Title: From the Honeycomb to the Kagome: What Can Variational Wave-functions Teach Us About Spin Liquids and How Can We Go Beyond Them?

Date: Dec 12, 2011 02:30 PM

URL: http://pirsa.org/11120057

Abstract: Although the typical physical system achieves an ordered state at low temperatures, spin liquids stay disordered even in their ground state. In addition to an increasing number of experimental candidates for spin liquids, recent numerical work from Meng, et. al and Yan, et. al. has supplied strong numerical evidence for natural Hamiltonians having spin liquid ground states. Their featureless nature, though, makes learning about these states particularly difficult. In this talk, we explore what variational ansatz can teach us about them. Additionally, we examine whether the canonical theoretical framework makes sense in the context of the best wave-functions. Finally, we look at what other tools we have to make sense of spin liquids.

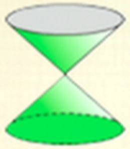
From the Honeycomb to the Kagome: What can Wave-functions teach us about spin liquids and how to go beyond them?

Bryan Clark, Princeton Center For Theoretical Science

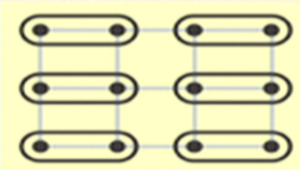
Collaborators: Dima Abanin, Shivaji Sondhi, Jesse Kinder, Eric Neuscamman, Michael Lawler, Garnet Chan

Perimeter: Dec. 12, 2011

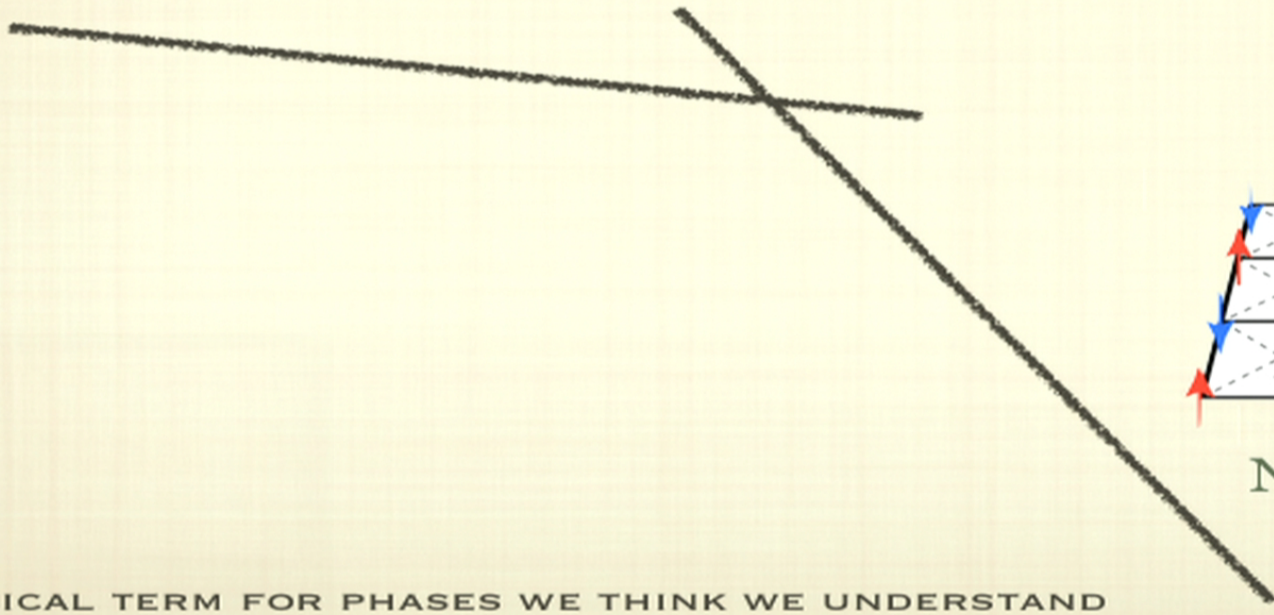
Boring Phases*

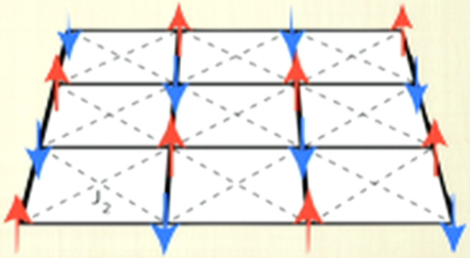


Semi-metal



Valence Bond Crystal



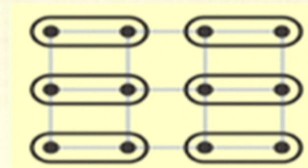


Neel State

* Technical term for phases we think we understand

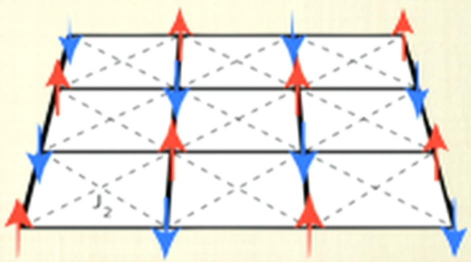
BORING PHASES*

Semi-metal



Valence Bond Crystal

Spin liquid



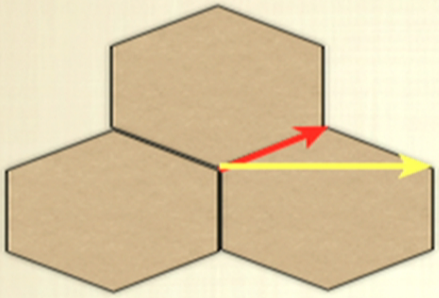
Neel State

* TECHNICAL TERM FOR PHASES WE THINK WE UNDERSTAND

The tale of 3 spin liquids...

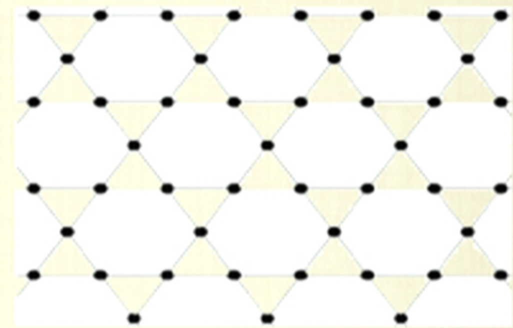
Heisenberg Model:

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j + \ldots$$



Honeycomb

Kagome



Yan, White, Huse

Hubbard Model:

$$H = -t \sum_{\langle i,j \rangle, s} a^{\dagger}_{is} a_{js} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Meng, et. al

$\frac{U}{t}$ 3.5 4.3

Why study spin liquids

Recent experimental evidence.

herbertsmithite

volborthite

vesignieite

$Na_4Ir_3O_8$

$EtMe_3Sb[Pd(dmit)_2]_2$

- Possible ground state of simple model.
- Relevance to high Tc
- Topological Order
- Not described by Fermi Liquid Theory nor Landau Theory for Phase Transitions.

