Resonating valence bond wavefunctions and interacting dimer models

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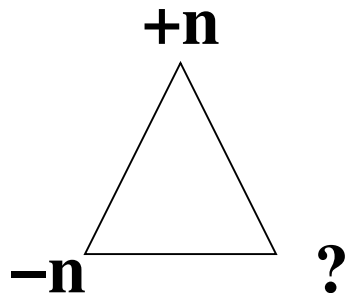
Antiferromagnetism in Mott insulators:

- Antiferromagnetic exchange interactions of magnetic ions in insulators:
  $E = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad J > 0$
- When is J>0, large? Difficult (quauntum chemistry) question, with thumb-rule answer: Goodenough-Kanamori-Anderson rules
  J.B. Goodenough, *Magnetism and the Chemical Bond (1963)*
  (exceptions known, *e.g.* Oles *et. al.* 2006)
- Sometimes possible to "measure" J: Inelastic neutron scattering in high field.
  e.g. $Yb_2Ti_2O_7$ Ross *et al.* PRX 2011

Triangles on my mind: Frustration and spin liquid behaviour

- Triangles $\rightarrow$ *frustrated* antiferromagnetism



  Competing interactions frustrate Neel order
- 'Quenching' of exchange allows new physics to take center-stage: Spin liquid regime $T_f \ll T \ll JS^2$
- Macroscopic degeneracy of *classical* minimum energy configurations.
- In spin liquid regime, spin correlations reflect this macroscopic degeneracy:
  No Bragg peaks in structure factor $\rightarrow$ correlated liquid state
- Physics of freezing at T_f: Classical order by disorder effects, subleading terms in energy, quantum effects $\sim JS$

$T = 0$: Quantum mechanical description of spin-liquids

- Resonating valence-bond (singlet) "soup"
  (Fazekas and Anderson 74)
  Each $S = 1/2$ spin paired into singlet with another—Partners swapped freely by quantum fluctuations

$$\Psi = \sum_{\text{pairings}} F((r_i r_j), (r_k, r_l) \dots) \prod (|\uparrow_i \downarrow_j\rangle - |\downarrow_i \uparrow_j\rangle) \dots$$

Projective constructions in specific contexts:

- Representing $S = 1/2$ by fermionic spinons:
  $\vec{S} = \sum_{\alpha=\uparrow,\downarrow} f^\dagger_\alpha \vec{\sigma}_{\alpha\beta} f_\beta$
  with projection: $\sum_{\alpha=\uparrow,\downarrow} f^\dagger_\alpha f_\alpha = 1$
- Projected BCS superconductor of spinons for cuprate Mott insulators (Anderson 87)
  (but experiments see AF order...)
- Projected Fermi-sea of spinons for (organic) triangular lattice magnets (Motrunich 2005; S. S. Lee & P. A. Lee 2005)
  (in broad agreement with experiment!)

Sign structure

- For *unfrustrated* couplings on *bipartite* lattices
  Sign structure is simple (Marshall's sign rule):

$$\sum_{\mathcal{P}} F((r_{A_1} r_{B_{\mathcal{P}(1)}}), (r_{A_2}, r_{B_{\mathcal{P}(2)}}) \dots) \prod (|\uparrow_{A_1} \downarrow_{B_{\mathcal{P}(1)}}\rangle - |\downarrow_{A_1} \uparrow_{B_{\mathcal{P}(1)}}\rangle) \dots$$

  with F positive
- Satisfied by projected Fermi sea on bipartite lattices
- Non-bipartite lattices: No simple sign structure.

Variational work

- Use factorizable F for square lattice antiferromagnet:

$$F = \prod f(\vec{r}_{A_1} - \vec{r}_{B_{\mathcal{P}(1)}}) f(\vec{r}_{A_2} - \vec{r}_{B_{\mathcal{P}(2)}})$$

- Long-range power-law tail in $f \rightarrow$ antiferromagnetism ($m^2 > 0$)
- Short-range $f \rightarrow$ short-range spin correlators (spin-liquid)
- Energy $\langle H_{\mathrm{sq}} \rangle = \langle \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \rangle$ depends only weakly on m^2
- "small" "deformations" of H_{sq} in spin-liquid phase(?)
  Liang, Doucot, Anderson (88)

The simplest (bipartite) RVB wavefunction: A surprise

- $f = 1$ for nearest-neighbour bonds, 0 otherwise
  $|\Psi\rangle = \sum_{\mathcal{D}} |\mathcal{D}\rangle$
  Each term $\leftrightarrow$ valid dimer cover $\mathcal{D}$ of bipartite lattice
  Square lattice case re-studied recently (Albuquerque & Alet 2010; Tang, Sandvik & Henley 2011)
- Spin-spin correlations very short-ranged ($\xi \sim$ few lattice spacings (as expected)
- The surprise—Bond-energy correlators decay very slowly:

