} s_i \cdot S_i + J_{AF}\sum_{\langle i,j\rangle} S_i \cdot S_j$
Heavy Fermions: J/t<<1
Manganites: |J/t|>8, J<0
J/t
A. Moreo et al., Cuprates: J/t~2
PRL84, 2690 (2000)
ITP, Nov. 2002

Two Orbitals plus Jahn-Teller phonons (Kanamori, Millis)

$$H = -\sum_{\langle i,j\rangle,a,b,\sigma} t_{ij}^{ab} c_{ia,\sigma}^{+} c_{jb,\sigma} - J_H \sum_{i,a,\sigma} S_i \cdot c_{ia,\sigma}^{+} \vec{\sigma}\, c_{ia,\sigma} +$$



$$+ g \sum_{i,a,\sigma} c_{ia,\sigma}^{+} Q^{ab}(i) c_{ib,\sigma} + \frac{k}{2} \sum_i tr\, Q^2(i)$$



$$Q = \begin{pmatrix} Q_3 & Q_2 \\ Q_2 & -Q_3 \end{pmatrix}$$

g: electron-phonon coupling

k: phonon stiffness

$$\lambda = g / \sqrt{k}$$

ITP, Nov. 2002

Computational Techniques

- Partition Function

phonons, t_{2g} spins, e_g electrons

$$Z = \int DQ \int DS\, tr_{e_g}\left(e^{-\beta H}\right)$$

$$S_i = \left(\sin\theta_i \cos\phi_i, \sin\theta_i \sin\phi_i, \cos\theta_i\right)$$

•Monte Carlo simulation over classical spins. Quantum itinerant electrons treated exactly.

•No sign problems. All temperatures and densities are accessible.

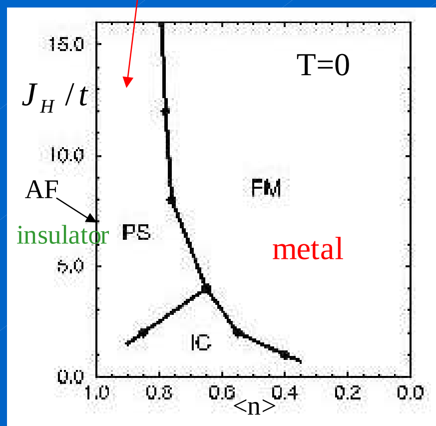
•Classical approximation tested in 1D comparing with Lanczos.

•Dynamical properties can be calculated straightforwardly.

ITP, Nov. 2002

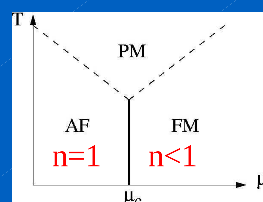
AF As observed experimentally (see later)

Results



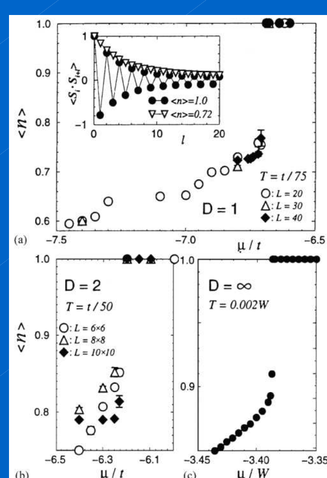
Yunoki et al. PRL80, 845 (1998).

- FM, AF , Phase Separation and Spin Incommensuration observed.
- No canted states in this model.



ITP, Nov. 2002

Monte Carlo and DMFT evidence of phase separation in 1-orbital model



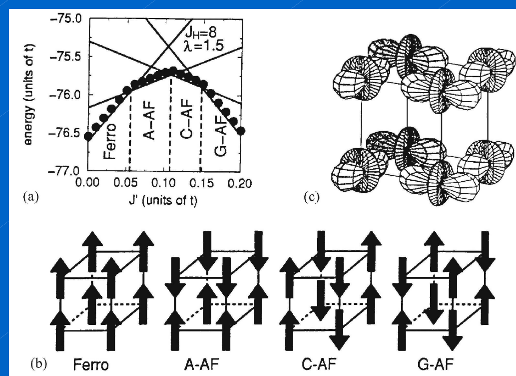
Phase separation manifests as a discontinuity in density vs. chemical potential.
It appears in all dimensions investigated .