Why study spin liquids

Recent experimental evidence.

herbertsmithite

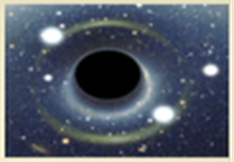
volborthite

vesignieite

$Na_4Ir_3O_8$

$EtMe_3Sb[Pd(dmit)_2]_2$

- ❑ Possible ground state of simple model.
- ❑ Relevance to high Tc
- ❑ Topological Order
- ❑ Not described by Fermi Liquid Theory nor Landau Theory for Phase Transitions.



Spin liquids ~~Black holes~~ have no hair

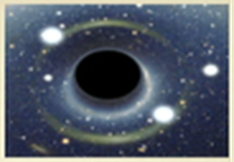
- No magnetic Order
- No Local Order Parameters
- No Symmetry Breaking

Makes it hard to identify and learn anything about.

Gapped + Topological **OR** Gapless

Spin liquids

~~Black holes~~ have no hair



- No magnetic Order
- No Local Order Parameters
- No Symmetry Breaking

Makes it hard to identify and learn anything about.

Gapped + Topological ?

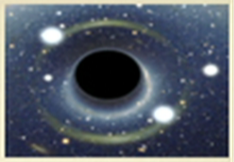
OR

Gapless

Torous:
4-fold degeneracy

Spin liquids

~~Black holes~~ have no hair



- No magnetic Order
- No Local Order Parameters
- No Symmetry Breaking

Makes it hard to identify and learn anything about.

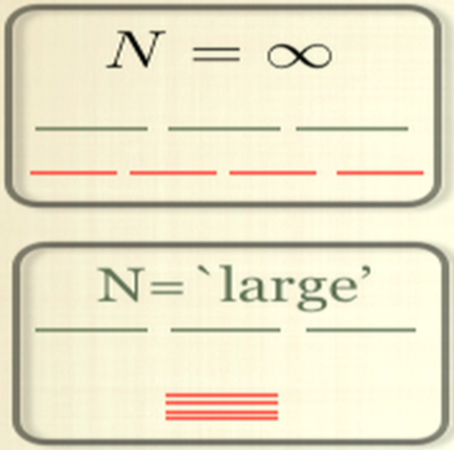
Gapped + Topological ? OR Gapless

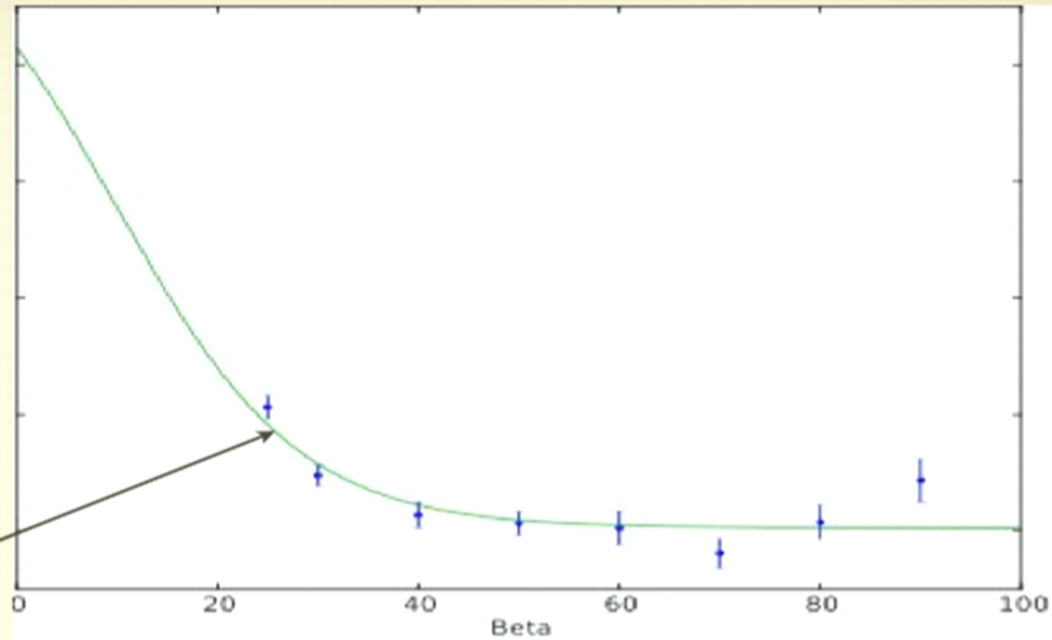
Hastings Theorem:
No symmetry Breaking
+
1 site / unit cell
$\Downarrow$
gapless or topological

Torous:
4-fold degeneracy

We'll always have QMC

Spectra:





Best Fit to Triplet: 0.11

Calculated Spin Gap (Meng, et. al): 0.11

Best Fit To Triplet + Extra State: >0.12

States below the Spin Gap aren't favored but not outright inconsistent with the data either.

Entropy

$$S(\beta) = S(0) - \left[\int_0^\beta E d\beta - \beta E(\beta)\right]$$

Spectra:

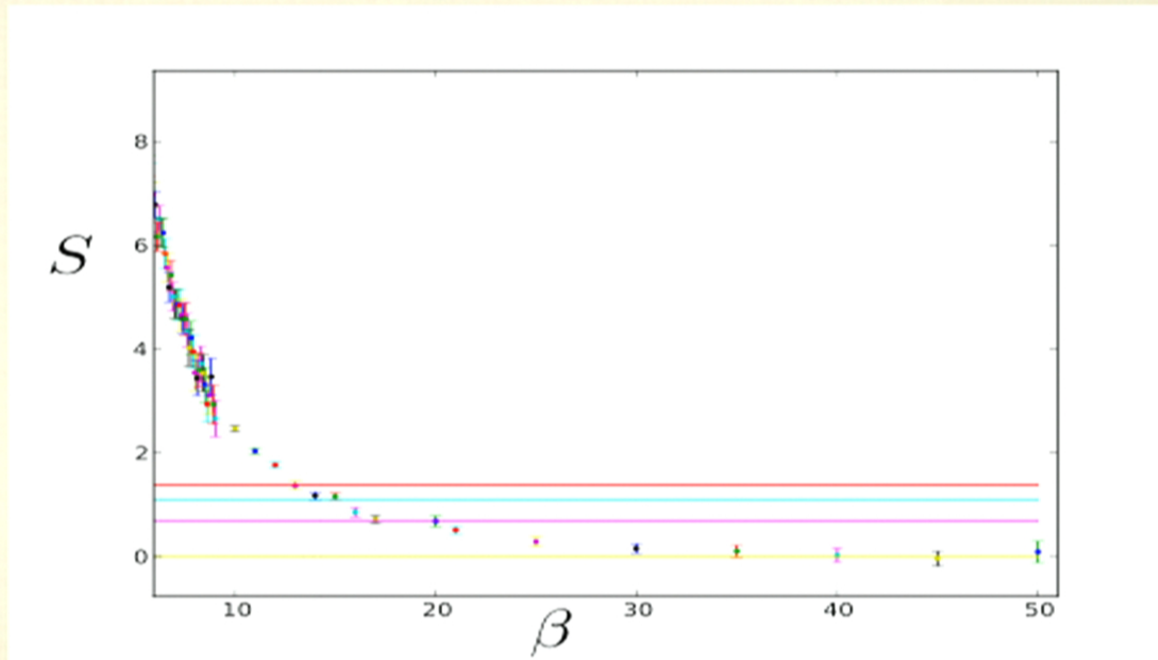
$N = \infty$

$S(0) = \ln(4)$

N=`large'

