Computational Studies of Models for Manganites and Cuprates

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Complexity in Strongly Correlated Electron Systems (Miniprogram). KITP, Santa Barbara, CA. (July 2005)

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Outline

- Brief review of spin fermion models and the Polynomial Expansion Method (PEM)
- Application 1: Two Orbital Model for Manganites
- Parallelization and Extensions of the TPEM
- Application 2: Spin fermion model for High Tc Superconductors
- Conclusions

Theoretical Overview: Spin Fermion Models

Complexity

Hubbard Models

Accurate Study?
No, because of the sign problem.
But Lanczos, DMRG, on small or 1 dimensional systems.

Spin-fermion Models

Model is accurate
if localized moments present.
Can be solved exactly by numerical methods that are polynomial in time

Classical models
(Ising, Heisenberg, etc)

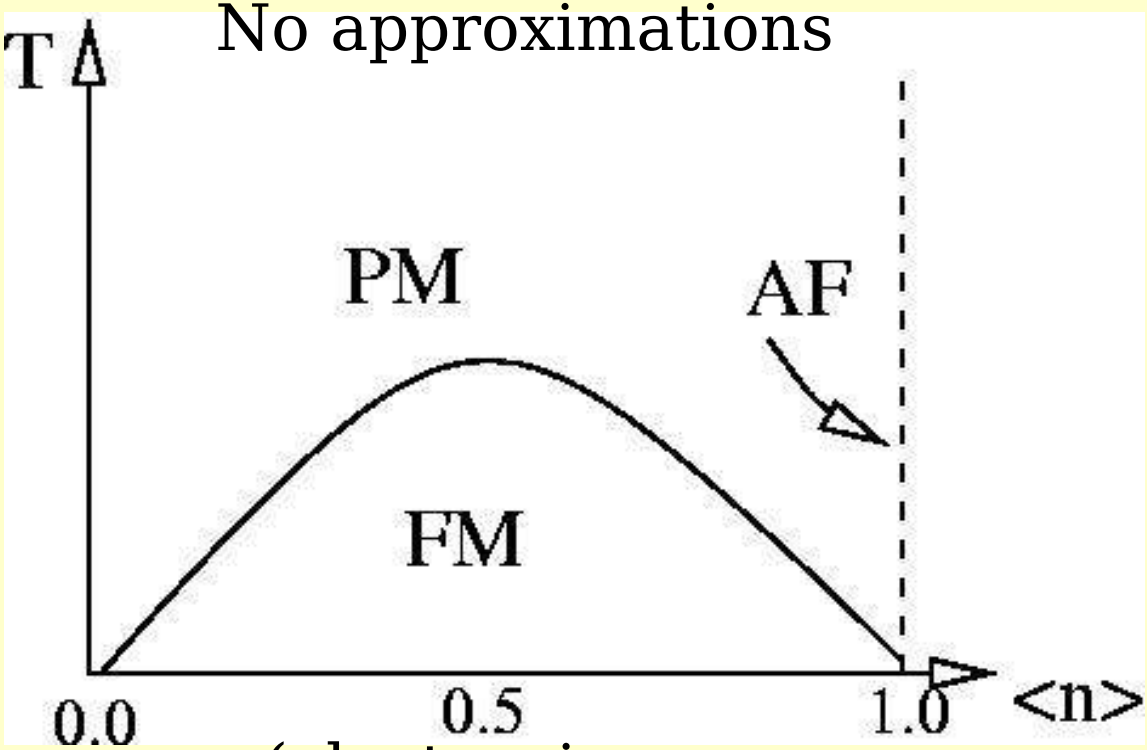
Easy to solve but
no electrons, no holes,
no spectral functions,
etc...

Spin Fermion Model for Manganites

$$H = -t \sum_{<ij>\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} - J_H \sum_{i\alpha\beta} c^{\dagger}_{i\alpha} c_{i\beta} \vec{S}_i \cdot \vec{\tau}_{\alpha,\beta}$$

No approximations

Local spin



(electronic density)

Manganite crystal

Computational Complexity

$$\hat{H} = \sum_{ij\alpha\beta} c^{\dagger}_{i\alpha} H_{i\alpha,j\beta}(\phi) c_{j\beta},$$

<---- SPIN-FERMION MODEL

$$Z = \int d\phi \sum_{n} \langle n | \exp(-\beta \hat{H}(\phi) + \beta\mu\hat{N}) | n \rangle$$

- Integration of the one-electron sector.
- Monte Carlo integration of Classical Fields
- Rigorously exact!
- Computational Complexity $O(N^4)$ (one matrix diagonalization per “spin-flip”, N*N_iterations diagonalizations ~ 216 * 10000 = 2,160,000!)

Theoretical Overview: Polynomial Expansion

Y. Motome and N. Furukawa, J. Phys. Soc. Japan 68, 3853 (1999)

$$A(\phi) = \int_{-1}^{1} F(x) D(\phi, x) dx,$$

Energy, Density, Action, Classical observables.

$$F(x) = \sum_{m=0}^{\infty} f_m T_m(x),$$

$$\mu_m(\phi) = \sum_{\nu=1}^{N_{dim}} \langle \nu | T_m(H(\phi)) | \nu \rangle,$$

$$A(\phi) = \sum_{m} f_m \mu_m(\phi)$$

- No diagonalization
- Matrix-vector prod. benefits from sparseness of H.

TPEM: Computational Complexities

[Y. Motome and N. Furukawa, J. Phys. Soc. Jpn. 73, 1482 (2004)]

N = number of sites
M = expansion cutoff
r = non-zeros per row of H
d = (r-1)/2
ε = threshold for product truncation

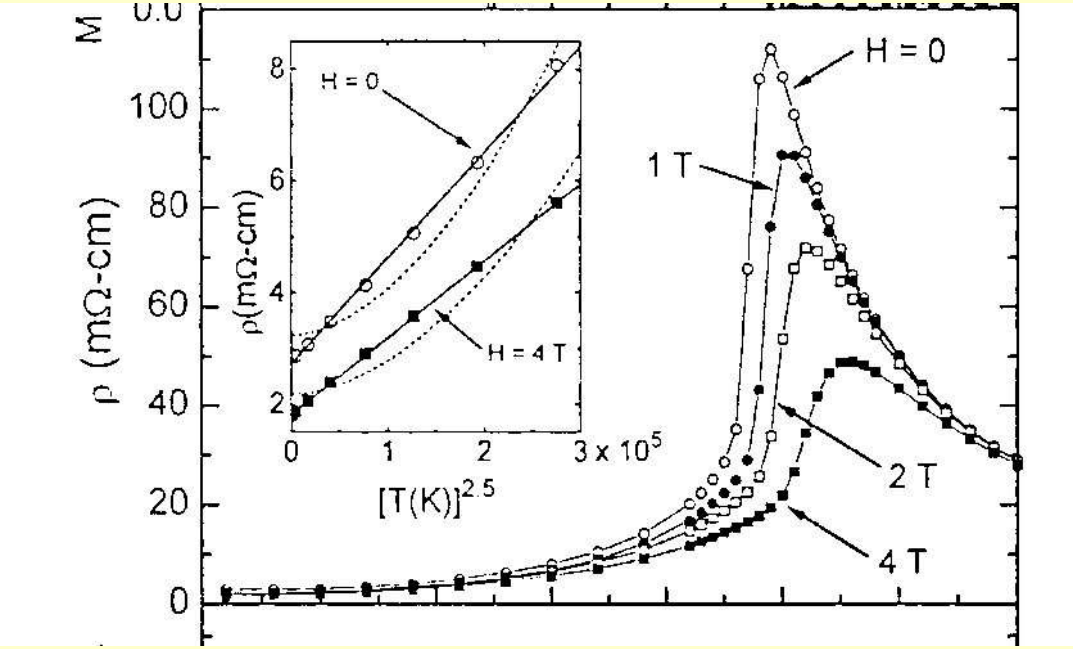
(Method does not introduce systematic errors, uncontrollable approx.)

Algorithm	|n;m>	Trace	Delta S	Total
Diag.	-------	------	$O(N^3)$	$O(N^4)$
full-PEM	O(MN)	O(N)	$O(MN^2)$	$O(MN^3)$
T-PEM(ε>0)	$O(M^{d+1})$	$O(M^d)$	$O(M^{2d+1})$	$O(M^{2d+1}N)$

Application 1: CMR Manganites

Outline:

- Spin fermion model
- Phase diagram from Numerical Simulations
- Conductance without chemical disorder
- Addition of chemical disorder

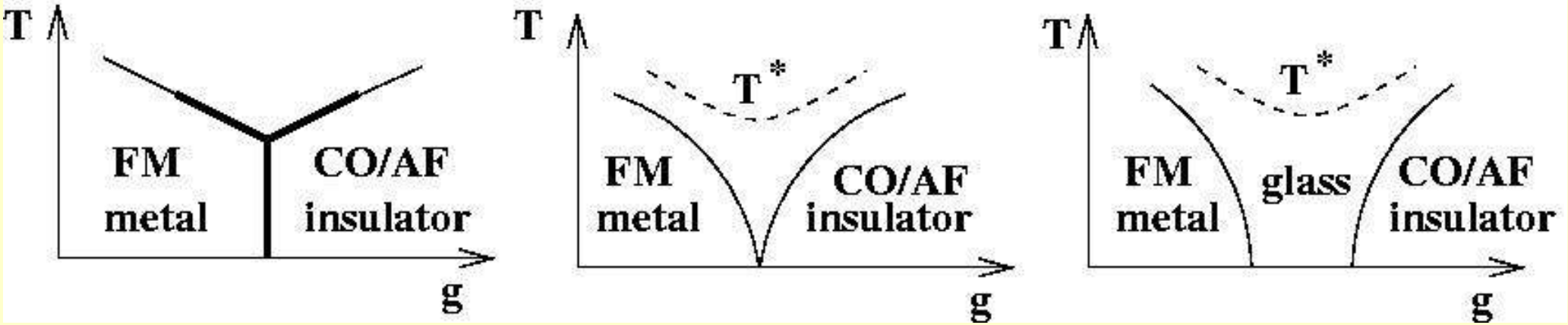


[Schiffer et al, PRL 75, 3336 (1995)]

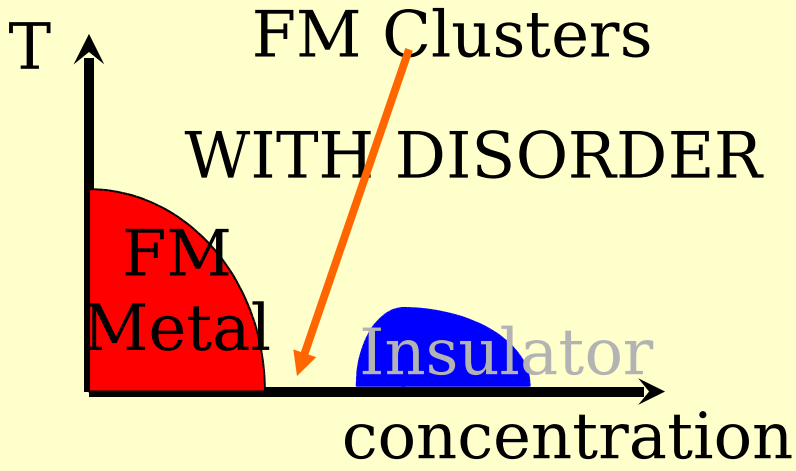
$La_{1-x}Ca_xMnO_3$

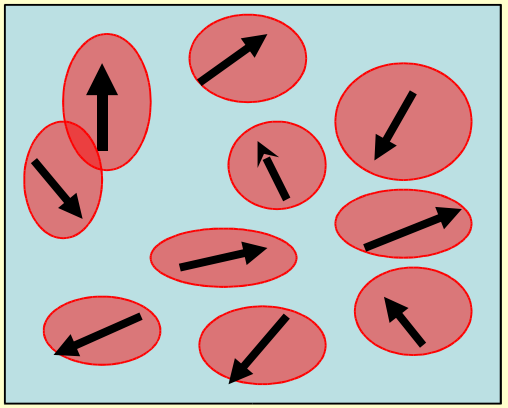
FM "Clusters" in CMR Manganites

[Dagotto, "Nanoscale Phase Separation and Colossal Magnetoresistance", Springer-Verlag. (2002).]