Yunoki, Furukawa, et al., PRL 98. See also Guinea, Arovas, …

Similar in spirit to the phase separation found in the t-J model, although there it involves SC and AF.

ITP, Nov. 2002

Orbital and Spin order at x=0



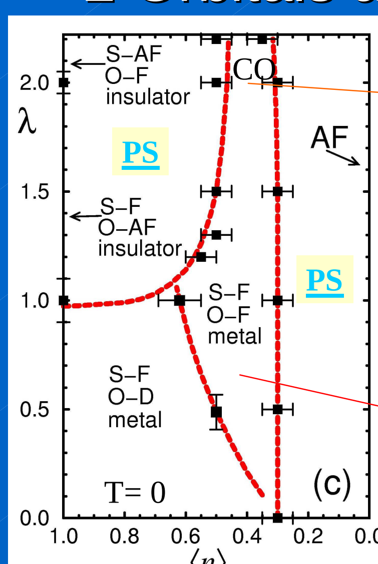
Hotta et al.
PRB 60, R15009 (1999)

Spin and orbital order at x=0

Many states close in energy => JAF is much relevant

ITP, Nov. 2002

2 Orbitals and J-T Phonons



Precursor of CE

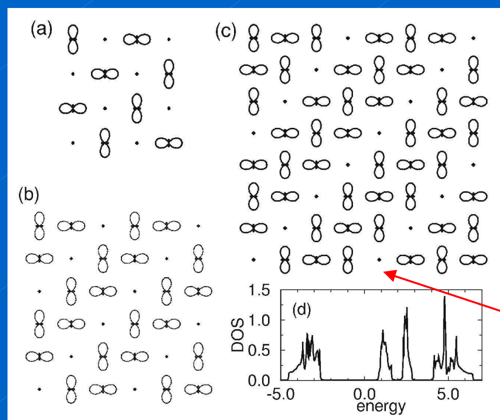
- All the stable phases observed experimentally are obtained.
- PS very prominent as in 1 orbital model.

Precursor of A-type AF

Yunoki et al.,
PRL 81, 5612 (1998)

ITP, Nov. 2002

Stripes exist as the ground state at large e-JT coupling



Ferromagnetic phase.

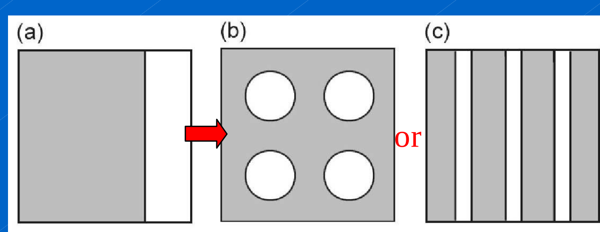
Hotta et al.
PRL86, 4922 (2001)

More about new phases later!

Pi-shift in orbital order. 1/r not needed.

ITP, Nov. 2002

Influence of 1/r Coulomb interaction



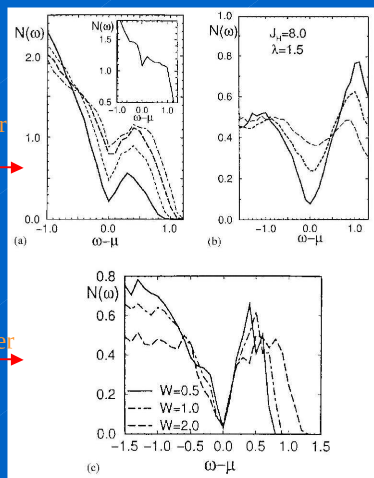
- Droplets, stripes or other nanometer size patterns may form (as in studies of high Tc and stripes, by many authors).
- In 1D the PS state evolved into CDW state with increasing repulsion (Malvezzi et al. PRB '99).

ITP, Nov. 2002

Pseudogap in simulations

No disorder

With disorder

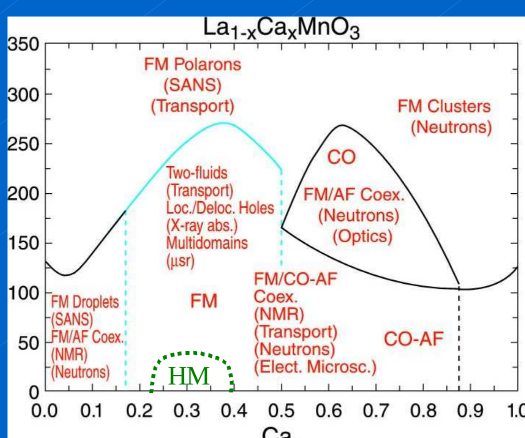


At intermediate temperatures dynamical clusters are found near the phase-separation critical temperature.
The clusters are metallic or insulating, inducing a Pseudogap.