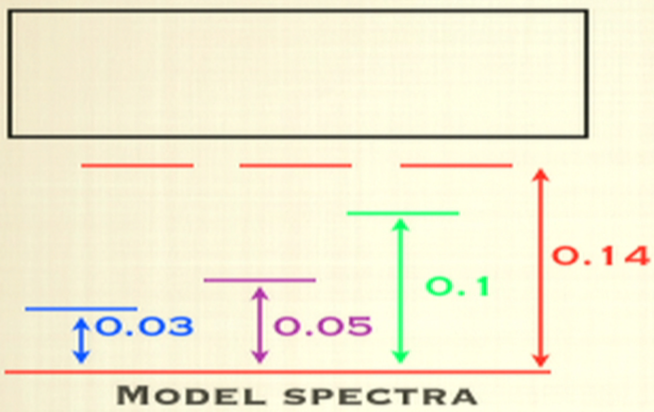
$S(\epsilon) \approx \ln(4)$

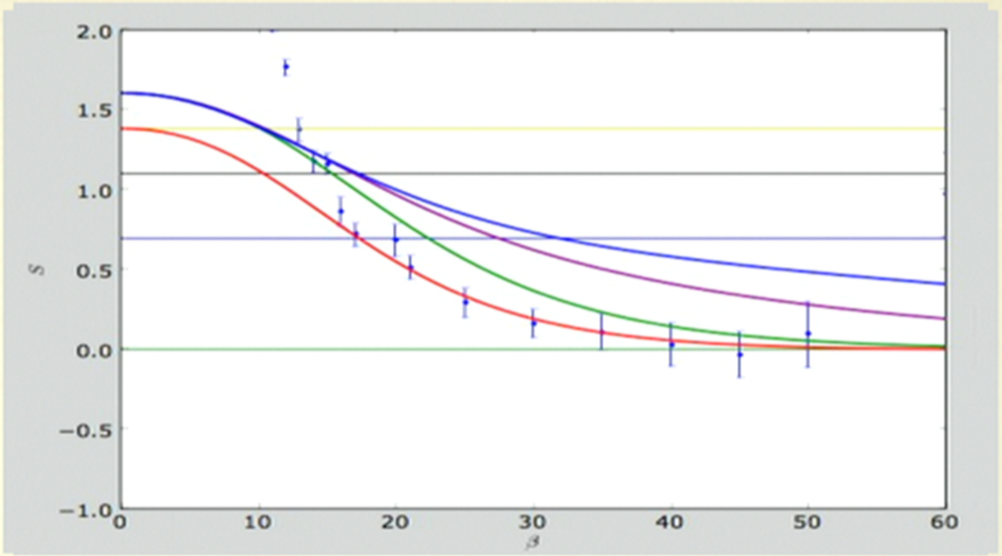
$S(0) = 0$



Can we quantify this?

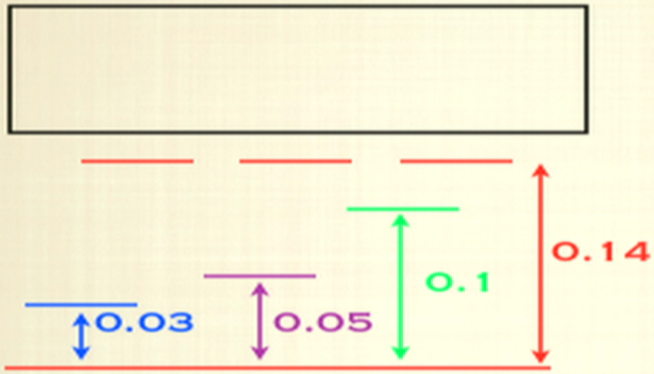
Quantification



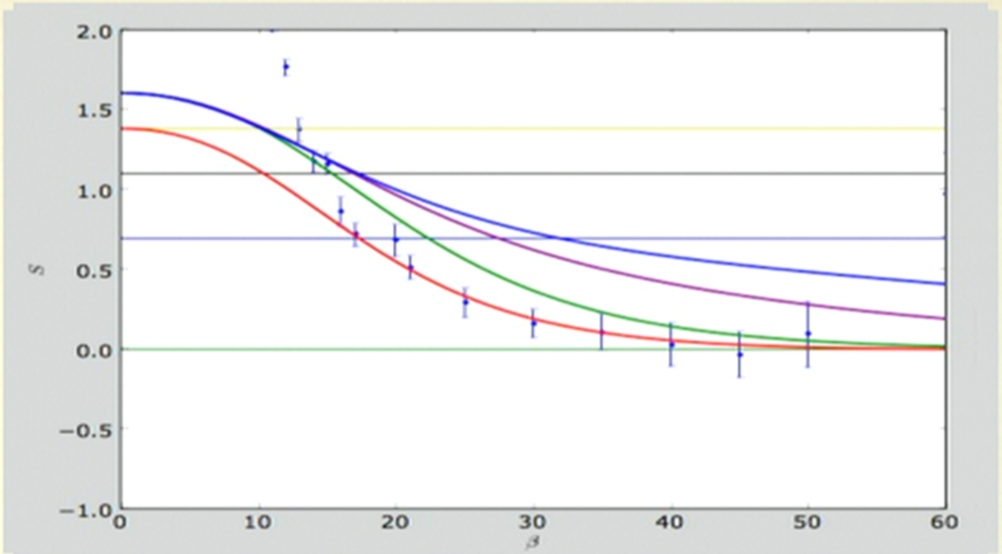


- No way to fix this Spectra!