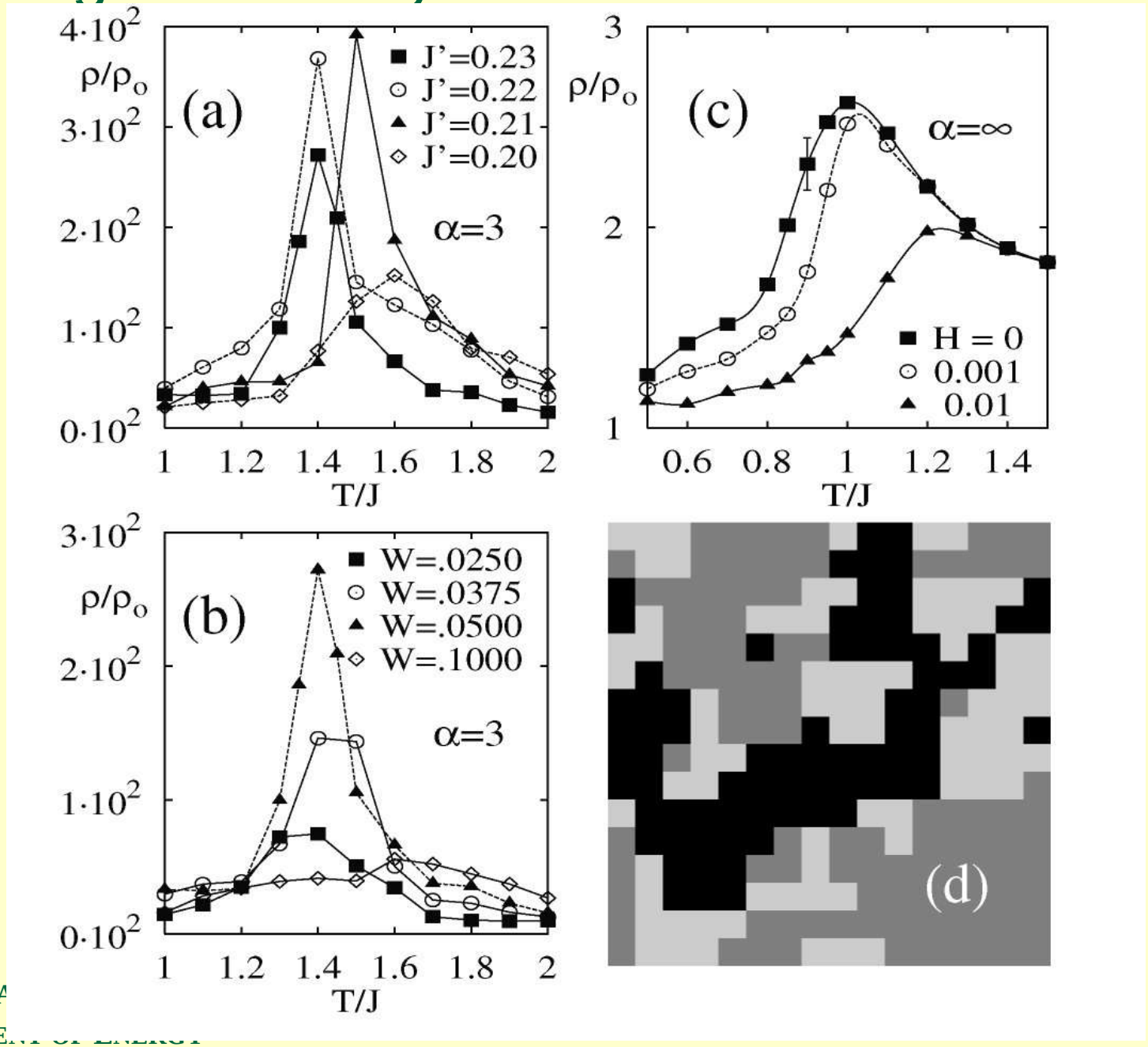
[Dagotto et al, Phys. Rep. 344, 1 (2001)]





CMR Manganites: Toy Model

J. Burgy et al., PRL 92 (2004)



Microscopic two-orbital Model for Manganites

[Dagotto, “Nanoscale Phase Separation and Colossal Magnetoresistance”, Springer-Verlag. (2002).]

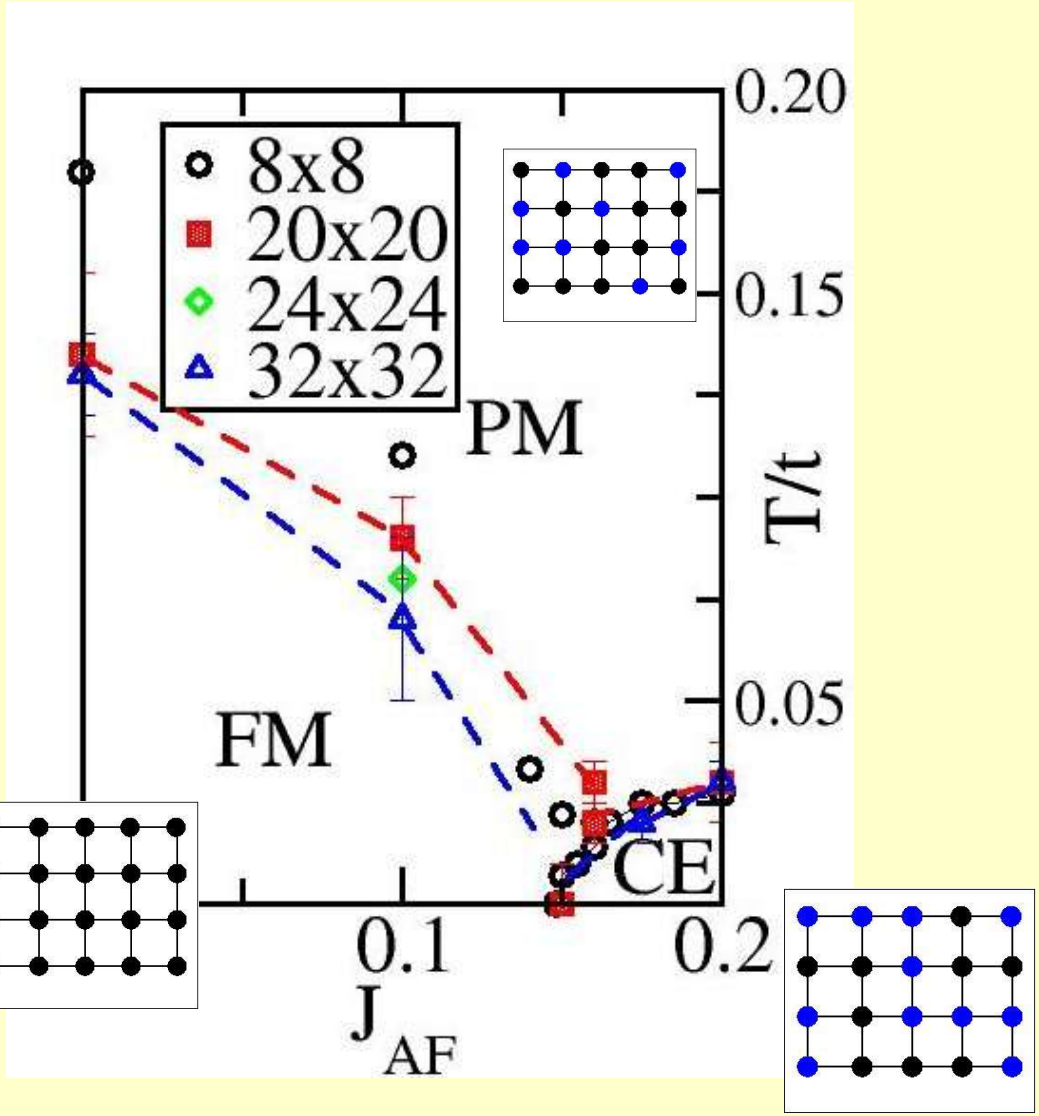
$$H_{2b} = \sum_{\gamma,\gamma',i,\alpha} t^{\alpha}_{\gamma\gamma'} \mathcal{S}(\theta_i, \phi_i, \theta_{i+\alpha}, \phi_{i+\alpha}) c^{\dagger}_{i,\gamma} c_{i+\alpha,\gamma'}$$
$$+ \lambda \sum_i (Q_{1i}\rho_i + Q_{2i}\tau_{xi} + Q_{3i}\tau_{zi})$$
$$+ \sum_i \sum_{\alpha=1}^{\alpha=3} D_\alpha Q^2_{\alpha i}.$$

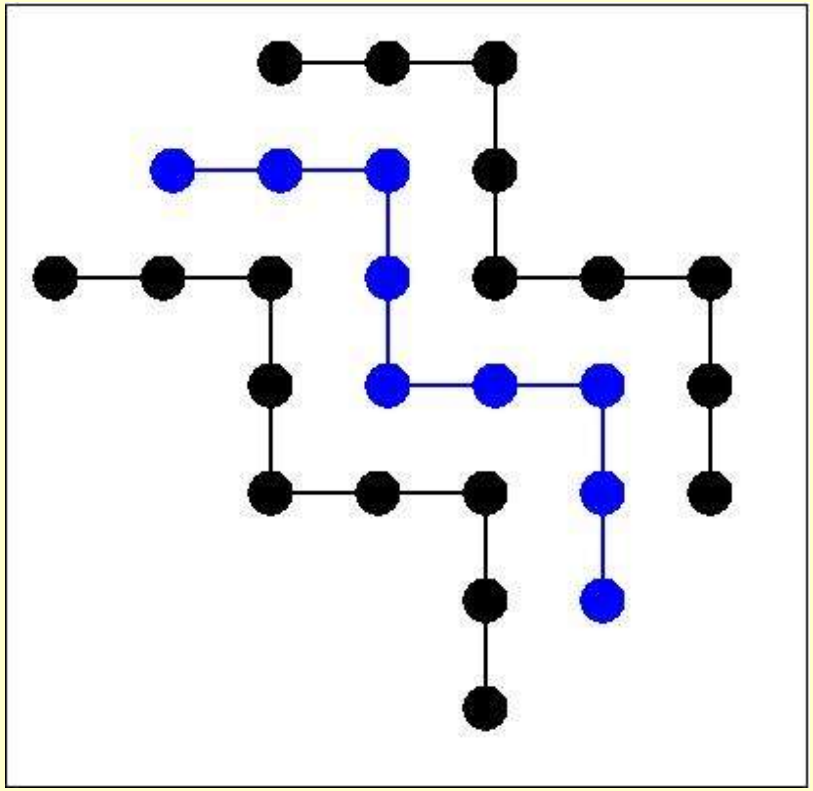
+JAF\sum_<ij> S_i * S_j

Two-orbital Model for Manganites

[C. Sen et al. unpublished]

