Complexity in Transition-Metal Oxides and Related Compounds

A. Moreo and E. Dagotto

Univ. of Tennessee, Knoxville

(on leave from FSU, Tallahassee)

NSF-DMR-0312333

Students and postdocs: H. Aliaga, G. Alvarez, J. Burgy, T. Hotta, C. Sen, Y. Yildirim, S. Yunoki

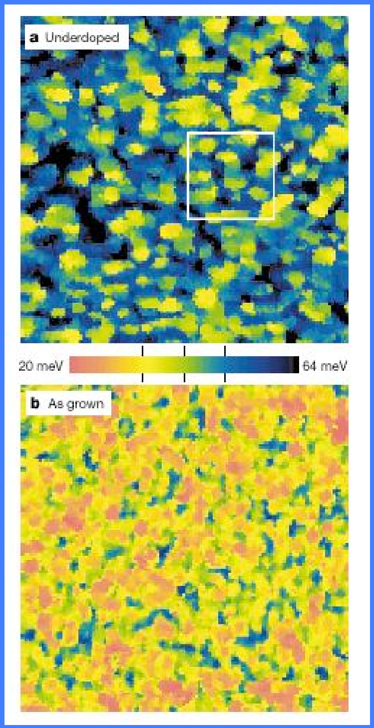
Many materials and theory simulations show signs of ``complexity''

- CMR manganites
- Underdoped High-Tc cuprates
- Ruthenates, cobaltites (also in diluted magnetic semiconductors?)

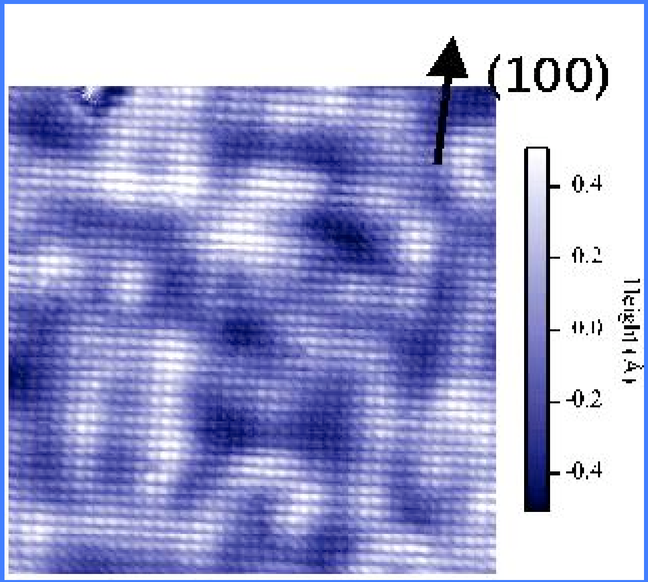
Common theme emerging:

Clustered states and dramatic effects as a result of small perturbations (complexity?)