Quantification



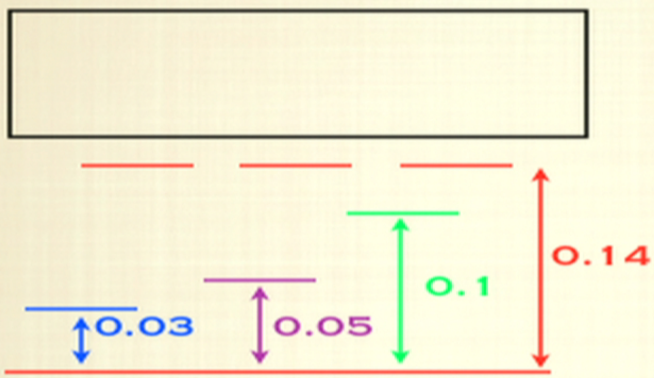
Model spectra



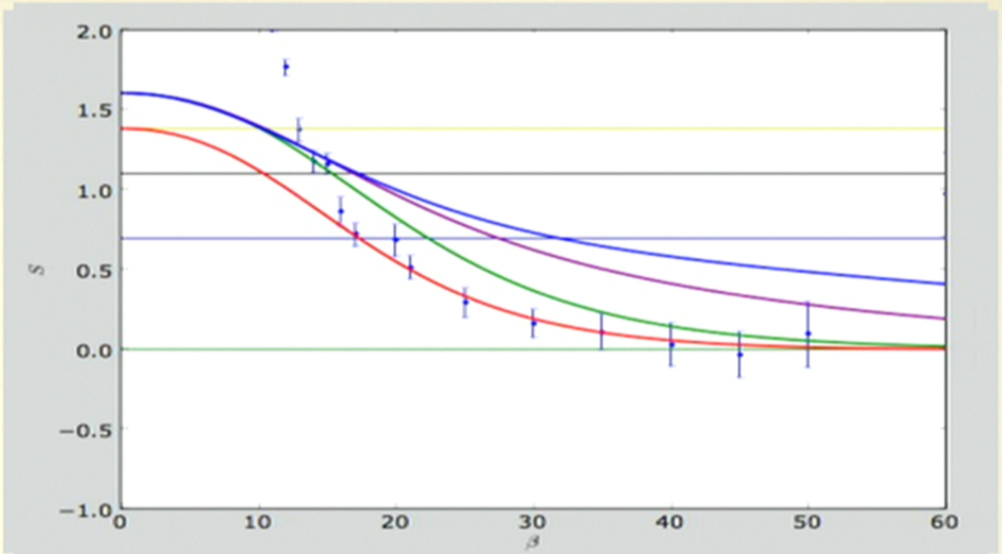
6x6 system

- No way to fix this spectra!

QUANTIFICATION



MODEL SPECTRA



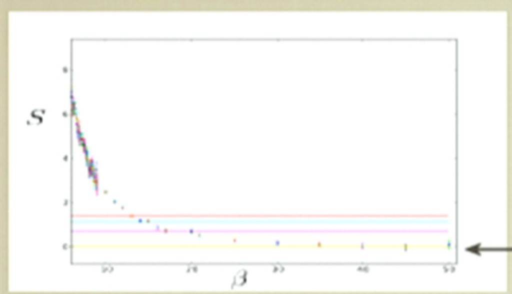
6X6 SYSTEM

- NO WAY TO FIX THIS SPECTRA!

Your QMC is Missing a State!

Your QMC is Missing a State!

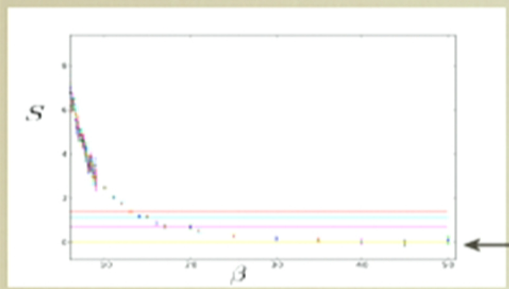
I.



Integrates to 0

Your QMC is Missing a State!

I.



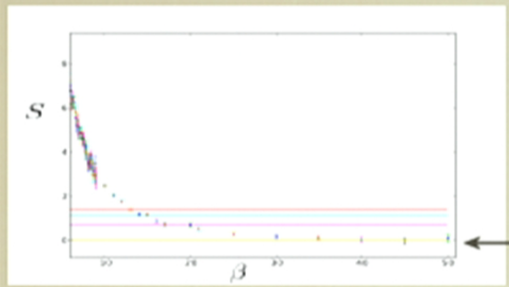
Integrates to 0

II.

Both high and low energy fit the same low lying spectra.

YOUR QMC IS MISSING A STATE!

I.



INTEGRATES TO 0

II.

BOTH HIGH AND LOW ENERGY FIT THE SAME LOW LYING SPECTRA.

III.

ANY SYSTEMATIC ERROR THROWS THIS RESULT OFF.

IV.

SCALE SET BY INFINITE T

IF YOU MISS THE STATE ENTIRELY OR YOU MISS THE LOW LYING STATES, YOU SHOULD NEVER GET S(T) BELOW LOG(2) FOR ANY T!

What about my Spin Liquid?

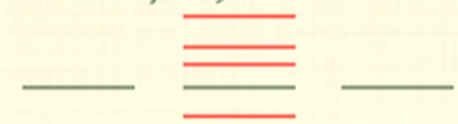
The Boring Possibility:

$$[N = \infty] \neq [N = 162]$$

The states decay exponentially but not fast enough

Lesson: Topological degeneracies are hard. The rest of this talk will be about other ways to learn about spin liquids.

N=72; N=162



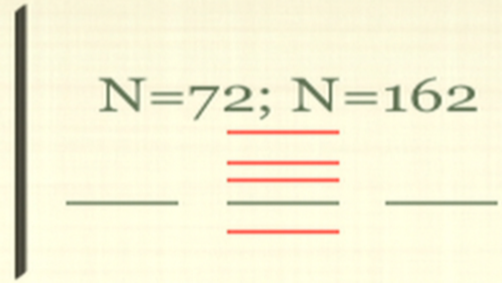
What about my Spin Liquid?

The Boring Possibility:

$$[N = \infty] \neq [N = 162]$$

The states decay exponentially but not fast enough

Lesson: Topological degeneracies are hard. The rest of this talk will be about other ways to learn about spin liquids.



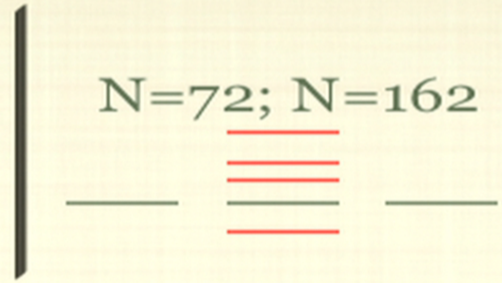
What about my Spin Liquid?

The Boring Possibility:

$$[N = \infty] \neq [N = 162]$$

The states decay exponentially but not fast enough

Lesson: Topological degeneracies are hard. The rest of this talk will be about other ways to learn about spin liquids.