Phase Diagram Without disorder

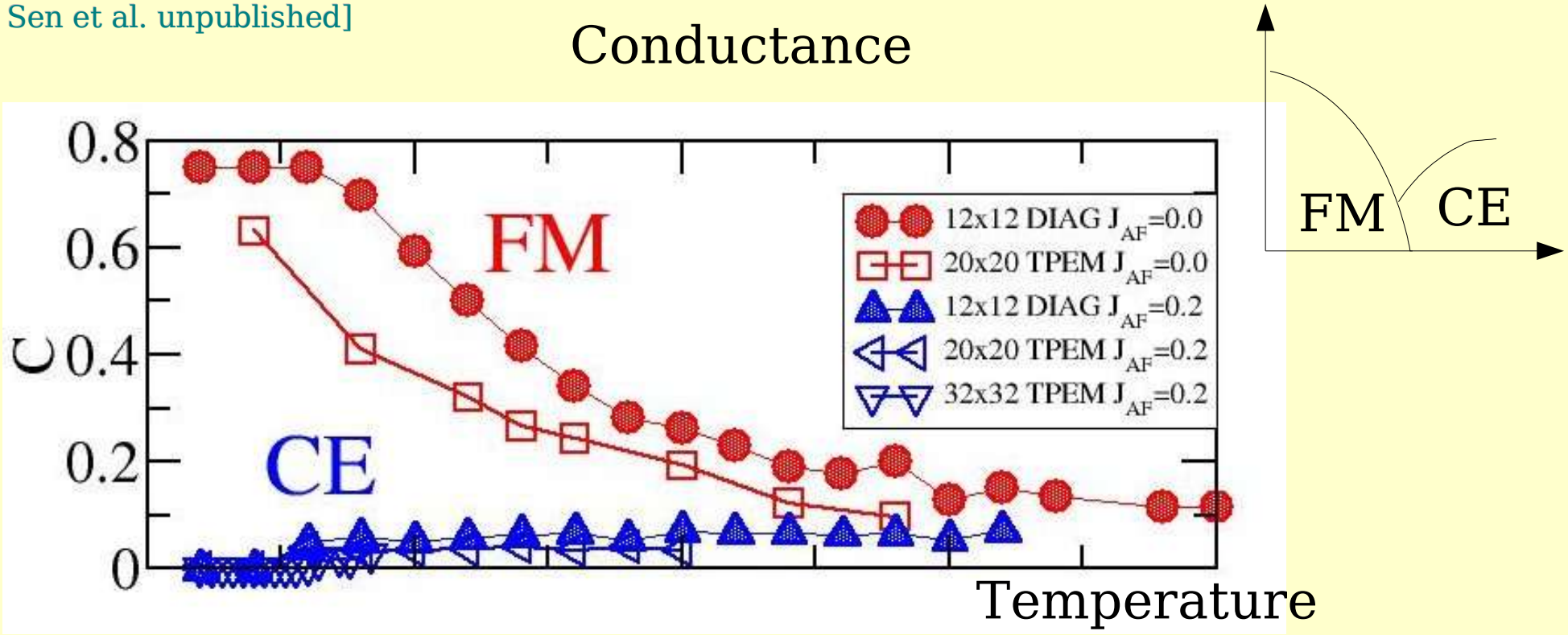




Magnetic CE-phase

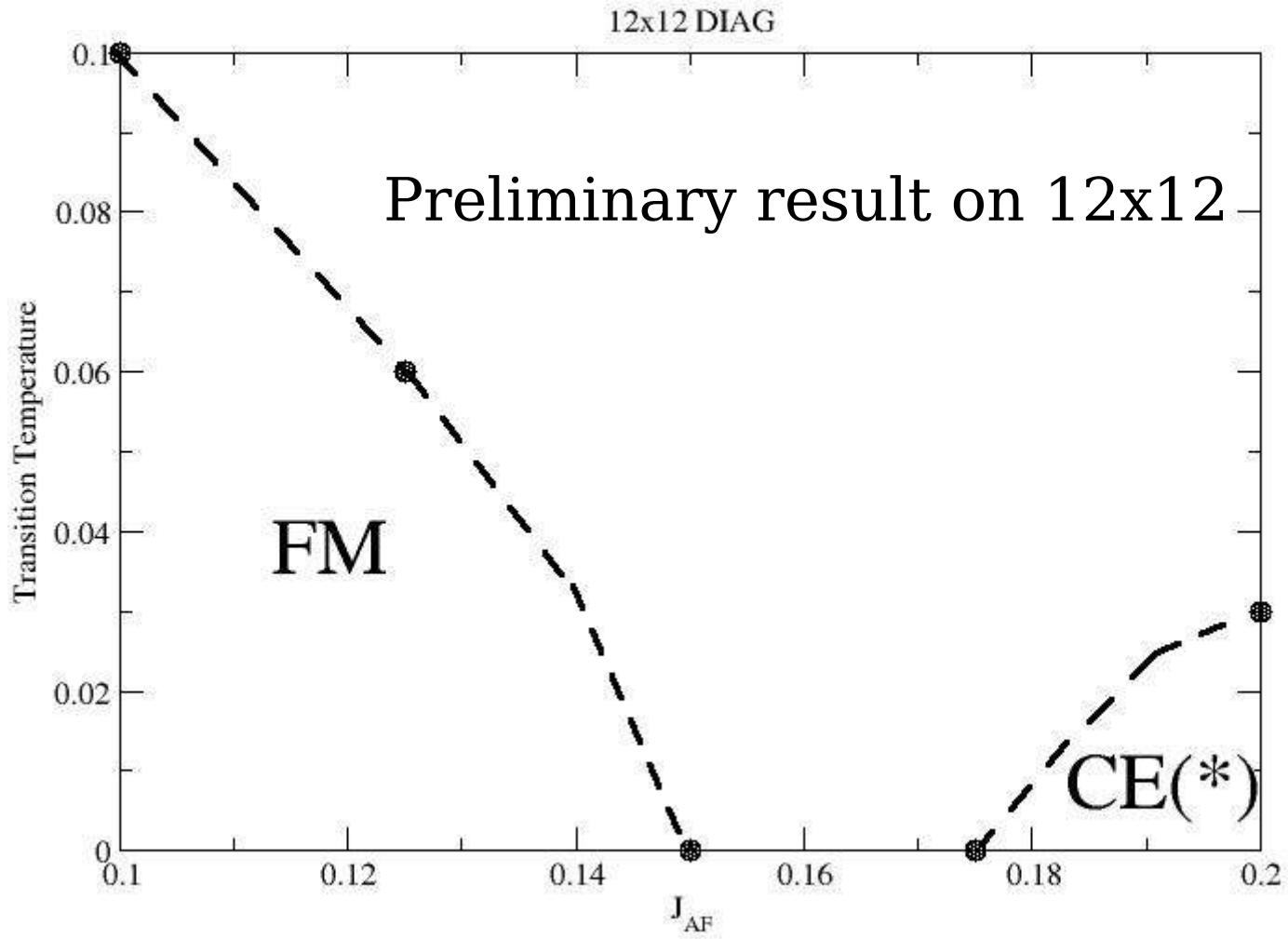
Two-orbital Model for Manganites

[C. Sen et al. unpublished]

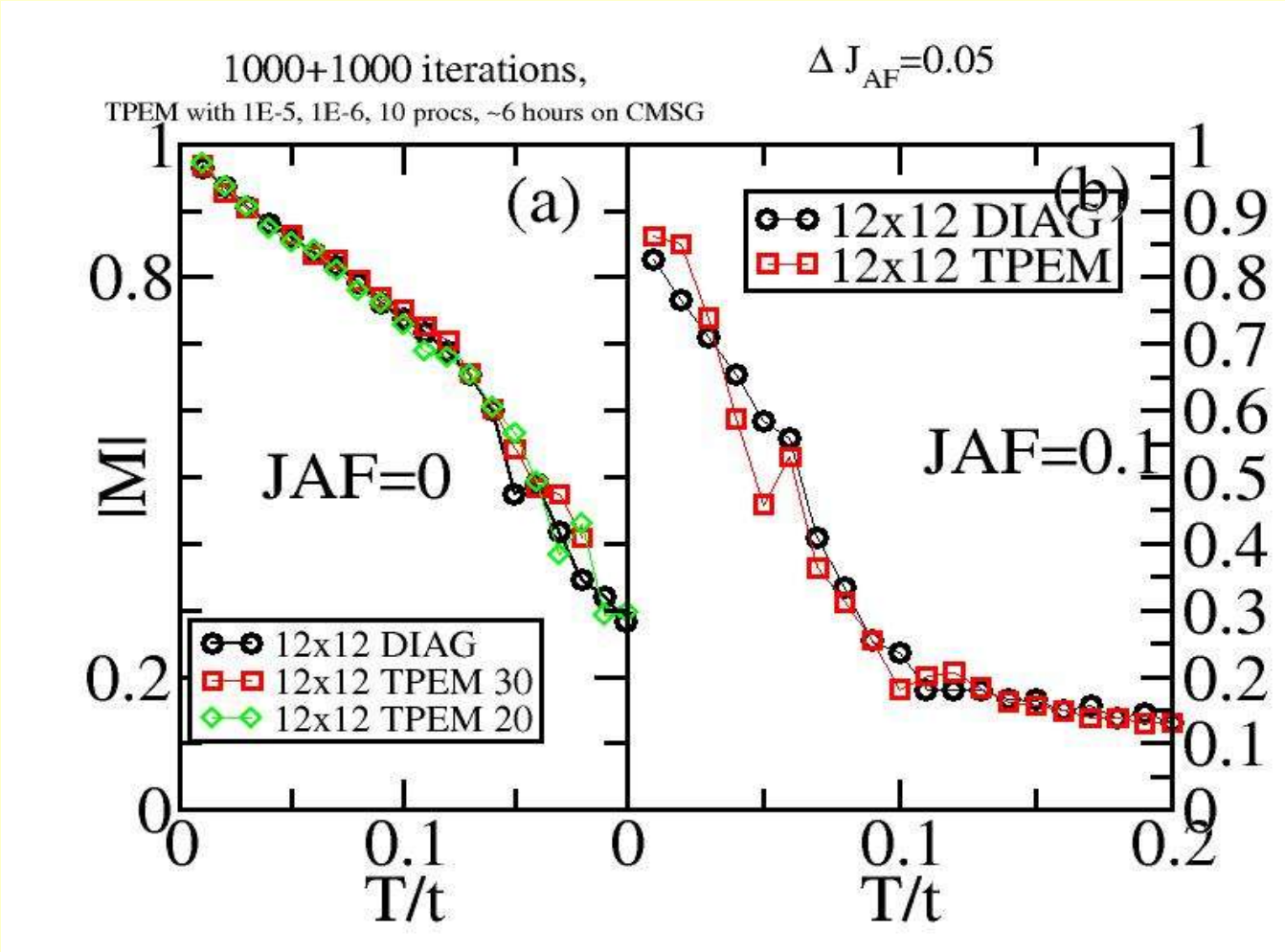


- Mesoscopic Conductance (Verges, et al.)
- Chemical Disorder has to be included.
- Study of Phonons with the TPEM : Spectrum bounds.
- But remember: this is a **exact numerical study**

Model for Manganites: TPEM & Chemical Disorder



TPEM: Disordered manganite systems



End of Manganites Part

Parallelization and Scalability of the PEM

$$\mu_m(\phi) = \sum_{\nu=1}^{N_{dim}} \langle \nu | T_m(H(\phi)) | \nu \rangle,$$

Independent terms in the expansion

TPEM: Scalability and Parallelization

N_{proc} = Number of processors.

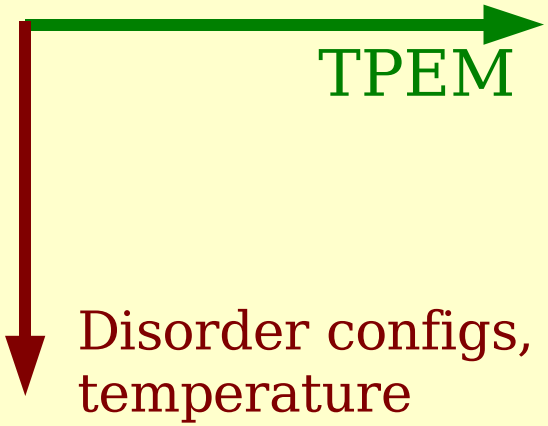
N_{dim} = Size of the one electron Hilbert space (OEHS).

- The PEM **without truncation** "scales" with N_{proc} up to N_{dim}. A "typical" 32x32 one-orbital model ==> 2048 procs.
- The **truncated PEM** "scales" with N_{proc} only up to the size of the truncated OEHS ~ 40-80 procs.