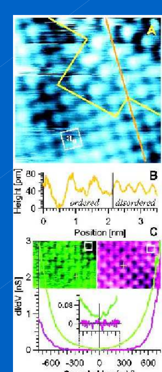
A.Moreo et al., PRL 83, 2773 (1999)

See also Dessau et al.
ARPES, bilayers
PG observed..

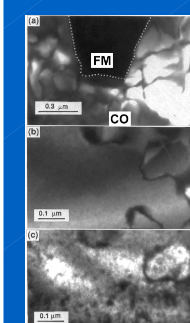
Experimental Evidence of Phase coexistence



A.Moreo et al.,
Science 283, 2034 (1999).

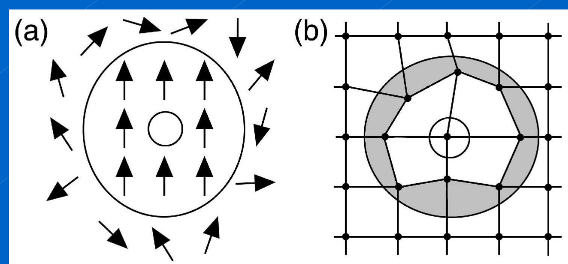


Renner et al.,
Nature ’02
BiCaMnO
STM



Uehara et al.,
Nature ’99
LaPrCaMnO
EM

Polarons or Larger Clusters?



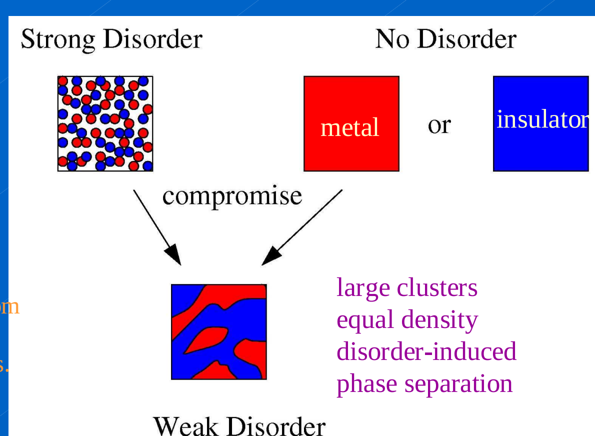
FM Polaron Lattice polaron

One carrier surrounded by a distortion.

Mn oxide experiments reveal far larger clusters, with many carriers inside. Polaron picture not suitable.

