Effects of Disorder in Double-Exchange Systems

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Outline

Effects of disorder in double-exchange systems on

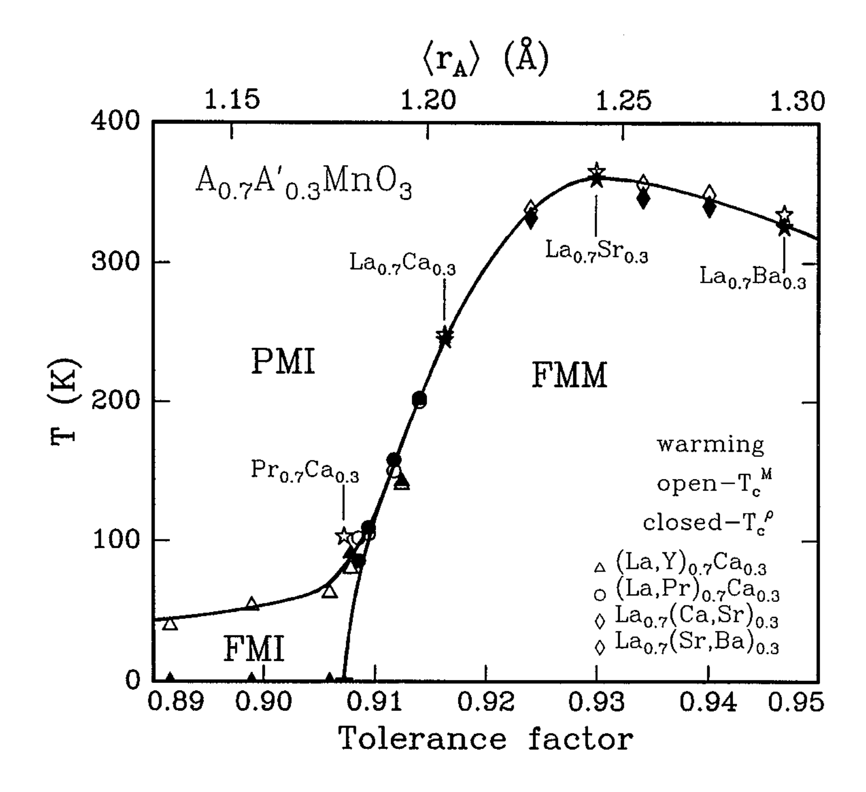
- T_C of ferromagnetic transition
  - 'world-record' Monte Carlo simulation
- spin excitation spectrum
  - anomalies such as broadening, softening, etc.
- competing phases
  - disorder-induced insulator-to-metal transition
  - origin of CMR

Disorder in CMR Manganites ?

Bandwidth Control ?

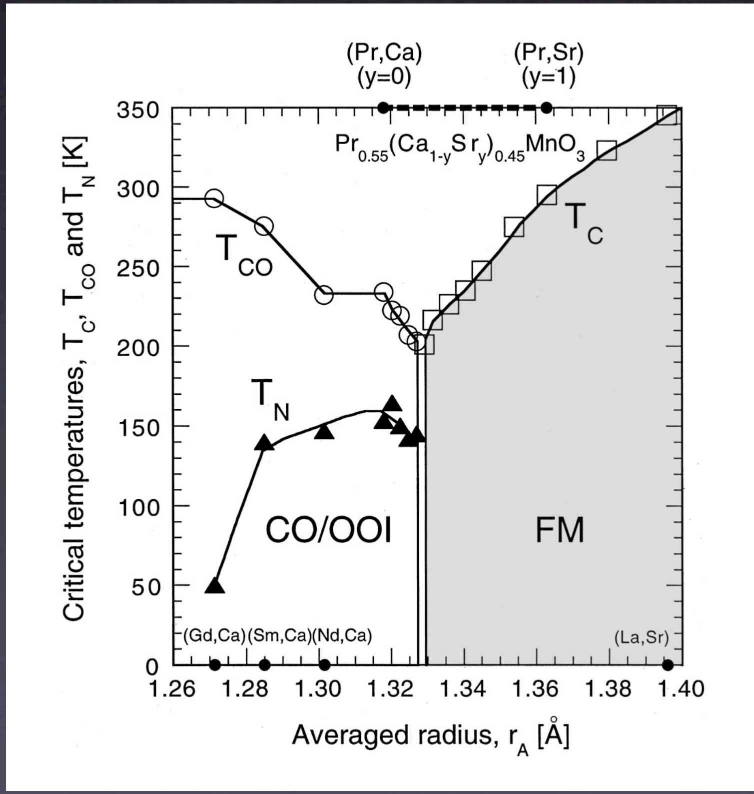
- ionic-radius control is often called 'bandwidth control' with changing the angle and length of Mn-O-Mn bonds

$A_{0.7}A'_{0.3}MnO_3$



Hwang *et al*., 1995

$Pr_{0.55}(Ca_{1-y}Sr_y)_{0.45}MnO_3$

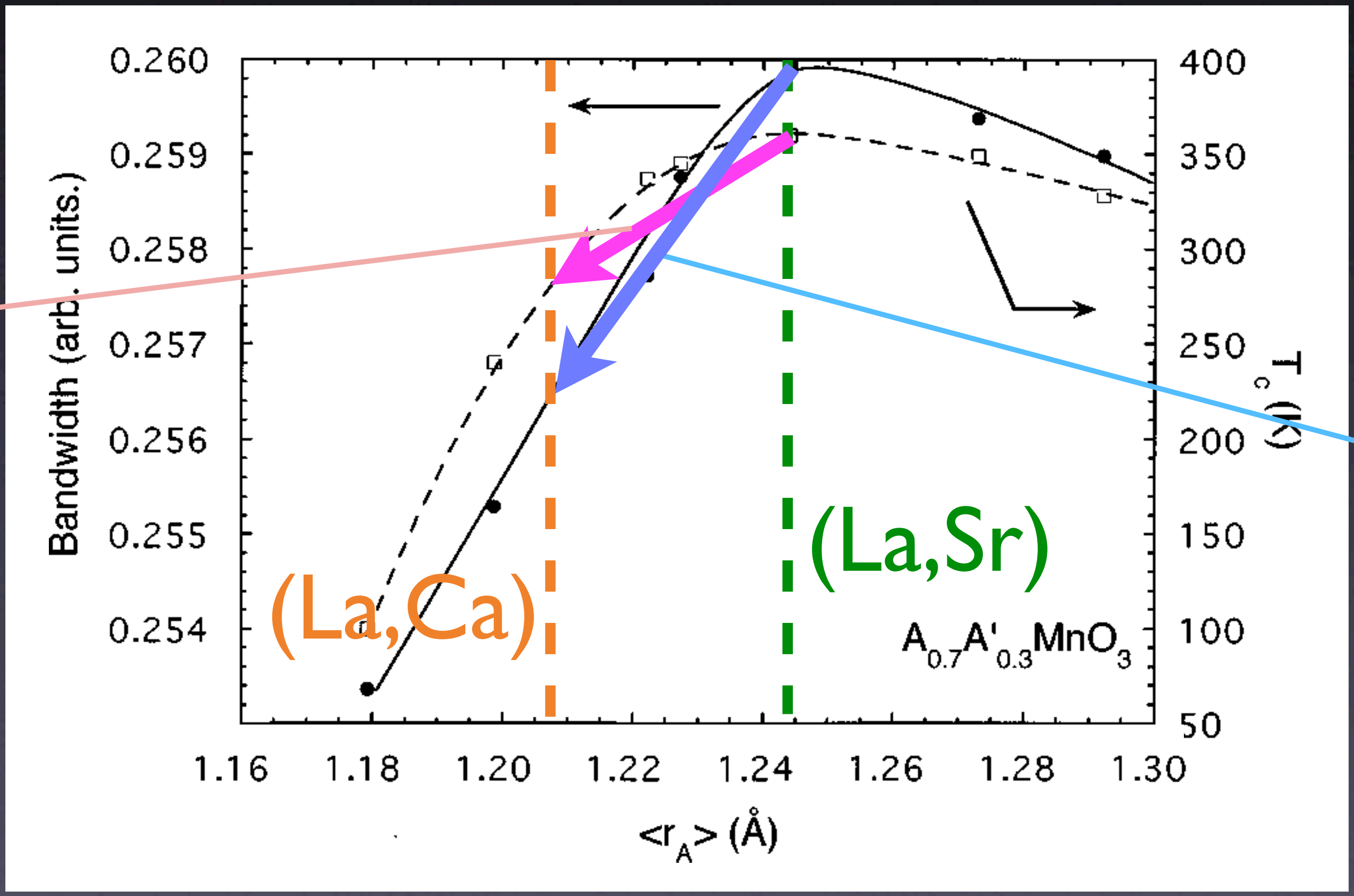


Tomioka and Tokura, 2002

'average' physics works ? - No.