NCCS Facility at ORNL

Parallelization and Truncation

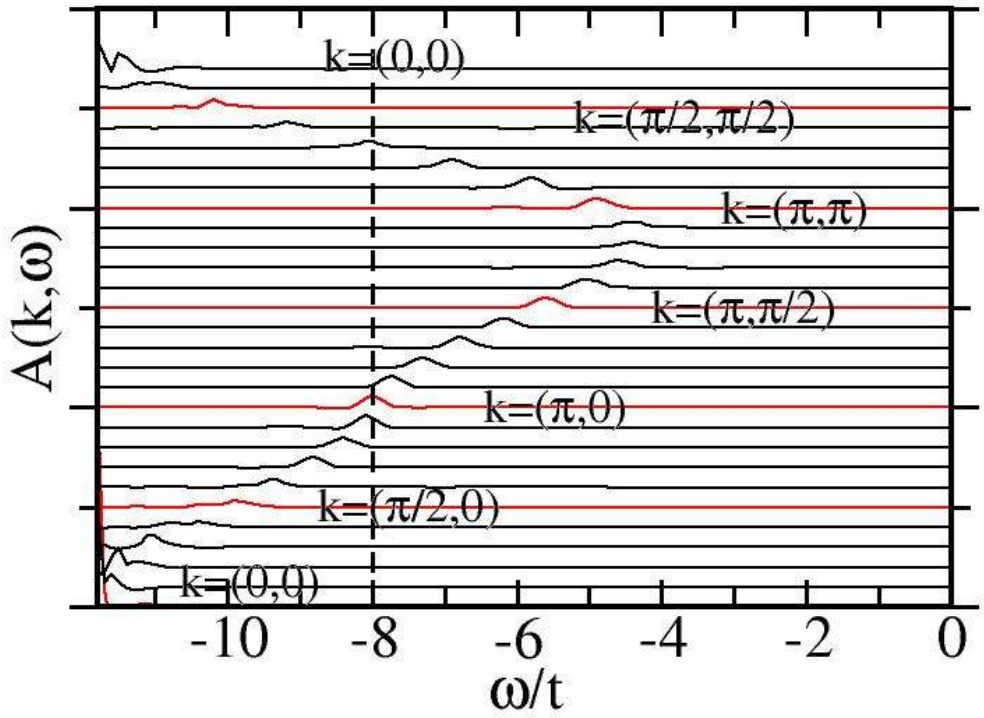
For the TPEM it is advantageous to use "double-parallelization": AxB processors, where A is for the TPEM parallelization and B processors is for various disorder configs., various temperatures, etc. ==> A~40-80, B~10-20, ==> "scales" up to 400-1600 pr.

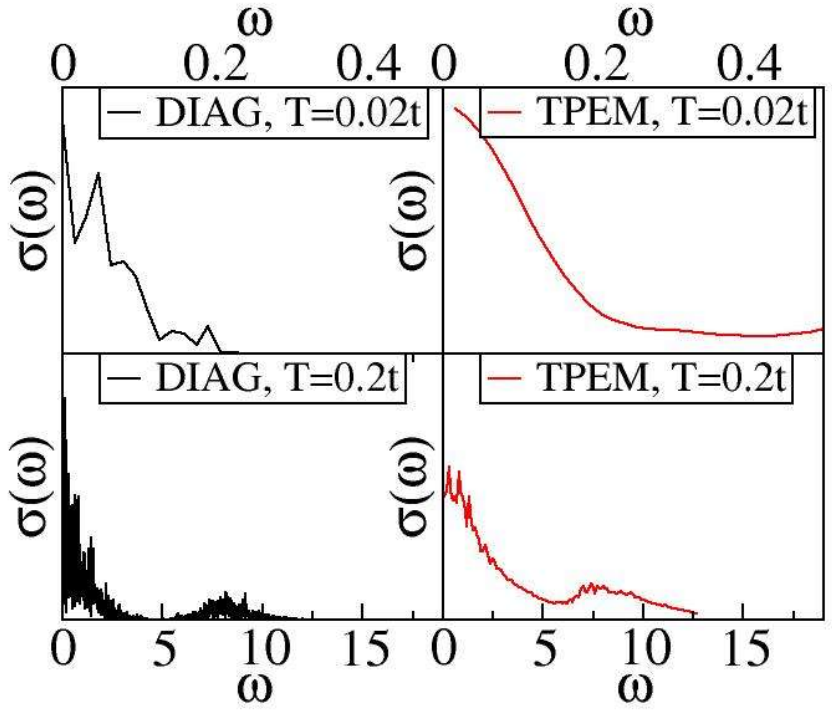


TPEM: Spectral Function and Optical Conductivity

$$A(\phi) = \int_{-1}^{1} F(x) D(\phi, x) dx,$$

Double exchange model for manganites





Comparision on 8x8, JH=4 <n>=0.5

20x20 lattice, JH=8, <n>=0.5 (FM g.s.)

[Alvarez and Schulthess, unpublished]

Spin Fermion Models: Software Toolkit

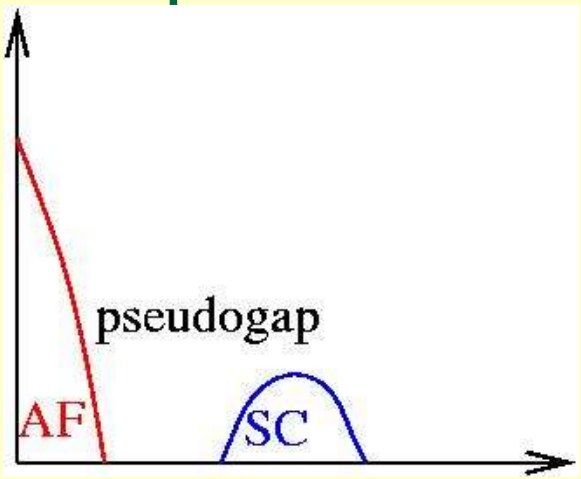
http://mri-fre.ornl.gov/spf

- High performance computing, optimizations.
- Flexible input, various models.
- Various geometries. (cubic, FCC, zincblende, etc)
- T/PEM implemented in a model independent way.
- Parallelization of the TPEM and grid parallelization.
- C++ and STL, perl for postprocessing.
- Integrated with the PSIMAG toolkit (http://mri-fre.ornl.gov/psimag)

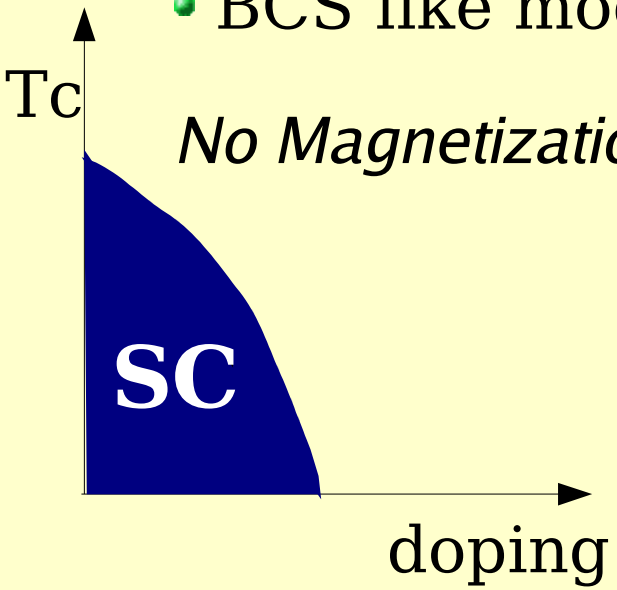
Partial Summary

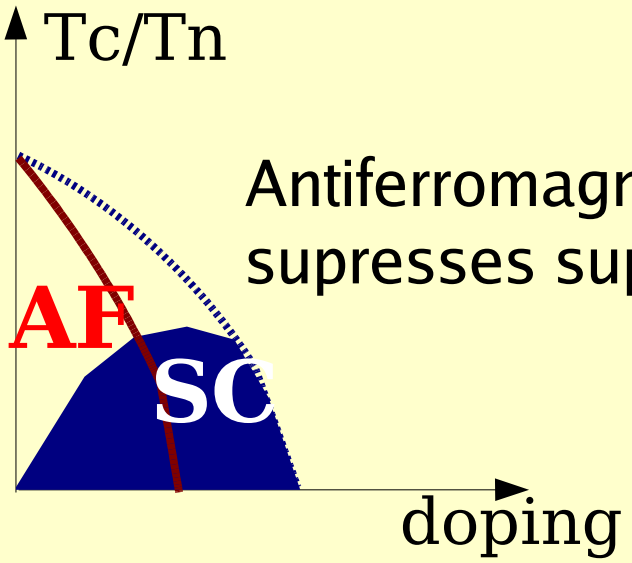
- The TPEM is becoming a standard way of studying spin-fermion models.
- Complexity is O(N), it is parallelizable and rigorously exact within numerical errors.
- Applicable to CMR manganites even in the CE phase and with chemical disorder.
- Spectral function and optical conductivity with the TPEM now possible.
- **GOAL: Unbiased numerical study of "spin-fermion" models with realistic band structure.**

Application 2: High Tc Superconductors



- Same carriers are responsible for both SC and AF.
- BCS like model with **d-wave symmetry**





The Spin Fermion Model

[G. Alvarez et al,
Phys. Rev. B 71, 014514 (2005)]

$$H_{\rm F} = -t \sum_{<\mathbf{ij}>,\sigma} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + H.c.) + 2 \sum_{\mathbf{i}} J_{\mathbf{i}} S^{z}_{\mathbf{i}} s^{z}_{\mathbf{i}} - \sum_{\mathbf{i}\sigma} \mu_{\mathbf{i}} n_{\mathbf{i}\sigma}$$
$$+ \frac{1}{D} \sum_{\mathbf{i},\alpha} \frac{1}{V_{\mathbf{i}}} |\Delta_{\mathbf{i}\alpha}|^2 - \sum_{\mathbf{i},\alpha} (\Delta_{\mathbf{i}\alpha} c_{\mathbf{i}\uparrow} c_{\mathbf{i}+\alpha\downarrow} + H.c.), \qquad (1)$$

(Derived from the extended Hubbard model)

Spin fermion model without explicit BCS pairing:

M. Moraghebi, S. Yunoki and A. Moreo, Phys. Rev. Lett. 88, 187001 (2002)

M. Moraghebi et al, Phys. Rev. B 63, 214513 (2001)

Computational Method

$$H_F = -t \sum_{<ij>,\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + H.c.) + 2 \sum_i J_i S^z_i s^z_i - \sum_{i\sigma} \mu_i n_{i\sigma}$$
$$+ \frac{1}{D} \sum_{i,\alpha} \frac{1}{V_i} |\Delta_{i\alpha}|^2 - \sum_{i,\alpha} (\Delta_{i\alpha} c_{i\uparrow} c_{i+\alpha\downarrow} + H.c.), \qquad (1)$$

- Local magnetization is treated as a classical field.
- D-wave SC order param. is a classical field.
- Fermions are quadratic and integrated out exactly at finite T
- Classical fields are integrated using a Monte Carlo method.