Recent Trends:
Inhomogeneities in Cuprates



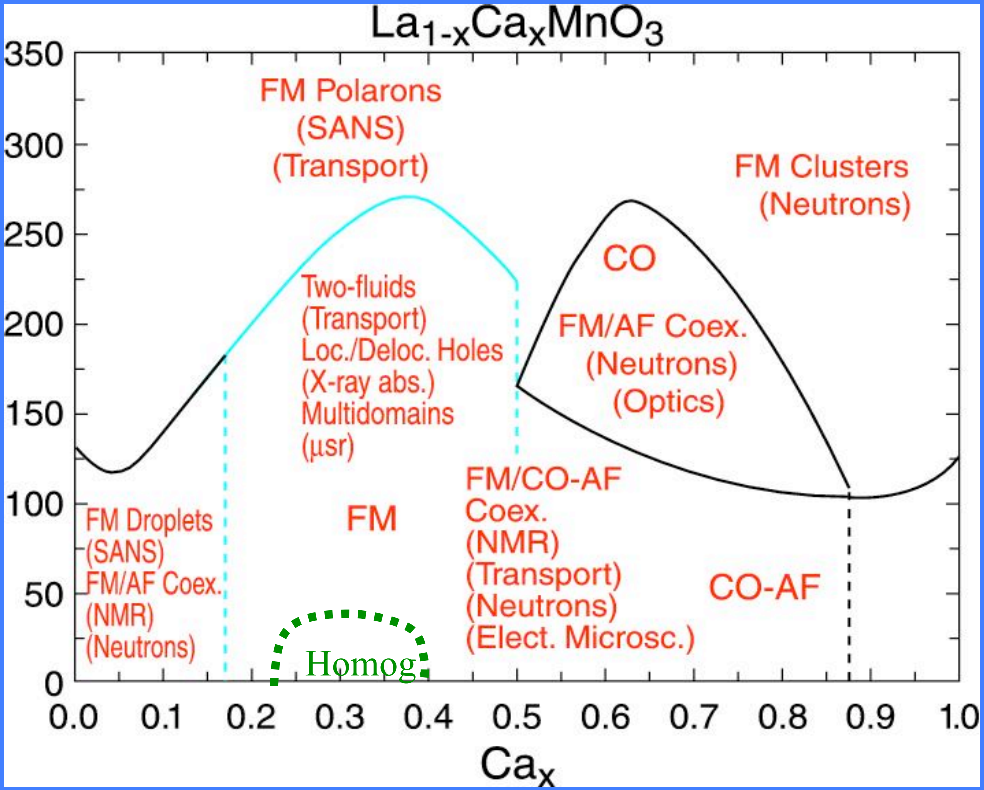
Ca2-x Nax Cu O2 Cl2



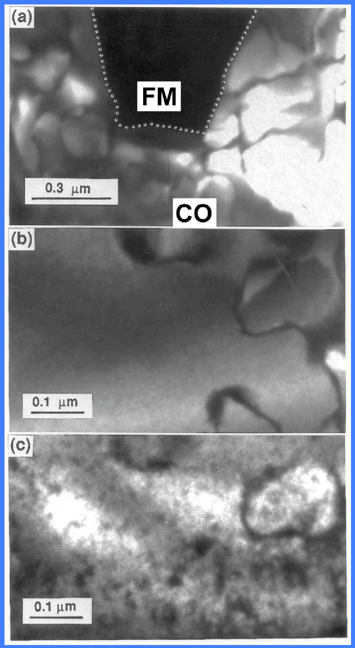
STM inhomogeneities. Nanoscale structures.
Large clusters and computational methods needed.

Phenomenological models beyond t-J/Hubbard may be crucial for underdoped region …