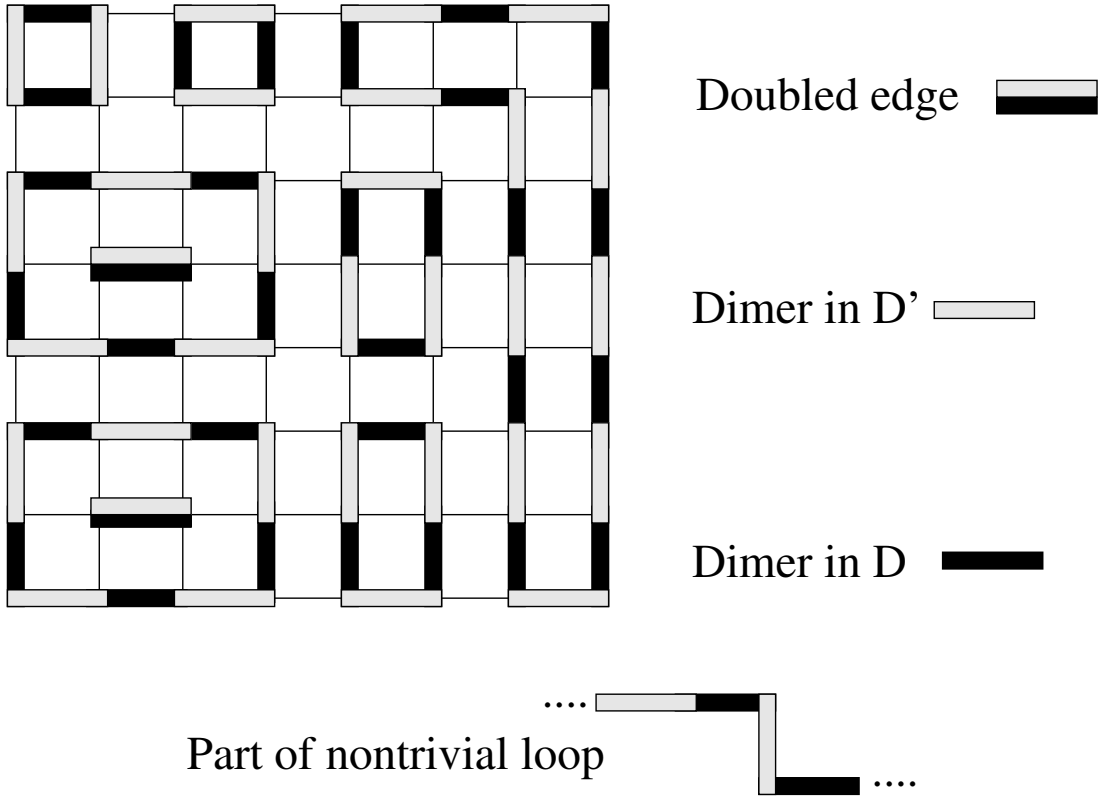
$$C_{E_x}(\vec{r}) \equiv \langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{0}+\hat{x}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\hat{x}} \rangle_c = \frac{(-1)^x}{|\vec{r}|^\alpha}$$

with $\alpha \approx 1.20$.
and similarly for C_{E_y}

Our goal: Understand this better

- Does the nnRVB state describe a critical system on the verge of valence-bond solid order?
- Can we quantitatively understand the power-law behaviour energy correlators?
- Is this special to the nnRVB state?
  Effect of adding longer-range valence bonds to the wavefunction?

Mapping to loop gas



Different terms *not* orthogonal $\langle \mathcal{D}' | \mathcal{D} \rangle = \langle \mathcal{D} | \mathcal{D}' \rangle = (2)^{n_d} (2)^{n_l}$

Implies $\langle \Psi | \Psi \rangle = \sum_{\mathcal{L}} w_{\text{loop}}(\mathcal{L})$ with $w_{\text{loop}}(\mathcal{L}) = (2)^{n_d(\mathcal{L})} (4)^{n_l(\mathcal{L})}$

(Sutherland 88)