Breakdown of 'Bandwidth Control' Picture

- change of T_C >> change of bandwidth W



ΔT_C~30%

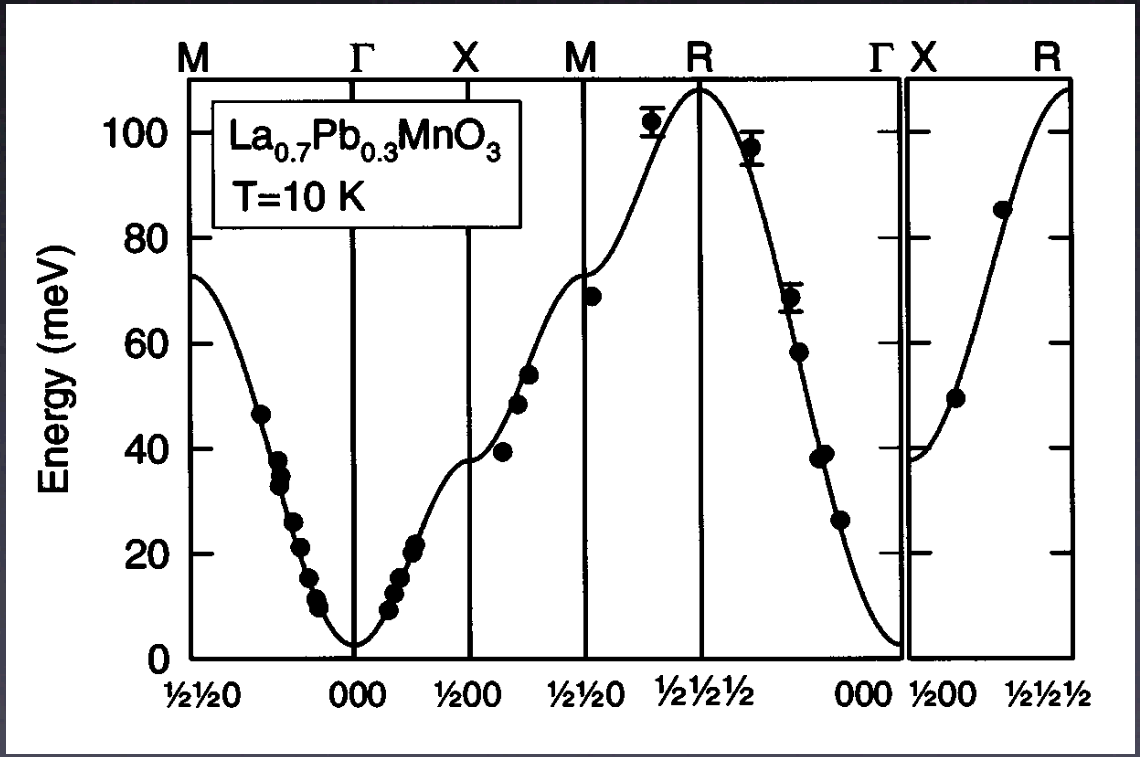
ΔW~2%

Radaelli *et al.*,1997

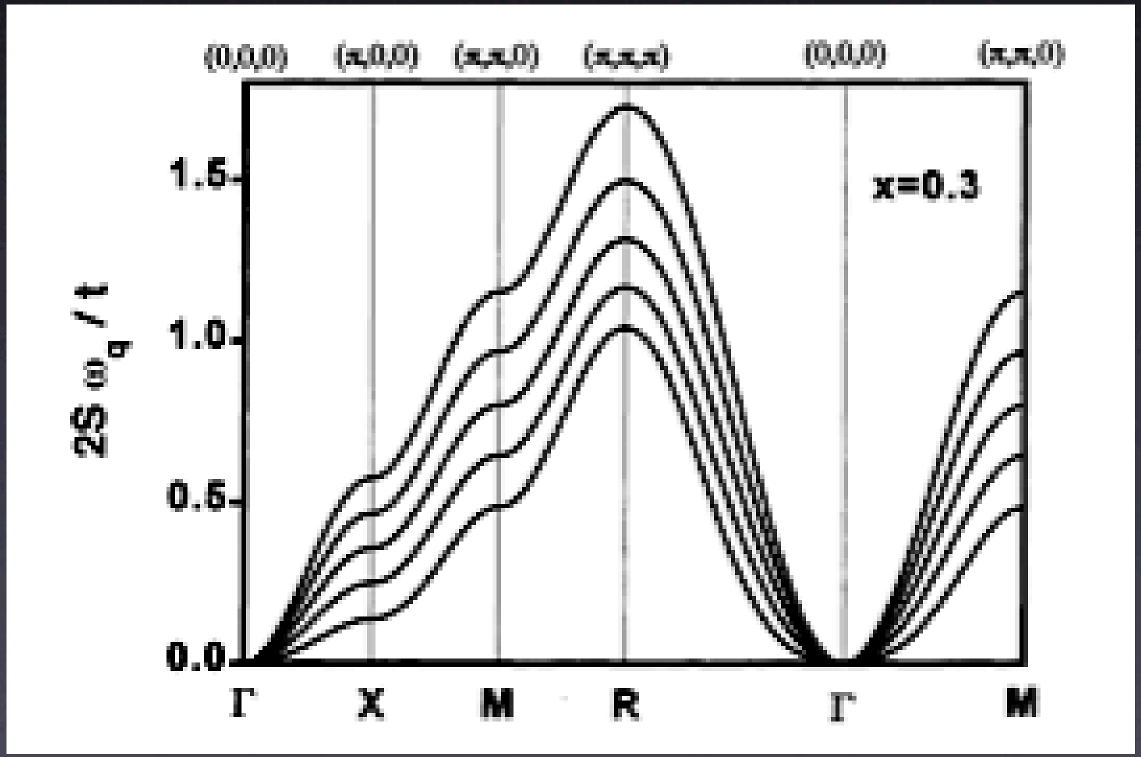
c.f. T_C scales to the bandwidth within
the double-exchange theory

Another Counterexample: Anomalies in Spin Excitation

- compounds with high T_C (wide bandwidth?)



Perring *et al.*,1997

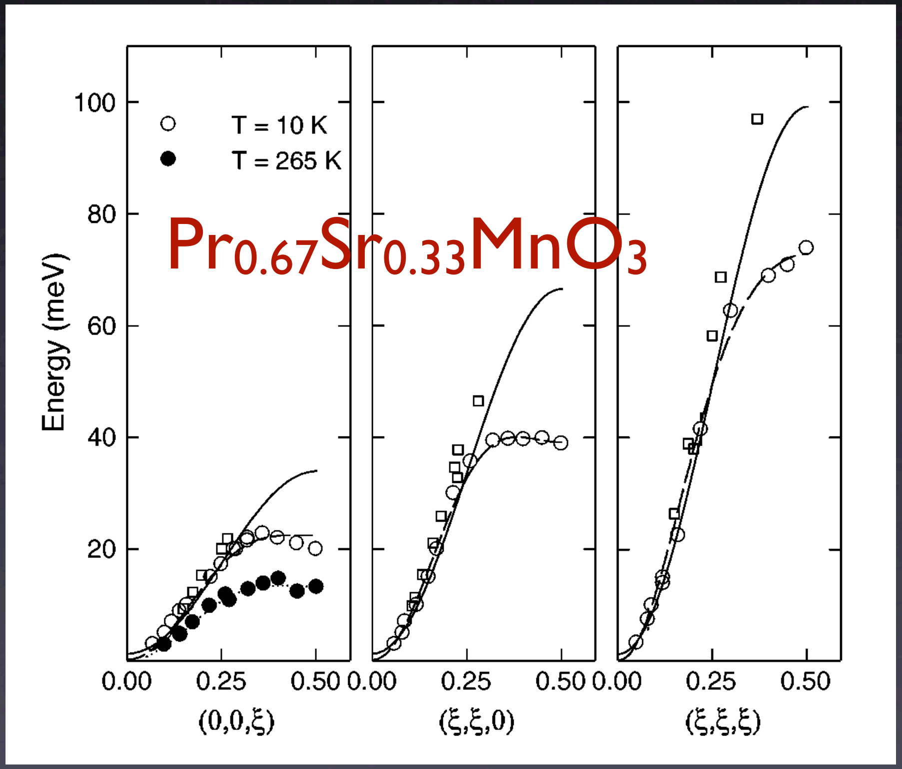


Furukawa, 1997

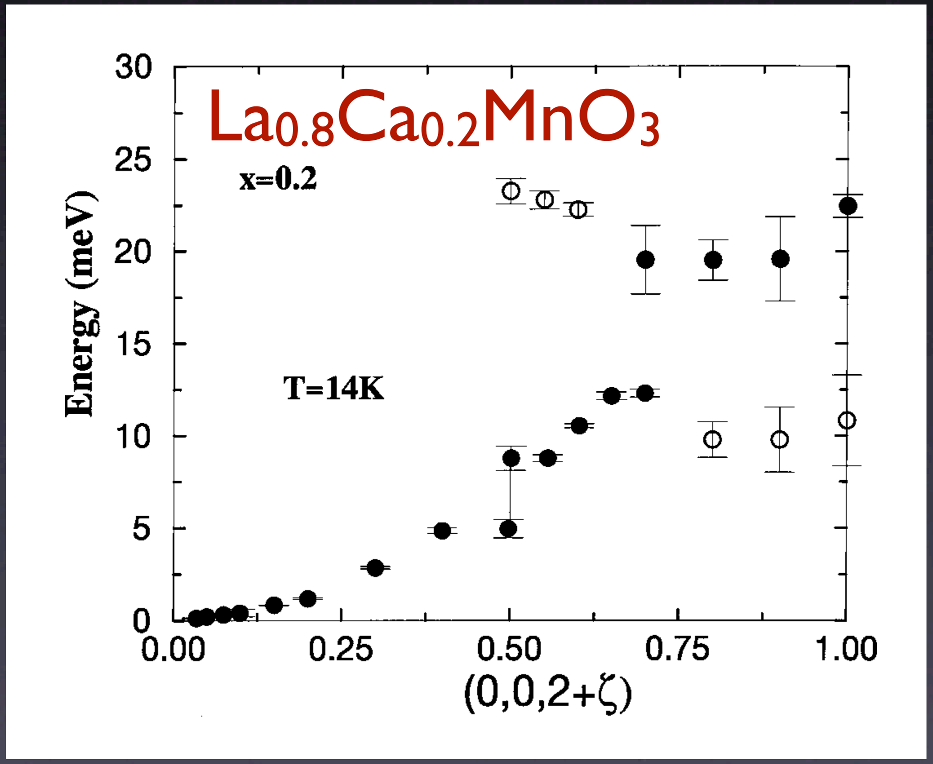
simple cosine-like dispersion
double-exchange theory is sufficient

Another Counterexample: Anomalies in Spin Excitation

- compounds with low T_C (narrow bandwidth?)



Hwang *et al.*, 1998

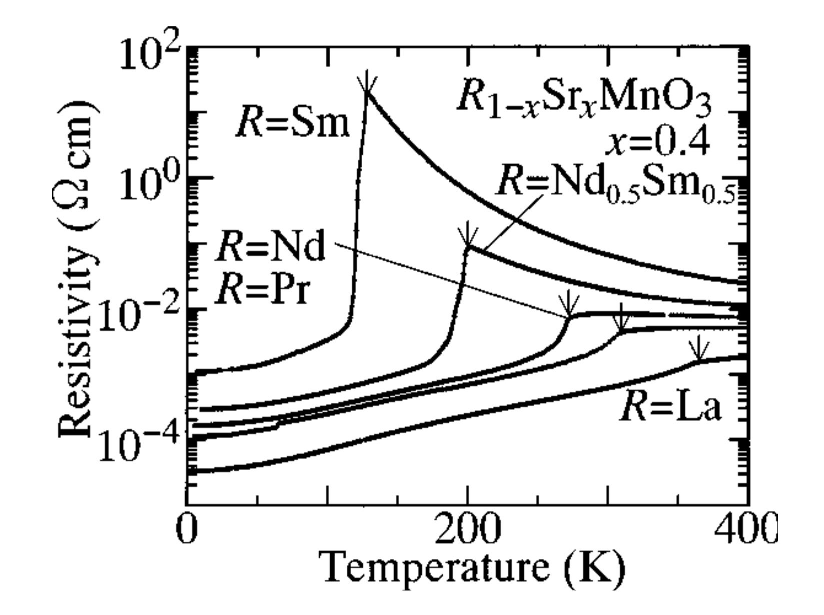


Biotteu *et al.*, 1997

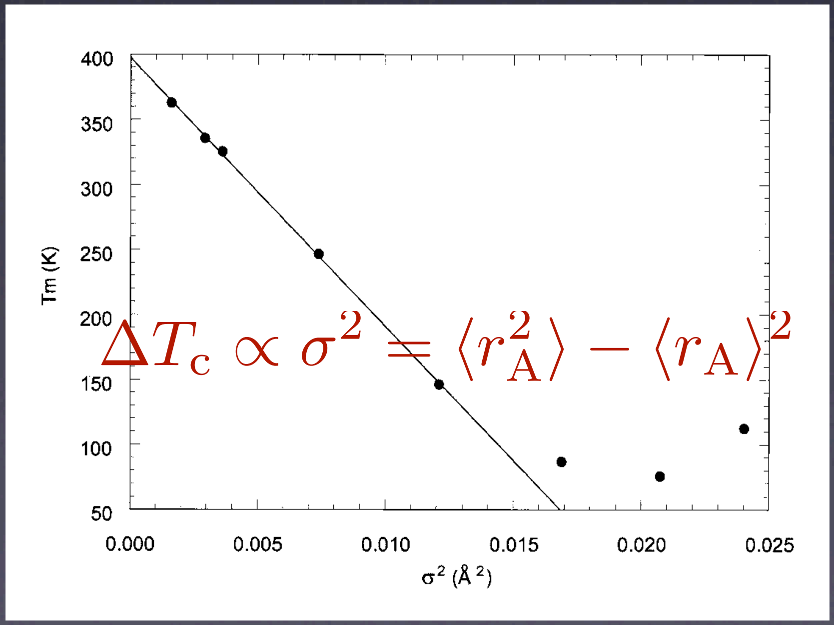
notable deviations from the simple cosine-like dispersion
anomalies: broadening, softening, anti-crossing, etc.

Disorder ?

