Computational Studies of Models for Manganites and Cuprates

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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

**Classical models**
(Ising, Heisenberg, etc)

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

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

**Easy to solve but**
no electrons, no holes, no spectral functions, etc...
Spin Fermion Model for Manganites

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

No approximations

Local spin

Manganite crystal

(electronic density)
Computational Complexity

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

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

- 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 \(\sim 216 \times 10000 = 2,160,000!\))
Theoretical Overview: Polynomial Expansion


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

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

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

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


\[ \star \text{No diagonalization} \]
\[ \star \text{Matrix-vector prod. benefits from sparseness of } H. \]
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.)*

<table>
<thead>
<tr>
<th>Algorithm</th>
<th></th>
<th>n;m&gt;</th>
<th>Trace</th>
<th>Delta S</th>
<th>Total</th>
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<td>O(N^3)</td>
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<td>O(MN)</td>
<td>O(N)</td>
<td>O(MN^2)</td>
<td>O(MN^3)</td>
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<tr>
<td>T-PEM(ε&gt;0)</td>
<td>O(M^{d+1})</td>
<td>O(M^d)</td>
<td>O(M^{2d+1})</td>
<td>O(M^{2d+1}N)</td>
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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


FM Clusters
WITH DISORDER

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CMR Manganites: Toy Model

J. Burgy et al., PRL 92 (2004)
Microscopic two-orbital Model for Manganites


\[ H_{2b} = \sum_{\gamma, \gamma', i, \alpha} t_{\gamma \gamma'}^{\alpha} S(\theta_i, \phi_i, \theta_i + \alpha, \phi_i + \alpha) c_{i, \gamma}^\dagger c_{i + \alpha, \gamma'} + \lambda \sum_i (Q_1 i \rho_i + Q_2 i \tau_{xi} + Q_3 i \tau_{zi}) \]

\[ + \sum_{\alpha=1}^{\alpha=3} D_{\alpha} Q_{\alpha i}^2 \]

+ JAF \sum <ij> S_i * S_j
Two-orbital Model for Manganites

Phase Diagram Without disorder

[C. Sen et al. unpublished]
Two-orbital Model for Manganites

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● Mesoscopic Conductance (Verges, et al.)
● Chemical Disorder has to be included.
● Study of Phonons with the TPEM: Spectrum bounds.
● But remember: this is an exact numerical study
Model for Manganites:
TPEM & Chemical Disorder

Preliminary result on 12x12
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

\[ N_{\text{proc}} = \text{Number of processors.} \]
\[ N_{\text{dim}} = \text{Size of the one electron Hilbert space (OEHS).} \]

- The PEM without truncation “scales” with \( N_{\text{proc}} \) up to \( N_{\text{dim}} \). A “typical” 32x32 one-orbital model \( \Rightarrow \) 2048 procs.
- The truncated PEM “scales” with \( N_{\text{proc}} \) only up to the size of the truncated OEHS \( \sim 40-80 \) procs.

NCCS Facility at ORNL

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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.

Cray XT3

Disorder configs, temperature
TPEM: Spectral Function and Optical Conductivity

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

Double exchange model for manganites

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

Comparison on 8x8, \( JH=4 <n>=0.5 \)

[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**

No Magnetization

Antiferromagnetism suppresses supercond.
The Spin Fermion Model

\[ H_F = -t \sum_{<ij>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + H.c.) + 2 \sum_i J_i S_i^z s_i^z - \sum_{i\sigma} \mu_i n_{i\sigma} \]

\[ + \frac{1}{D} \sum_{i,\alpha} \frac{1}{V_i} |\Delta_{i\alpha}|^2 - \sum_{i,\alpha} (\Delta_{i\alpha} c_{i\alpha}^\dagger c_{i+\alpha\downarrow} + H.c.), \quad (1) \]

(Derived from the extended Hubbard model)

Spin fermion model without explicit BCS pairing:


Computational Method

\[
H_F = -t \sum_{\langle ij \rangle, \sigma} (c_i^\dagger c_j \sigma + H.c.) + 2 \sum_i J_i S_i^z s_i^z - \sum_{i \sigma} \mu_i n_{i \sigma}
\]

\[
+ \frac{1}{D} \sum_{i, \alpha} \frac{1}{V_i} |\Delta_{i \alpha}|^2 - \sum_{i, \alpha} (\Delta_{i \alpha} c_i^\uparrow c_{i+\alpha}^\downarrow + H.c.), \quad (1)
\]

- 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.


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RAM (CCS at ORNL)
Phase Diagram without Disorder

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

Addition of Chemical Disorder

\[ \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \]

Sr\(^{2+}\) replaces La\(^{3+}\)

\[
H_F = -t \sum_{\langle ij \rangle, \sigma} (c_i^{\dagger} c_j + H.c.) + 2 \sum_i J_i S_i^z S_i^z - \sum_{i, \sigma} \mu_i n_i \sigma \\
+ \frac{1}{D} \sum_{i, \alpha} \frac{1}{V_i} |\Delta_{i\alpha}|^2 - \sum_{i, \alpha} (\Delta_{i\alpha} c_i^{\dagger} c_{i+\alpha} + H.c.), \quad (1)
\]
Phase Diagram with Disorder

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

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Spectral Density: No Disorder

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

"stripes" ground state

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

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

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

(M. Mayr et al., cond-mat/0503727)

[Yoshida et al, PRL 91 (2003)]
Ground state with SC Clusters

Approximation: Guinzburg-Landau Model used.
Multilayers

Approximation: Guinzburg-Landau Model used.

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Multilayers: $T_c$

Approximation: Guinzburg-Landau Model used.

Percolation “easier” with 2 or more layers


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Effect of an external “field”

Approximation: Guinzburg-Landau Model used.
Giant Proximity Effect

Approximation: Guinzburg-Landau Model used.

Giant Proximity Effect

Structure behaves as a Josepsson junction between $T_c'$ and $T_c$ for a barrier thickness as large as 20nm


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-$\sigma$ 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

T

SC Clusters
WITH DISORDER

SC carriers

AF

FM Clusters
WITH DISORDER

FM Metal
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.