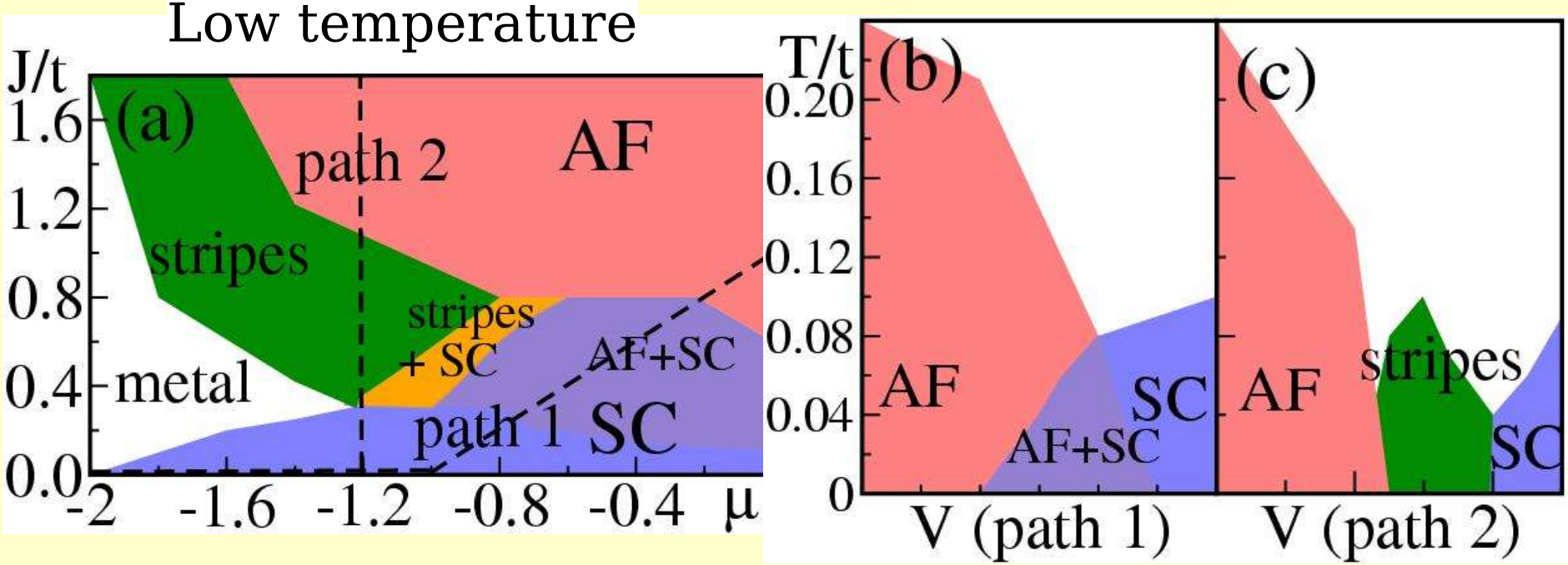
RAM (CCS at ORNL)

[Dagotto, "Nanoscale Phase Separation and Colossal Magnetoresistance", Springer-Verlag. (2002).]

Phase Diagram without Disorder

Temperature Dependence

Low temperature

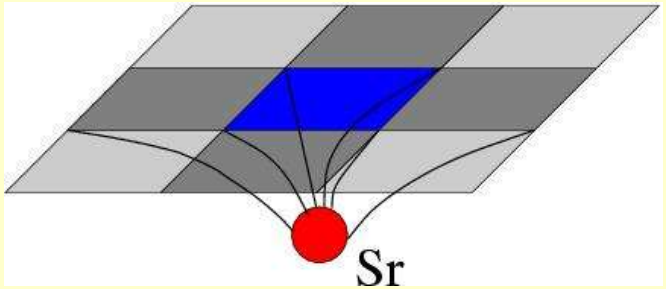


- Robust Coexistence AF+SC
- Different paths from AF to SC

[G. Alvarez et al,
Phys. Rev. B 71, 014514 (2005)]

Addition of Chemical Disorder

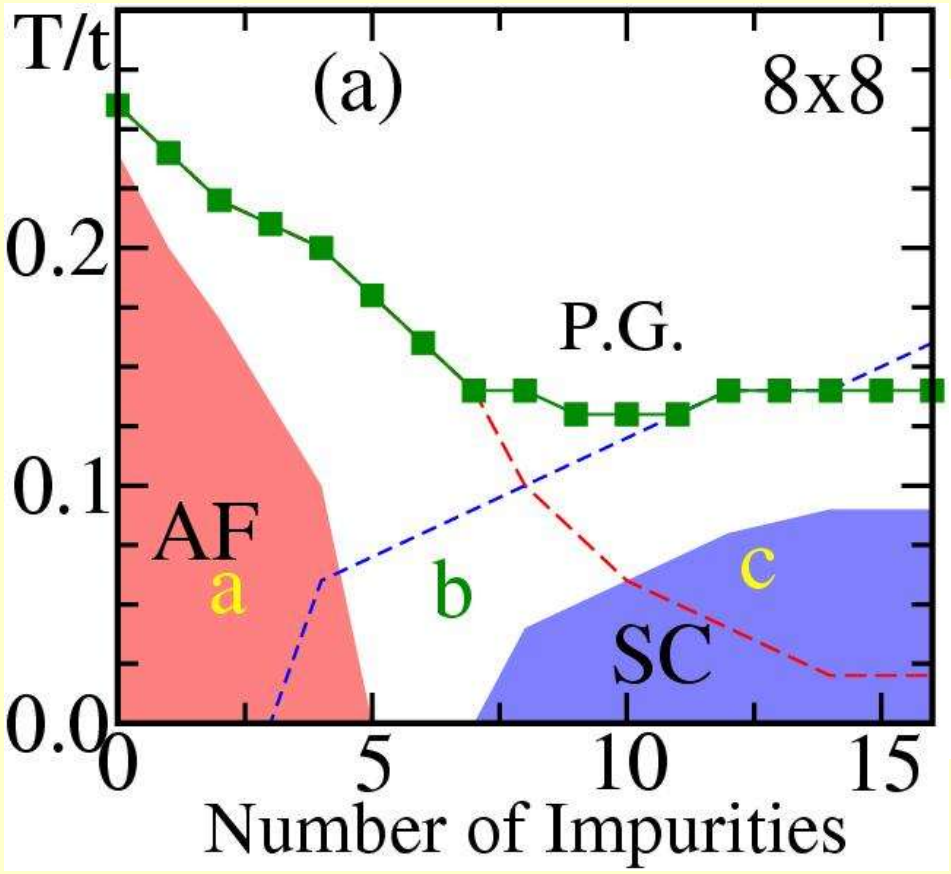
$La_{2-x}Sr_xCuO_4$

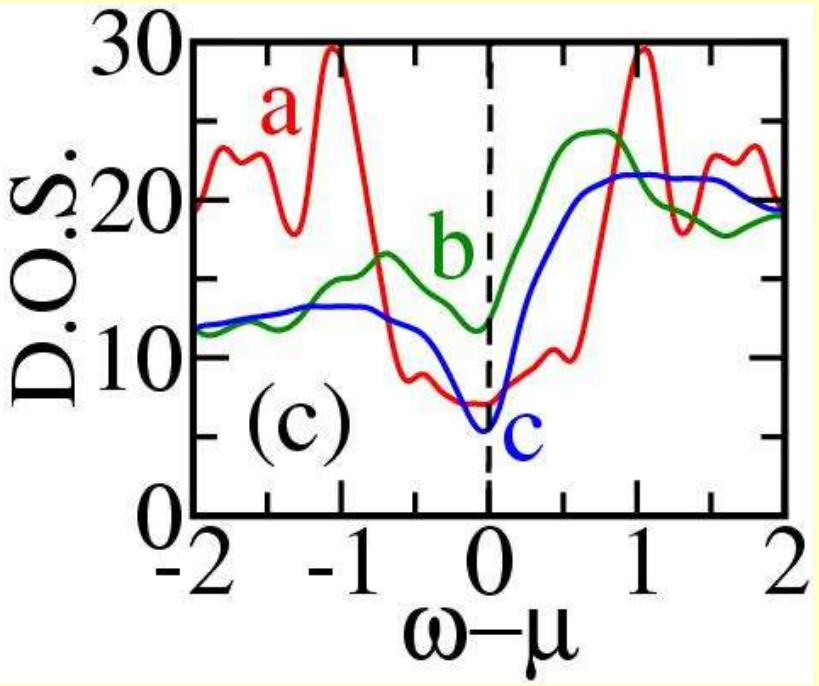


Sr^{2+} replaces La^{3+}

$$H_{\rm F} = -t \sum_{<\mathbf{ij}>,\sigma} (c^{\dagger}_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} + H.c.) + 2 \sum_{\mathbf{i}} J_{\mathbf{i}} S^z_{\mathbf{i}} s^z_{\mathbf{i}} - \sum_{\mathbf{i}\sigma} \mu_{\mathbf{i}} n_{\mathbf{i}\sigma}$$
$$+ \frac{1}{D} \sum_{\mathbf{i},\alpha} \frac{1}{V_{\mathbf{i}}} |\Delta_{\mathbf{i}\alpha}|^2 - \sum_{\mathbf{i},\alpha} (\Delta_{\mathbf{i}\alpha} c_{\mathbf{i}\uparrow} c_{\mathbf{i}+\alpha\downarrow} + H.c.), \qquad (1)$$

Phase Diagram with Disorder

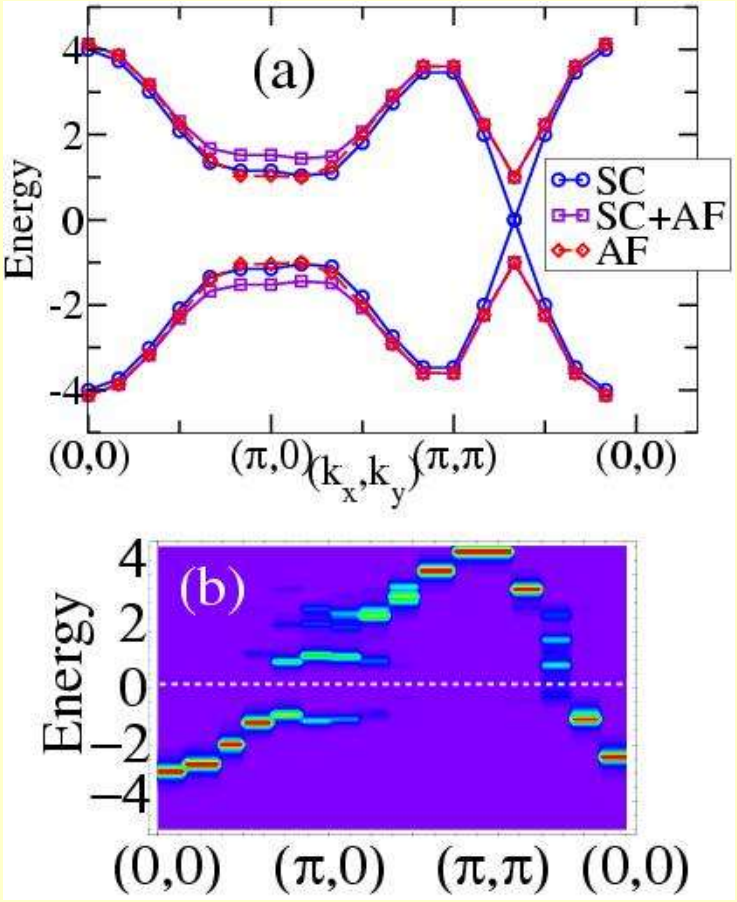




[G. Alvarez et al,
Phys. Rev. B 71, 014514 (2005)]

- Disorder opens a region of no long range order
- A pseudo-gap in the DOS is observed in this region below Tpg
- Tpg is related to AF/SC short range order.