- residual resistivity increases as T_C decreases although the specific heat does not show any significant mass enhancement (Coey *et al.*, 1995)
- T_C scales to the standard deviation of A-site ionic radii for a constant average radius
- sample dependence of spin excitation spectra (Perring *et al.*, 2000, Furukawa and Hirota, 2000)



Saitoh *et al.*, 1999

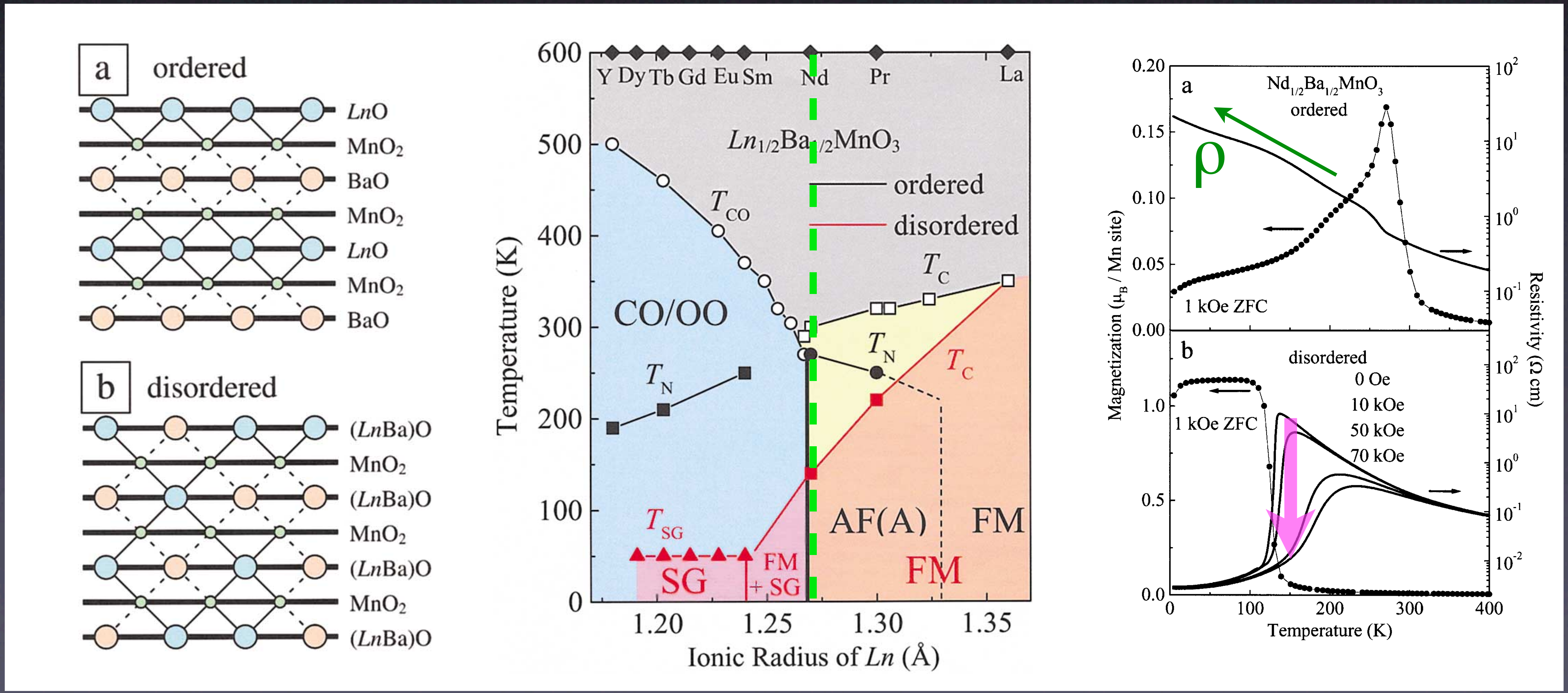


Rodriguez-Martinez and Attfield, 2000

Yes, Disorder !

new ‘*disorder-controllable*’ compounds

- A-site ordered/disordered compounds $A_{1/2}Ba_{1/2}MnO_3$
- disorder-induced insulator-metal transition and CMR



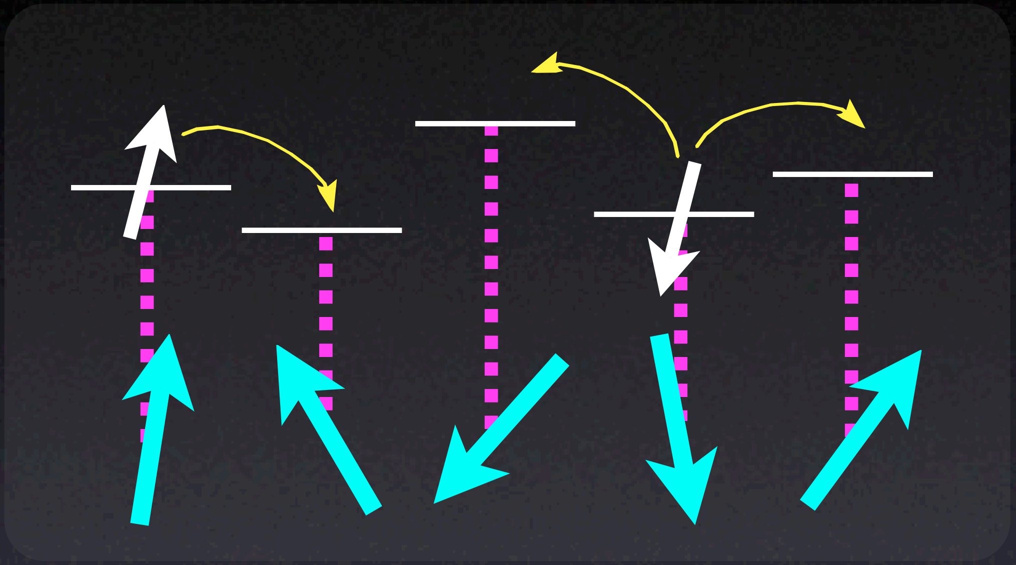
Akahoshi *et al.*, 2003

Our Strategy...

- complexity - itinerant electrons, Hund's coupling, degenerate orbitals, Jahn-Teller distortion, strain, etc.
- On top of those, there must be disorder: too much to begin with...
- We restart from a minimal model with disorder to examine how far we can reach and what is beyond.

DE model with Disorder

- single band
- strong Hund's-rule coupling
- classical localized spins
- on-site potential disorder



$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \mathrm{H.c.}) - J_\mathrm{H} \sum_i \vec{\sigma}_i \cdot \vec{S}_i + \sum_i \varepsilon_i n_i$$

$$\to - \sum_{\langle ij \rangle} (\tilde{t}_{ij} \tilde{c}_i^\dagger \tilde{c}_j + \tilde{t}_{ji} \tilde{c}_j^\dagger \tilde{c}_i) + \sum_i \varepsilon_i \tilde{n}_i$$

$$\tilde{t}_{ij} = t \Big\{ \cos\frac{\theta_i}{2} \cos\frac{\theta_j}{2} + \sin\frac{\theta_i}{2} \sin\frac{\theta_j}{2} \mathrm{e}^{-i(\phi_i - \phi_j)} \Big\}$$

- We will add breathing-type phonons to describe phase competitions later.

Curie Temperature T_C

Monte Carlo Simulation

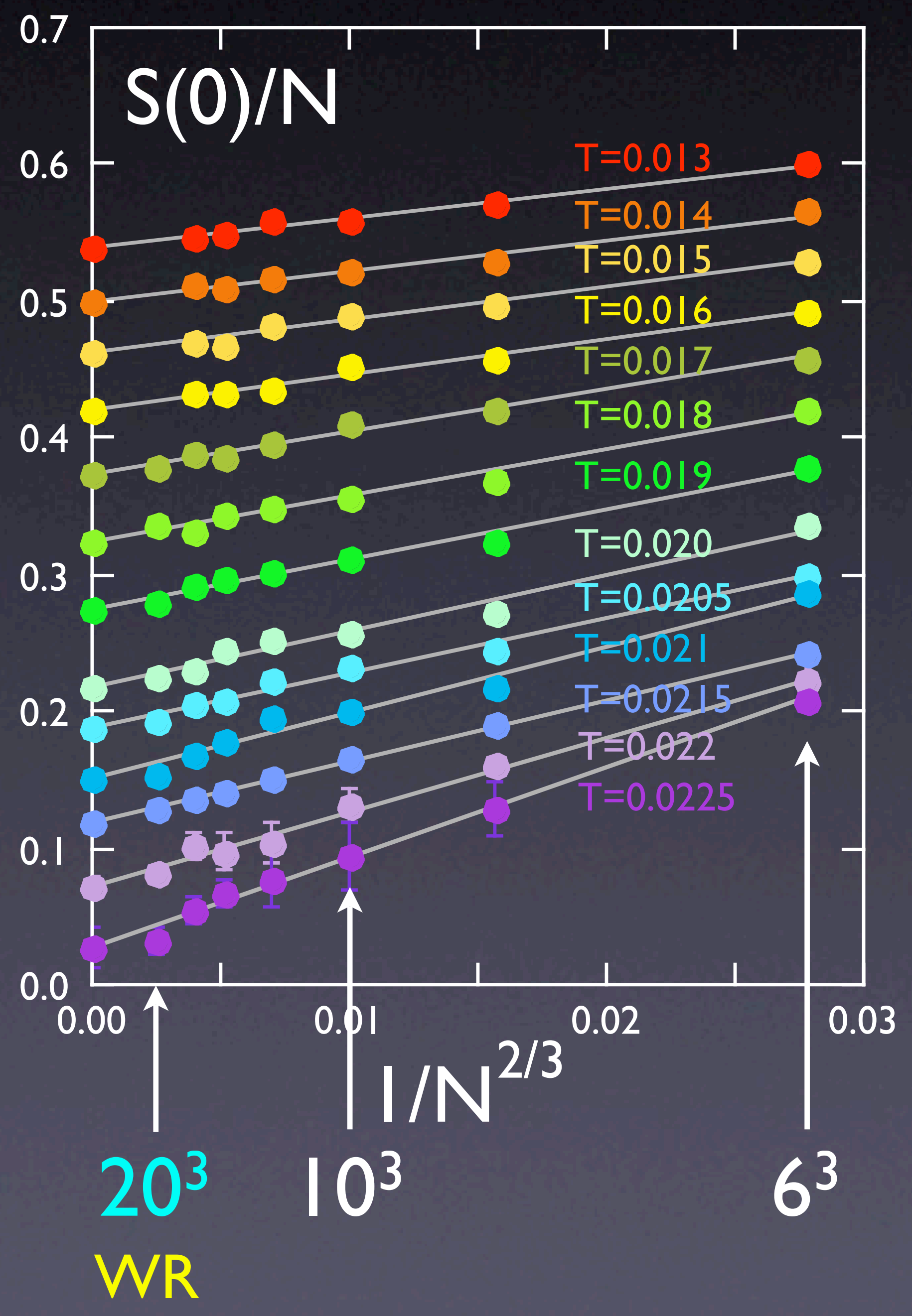
- truncated polynomial expansion Monte Carlo (Motome and Furukawa, 1999, 2001, 2004)
  - Chebyshev polynomial expansion for DOS
  - Order N algorithm (cpu time ∝ system size N)
  - easy to implement parallel computation