ITP, Nov. 2002

Disorder effects are very important near a first-order transition

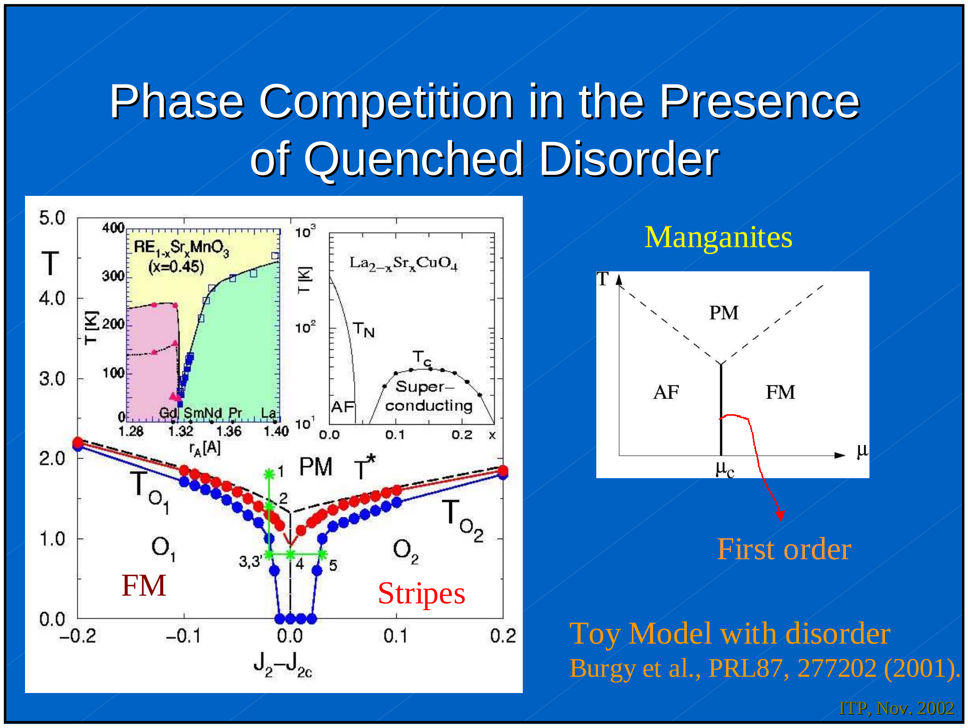


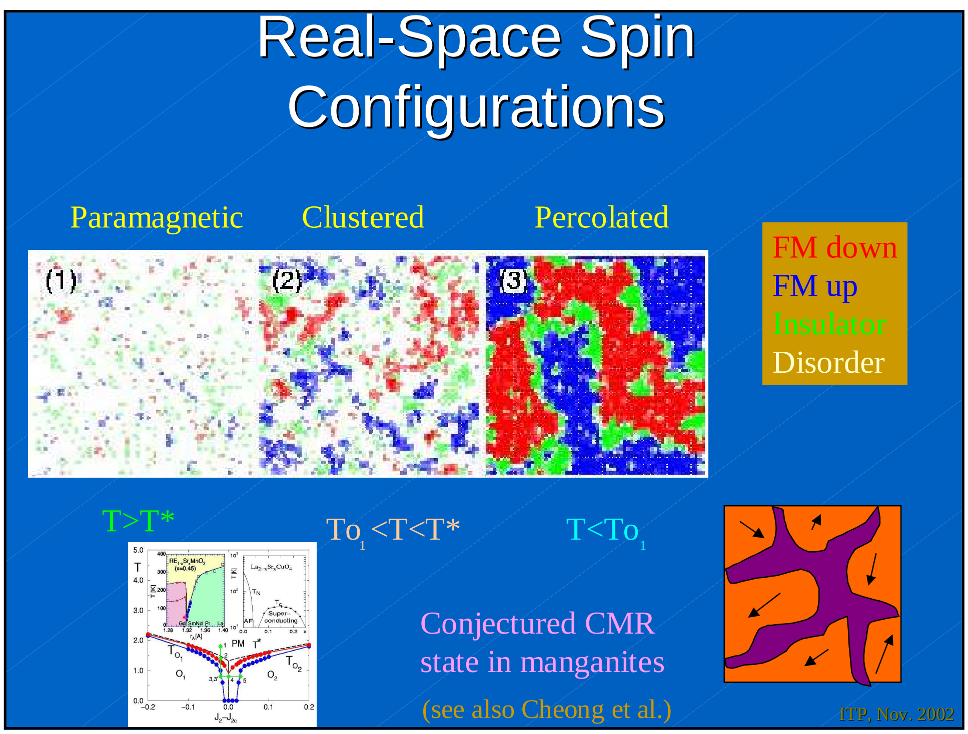
Disorder due to chemical doping => random hopping and Coulomb centers.

Imry-Ma Wortis

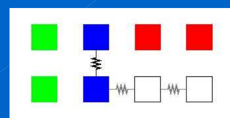
Warning: Cluster size is disorder strength dependent!

ITP, Nov. 2002

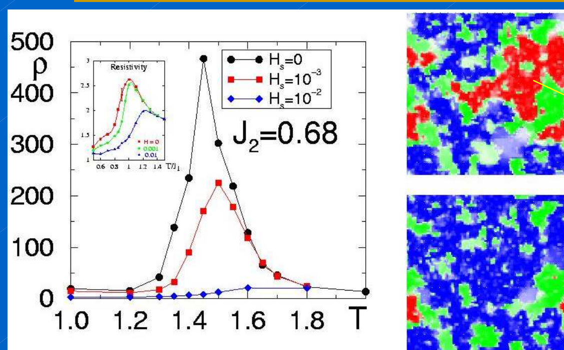

Phase Competition in the Presence of Quenched Disorder
$RE_{1-x}Sr_xMnO_3$ (x=0.45)
$La_{2-x}Sr_xCuO_4$
T [K]
r_A[A]
T_N
T_C
Super–conducting
AF
PM
T^*
T_{O_1}
T_{O_2}
O_1
O_2
FM
Stripes
J_2-J_{2c}
Manganites
T
PM
AF
FM
μ
μ_c
First order
Toy Model with disorder
Burgy et al., PRL87, 277202 (2001).
ITP, Nov. 2002