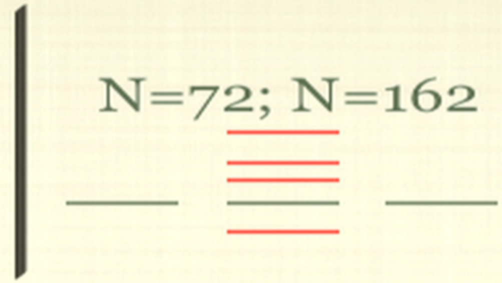
What about my Spin Liquid?

The Boring Possibility:

$$[N = \infty] \neq [N = 162]$$

The states decay exponentially but not fast enough

Lesson: Topological degeneracies are hard. The rest of this talk will be about other ways to learn about spin liquids.



The Exotic Possibility:

This isn't a spin liquid!

But ... there is no symmetry breaking

A new(ish) animal!

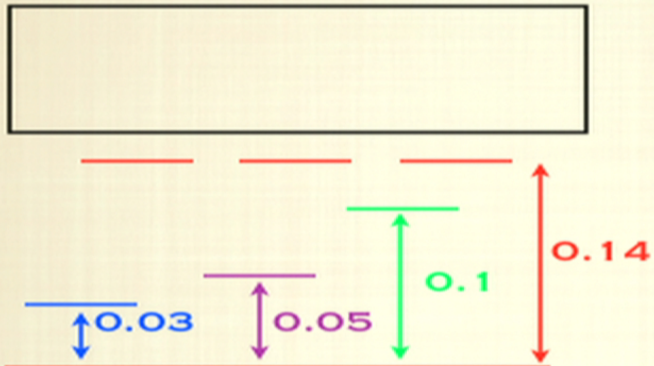
Where are we so far?

We can't find the topological degeneracy on the most numerically convincing spin liquid either because (a) it's not there or (b) it's hard to find.

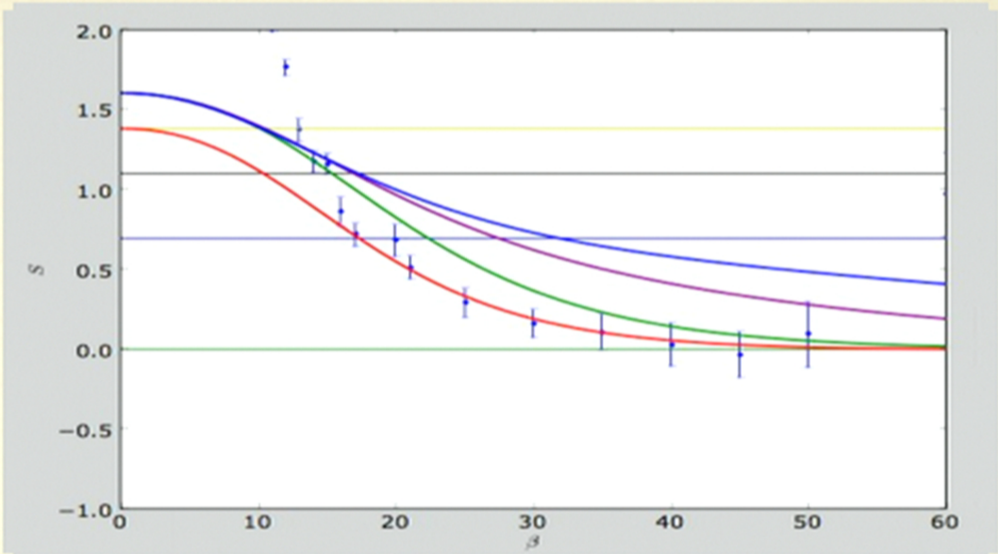
The second two "tales" are about spin systems and wave-functions.

- Does the analytically suggested wave-functions work?
- If so, which "spin-liquid" am I?

QUANTIFICATION



MODEL SPECTRA



6X6 SYSTEM

- NO WAY TO FIX THIS SPECTRA!

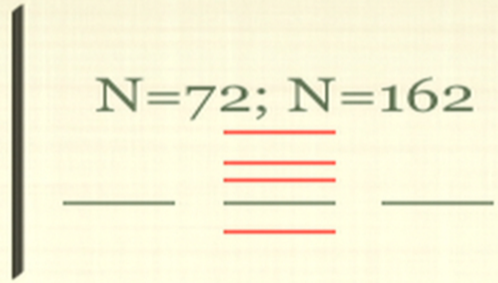
What about my Spin Liquid?

The Boring Possibility:

$$[N = \infty] \neq [N = 162]$$

The states decay exponentially but not fast enough

Lesson: Topological degeneracies are hard. The rest of this talk will be about other ways to learn about spin liquids.



Other

Some gap is off?

The Exotic Possibility:

This isn't a spin liquid!

But ... there is no symmetry breaking

A new(ish) animal!

Where are we so far?

We can't find the topological degeneracy on the most numerically convincing spin liquid either because (a) it's not there or (b) it's hard to find.

The second two "tales" are about spin systems and wave-functions.

- Does the analytically suggested wave-functions work?
- If so, which "spin-liquid" am I?

This Talk's Approach

Approach 1

Simple at the cost of accuracy.

Wave function form itself useful

$$\Psi_{PBCS} = P\prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow})|0\rangle$$

"Spin Liquid if from symmetric H"

MAke direct Connection to Analytics

Approach 2

Mimic Exact Diagonalization: DMRG, Huse-Elser, Quantum Chemistry, DMC, ...

Wave-function itself not insightful

$$[0.3, 0.12, 0.6, 0.9, 0.88, \ldots]$$

Learn things by probing correlations:

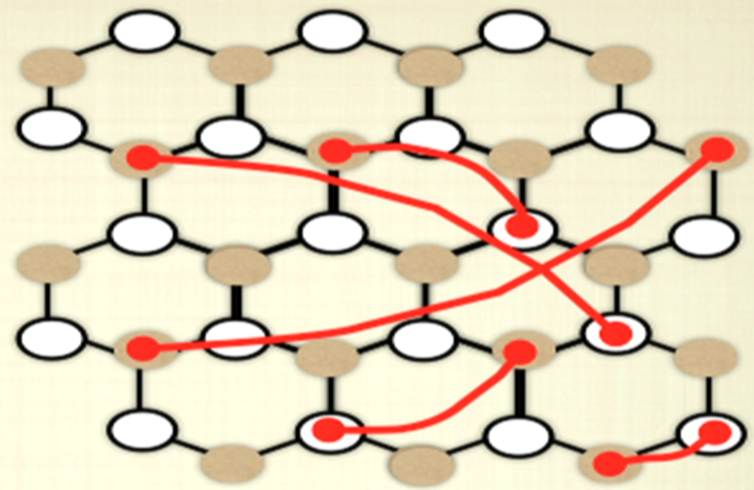
$$n(R - R') = \Psi(R)\Psi^*(R')$$

RVB

RVB wave functions

$$\Psi = \sum_{dim.covering} \prod_{[ij]} \phi(r_i - r_j) | \uparrow_i \downarrow_j - \uparrow_j \downarrow_i \rangle$$

Note: Only showing some of the dimers



GAPPED SPIN LIQUIDS: PRIMARILY SHORT RANGE RVB SINGLETS. FINITE COST TO BREAK THEM.