Spectral Density: No Disorder

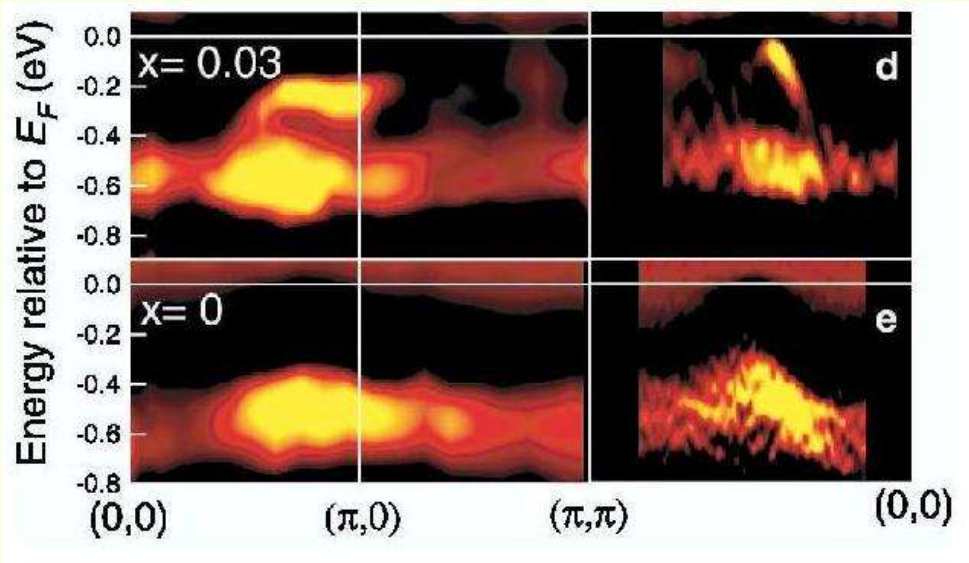


"stripes" ground state

[M. Mayr et al., cond-mat/0503727]

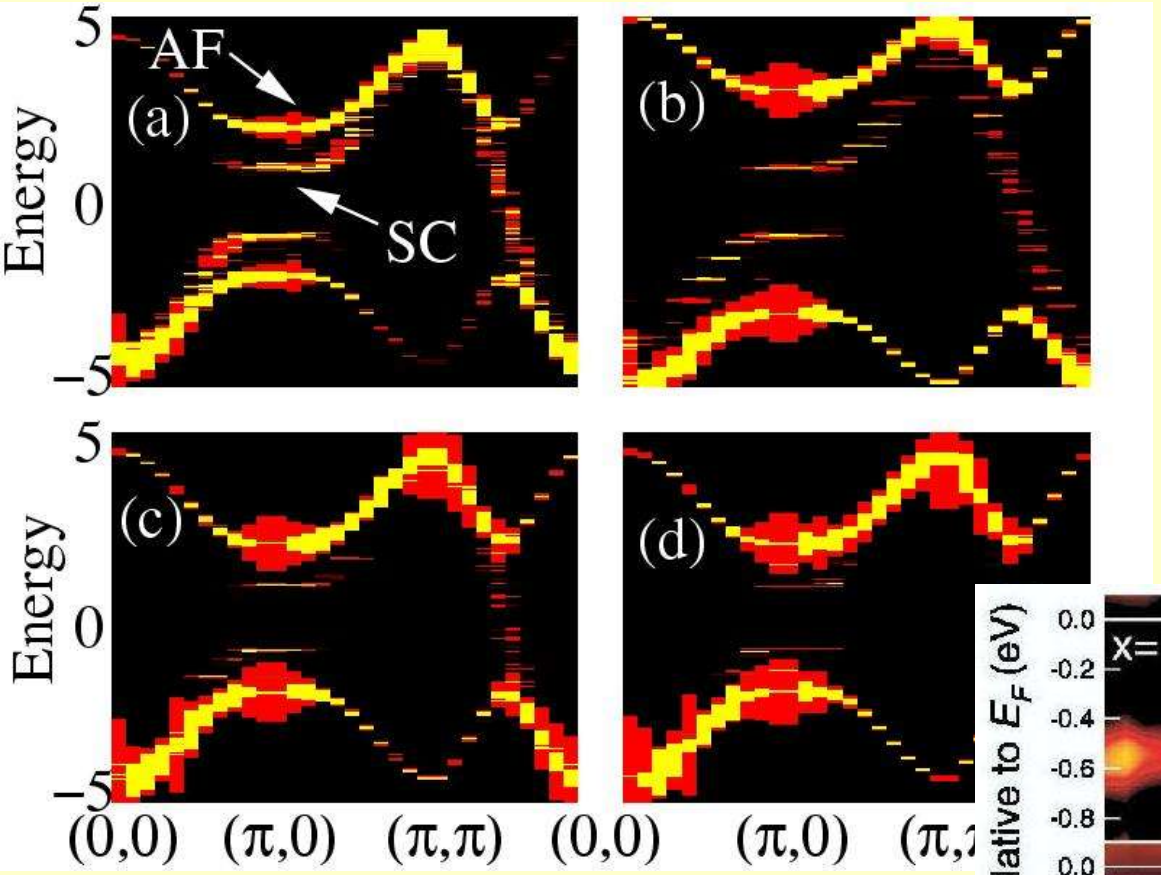
Without disorder the spectral function of the model does not reproduce the observed flat band in ARPES.

[Yoshida et al, PRL 91 027001 (2003)]

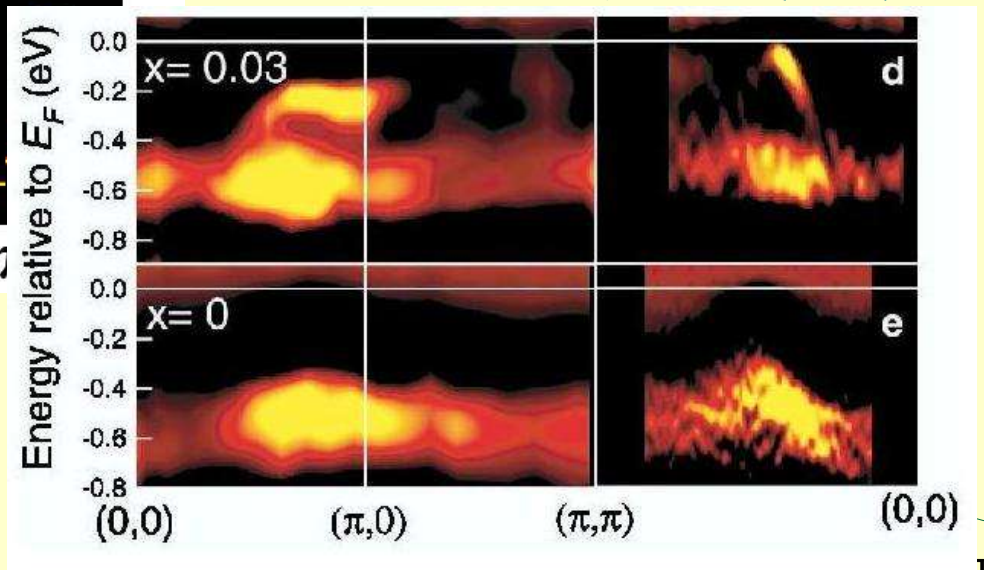


Spectral Functions

With disorder the spectral function shows a flat band originating from SC cluster.

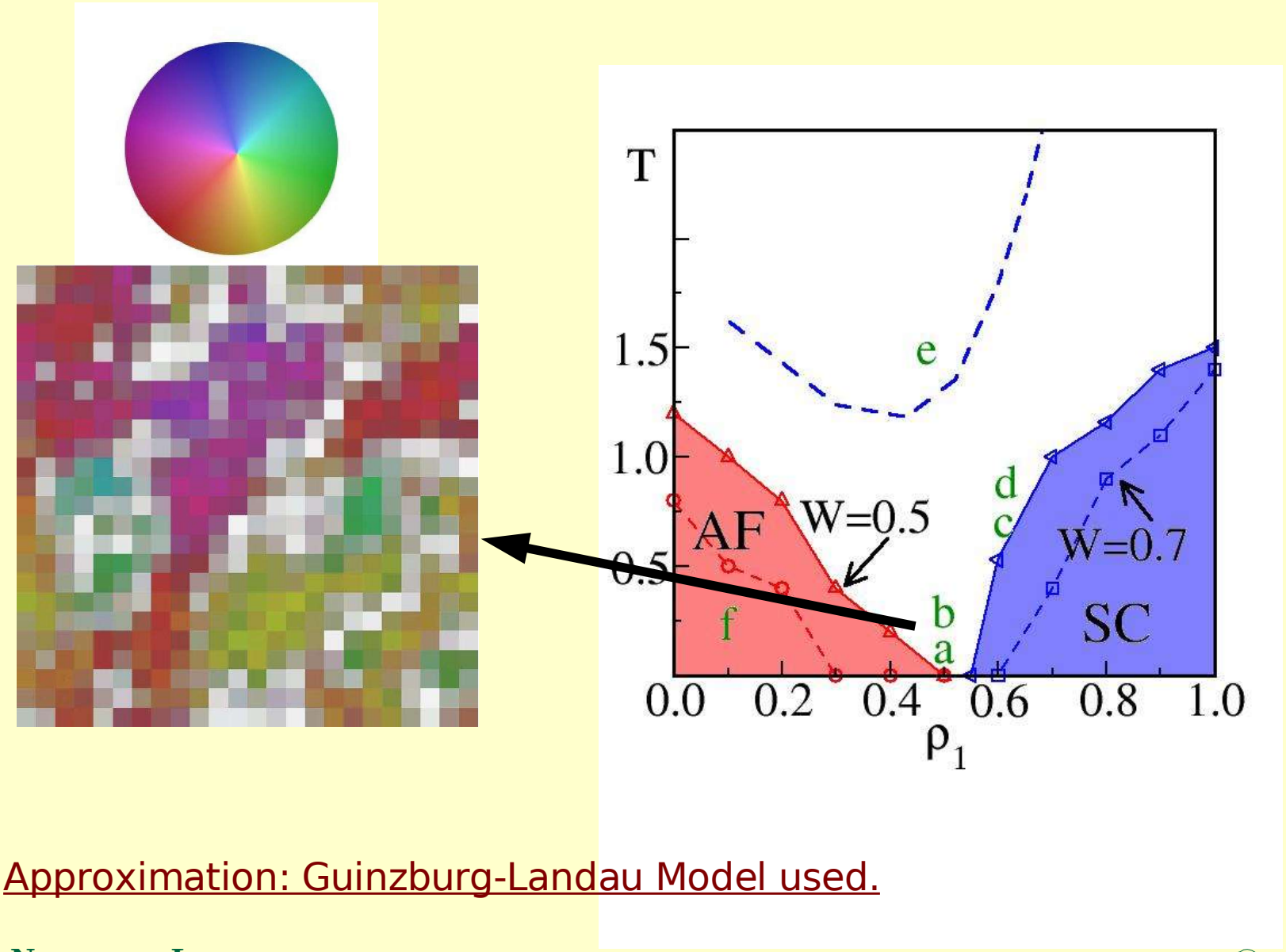


[Yoshida et al, PRL 91 (2003)]



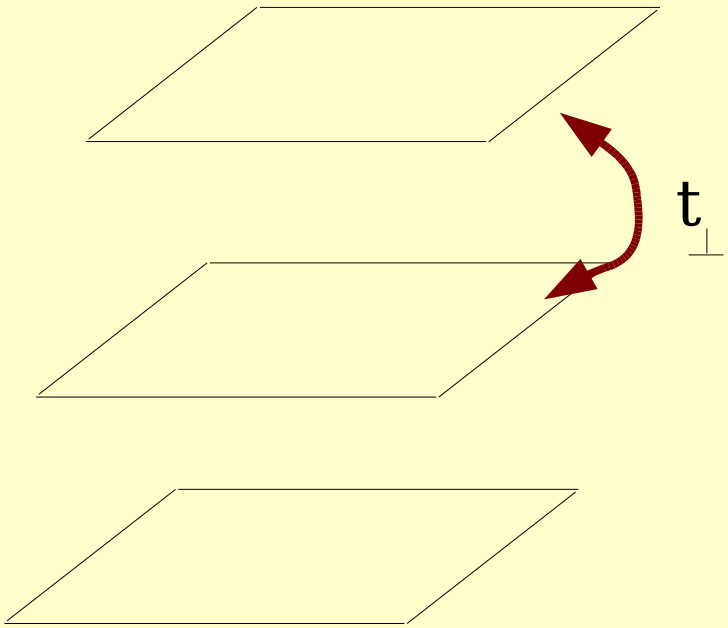
[M. Mayr et al., cond-mat/*0503727*]

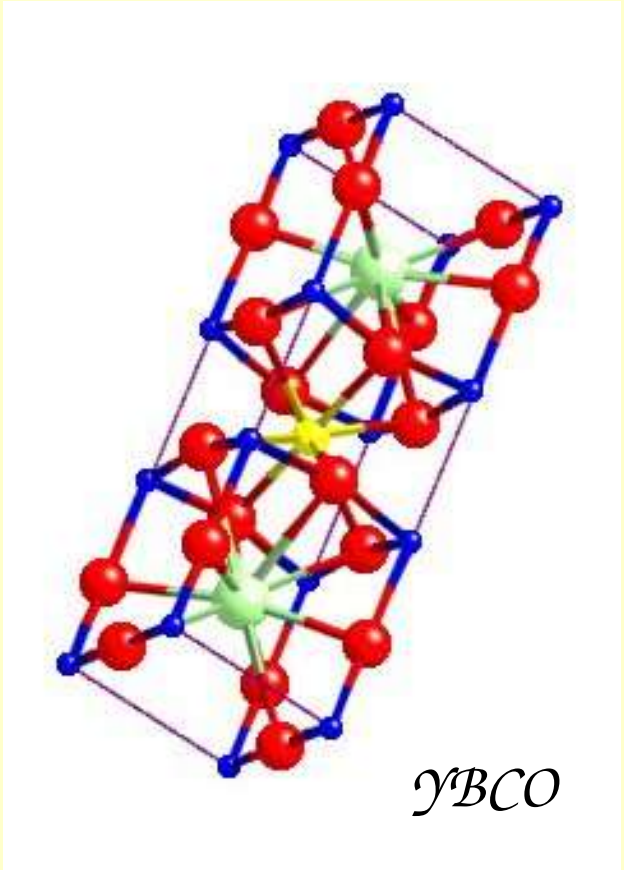
Ground state with SC Clusters



Approximation: Guinzburg-Landau Model used.