Real-Space Spin Configurations
Paramagnetic
Clustered
Percolated
(1)
(2)
(3)
FM down
FM up
Insulator
Disorder
T>T*
To_1<T<T*
T<To_1
Conjectured CMR state in manganites
(see also Cheong et al.)
ITP, Nov. 2002

CMR effect



Resistor Network: FM up FM down Insulator Disorder



H=0

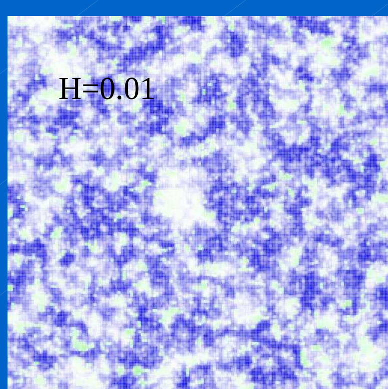
Rotates easily

H=0.01

MR ratios as large as 1000% at Hs=0.01 (Burgy et al.,PRL 87, 277202 (2001)).

ITP, Nov. 2002

Evolution with Magnetic Field



10 seconds movie

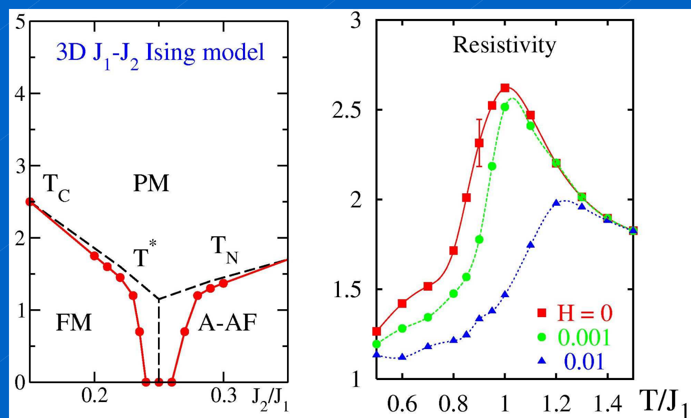
$$\Delta H = 0.001$$

0.1% of natural scale
0.001t~1 Tesla

M=0 at H=0 , but
M grows rapidly
with increasing H due
to easy cluster rotation.

ITP, Nov. 2002

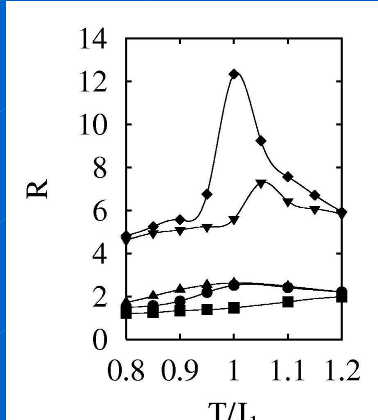
Similar results in 3D



Qualitatively as in experiments, but with smaller intensity than in 2D..
Are longer range interactions needed? (strain, Coulomb)

ITP, Nov. 2002

Results in 3D, including long-range correlations



Top: long-range 1/r^3 interaction H=0.0 and 0.01

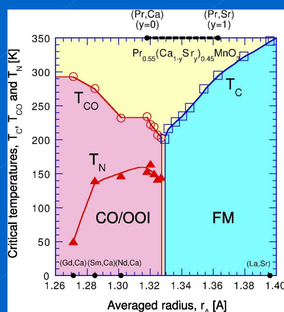
Bottom: Short-range, H=0.0, 0.001, and 0.01

Work in progress, J.Burgy et al. See also K. Yang, cond-mat.

ITP, Nov. 2002

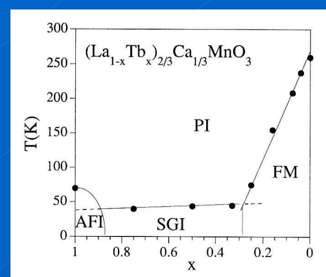
Experimental Test of Predictions

T*>Tc



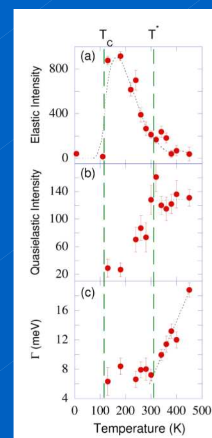
“Weak” disorder

Tomioka et al.