GAPLESS SPIN LIQUIDS: RVB SINGLETS OF ALL SIZE. ARBITRARY SMALL COST TO BREAK LONG BONDS.

THIS WAVE FUNCTION IS HARD TO WORK WITH EXPLICITLY BECAUSE THE BASIS IS NON-ORTHOGONAL

Gapped Spin Liquids

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

Another perspective

Schwinger-Fermion + Mean Field $S_i = \frac{1}{2} f_{i\alpha} \vec{\sigma}_{\alpha\beta} f_{i\beta}$ $\quad f^\dagger_{i\alpha} f_{i\alpha} = 1 \quad f_{i\alpha} f_{i\beta} \epsilon_{\alpha\beta} = 0$

$$H_F = -t \sum_{\langle i,j \rangle, s} f^\dagger_{is} f_{js} + \sum_{ij} \Delta_{ij} (f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}) + h.c.$$

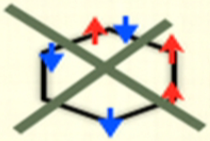
Solve mean field Hamiltonian and implement constraint by projection.

$$\Psi_{PBCS} = P \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) |0\rangle$$

$$\langle R | \Psi_{PBCS} \rangle = \det M$$

$$M_{ij} = \phi(\vec{r}_{\uparrow,i} - \vec{r}_{\downarrow,j}) \equiv \phi(\vec{r}_{ij})$$

Project out double and zero occupancy.



Gapped Spin Liquids

$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

<u>Another perspective</u>

Schwinger-Fermion + Mean Field $S_i = \frac{1}{2} f_{i\alpha} \vec{\sigma}_{\alpha\beta} f_{i\beta}$ $\quad f^\dagger_{i\alpha} f_{i\alpha} = 1 \quad f_{i\alpha} f_{i\beta} \epsilon_{\alpha\beta} = 0$

$$H_F = -t \sum_{\langle i,j \rangle, s} f^\dagger_{is} f_{js} + \sum_{ij} \Delta_{ij} (f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}) + h.c.$$

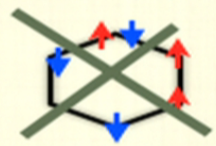
Solve mean field Hamiltonian and implement constraint by projection.

$$\Psi_{PBCS} = P \prod_k (u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow}) |0\rangle$$

$$\langle R | \Psi_{PBCS} \rangle = \det M$$

$$M_{ij} = \phi(\vec{r}_{\uparrow,i} - \vec{r}_{\downarrow,j}) \equiv \phi(\vec{r}_{ij})$$

Project out double and zero occupancy.



RVB wave functions

$$\Psi = \sum_{dim.covering} \prod_{[ij]} \phi(r_i - r_j) | \uparrow_i \downarrow_j - \uparrow_j \downarrow_i \rangle$$

These are (almost) the same.

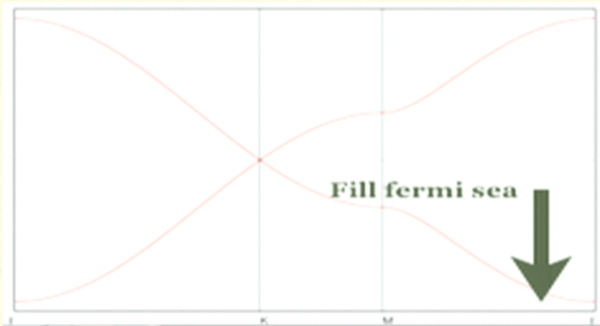
(up to a sign we can often gauge away)

GAPLESS SPIN LIQUIDS

We need a state with long range RVB singlets.

$$H_F = -t \sum_{\langle i,j \rangle, s} f^\dagger_{is} f_{js}$$

Solve mean field and project.