Physical observables in the loop gas language

- Basic point: Action of $P_{AB} = \frac{1}{4} - \vec{S}_A \cdot \vec{S}_B$
  - Gives back state with amplitude 1 if $\langle AB \rangle$ has singlet on it
  - If no singlet on $\langle AB \rangle$: Forms $\langle AB \rangle$ singlet and reconnects partners, but with amplitude $1/2$
- Use to show:
  - $\langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{r}} \rangle \sim \mathrm{Prob}(l[\vec{0}] = l[\vec{r}])$
  - $$C_{E_x}(\vec{r}) \sim \mathrm{Prob}(l[\vec{0}] = l[\vec{0} + \hat{x}] \;\&\; l[\vec{r}] = l[\vec{r} + \hat{x}]) - \mathrm{Prob}(l[\vec{0}] = l[\hat{x}])\mathrm{Prob}(l[\vec{r}] = l[\vec{r} + \hat{x}])$$

    (dominant contribution at large $|\vec{r}|$)
- Short-range $\langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{r}} \rangle \rightarrow$ Short-loop phase of loop model
- If loops are short, why is C_{E_x} a slow power-law?

The key point: Correlations between loops

- Loop model is at full-packing
- Full packing constraint apparently introduces very strong correlations between loops
- Need to understand these correlations

Understanding correlations: Generalize nnRVB state to SU(g)

$$
\begin{aligned}
|\Psi(g)\rangle &= \sum_{\mathcal{D}} |\mathcal{D}\rangle_g \text{ , where} \\
|\mathcal{D}\rangle_g &= \prod_{e\in\mathcal{D}} |\Phi_0(g)\rangle_e
\end{aligned}
$$

with

$$
|\Phi_0(g)\rangle_e = \sum_{m=-S_g}^{S_g} (-1)^{(S_g-m)} |S^z_{e_A} = m, S^z_{e_B} = -m\rangle
$$

Singlet generalized to $SU(g)$: A sublattice carries fundamental ($g \times g$ matrices) representation. B-sublattice has complex-conjugate. Using equivalent spin-S_g language ($S_g = \frac{g-1}{2}$)

Understanding correlations: Loop gas at general g

- If g increases, gas likes to have more loops
- So long loops disfavoured (full-packing, hard-core constraints)
- In limit of large g, all loops of minimum size
  Doubled edges at full-packing

The $g = \infty$ limit is non-trivial

- Doubled edges at full-packing maps to fully-packed dimer model
- Bipartite dimer models known to have long-range power-law correlations between dimers due to full-packing and hard-core constraints
- Basic idea:
  Loop gas at $g = 2$ “inherits” these correlations

Aside: Fully-packed square lattice dimer model

- Hard-core constraint $\rightarrow$ Divergence-free "magnetic" field (2d)
- $\Delta \cdot \mathbf{B} = 0$ solved by $B_\mu = \epsilon^{\mu\nu}\Delta_\nu h$
- Action for height field

$$S = \pi\rho \int d^2 r (\nabla h)^2 + \sum_{p=4,8,12\ldots} y_p \int d^2 r \cos(2\pi p h) + \ldots$$

- y_p irrelevant for $0 < \rho^* \leq 4$.
- Power-law correlations for dimers.
  Usual dimer model has $\rho^* = \frac{1}{2}$

From $g = \infty$ to finite g: Classical "Schrieffer-Wolff"

- Each non-trivial loop in $\mathcal{L} \rightarrow$ two sequences of doubled-edges on alternating edges.
- $\mathcal{L}$ with n_l non-trivial loops and n_d doubled edges $\rightarrow 2^{n_l(\mathcal{L})}$ different loop configurations made up purely of doubled edges ($\equiv$ dimers)
- $\mathcal{L} \rightarrow 2^{n_l(\mathcal{L})}$ dimer configurations $\mathcal{D}_\alpha$ ($\alpha = 1, 2 \ldots 2^{n_l(\mathcal{L})}$).

Classical "Schrieffer-Wolff": More details

- $w_{loop}(g, \mathcal{L})$ distributed equally among these $\mathcal{D}_\alpha$.
- Each of these $2^{n_l(\mathcal{L})}$ different configurations $\mathcal{D}_\alpha$ acquire an additional weight $w(g, \mathcal{L})/2^{n_l(\mathcal{L})}$.
- Resulting $w_{dimer}(g, \mathcal{D})$:

$$w_{dimer}(g, \mathcal{D}) \quad = \quad \sum_{\mathcal{L}|\mathcal{D}} \frac{w_{loop}(g, \mathcal{L})}{2^{n_l(\mathcal{L})}}$$

  $\mathcal{L}|\mathcal{D}$: all loop configurations $\mathcal{L}$ obtained from the overlap of $\mathcal{D}$ with any other fully-packed dimer configuration $\mathcal{D}'$.
- Energy $V(g, \mathcal{D})$ of a dimer configuration $\mathcal{D}$ in this classical interacting fully-packed dimer model:

$$V(g, \mathcal{D}) = -\log\left(w_{dimer}(g, \mathcal{D})\right)$$

Classical Schrieffer-Wolff: Cleaner formulation

- $$w_{dimer}(g, \mathcal{D}) \quad = \quad \langle \Psi(g) | \mathcal{D} \rangle_g$$