Recent Trends: Inhomogeneities in Manganites

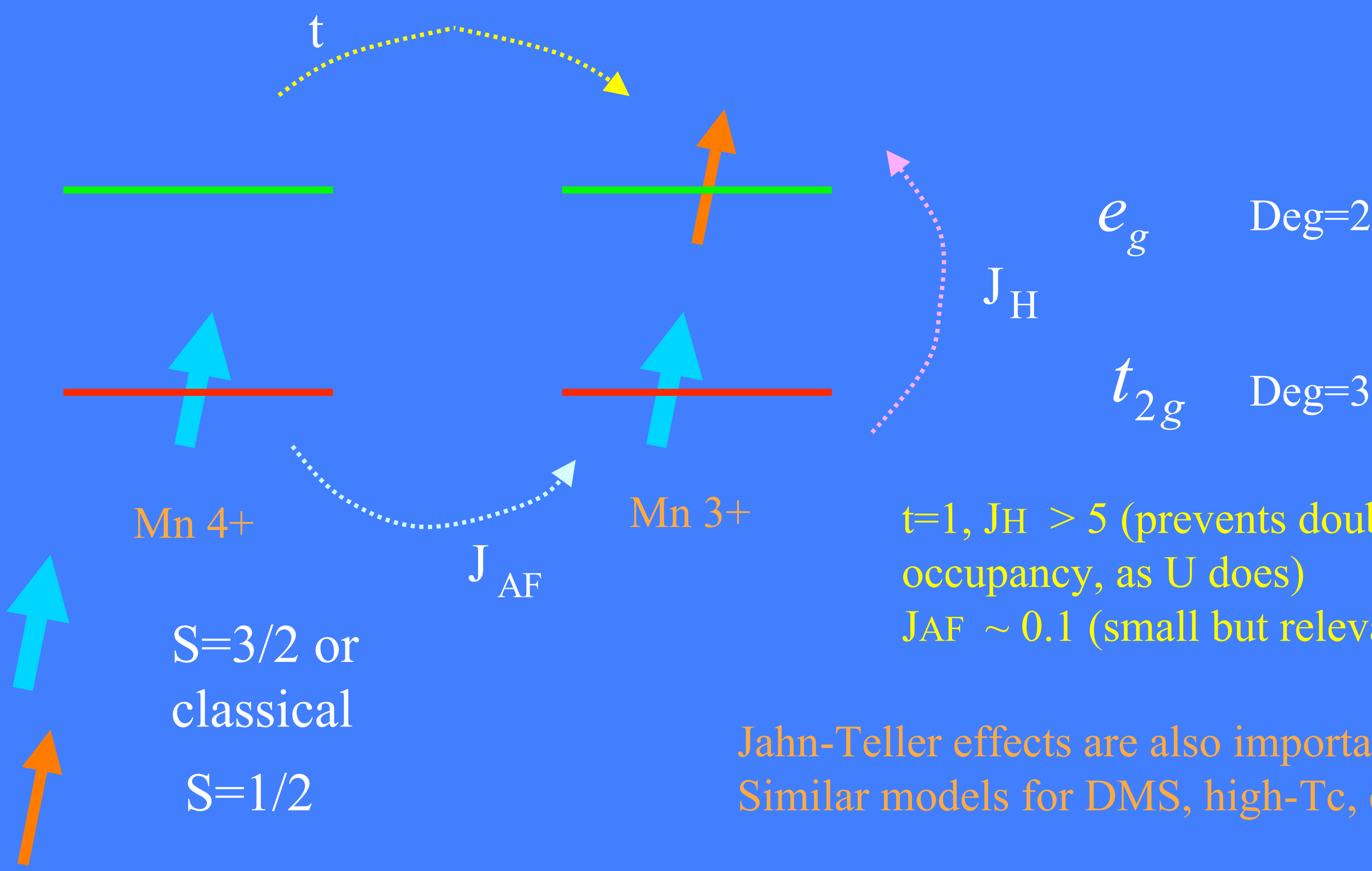


A. Moreo, S. Yunoki and E. D., Science 283, 2034 (1999).



Uehara et al., Nature '99 LaPrCaMnO EM

Main couplings in ``spin fermion'' like models

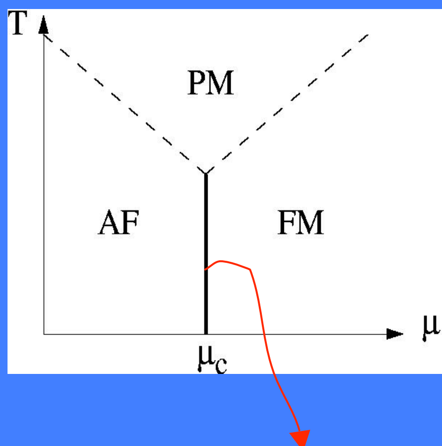


t=1, J_H > 5 (prevents double occupancy, as U does)
J_{AF} ~ 0.1 (small but relevant)

Jahn-Teller effects are also important
Similar models for DMS, high-Tc, etc.

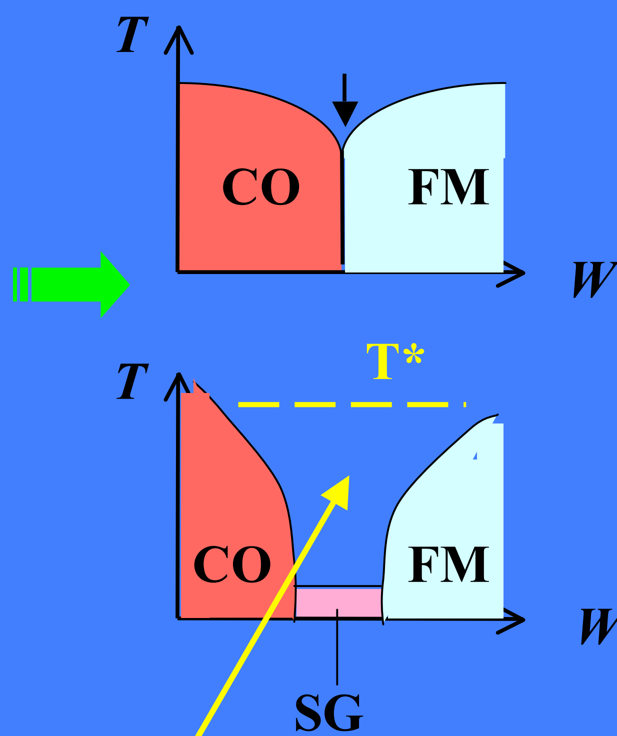
Summary of huge MC theory effort : ``Phase Separation causes CMR effect''