$$\Psi_{\rm gutz} = \det M$$

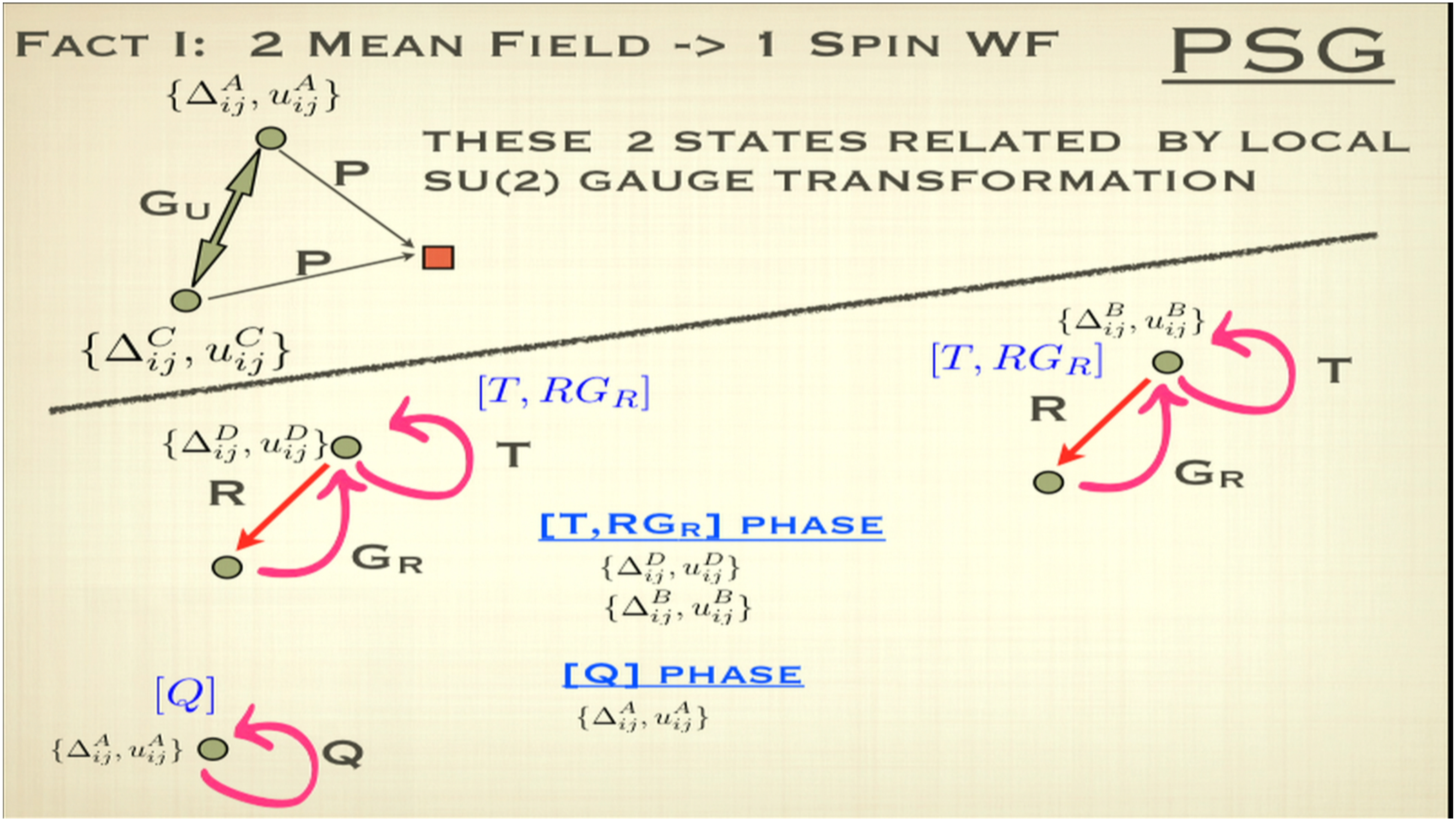
$$M_{ij} = \phi_i(r_j)$$

$$\phi_i(\vec{r}) = -t e^{ik_{ix} r_x/\sqrt{3}} \left[1 + 2e^{-i\frac{k_{ix} r_x \sqrt{3}}{2}} \cos\left(\frac{k_{iy} r_y}{2}\right) \right]$$

Projected Gutzweiller: $P\,\Psi_{\rm gutz}$

Not surprising this is gapless since projected a state with no gap.

Zero parameter wave function!


FACT I: 2 MEAN FIELD -> 1 SPIN WF
PSG
$\{\Delta_{ij}^A, u_{ij}^A\}$
THESE 2 STATES RELATED BY LOCAL SU(2) GAUGE TRANSFORMATION
P
GU
P
$\{\Delta_{ij}^C, u_{ij}^C\}$
$\{\Delta_{ij}^B, u_{ij}^B\}$
$[T, RG_R]$
T
R
GR
$[T, RG_R]$
$\{\Delta_{ij}^D, u_{ij}^D\}$
T
R
GR
[T,RGR] PHASE
$\{\Delta_{ij}^D, u_{ij}^D\}$
$\{\Delta_{ij}^B, u_{ij}^B\}$
$[Q]$
$\{\Delta_{ij}^A, u_{ij}^A\}$
Q
[Q] PHASE
$\{\Delta_{ij}^A, u_{ij}^A\}$

Degeneracy at the Mean Field

(Typical) Process:

- Pick parameters in Mean Field H
- Evaluate the Energy
- Pick Better Parameters

Degeneracy at the Mean Field

(Typical) Process:

- Pick parameters in Mean Field H
- Evaluate the Energy
- Pick Better Parameters

Obstacle:

Single Particle BDG Spectra:

Which of the 3 states do you use to fill the Fermi sea?

Particularly bad in the Kagome where sometimes you have macroscopic degeneracy!

Typical Solution: Give Up!

Solutions Begat Problems

$$\Phi[i,j] = \begin{bmatrix} 0.2 & 0.2 & 1.4 \\ 0.2 & 4.2 & 3.3 \\ 1.4 & 3.3 & 0.3 \end{bmatrix}$$

Am I A Spin Liquid?

Which one?

Solutions Begat Problems

$$\Gamma = \begin{bmatrix} \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger & \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \\ \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi} & \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \end{bmatrix}$$

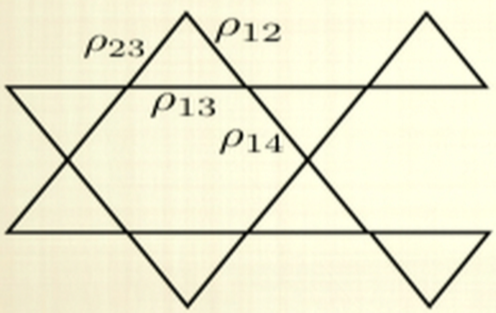
$$\Phi[i,j] = \begin{bmatrix} 0.2 & 0.2 & 1.4 \\ 0.2 & 4.2 & 3.3 \\ 1.4 & 3.3 & 0.3 \end{bmatrix}$$

Am I a spin liquid?

Which one?

Anomalous Density Matrix

$$\rho \equiv \frac{\langle\Omega|\Psi\cdot\Psi^\dagger|\Omega\rangle}{\langle\Omega|\Omega\rangle} = \frac{1}{\langle\Omega|\Omega\rangle}\begin{pmatrix} \langle\Omega|f_\uparrow\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\uparrow\cdot f_\downarrow|\Omega\rangle \\ \langle\Omega|f_\downarrow^\dagger\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\downarrow^\dagger\cdot f_\downarrow|\Omega\rangle \end{pmatrix}$$



$$\rho_{ij} = \begin{pmatrix} -A_{ij}^* & B_{ij} \\ B_{ij}^* & A_{ij} \end{pmatrix}$$

$$|\rho_{ij}| = \sqrt{\det \rho_{ij}} \longleftarrow$$ Gauge Invariant

If a spin liquid, all bonds are identical

SOLUTIONS BEGAT PROBLEMS

$$\Gamma = \begin{bmatrix} \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger & \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \\ \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi} & \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \end{bmatrix}$$

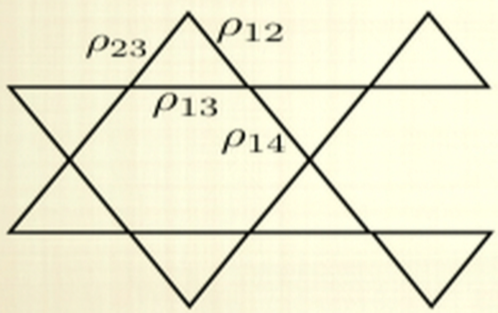
$$\Phi[i,j] = \begin{bmatrix} 0.2 & 0.2 & 1.4 \\ 0.2 & 4.2 & 3.3 \\ 1.4 & 3.3 & 0.3 \end{bmatrix}$$

AM I A SPIN LIQUID?

WHICH ONE?