- $$\mathcal{Z}_{loop} = \mathcal{Z}_{dimer} = \sum_{\mathcal{D}} w_{dimer}(g, \mathcal{D})$$

Cluster expansion for $V(g, \mathcal{D})$

- Natural decomposition of $V(g, \mathcal{D})$: Sum of n-body potential energies $V_n(\mathcal{D}_n)$ of subconfigurations $\mathcal{D}_n$ consisting of n distinct dimers from $\mathcal{D}$:

$$V(g, \mathcal{D}) = \sum_n \sum_{\mathcal{D}_n \in \mathcal{D}} V_n(\mathcal{D}_n)$$

- V_n determined recursively from $w_{dimer}^{\mathcal{G}_n}(g, \mathcal{D}_n)$ of $\mathcal{D}_n$ in the interacting dimer model on the finite subgraph $\mathcal{G}_n(\mathcal{D}_n)$ of the square lattice
  - Calculated from loop model defined on $\mathcal{G}_n(\mathcal{D}_n)$
  - Subgraph $\mathcal{G}_n(\mathcal{D}_n)$: $2n$ vertices covered by dimers in $\mathcal{D}_n$ + all allowed edges between these vertices

Cluster expansion: Details

- V_n obtained recursively

$$-\log\left[w_{dimer}^{\mathcal{G}_n}(g,\mathcal{D}_n)\right] = V_n(\mathcal{D}_n) + \sum_{m=1}^{n-1} \sum_{\mathcal{D}_m \in \mathcal{D}_n} V_m(\mathcal{D}_m)$$

$\mathcal{D}_m \in \mathcal{D}_n$: all m-dimer subconfigurations $\mathcal{D}_m$ of $\mathcal{D}_n$
and $\mathcal{G}_m(\mathcal{D}_m)$: corresponding subgraphs of $\mathcal{G}_n(\mathcal{D}_n)$.

- V_1 () $= V_1$ () $= -\log(g)$. (1)

non-interacting dimer model in large-g limit

Leading non-trivial order in g^{-1}

- $V_2\left(\square\right) = V_2\left(\square\right) = -\log(1+g^{-1})$

- Classical interacting dimer model with aligning interaction between parallel dimers on the same plaquette
- Luckily: Well-studied in past numerical work (Alet et al 2006, Papanikolaou et al 2007)
- Read off results...

Behaviour of classical model

- As V_2 increased fro zero, stiffness ρ^* in height description increases
  Eventually, transition to columnar ordered state
  ((Alet et al 2006, Papanikolaou et al 2007)
- Transition not relevant for our purposes—V_2 small in our case
- Read of magnitude of ρ^*, and prediction for energy energy correlators

“Operator correspondence”

- Need to know how to transform energy correlator to dimer variables
- Formal rule:

$$\bar{\mathcal{P}}_{\hat{O}}(\mathcal{D}) = \frac{1}{w_{dimer}(g,\mathcal{D})} \sum_{\mathcal{L}|\mathcal{D}} \frac{w_{loop}(g,\mathcal{L})\mathcal{P}_{\hat{O}}(\mathcal{L})}{2^{n_l(\mathcal{L})}} \ , \qquad (2)$$

$\mathcal{P}_{\hat{O}}(\mathcal{L})$: contribution of $\mathcal{L}$ to $\langle\Psi(g)|\hat{O}|\Psi(g)\rangle$ in loop-gas language

- For leading long-distance behaviour: Replace energy density by dimer occupation

Reality check: Set $g = 2$

Dimer-dimer correlators at $V_2 = \log(\frac{3}{2})$ (with attractive sign)

$$C_{E_x}(\vec{r}) \equiv \langle \vec{S}_{\vec{0}} \cdot \vec{S}_{\vec{0}+\hat{x}} \vec{S}_{\vec{r}} \cdot \vec{S}_{\vec{r}+\hat{x}} \rangle_c = \frac{(-1)^x}{|\vec{r}|^\alpha}$$

with $\alpha \approx 1.22$!

Compares well with exact numerics finding $\alpha \approx 1.20$

Adding further neighbour bonds

- Stick to bipartite valence bonds
  $g = \infty$: Bipartite but non-planar dimer model
  Power-law dimer correlations *not* destroyed (Sandvik & Moessner 2000)
- nnRVB wavefunction represents a point in a critical phase(?) with variable α
  Caveat Emptor: No detailed understanding of dimer interactions + longer-range dimers

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