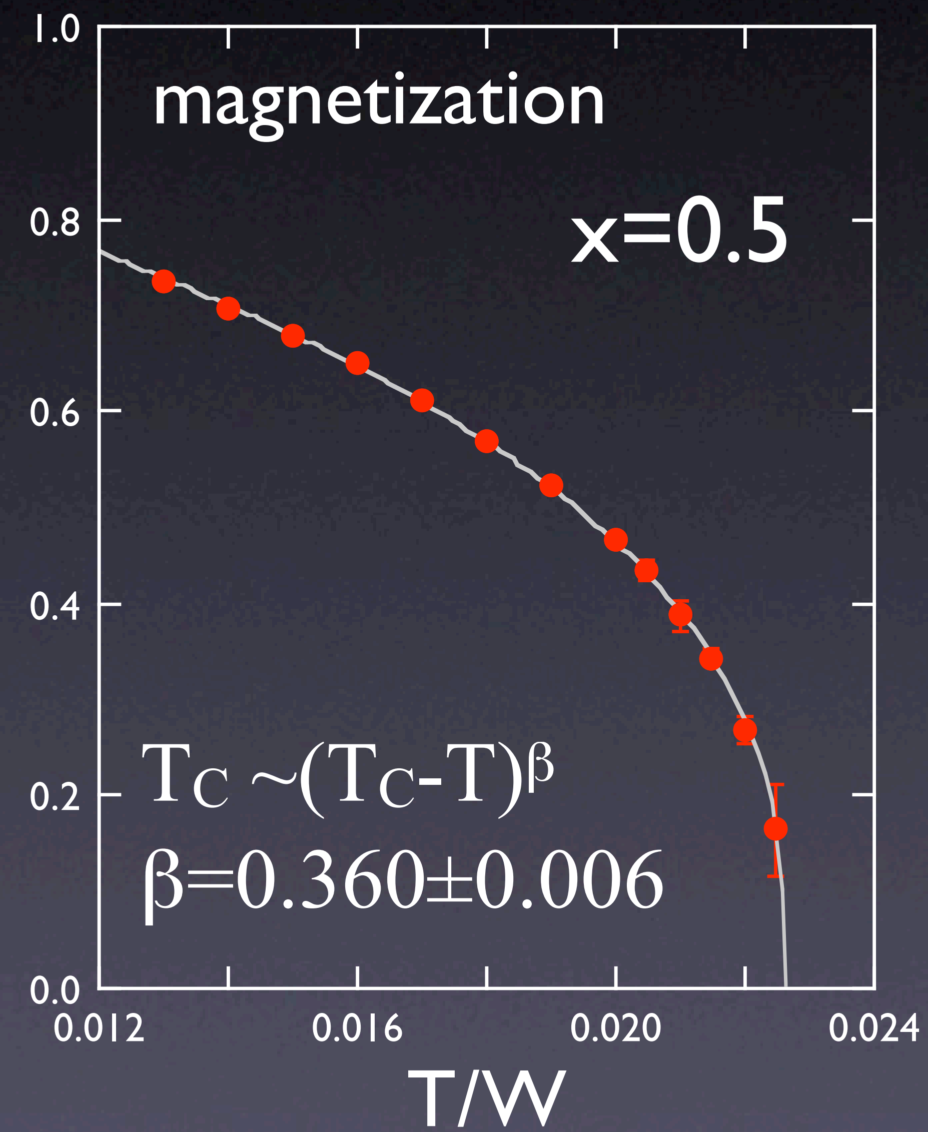
system size	conventonal MC: $O(N^4)$	t-PEMC: O(N)
8x8x8	2.5 years	2.4 days
12x12x12	300 years	8 days
16x16x16	9500 years	21 days

CPU time for 10000 MC steps on Athlon™ MP 1500+ (N_{PE}=1)

How does it work?

- in the clean limit (without disorder)

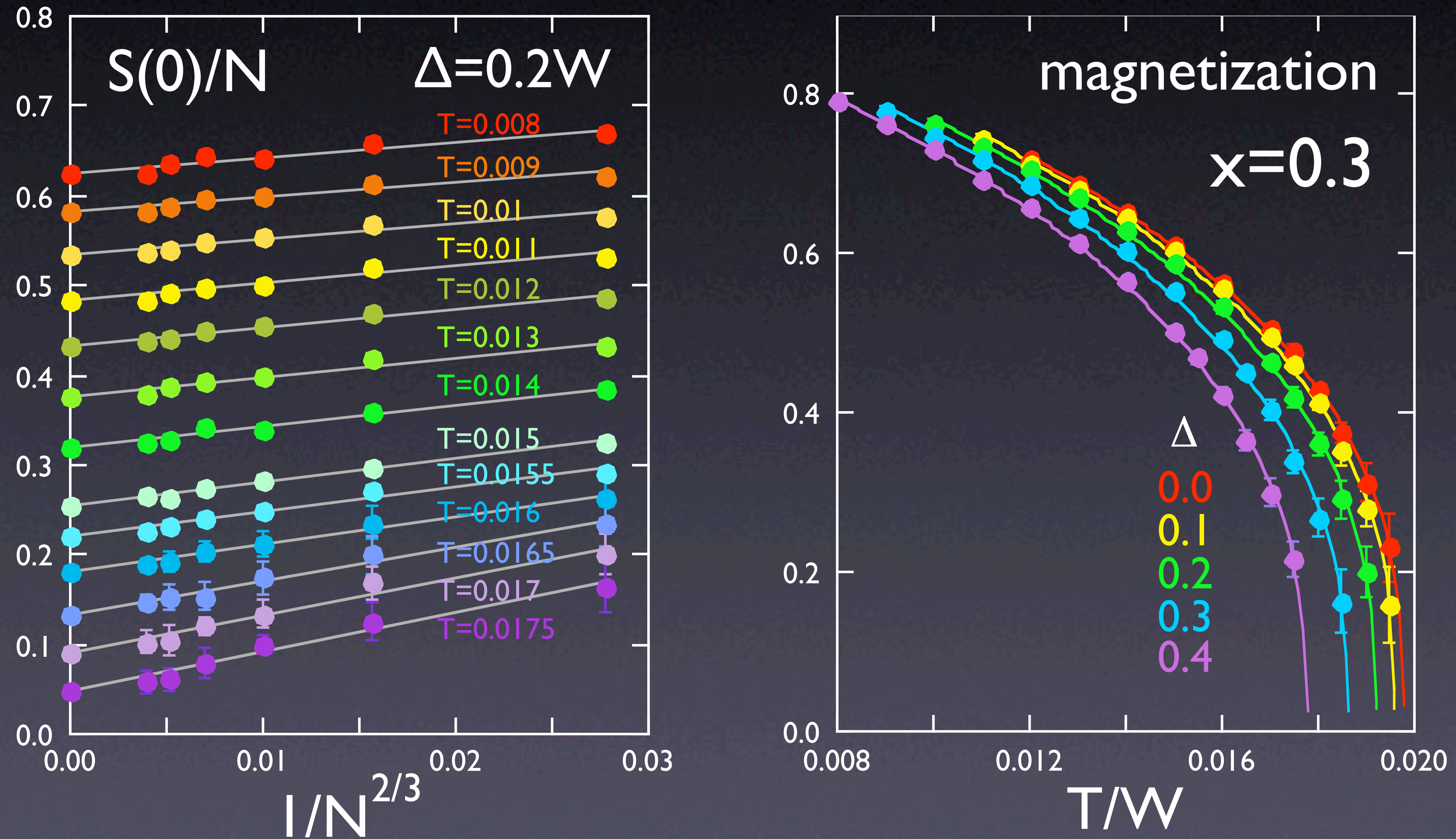




Heisenberg univ. class

How does it work?

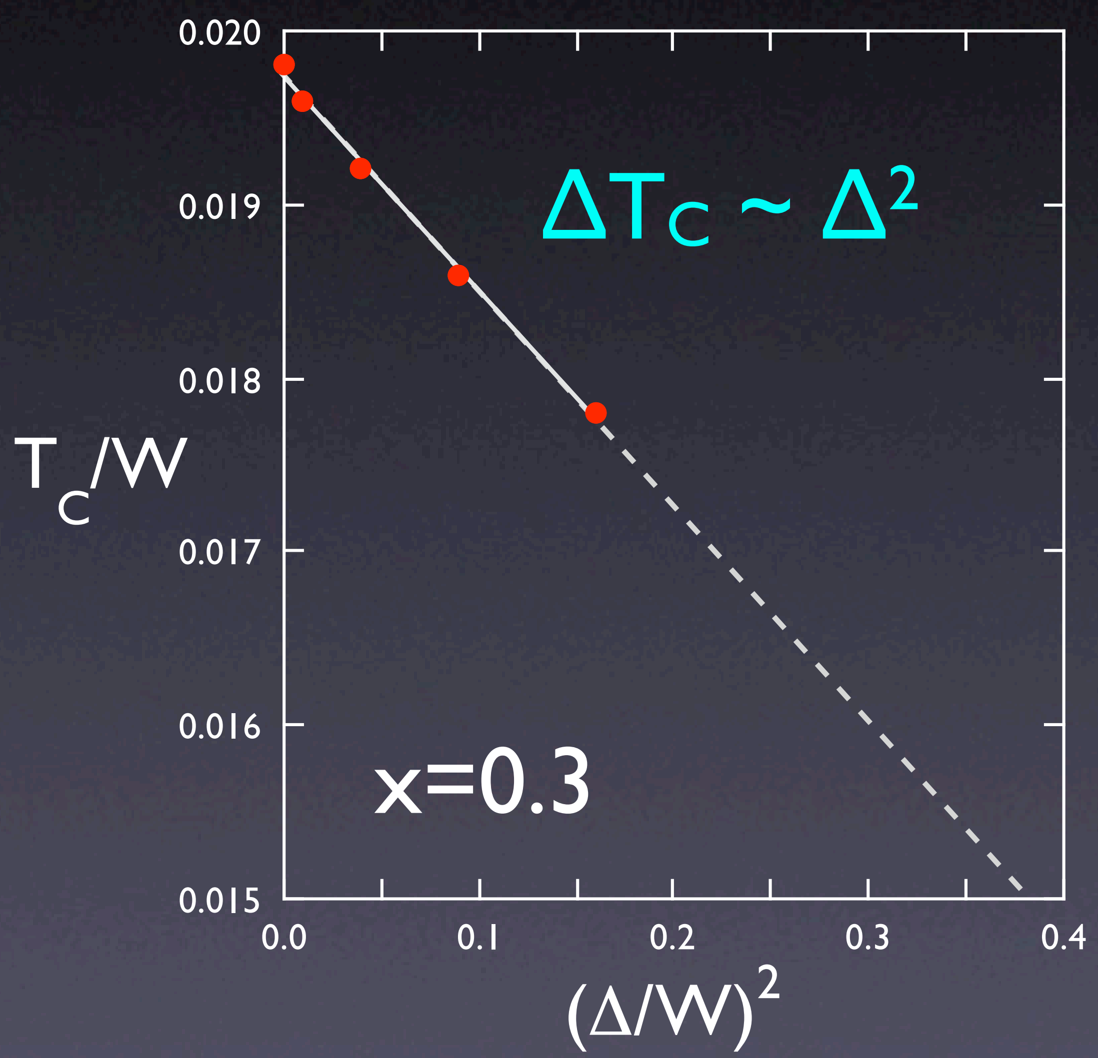
- dirty case (with disorder)



binary disorder $\varepsilon_i = \pm\Delta$

Heisenberg univ. class
(disorder is irrelevant)

Suppression of T_C by Disorder



- reduction of T_C scales to Δ^2
- 30% reduction is achieved at Δ~0.4-0.5W, which corresponds to ~0.5eV

  c.f. Pickett and Singh, 1997

- drawback: transition is always continuous
  - ✓ phonons?