Multilayers

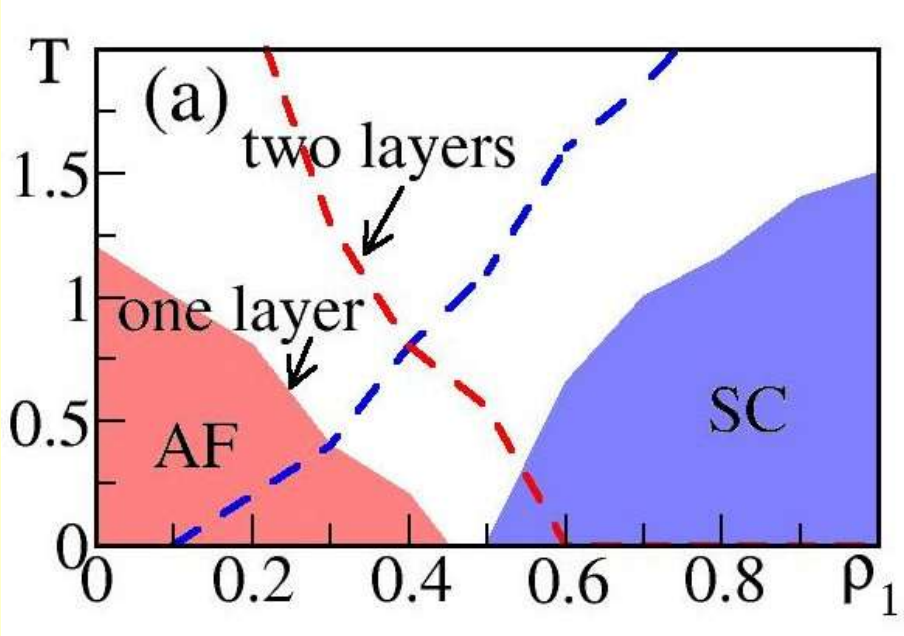




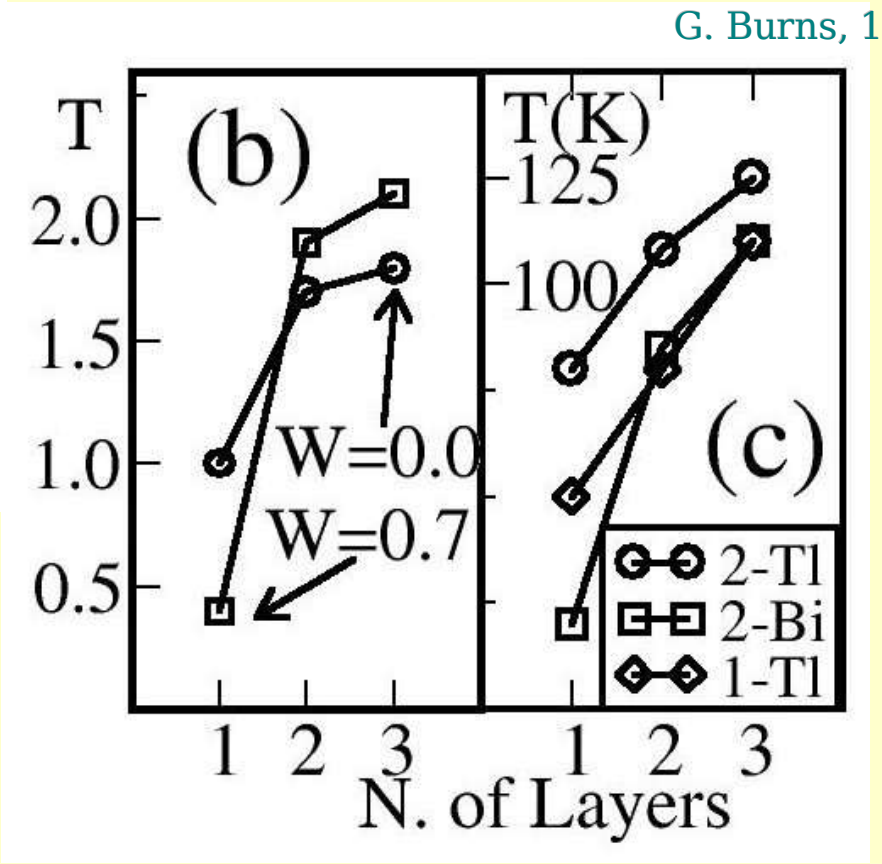
Approximation: Guinzburg-Landau Model used.

Multilayers: Tc

Approximation: Guinzburg-Landau Model used.



G. Burns, 1992

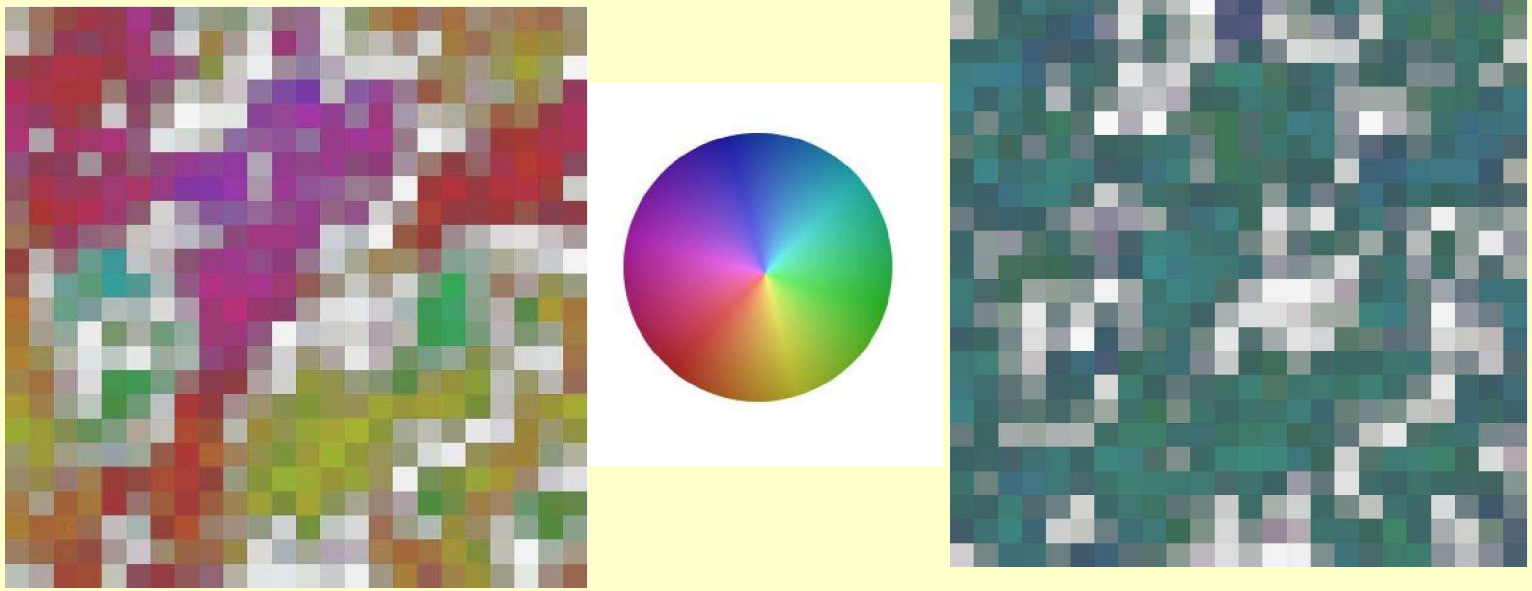


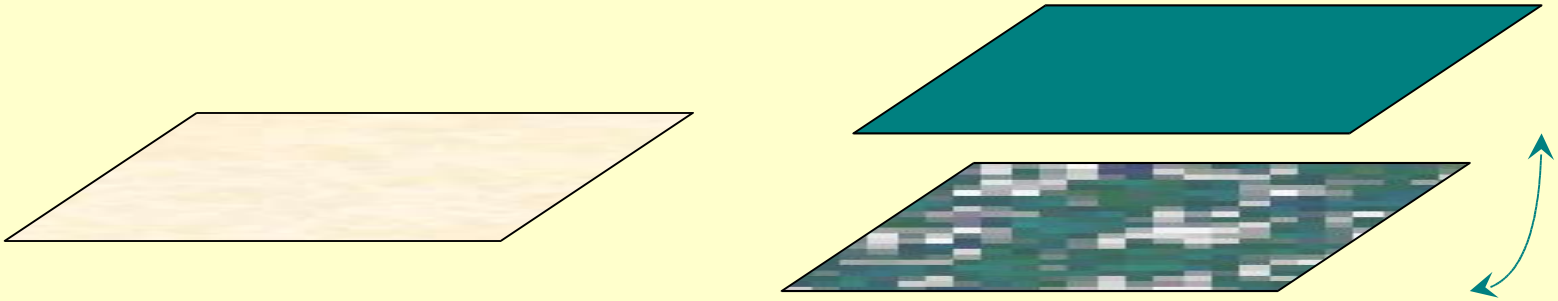
Percolation “easier” with 2 or more layers

[G. Alvarez et al,
Phys. Rev. B 71, 014514 (2005)]

Effect of an external “field”

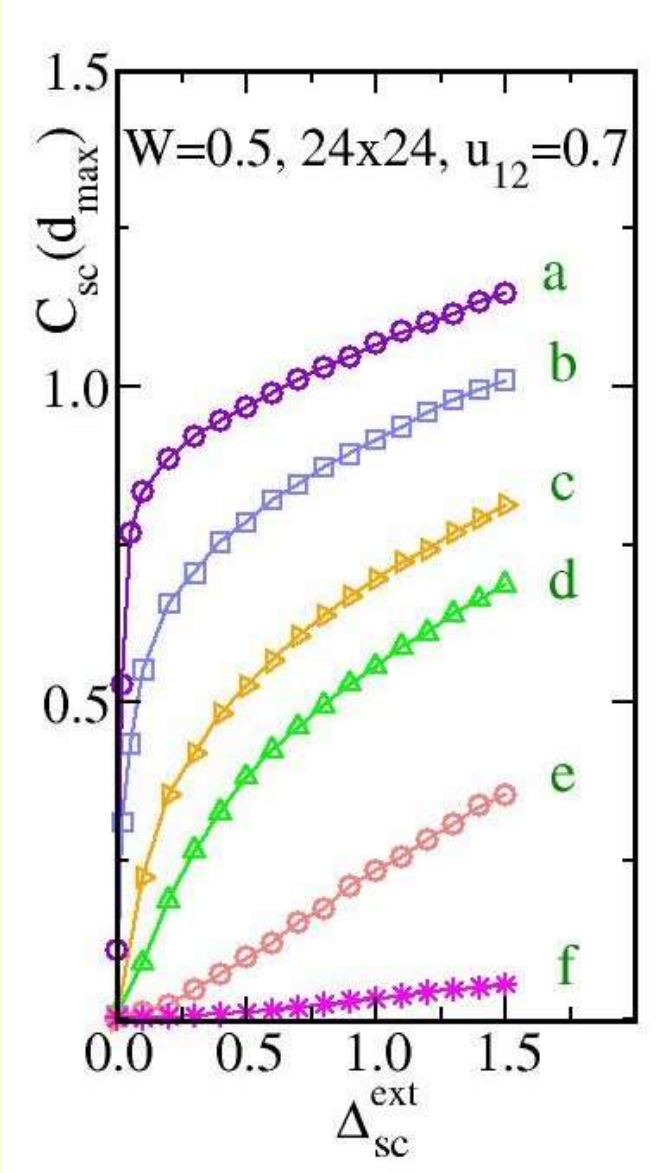
Approximation: Guinzburg-Landau Model used.