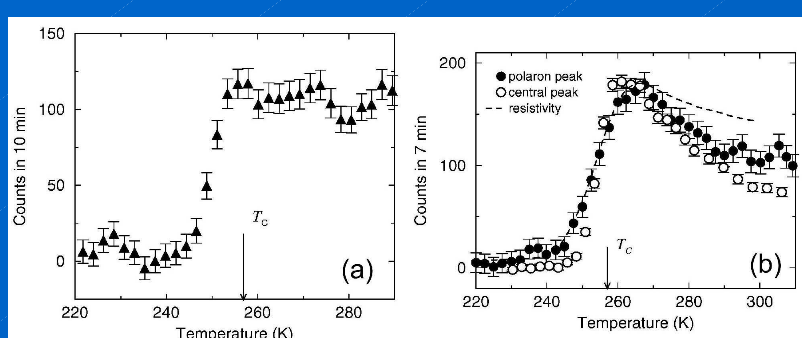
“Strong” disorder

De Teresa et al.



Argyriou et al.

``Correlated polarons'' (a.k.a. short-range charge order) above Tc

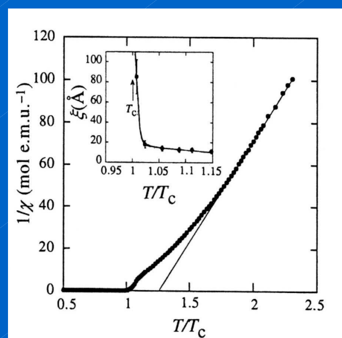


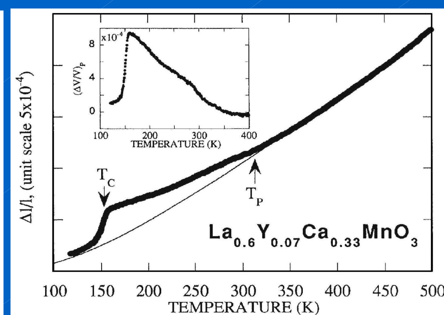
Uncorrelated polarons
Nearly T-independent

Correlated polarons
Follows resistivity vs. T

Results from Adams et al., PRL 85, 3954 (2000).

Additional evidence of T*





LCMO

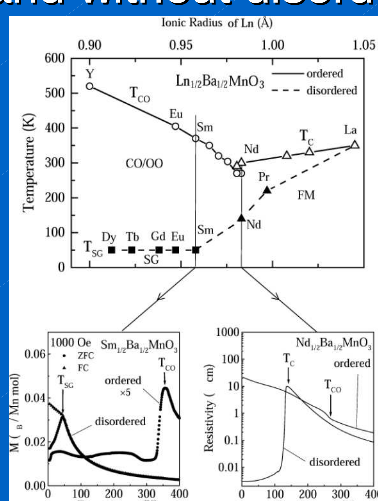
Thermal expansion

From De Teresa, Ibarra et al.

ITP, Nov. 2002

Experimental phase diagrams with and without disorder

Dramatic changes with and without disorder. CO phase affected the most.



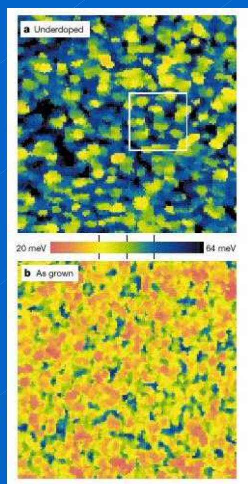
Tokura et al. 2002

ITP, Nov. 2002

High Tc Cuprates

STM Gap Maps

560A x 560A



Underdoped Bi-2212, Tc=79K

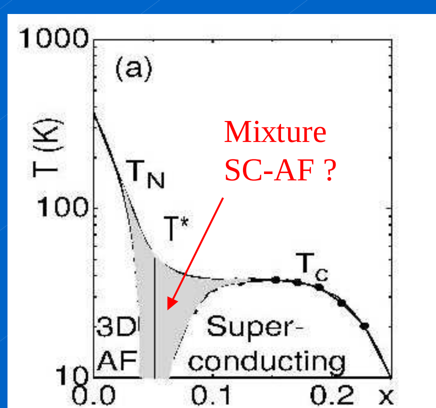
Overdoped Bi-2212

- Mixture of two different short-range electronic orders?
- Long-range characteristics of granular SC?
- SC domains ~3nm.