Spin Excitation Spectrum

Spin-wave Approximation

- Holstein-Primakoff transformation

$$S_i^z = S - a_i^\dagger a_i, \;\; S_i^x = \sqrt{S/2}(a_i^\dagger + a_i), S_i^y = \sqrt{S/2}(a_i^\dagger - a_i)$$

- in the lowest-order of 1/S expansion:

$$\langle \tilde{t}_{ij}\tilde{c}_i^\dagger \tilde{c}_j + \tilde{t}_{ji}\tilde{c}_j^\dagger \tilde{c}_i \rangle \to 2SJ_{ij}(a_i^\dagger a_j + a_j^\dagger a_i - a_i^\dagger a_i - a_j^\dagger a_j)$$

$$J_{ij} = \tilde{t}_{ij}\langle \tilde{c}_i^\dagger \tilde{c}_j \rangle / 4S^2$$

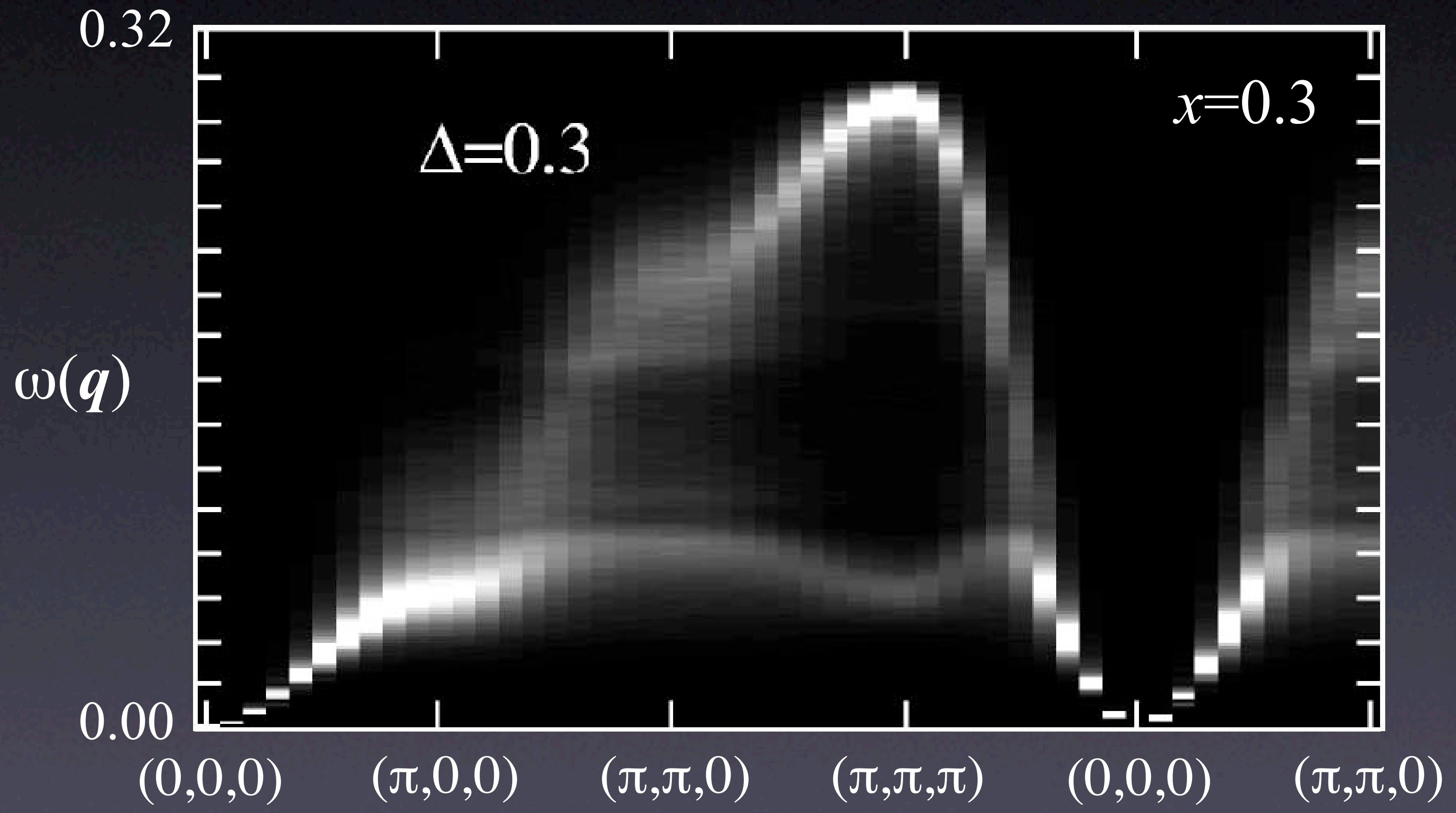
effective exchange interaction induced by itinerant electrons

equivalent to the spin-wave Hamiltonian for Heisenberg model

- spin excitation spectrum is obtained by eigenvalues/vectors of the spin-wave Hamiltonian

$$A(\vec{q},\omega) = \sum_l \left|\langle q|l\rangle\right|^2 \delta(\omega - \omega_l) \qquad H_{\rm sw}|l\rangle = \omega_l |l\rangle$$

Spin Excitation Spectrum: Disorder Strength Dependence



disorder induces broadening, branching, softening, ...

Origin of Anomalies: Friedel Oscillation in Half-metal

- features of spin-excitation anomalies:
  - robust against various types of disorder
  - more apparent in lower dimensions
  - correlation with Fermi wave number