Clean limit :



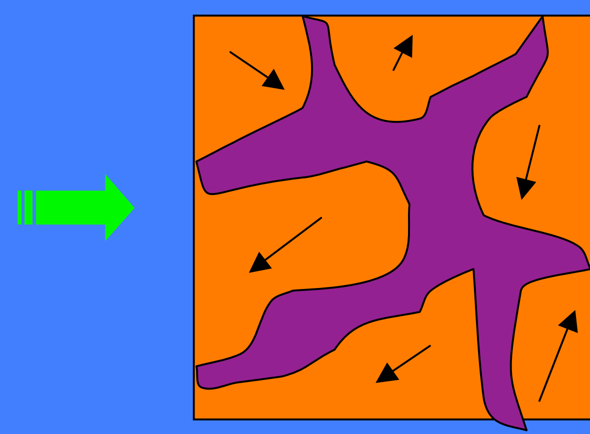
First order

Disorder added :



Mixture of competing phases

CMR origin:

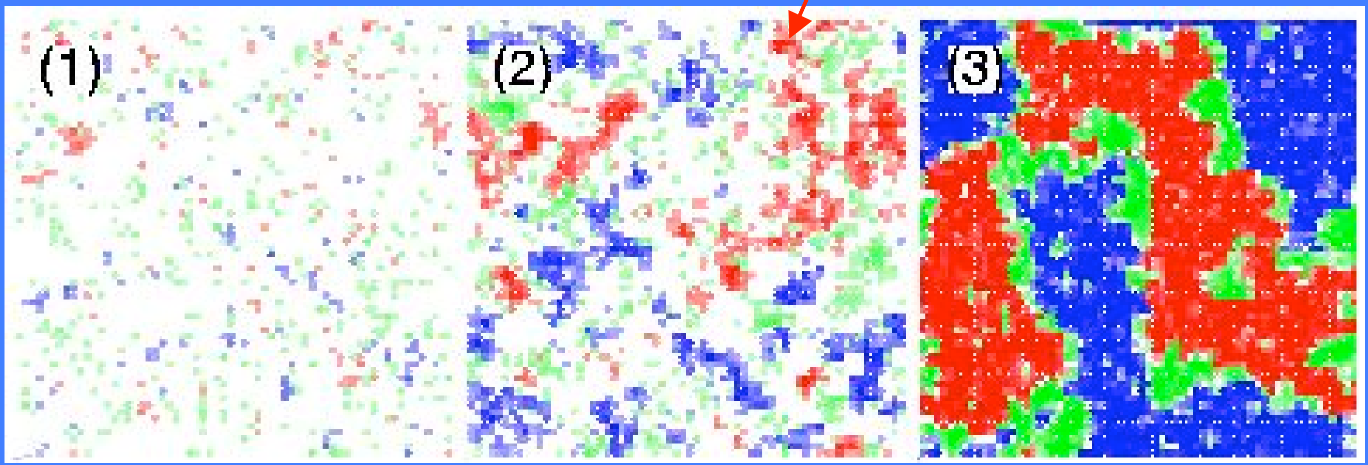


Preformed nanoclusters rapidly orient their moments in a magnetic field. Huge CMR effects found in MC studies (see Phys. Reports 344, 1 (2001)).

