Contractor Renormalization for the 2D Hubbard and Frustrated Heisenberg Models

Collaborators:
Ehud Altman, Erez Berg, Technion

Outline

1. Renormalization and Effective Hamiltonians
2. Contractor Renormalization
3. 2-D Hubbard $\Rightarrow$ Plaquette Boson-Fermion Model
4. Quantum Frustration: Checkerboard and Pyrochlore lattices

References:
Cuprates:

Pyrochlores: E. Berg, E. Altman and A. Auerbach, cond-mat/0206384; PRL submitted.
The Cuprate Problem

Effective Hamiltonian which includes:

1. Tightly bound d-wave pairs
2. Antiferromagnetic correlations

Can we get this from a strong repulsively interacting electrons model?

Problem: Quantum Frustration

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j = J \sum_{\text{tet}} S_{\text{tet}}^2 + \text{const} \]

Pyrochlore  Checkerboard

Extensive number (N/2) degrees of freedom in classical GS manifold

Spinwave theory is poorly controlled
Highly frustrated magnets

\[ H = J \sum_{\langle ij \rangle} S_i \cdot S_j \]

\[ H_{\text{eff}} = ? \]

Strong Quantum fluctuations (spin-\(1/2\))?

Spin-\(1/2\) Checkerboard Antiferromagnet

Exact diagonalization
(\text{Palmer and Chalker, 2001})

How to describe ground state and low energy singlets?
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**k-Space Renormalization (Shankar)**

Eliminate high momenta single particle states

\[ Z_{micro} = \int D^2 \bar{z} \exp\left(-\int d\tau \bar{z} \partial_\tau z - H(\bar{z}, z)\right) = \int D^2 \bar{z}_{k<K'} \exp(-S(\bar{\tau}'), \tau)] \]

\[ S_{K'} \approx \sum_{k<K'} \left(i\omega - \epsilon_k - \Sigma(k, \omega)\right) \bar{z}_k z_k - \int \bar{z}_k \bar{z}_{k'} \bar{z}_{k''} \bar{z}_{k+k'-k''} + \ldots \]

"Effective Hamiltonian"

Renormalization group: \( S(K) \rightarrow S(K') \)

Couplings flow: \( f(K), \Sigma(K) \)

**Provision:** \( S(K') \) should be similar to \( S(K) \)

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**Renormalization by Canonical Transformation**

\[ H = -t \sum_{ij} c_i^+ c_j + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

Schrieffer-Wolff ->

\[ H^{eff} \approx \frac{4t^2}{U} \sum_{ij} S_i \cdot S_j + O(t/U, E/U) \]

**Advantages**

1. Reduced Hilbert Space \( \mathcal{S} = \{ c_i^+ \bar{\sigma}_{j\nu} c_{j\nu} \} \)
2. Bosonic degrees of freedom
3. Better mean field approximations for Heisenberg than for the Hubbard Model

**Problems:**

1. Pertubative limit of \((t/U)\ll 1\)
2. \( H(E) \) is not really a Hamiltonian

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Direct Numerical Correlations

Need $L > \xi_{\text{correlation}}$

\[ \text{Simulation time is } \approx \exp\left( L^d \right) \]

If $\xi$ is large, it is futile to try to extract thermodynamic correlations

What are numerics good for?

Emerging Low Energy Degrees of Freedom

GeV quarks&leptons  MeV nucleons  eV atoms  0.1 eV chemical bonds

The Captain's Weight

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**Numerical Renormalization**

Need only $L > \xi_{\text{coherence}}$!

$\xi_{\text{coherence}} = \text{size of “atoms”}$

How do we identify “atoms” and calculate effective couplings??