- Friedel oscillation in half-metallic systems

disorder → $2k_F$ charge oscillations

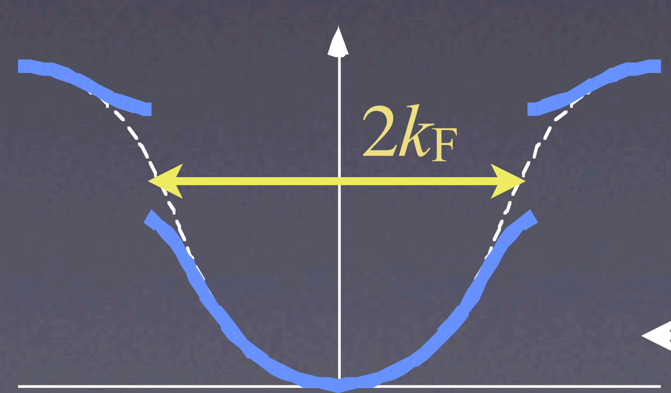
Friedel oscillation

↕ half metal

$2k_F$ spin oscillations

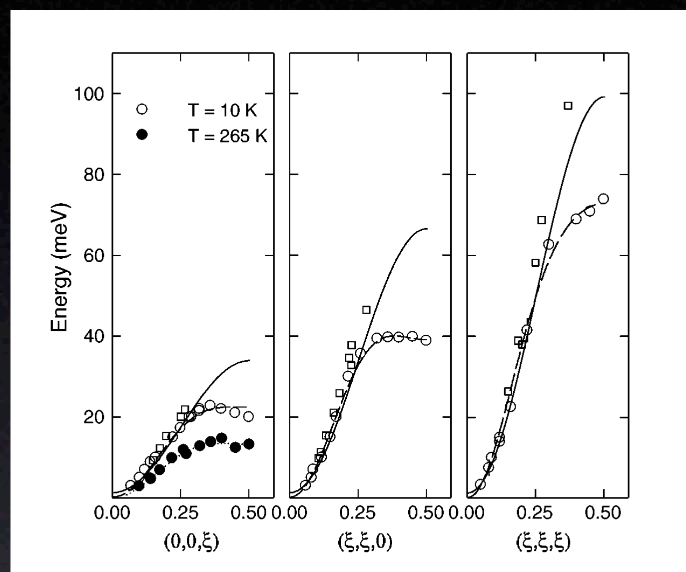
↓

← scattering of magnons

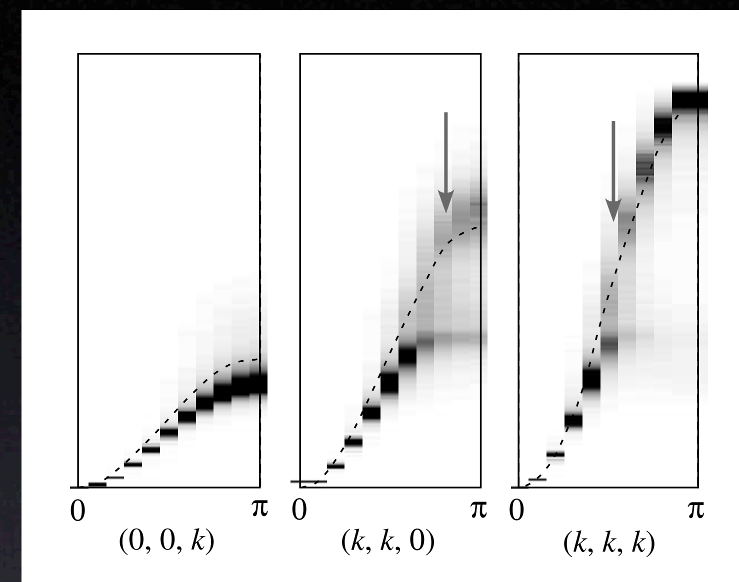


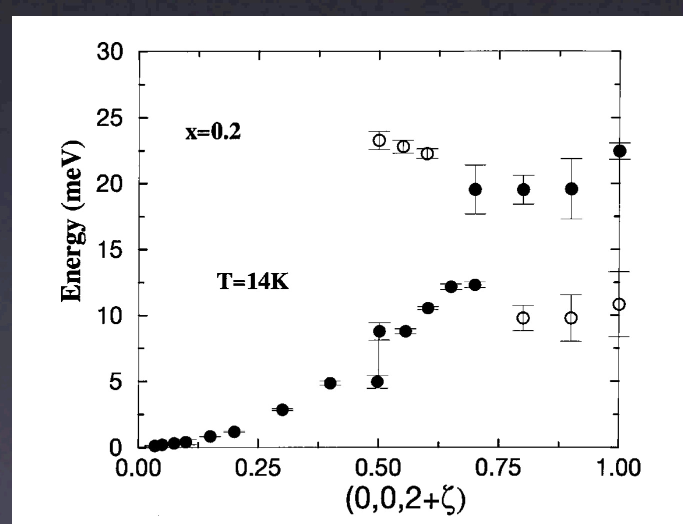
anti-crossing at k_F

Comparison with Experiments

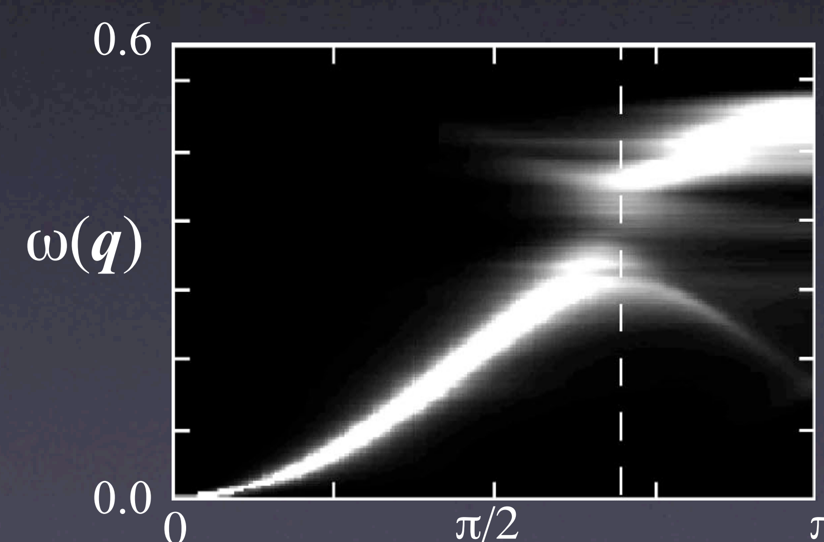


Hwang *et al.* 1998





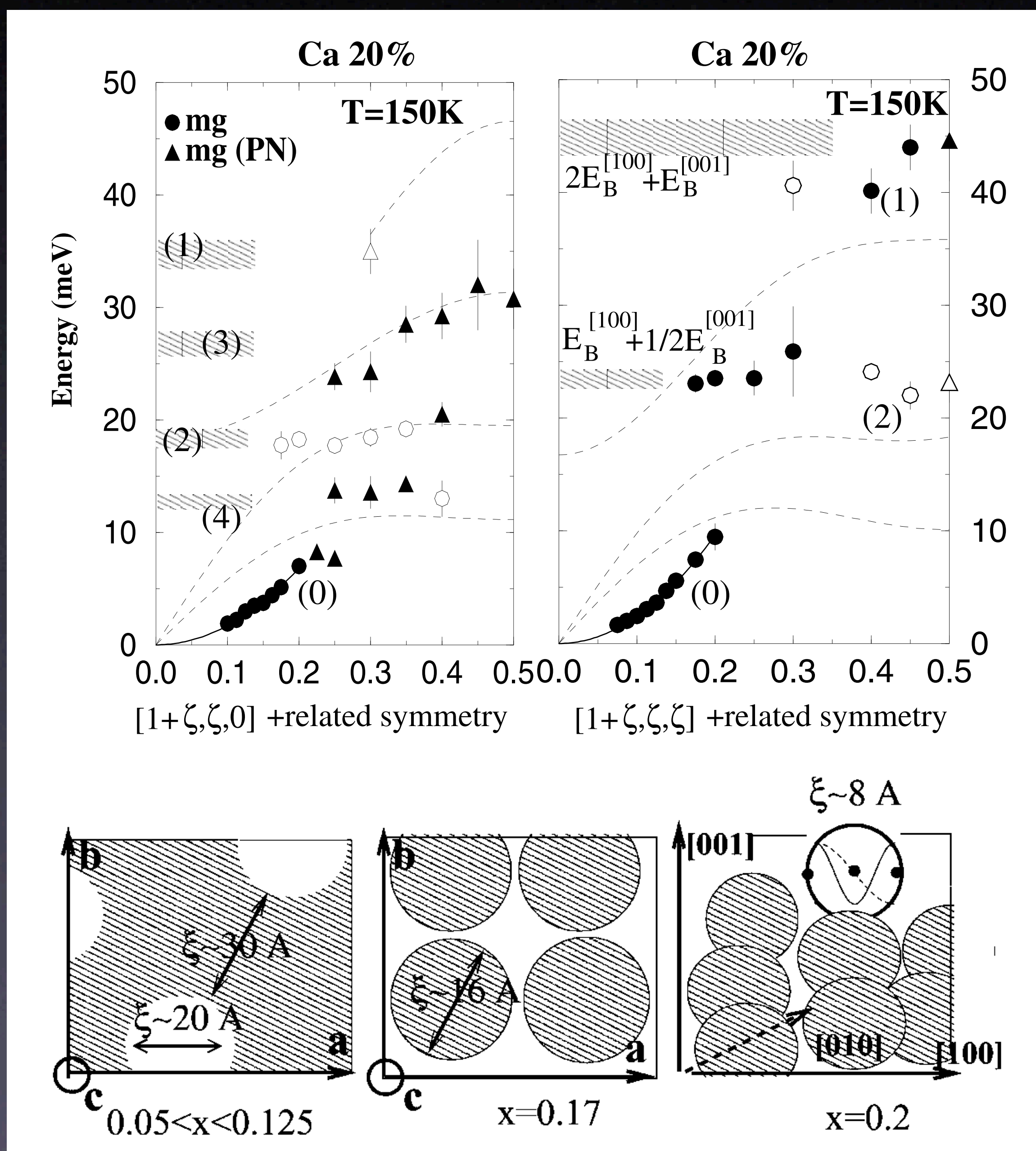
Biotteau *et al.* 2001



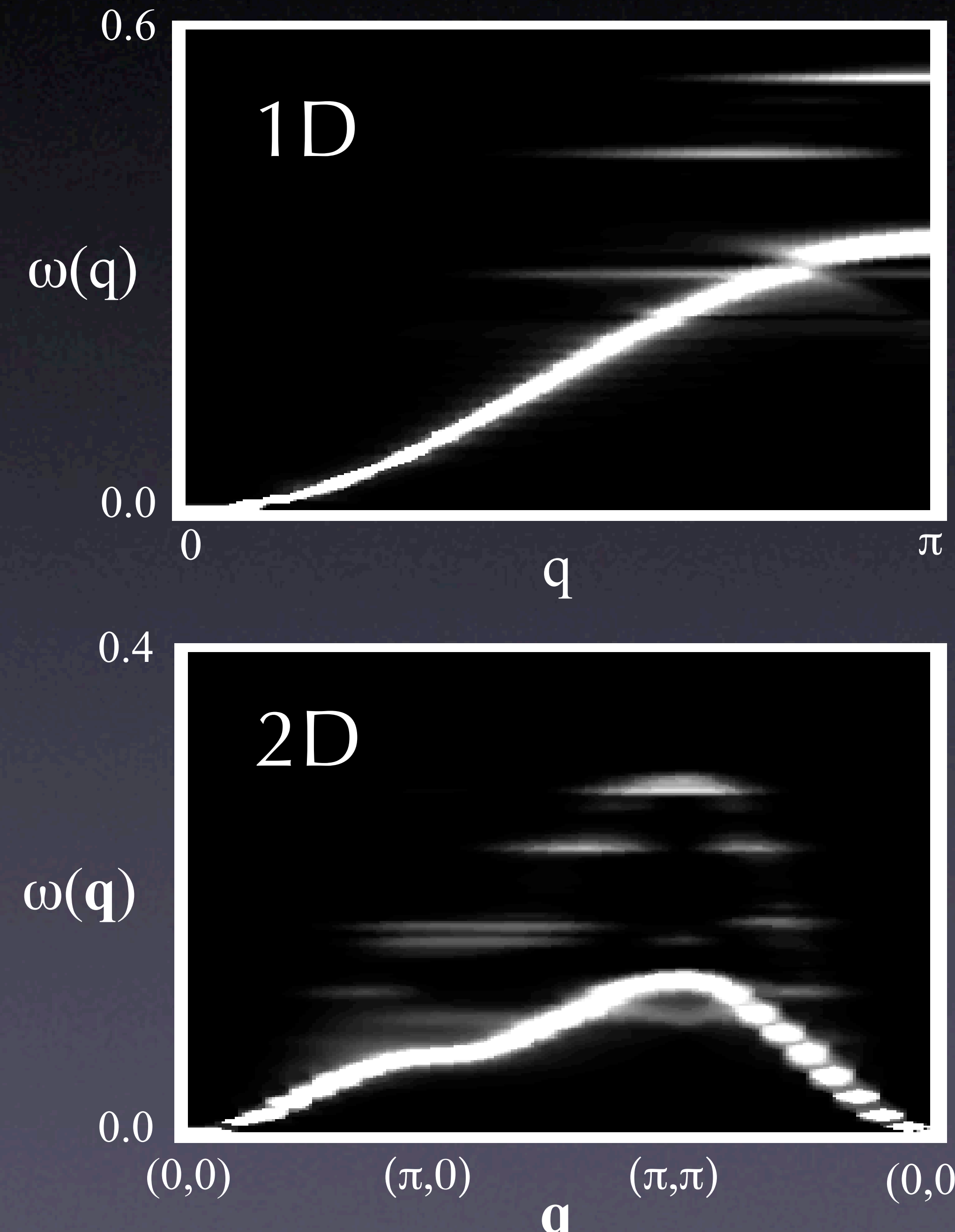
- other theoretical proposals: super-exchange interactions between localized spins (Solovyev and Terakura 1999), orbital fluctuations (Khaliullin and Lilian, 2000), electron-phonon coupling (Furukawa, 1999), electron-electron correlations (Kaplan and Mahanti, 1997; Golosov, 2000; Shannon and Chubukov, 2002)

Extension to Droplet States

(... in progress)



Hennion *et al.* 2005



in collaboration with T. Ziman, O. Cepas (ILL) and G. Bouzerar (CNRS)

Competing Phases

FM vs COI Model

- minimal model to describe the phase competition between FM and COI

$$H = -t \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}) - J_{\mathrm{H}} \sum_{i} \sigma_i^z S_i$$

double-exchange FM

$$- g \sum_i x_i (n_i - \frac{1}{2}) + \frac{1}{2} \sum_i x_i^2 + \frac{\lambda}{2} \sum_{\langle ij \rangle} x_i x_j + \sum_i \varepsilon_i n_i$$

electron-phonon coupling (breathing mode)

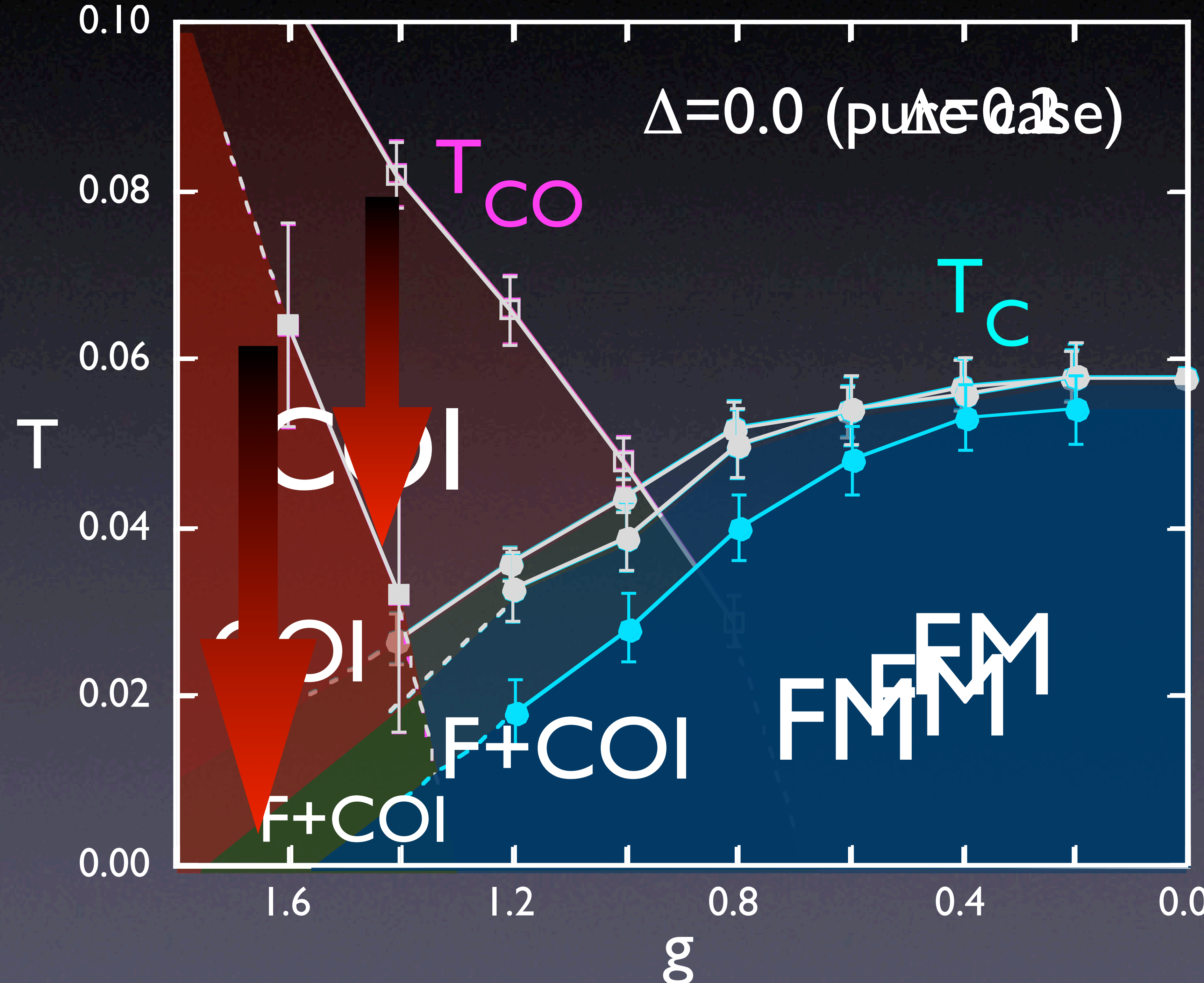
elastic energy (classical)

quenched disorder (on-site randomness)