Real-Space Spin Configurations

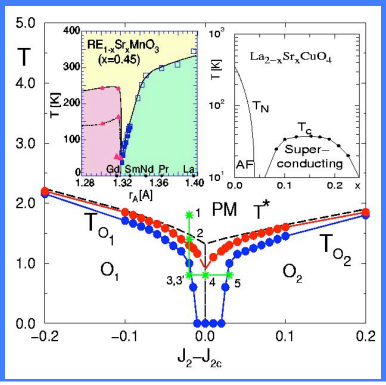
Quasi-static

Paramagnetic | Clustered | Percolated



FM down
FM up
Insulator
Disorder

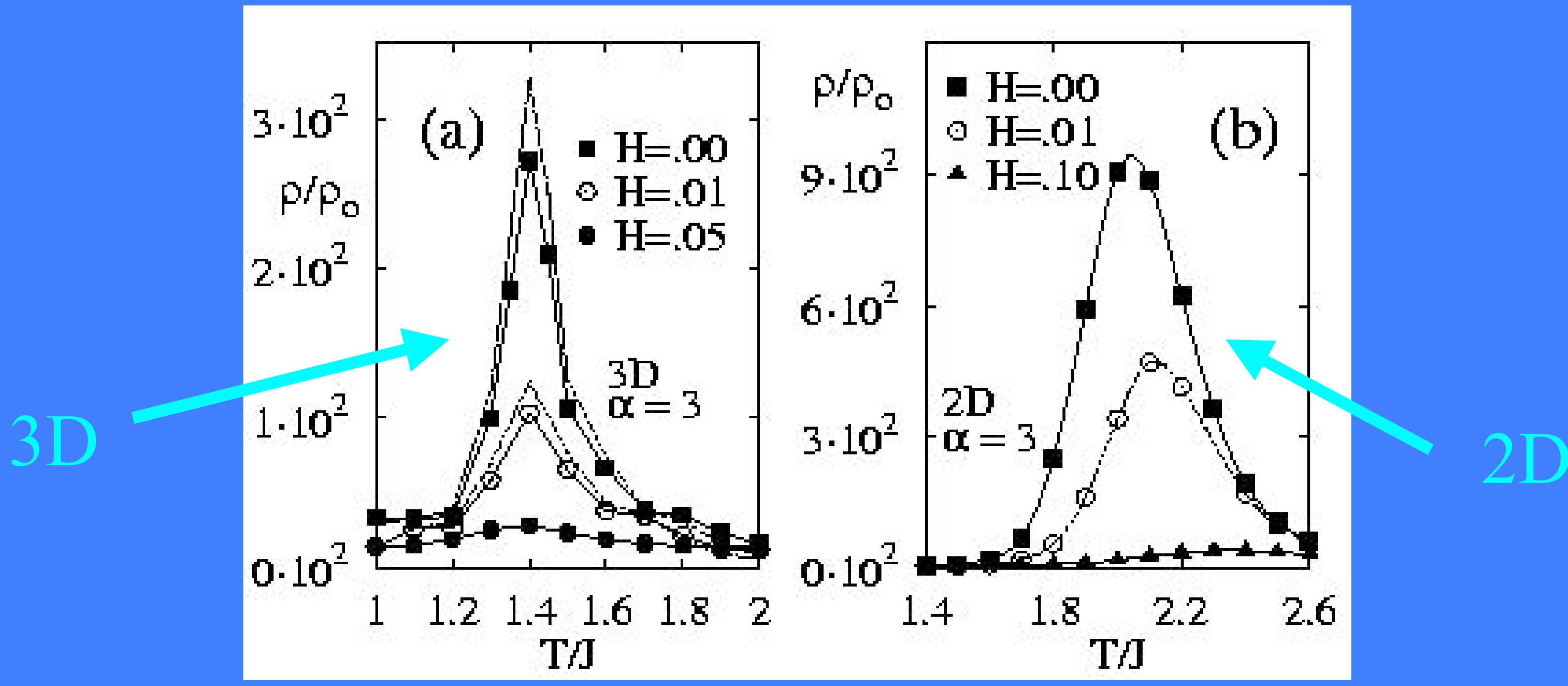
$T>T^*$ | $To_1<T<T^*$ | $T<To_1$



Clean-limit Tc.

Resistivity with correlated disorder to mimic cooperative JT distortions

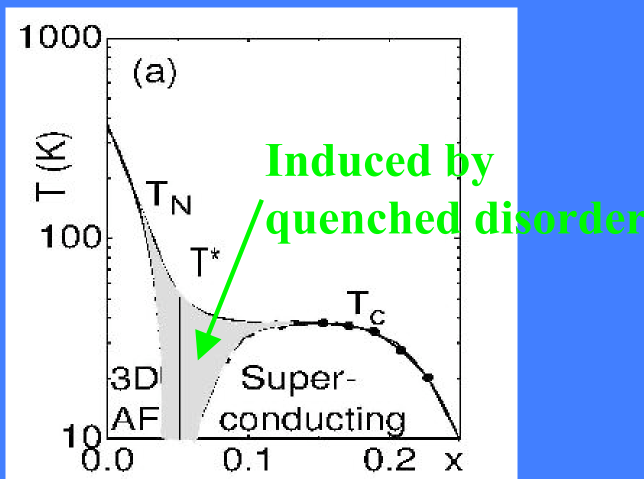
(J. Burgy et al., PRL 92, 097202 (2004); J. Burgy et al., PRL 2001)