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**Contractor Renormalization (CORE)**

Morningstar-Weinstein, PRD (1996)

**Step I:** Divide lattice to disjoint blocks

Truncate:

$N \rightarrow M$ lowest states per block $\{ |\phi_i \rangle \}_{i=1}^M$

“atoms”
**Step II: $H^{ren}$ for a particular cluster of $N$ blocks**

Reduced Hilbert space: $|\alpha\rangle = |\phi_1, \phi_2, \ldots, \phi_N\rangle$ (dim = $M^N$)

3. Orthonormalize from ground state up. (Gramm-Schmidt)

$$\varepsilon_n, |n\rangle, \sum P_\alpha |n\rangle \rightarrow |\psi_n\rangle$$

$$H^{ren}_{(1,\ldots,N)} \equiv \sum_{n=1}^{M^N} \varepsilon_n |\tilde{\psi}_n\rangle \langle \tilde{\psi}_n|$$

$$h_{(1,\ldots,N)} \equiv H^{ren}_{(1,\ldots,N)} - \sum_{i_1,\ldots,i_L} h_{i_1,\ldots,i_L}^{conn, subclus}.$$
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Test: 1D Heisenberg

\[ JS_i \cdot S_{i+1} \rightarrow E_0 / N = \sum_r h_0^r \]

C.J. Morningstar & M. Weinstein hep-lat/000202

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<thead>
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<th>Range (size)</th>
<th>Energy Density</th>
<th>CIRE</th>
<th>Padé [N/M]</th>
<th>Energy Density</th>
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</tbody>
</table>


Hubbard Plaquette States

0 holes 1 hole 2 holes

<table>
<thead>
<tr>
<th>(π,π) Triplet</th>
</tr>
</thead>
<tbody>
<tr>
<td>(π,π) D-wave hole pair</td>
</tr>
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</table>

AFmagnet and Superconductor degrees of freedom!
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Coupling Plaquettes (CORE)

"Plaquette Boson Fermion Model of Cuprates"

Coupling plaquettes: Failure of perturbative approach

Pair hopping: \( J_C \propto \frac{t'^2}{\Delta_b} \)
Fails for \( t' > \Delta_b \)

Energy of 2 holes on the cluster

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Good convergence of the cluster expansion!

\[ \frac{\langle h_{ijk} \rangle}{\langle h_{ij} \rangle} \sim 10^{-1} - 10^{-2} \]

\[ H_{\text{approx}} \]

\[ H_{(1,2,3)} \]

\[ \downarrow \]

Short coherence length!

S.H. Pan et al (PRL 00)

Pairs keep their integrity on the full lattice!!

Pair Integrity

Pair correlations in t-J model by DMRG (White & Scalapino)

Hole pairs stay tightly bound in larger clusters

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Four Boson Model

\[ \mathcal{H}^b = (\epsilon_b - 2\mu) \sum_i b_i^\dagger b_i - J_b \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{H.c.}) \]

\[ \mathcal{H}^t = \epsilon_t \sum_{i\alpha} t_{i\alpha}^\dagger t_{i\alpha}^\dagger - J_t \sum_{\alpha(\alpha\beta)} (t_{\alpha\beta}^\dagger t_{\alpha\beta} + \text{H.c.}) - \frac{J_H}{2} \sum_{\alpha(\alpha\beta)} (t_{\alpha\beta}^\dagger t_{\alpha\beta} + \text{H.c.}) \]

Projected SO(5) Theory
S-C Zhang, J.P. Hu, E. Arrigoni, W. Hanke, A. Auerbach, PRB60, (99)

Numerics:
Dorneich, Hanke, Arrigoni, Troyer, Zhang, (02)

Similar scale for pair and magnon hopping!

Small superfluid density

\[ H = \frac{1}{2} \rho \int d^2 x \left( \nabla^2 + iA \right) \rho \]

Ginzburg-Landau

\[ \rho_c \propto \frac{1}{\lambda^2} \]

Uemura’s Plot (89)

BCS

\[ \rho_c = \frac{\hbar^2 n_e^2}{2m} \approx \epsilon_r \approx kT \]

\[ T_c = \frac{\hbar}{m} e^{-\lambda} = 10^3 \text{eV} \]

\[ n_e = \frac{\gamma}{\omega_c} \]

\( T_c, \rho_c, n_e \) unrelated

BEC of real-space pairs
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Plaquetized Lattice?

\[ x = 0.125 \]

\[ Q = (\frac{\pi}{4}, 0) + (0, \frac{\pi}{4}) \]

\[ \langle b_r \rangle \propto e^{iQr} \]

Stripes,

or Plaquetized order parameter?