2D, $\langle n \rangle = 0.5$, $J_{\mathrm{H}} = \infty$, S_i: Ising spin, $\lambda = 0.1$, $\varepsilon_i = \pm\Delta$

- Monte Carlo simulation for thermodynamics
  - distinguish: long-range order vs short-range correlation

Phase Diagram

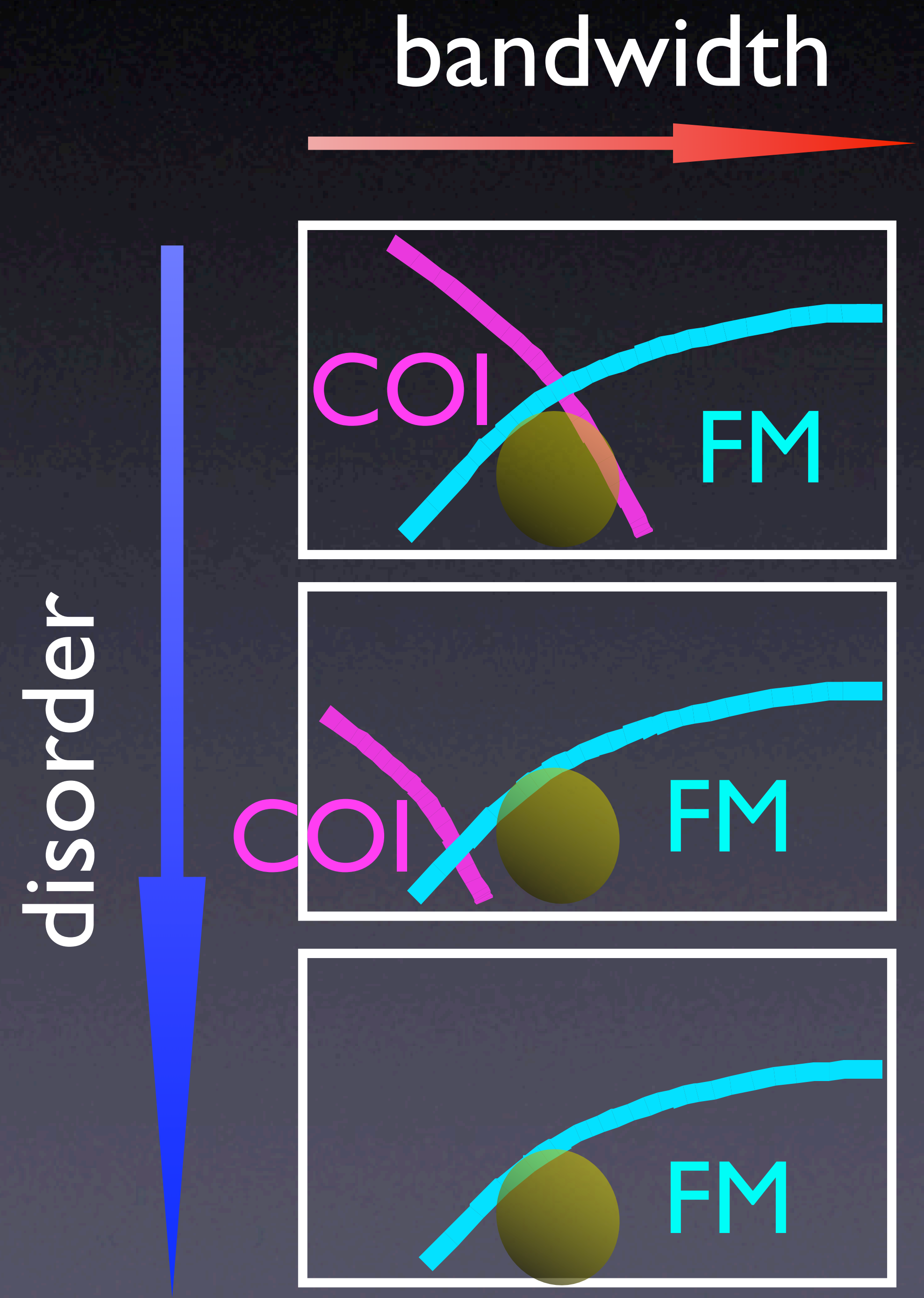


multicritical behavior (FM vs COI)

COI is fragile against disorder

COI vanishes FM is robust

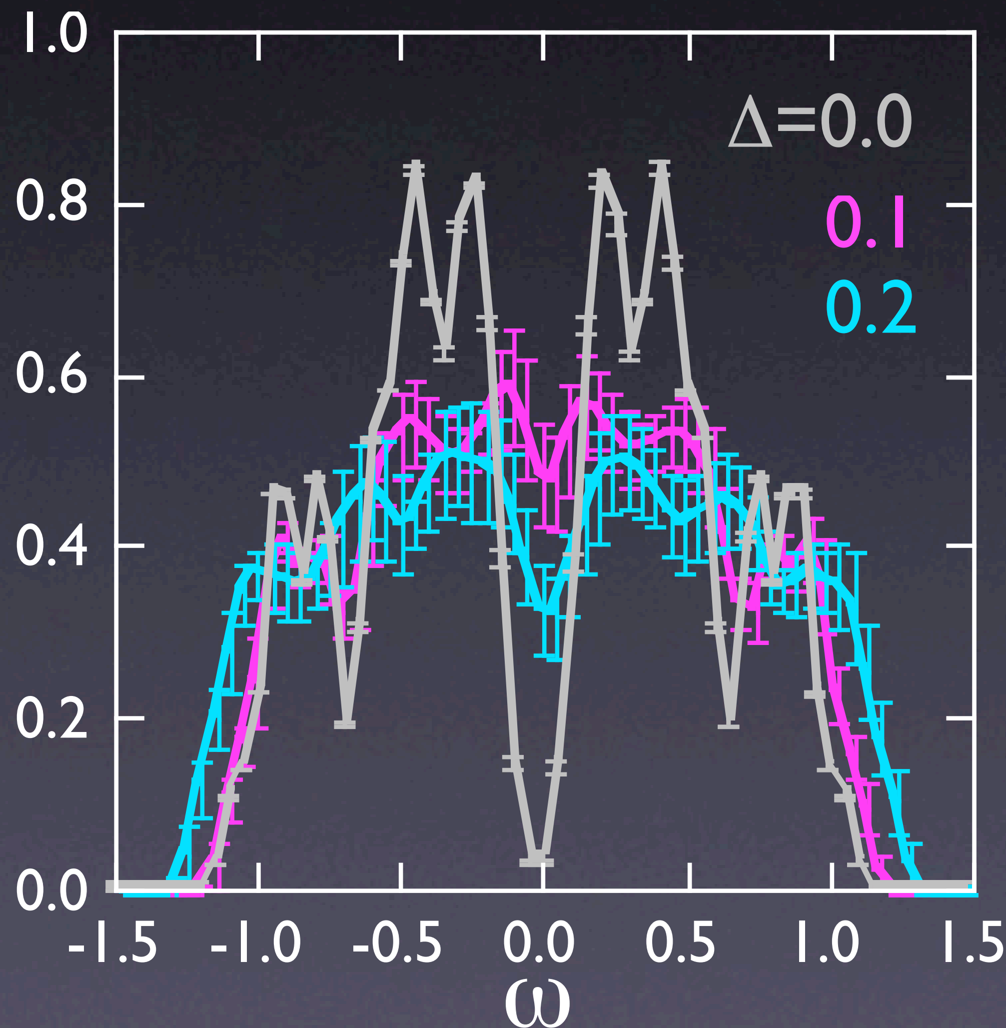
Asymmetric Change of Phase Diagram



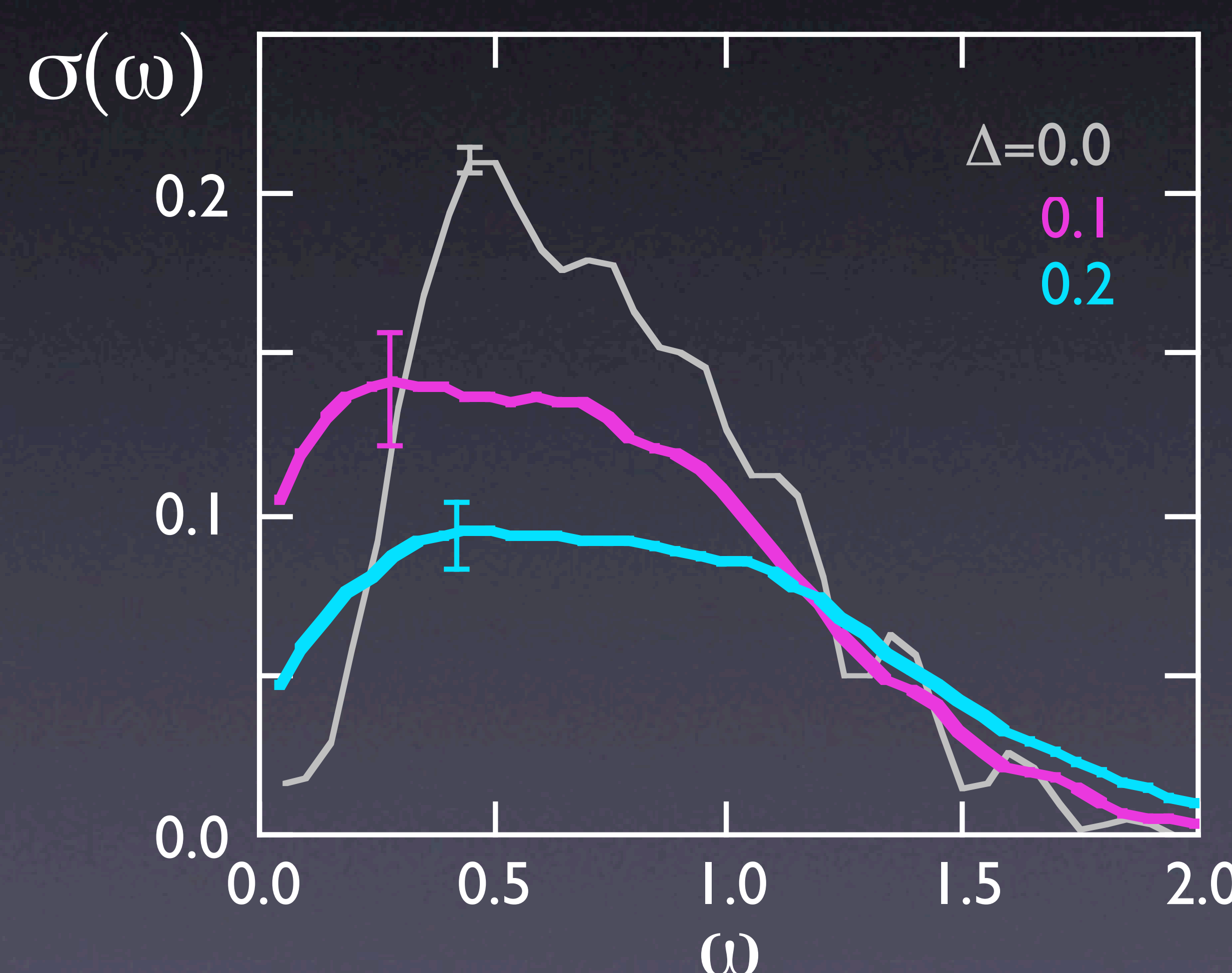
- COI is fragile against the disorder while FM is robust
- The multicritical point shifts to enlarge FM region
- disorder-induced insulator-to-metal transition