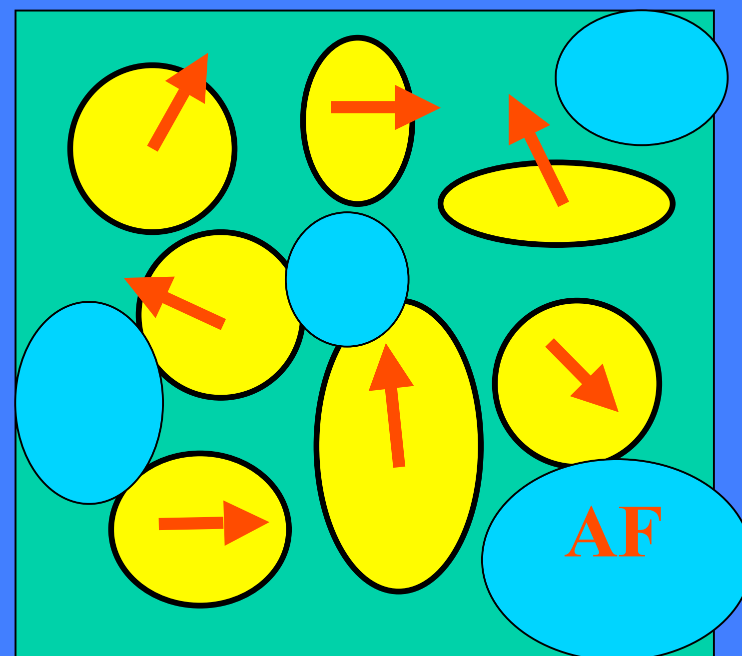
CMR in 3D and 2D are very similar
if ``elasticity'' is incorporated.

Similar effect in Cuprates?

(Alvarez et al., cond-mat/0401474)



Theory:
Bi, tri, or tetracritical
in clean limit.

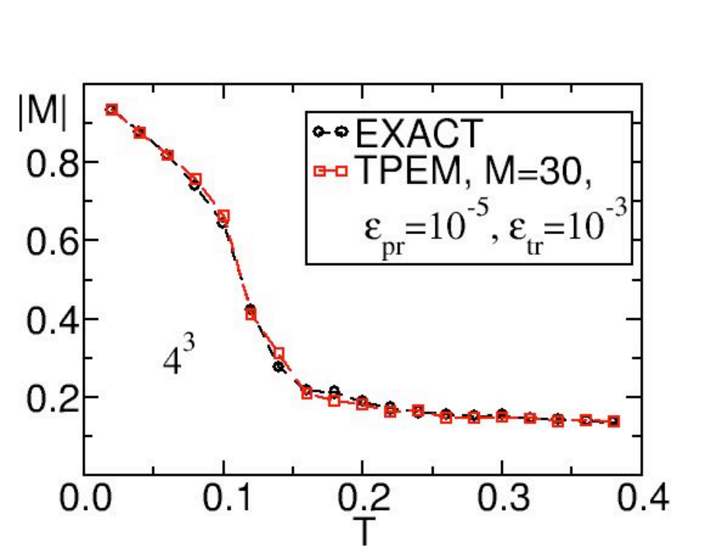


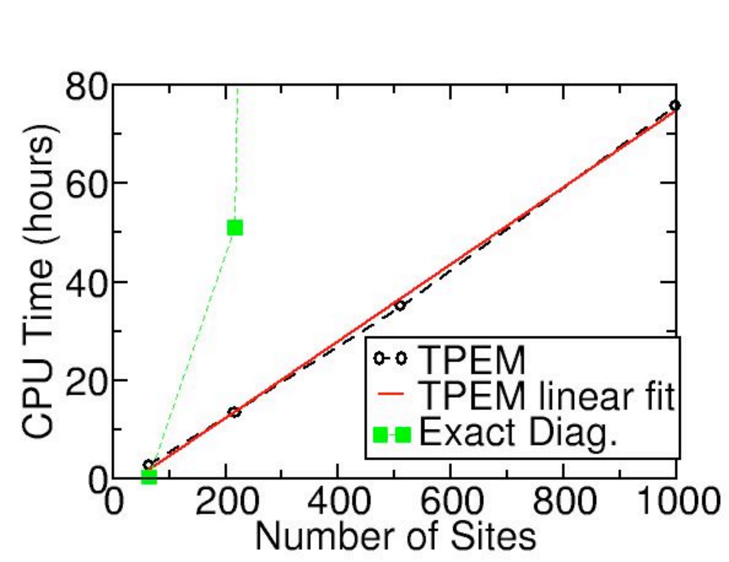
Proposed: Random orientation of the local SC phase in glassy underdoped region
Giant effects are possible in many materials