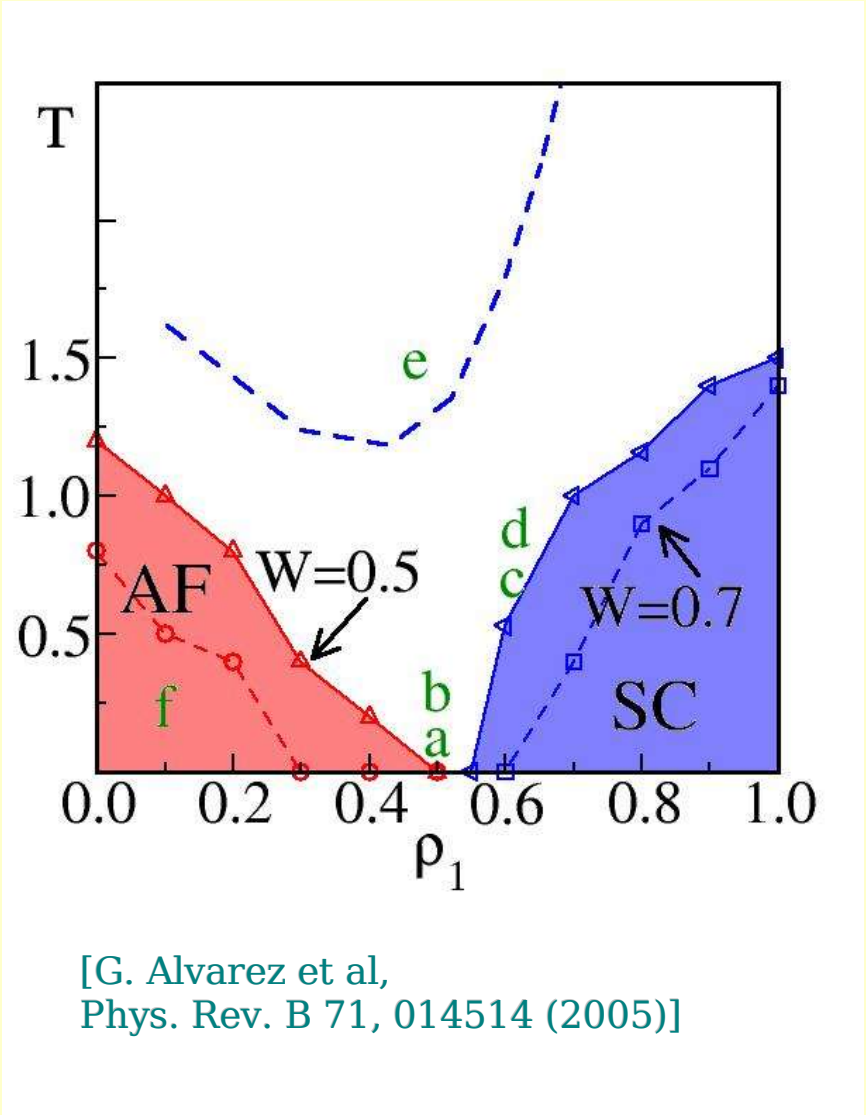




Giant Proximity Effect

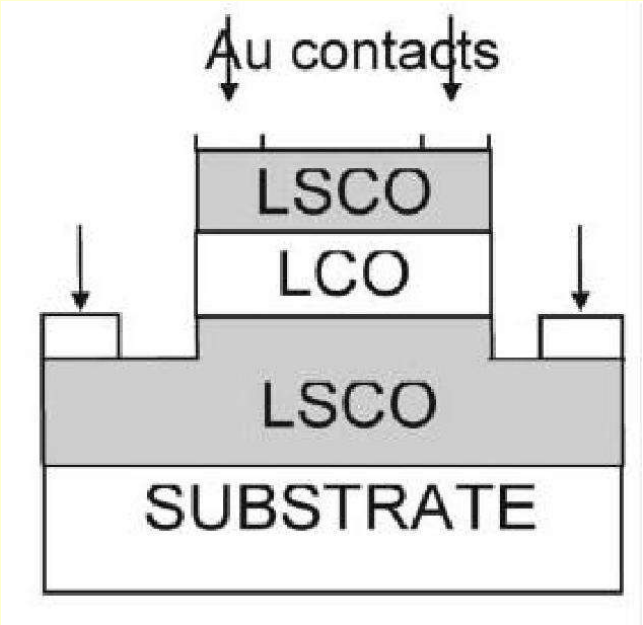
Approximation: Guinzburg-Landau Model used.





[G. Alvarez et al,
Phys. Rev. B 71, 014514 (2005)]

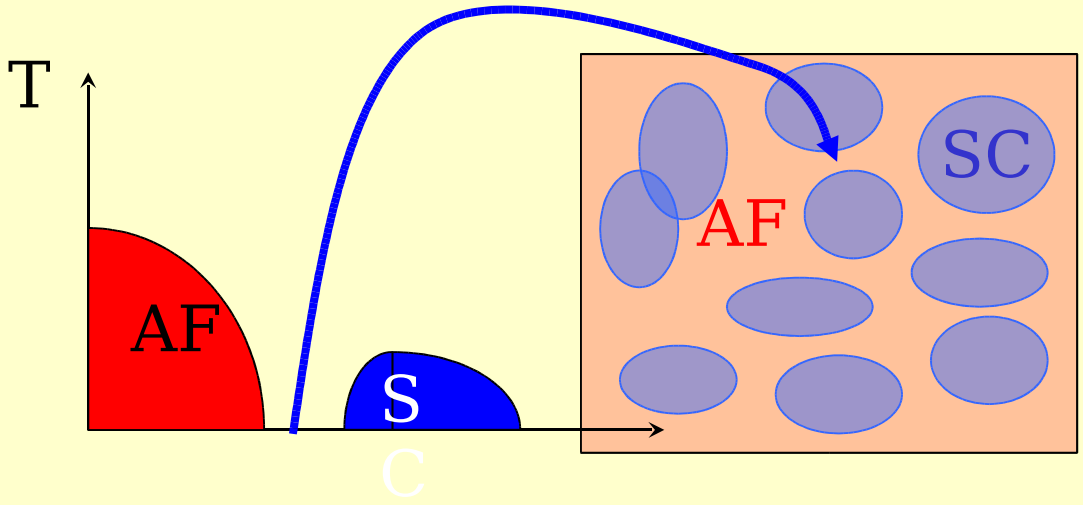
Giant Proximity Effect



Structure behaves as a Josepson junction between Tc' and Tc for a barrier thickness as large as 20nm

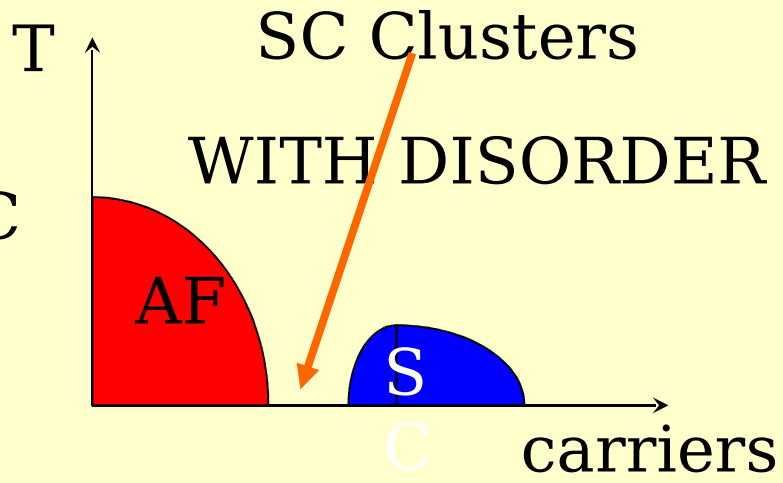
[G. Alvarez and E. Dagotto, Physics World Magazine, Dec. 2004]

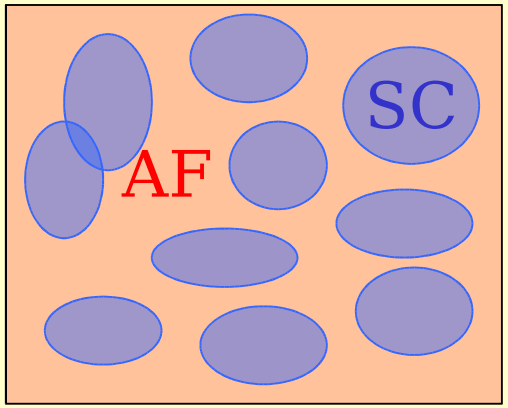
FIG. 1. Trilayer $SN'S$ devices studied in this work and their transport characteristics. Inset: The device geometry. The top and bottom HTS electrodes were made of LSCO. The barriers were made of LCO, and their thickness was varied from 13 to 200 Å. The circular mesa diameter was varied from 10 to 80 mm. Gold contacts allowed for 4-point contact transport measurements. Main panel: The current density as a function of voltage dependence (the j-V characteristics), at $T = 6.4$ K, for a set of ten sandwich junctions on the same chip. The plot illustrates very good device uniformity; in the best such set, the 1-σ spread in j_c was merely 2.5%. In the particular set shown here, the LCO barrier was 100 Å thick.



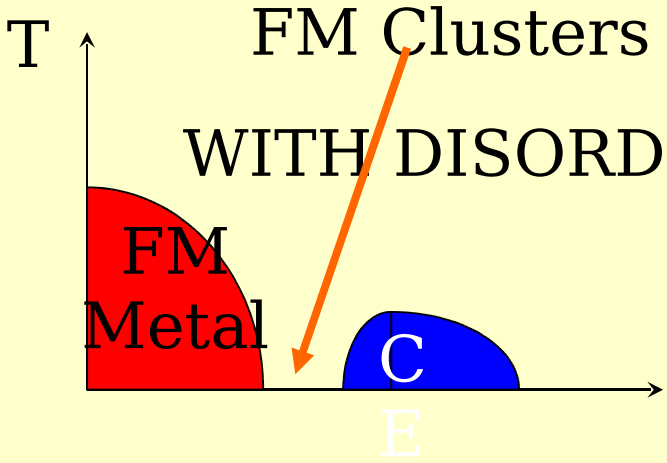
Magnetic Oxides: Formal Similarities

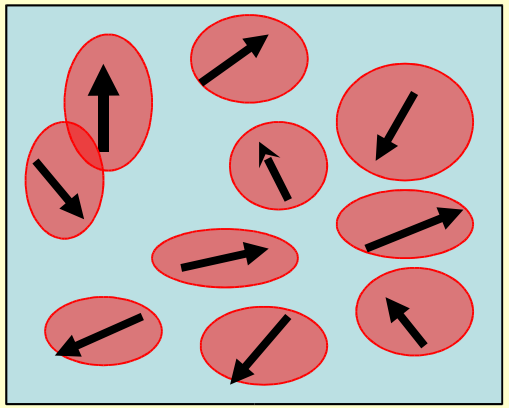
High Tc SC





CMR Manganites





Summary for HTSs Simulations:

- A spin-fermion model for HTSs was studied with unbiased numerical techniques.
- The model's phase diagram is non-universal.
- Adding disorder produces a ground state with “SC clusters”.
- ARPES spectra for LSCO presents two distinctive branches near the X point. This is reproduced with our model when disorder is present.
- Spin fermion model supports a mixed phase description of high temperature superconductors.