Disorder-Induced Insulator-to-Metal Transition

density of states

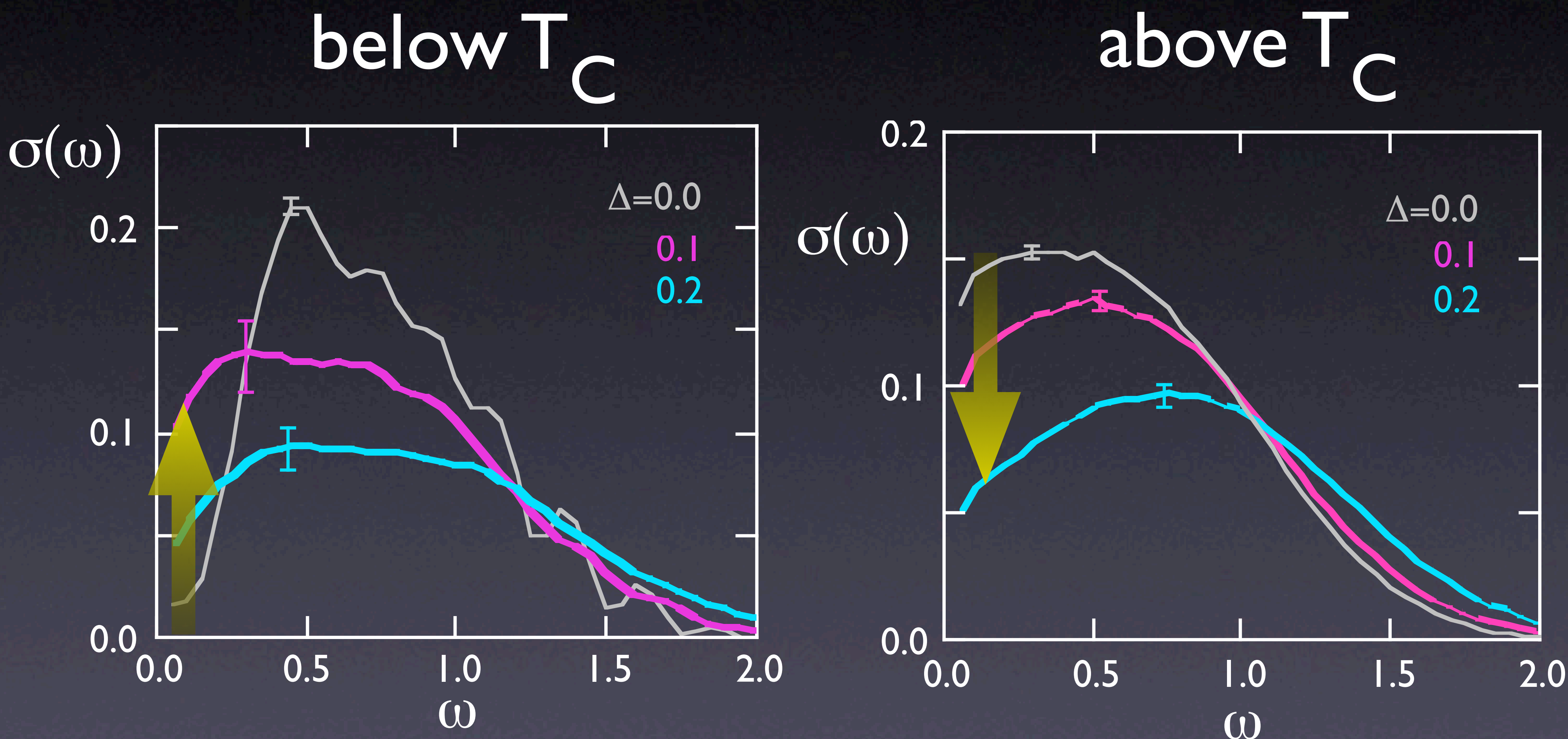


optical conductivity



see also Sen, Alvarez and Dagotto, 2004

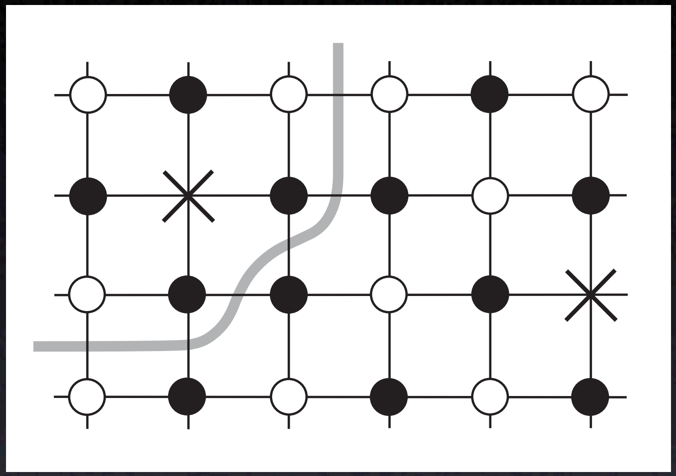
Contrastive Effects of Disorder



- Disorder makes the system metallic below T_C but insulating above T_C

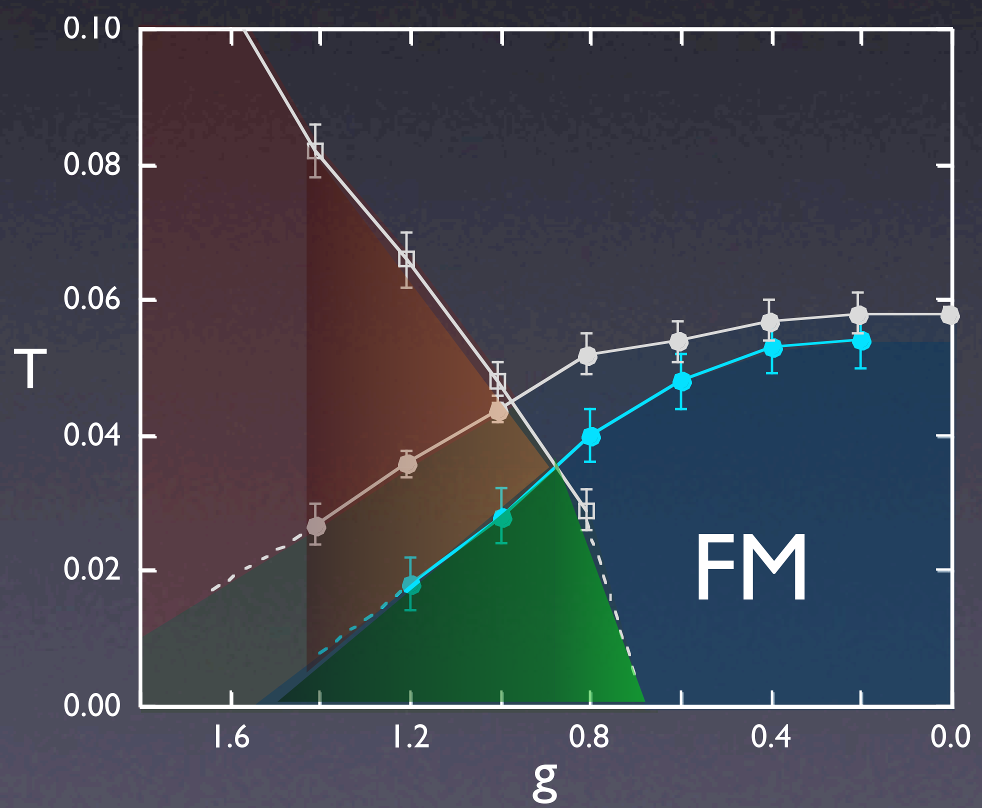
Role of Disorder

- pinning to commensurate CO
  - antiphase boundaries kill LRO
- domain walls: extra entropy



CO short-range correlation

insulating state with charge pseudo gap



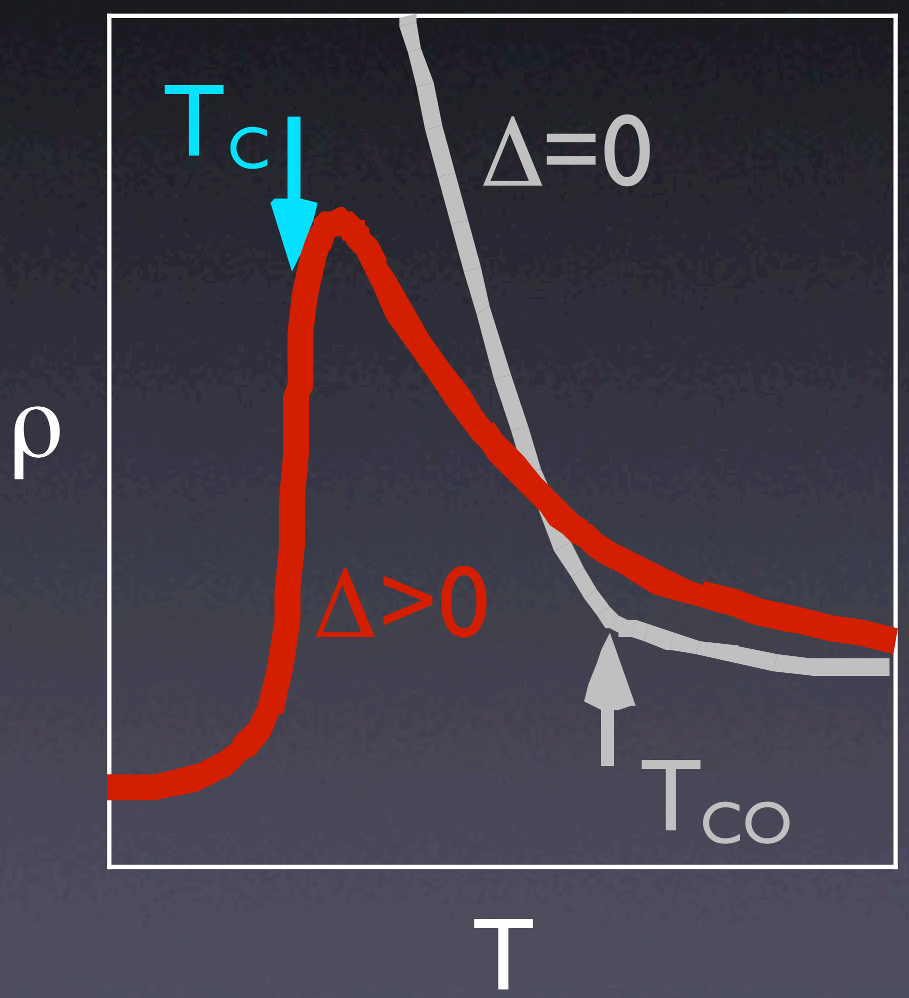
CO LRO is never stabilized

FM overtakes in the energy competition

re-entrant behavior from high-T insulating to low-T metallic state

Origin of CMR ?

- Re-entrant behavior gives a good motive to cause the enhanced CMR
- direct (numerical) confirmation is needed
- extention to more realistic models including orbitals, Jahn-Teller, etc.
  - ✓ pinning to orbital order/ cooperative Jahn-Teller



Summary

- Monte Carlo study of T_C
  - rapid decrease of T_C by introducing disorder
- spin excitation anomalies
  - Friedel oscillation in half-metallic systems
- phase competition between FM and COI
  - disorder-induced insulator-to-metal transition and CMR