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Back to the Pyrochlores:

Goal: \( H_{\text{eff}} \) in terms of lowest tetrahedron states
**Tetrahedron eigenstates**

\[ H(\begin{array}{c}
\circ
\end{array}) = JS_{\text{tot}}^2 + c \]

**Effective Hamiltonian**

\[ H_{\text{eff}} = \sum_i h_i(\begin{array}{c}
\circ
\end{array}) + \sum_j h_j \left\{ \begin{array}{c}
\circ
\end{array} \right\} \]

\[ \Rightarrow H_{\text{eff}} = -J_1 \sum_{\langle ij \rangle} (\vec{S}_i \cdot \hat{\Omega}_{ij}) \left( \vec{S}_j \cdot \hat{\Omega}_{ij} \right) - h_1 \sum_i S_i^z \]

\[ J_1 \approx J/2 \]

\[ h_1 \approx J/4 \]

\[ \hat{\Omega}_{\text{Vertical}} = \leftarrow \quad \hat{\Omega}_{\text{Horizontal}} = \rightarrow \]
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**Mean Field solution**

- Energy per plaquette as a function of \( \theta/\pi \)
- Direction of pseudospins

**Thermodynamics**

- Crossed plaquettes are symmetric with respect to the degenerate ground states!
- Singlet Excitations
- Ising Domain walls
- Palmer and Chalker (2001)
- Spin flip excitation energy \( \sim J/2 \)
- Number of low singlet excitations grows linearly with size

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Quantum Pyrochlore Antiferromagnet

No MF order down to zero temperature!

Villain (79);
Moessner and Chalker (98);

Spectrum of a finite cluster of the spin-\(1/2\) Pyrochlore

First CORE Step

First stage: Tetrahedral clustering

Pseudospins defined on a FCC lattice

Effective 3-body hamiltonian

\[
H_{\text{eff}} \approx J_3 \sum_{\langle i,j,k \rangle} \left( \frac{1}{2} + \vec{S}_i \cdot \vec{e}_{ijk} \right) \left( \frac{1}{2} + \vec{S}_j \cdot \vec{e}_{ijk} \right) \left( \frac{1}{2} + \vec{S}_k \cdot \vec{e}_{ijk} \right)
\]

Perturbative Expansion: Harris, Berlinsky, Bruder (92)

MF level: four sublattice “Order”

Remaining macroscopic degeneracy!
**Second CORE step**

Second stage: “Super Tetrahedral” clustering

Basic block: “supertetrahedron”

Spectrum of a single block:

- Pseudospin - ½

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**Mean Field Solution**

\[ H_{\text{eff}} = J \sum_{\langle ij \rangle} (\hat{S}_i \cdot \hat{c}_{ij})(\hat{S}_j \cdot \hat{c}_{ij}) + J_b \sum_{\langle ij \rangle} (\hat{S}_i \cdot \hat{c}_{ij})(\hat{S}_j \cdot \hat{c}_{ij}) + \ldots \]

Mean field ground state:

Supertetrahedron pseudospins

- Ground state: 6 fold degeneracy, rotational and translational symmetry breaking
- Coherence length: ~ single supertetrahedron
- Domain wall excitations
Summary

1. CORE renormalizes a microscopic Hamiltonian to an effective Hamiltonian, non perturbatively.

2. The truncation error can be controlled by a short coherence length ("atom size").

3. Applying CORE to the Hubbard Model yields an effective Plaquette Boson Fermion Model.

4. Applying CORE to the Pyrochlore yields a lattice symmetry breaking ground state and very low lying singlet excitations.

Future:
Development of larger scale CORE computations (S. Capponi)
Explore the PBFM.
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**Pair Binding on a Plaquette**

\[ \Delta \equiv E_2 - 2E_3 + E_4 < 0 \]

Pair binding was found for Hubbard and t-J clusters close to half filling!