New algorithms under development

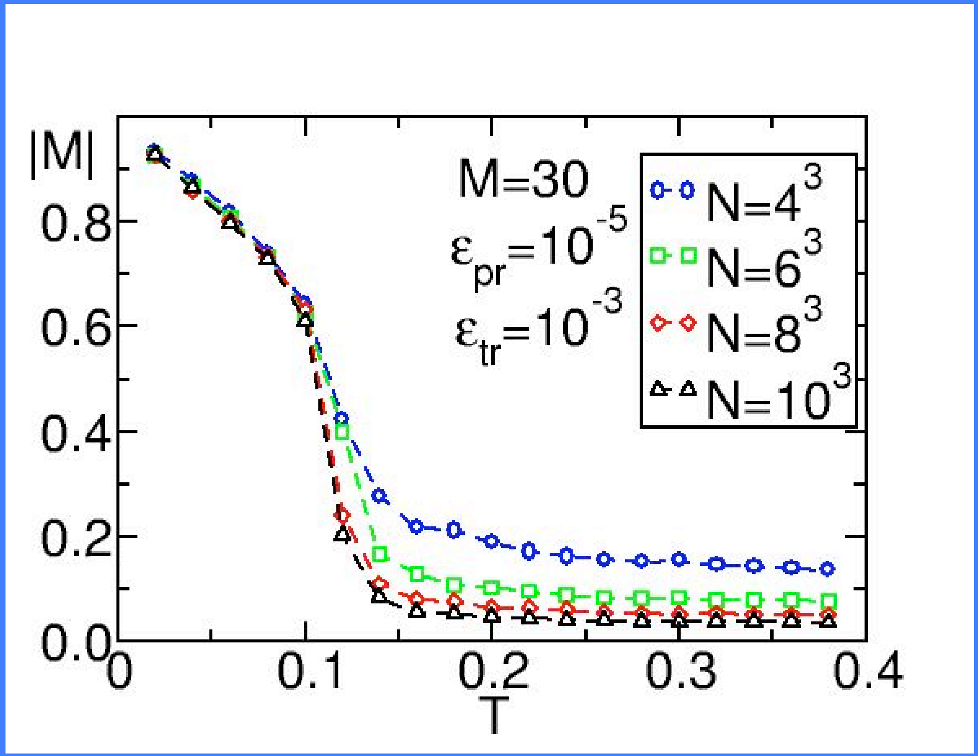
Current technique scales as N^4. Strong limitations in 3D. CMR only observed in ``toy models'' thus far.

New method (Furukawa et al.) is of order N. Focus on DOS, obtained via a Chebyshev polynomial expansion. Works in localized electron basis, uses local nature of MC updates, and sparse Hamiltonian.





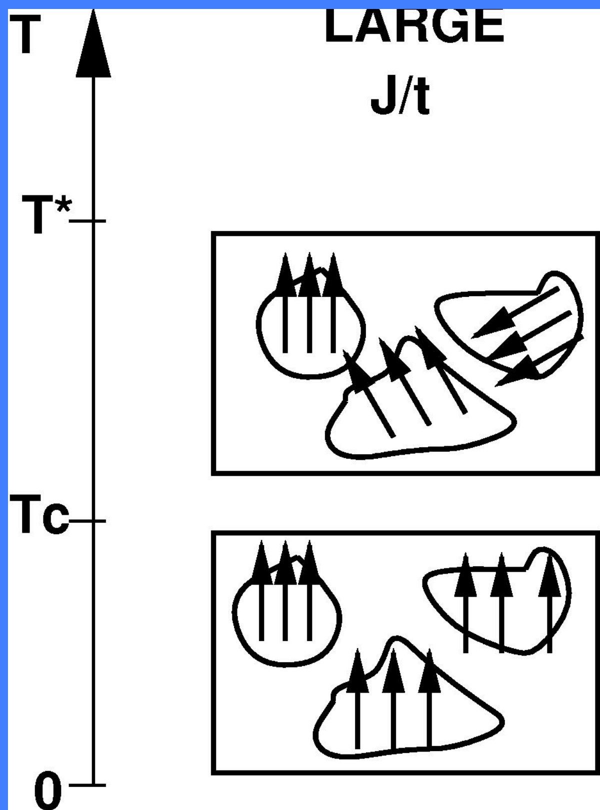
1000 sites can be easily reached



Critical exponents can be found?