Lang et al., Nature '02.

ITP, Nov. 2002

CMR-motivated Speculations for Cuprates:

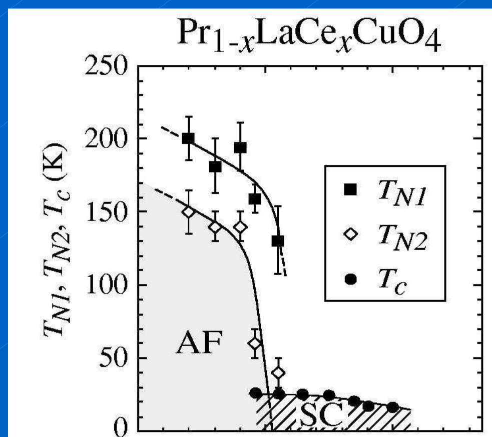


- First-order AF-SC transition in clean limit? Similar ideas in SO(5) context. Tetracriticality is another possibility (Sachdev).
- Percolative transition?
- T* as a Griffiths T?
- 'Colossal" Effects in underdoped regime? Proximity effect?
- Coexistence in ARPES data? (Fujimori)

Burgy et al, PRL 87, 277202 (2001)

ITP, Nov. 2002

First-order SC—AF transition in electron-doped systems?



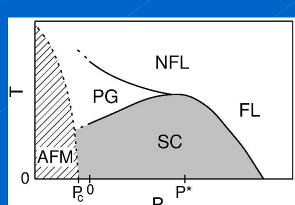
M. Fujita et al.,
cond-mat/0203320
muSR and suscept.
(Blumberg's talk)

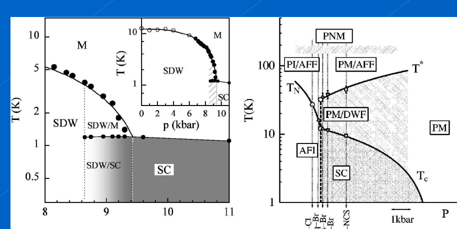
Heavy fermions
and organic SC
have similar
features.

Brown's talk

ITP, Nov. 2002

Heavy Fermions and Organic SC have similar features





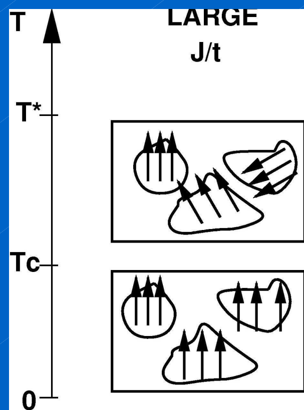
Ce-based heavy fermion
(Los Alamos)

Organic superconductors:
SDW/SC coexistence or
First-order SC-SDW transition

ITP, Nov. 2002

T* in diluted magnetic semiconductors as well?

Mn-doped GaAs; x=0.1;Tc = 110K. Spintronics?
Model: carriers interacting with Mn-spins locally



Monte Carlo simulations

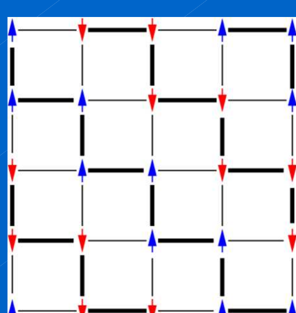
Clustered state, insulating

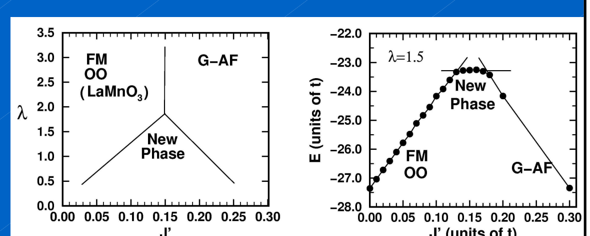
FM state, metallic

Alvarez et al., PRL to appear. See also Mayr et al., PRB 2002

ITP, Nov. 2002

Very recent developments: New `` E-phase” in undoped limit





Hotta et al., cond-mat
See also Kimura et al. (experiments).

ITP, Nov. 2002