(Hirsch et al., Fye et al. 89.)

**Is this the Pairing Mechanism?** \( U/t \)

**Test: Tight Binding models**

2D

![Diagram](image-url)
Fermion holes

\( \mathcal{H}_{\text{fermion holes}} = \sum_{k_x} (\varepsilon_k^f - \mu) \hat{f}_{k_x \uparrow} \hat{f}_{k_x \downarrow} \)

\( \varepsilon_k^f = t' \left( \cos k_x + \cos k_y \right) + t' \left( \cos k_x - \cos k_y \right) \)

Plaquette fermions

Non Interacting, Tight Binding
Contractor Renormalization for the 2D Hubbard and Frustrated Heisenberg Models

Fig. 4(color). Full Brillouin zone plots of $\Delta n_k/\Delta T$ for the $t$-$J$ model. The color scale is the same for both plots. Orange, yellow, and green are negative, with a minimum value of $\Delta n_k/\Delta T = -0.08J^{-1}$. Blue, violet, and red are positive, with a maximum value of $\Delta n_k/\Delta T = 0.15J^{-1}$. The plots correspond to different temperatures; left: $T = 0.5J$; right: $T = 0.3J$. In the right plot the solid curve is the $T = 0$ tight-

Plaquette Boson – Fermion Model

$$H^{PBFM} = H^{bosons} + H^{fermions} + H^{bf}$$

$$\mathcal{H}^{bf} = g_b \sum_{k,q} (d_{k+q/2}^\dagger b_q f_k f_{-k+q} + H.c.)$$

STM Differential Conductance (nS)

In vortex out of vortex

Hole fermions at $q = (\pm \pi, \pm \pi)$

$S.H. Pan et al. (PRL 00)$

Pseudogap

$$\Delta_{pg} = E_{k^*} - \mu(x,T)$$

$$\mu(x) - \mu(0) = \frac{x}{2k_x + k_y}$$

Superconducting gap

$$\Delta^s = g_s \langle b \rangle$$

$$E_i = \sqrt{(\epsilon_i - \mu) + (\Delta^s)^2}$$

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**Numerical support**

Static and dynamical properties of doped Hubbard clusters

E. Dagotto, A. Moreo, F. Ortolani, D. Poilblanc, and J. Riera

4X4 cluster

- Holes in pockets
- 3 pairs in a condensate
- Pair condensate

**The problem of Two Gaps**

Pseudogap **decreases** with doping (measures chemical potential)

\[
\mu(x) - \mu(0) = \frac{x}{(2k_x + k_y)}
\]

\[
\Delta_{kg}^{\text{pg}} \equiv E_{k_T} - \mu(x, T)
\]

Coherence gap **increases** with doping (measures hole pairs order parameter)

\[
\Delta_{kg}^{\text{SC}} = g_d \langle \Phi \rangle
\]

Prediction: \(\Delta_{SC} \propto \sqrt{T_C}\)
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Short coherence length

\[ \xi \sim 20 \text{ Å} \sim 5a \]

Phase diagram (Monte Carlo)

Phase diagram and dynamics of the projected SO(5)-symmetric model of high-\(T_c\) superconductivity

A. Doniach\textsuperscript{1}, W. Haule\textsuperscript{1}, E. Arrigoni\textsuperscript{1}, M. Troyer\textsuperscript{2} and S.C. Zhang\textsuperscript{3}

Dispersion of the \((\pi, \pi)\) triplet

Experiment

Uemura\textsuperscript{3} plot

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Contractor Renormalization for the 2D Hubbard and Frustrated Heisenberg Models

\[ h_{ijk} \approx J_3 \left( \frac{1}{2} + \vec{S}_j \cdot \vec{e}_{jk} \right) \left( \frac{1}{2} + \vec{S}_j \cdot \vec{e}_{jk} \right) \left( \frac{1}{2} + \vec{S}_k \cdot \vec{e}_{jk} \right) \]