T* in diluted magnetic semiconductors as well?

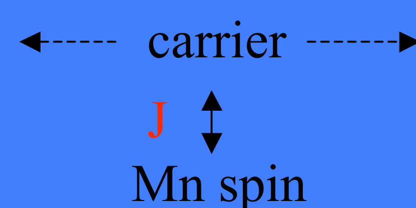
Mn-doped GaAs; x=0.1;Tc = 110K. Spintronics? Model: carriers interacting with randomly distributed Mn-spins locally



Monte Carlo simulations very similar to those for manganites.

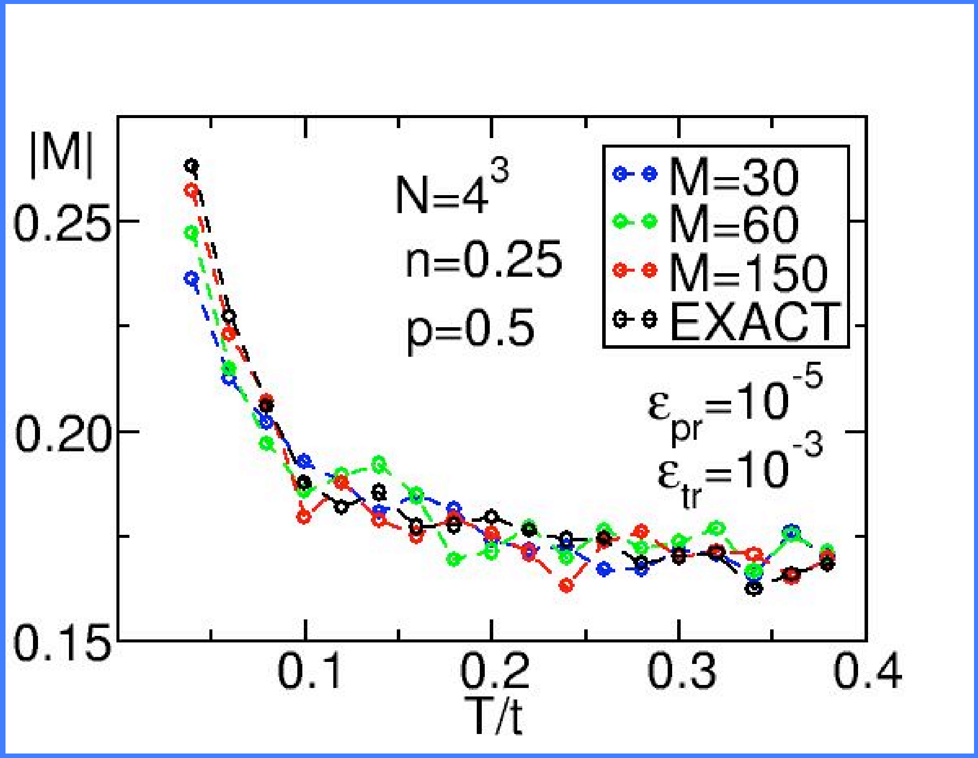
Clustered state, insulating

FM state, metallic



Alvarez et al., PRL 89, 277202 (02). See also Mayr et al., PRB 2002

Applications to Diluted Magnetic Semiconductors in preparation



DMS models also have itinerant electrons in interaction with localized classical spins (many bands can be studied).

Summary:

Many problems of current interest need the simulation of systems of fermions in interaction with classical dof

Complex behavior and self-generated nanostructures emerge

(i) Direct exact diagonalization: N^4

(ii) Polynomial expansion method (PEM) for sparse Hamiltonians: N^3

(iii) Further improvements: local basis, local MC updates: N

Near future: multiband DMS and realistic manganite simulations in percolative regime.