ANOMALOUS DENSITY MATRIX

$$\rho \equiv \frac{\langle\Omega|\Psi\cdot\Psi^\dagger|\Omega\rangle}{\langle\Omega|\Omega\rangle} = \frac{1}{\langle\Omega|\Omega\rangle}\begin{pmatrix} \langle\Omega|f_\uparrow\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\uparrow\cdot f_\downarrow|\Omega\rangle \\ \langle\Omega|f_\downarrow^\dagger\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\downarrow^\dagger\cdot f_\downarrow|\Omega\rangle \end{pmatrix}$$



$$\rho_{ij} = \begin{pmatrix} -A_{ij}^* & B_{ij} \\ B_{ij}^* & A_{ij} \end{pmatrix}$$

$$|\rho_{ij}| = \sqrt{\det\rho_{ij}}$$ ⟵ GAUGE INVARIANT

IF A SPIN LIQUID, ALL BONDS ARE IDENTICAL

FLUXES: $W_{ij} = -i\rho_{ij}/|\rho_{ij}|$

$$\phi_{ijk\ldots l} = i^{N_{\mathrm{loop}}} W_{ij}\cdot W_{jk}\cdot\ldots\cdot W_{li}$$

$$\theta = 2\arccos((\mathrm{Tr}\Phi_{ijk\ldots l})/2)$$

DIFFERENT SPIN LIQUIDS HAVE DIFFERENT FLUXES

Solutions Begat Problems

$$\Gamma = \begin{bmatrix} \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger & \frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \\ \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi} & \Phi\frac{\mathbb{I}}{\mathbb{I}+\Phi^\dagger\Phi}\Phi^\dagger \end{bmatrix}$$

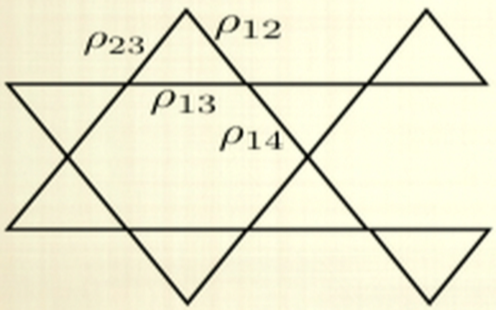
$$\Phi[i,j] = \begin{bmatrix} 0.2 & 0.2 & 1.4 \\ 0.2 & 4.2 & 3.3 \\ 1.4 & 3.3 & 0.3 \end{bmatrix}$$

Am I a Spin Liquid?

Which one?

Anomalous Density Matrix

$$\rho \equiv \frac{\langle\Omega|\Psi\cdot\Psi^\dagger|\Omega\rangle}{\langle\Omega|\Omega\rangle} = \frac{1}{\langle\Omega|\Omega\rangle}\begin{pmatrix} \langle\Omega|f_\uparrow\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\uparrow\cdot f_\downarrow|\Omega\rangle \\ \langle\Omega|f_\downarrow^\dagger\cdot f_\uparrow^\dagger|\Omega\rangle & \langle\Omega|f_\downarrow^\dagger\cdot f_\downarrow|\Omega\rangle \end{pmatrix}$$



$$\rho_{ij} = \begin{pmatrix} -A_{ij}^* & B_{ij} \\ B_{ij}^* & A_{ij} \end{pmatrix}$$

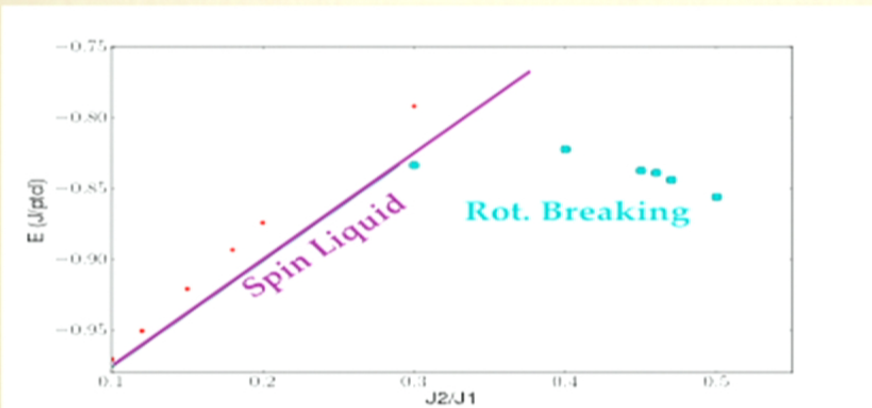
$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$ ⟵ Gauge Invariant

If a spin liquid, all bonds are identical

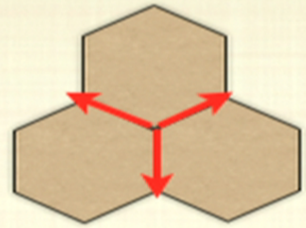
NOT ALL Φ ARE SPIN LIQUIDS!

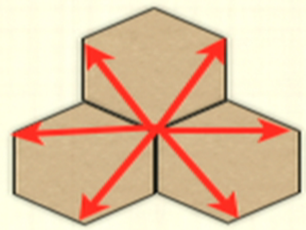
Optimizing $\phi(\vec{r}_{ij})$

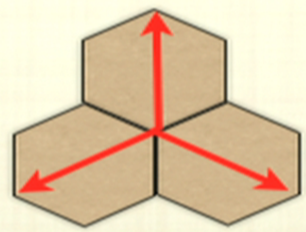
$$\phi(\vec{r}_{ij}) \equiv \phi(-\vec{r}_{ij})$$

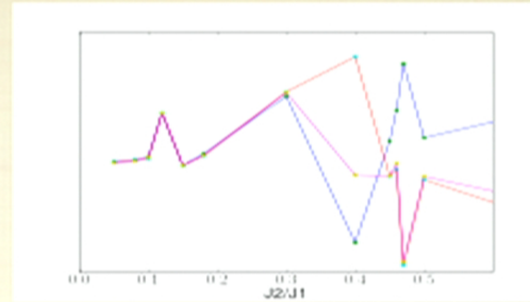


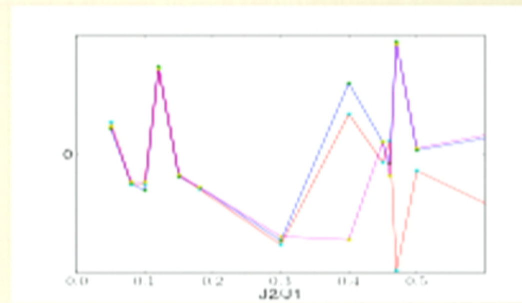
At $\frac{J_2}{J_1} \approx 0.3$, the rotational symmetry breaks.

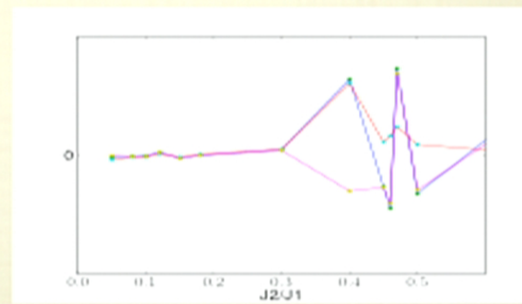












The story so far...

We want to think about spin liquids from a wave-function perspective. This means thinking about PBCS (which encompass spin liquids + more). There are technical issues with this we've overcome ...

Next:

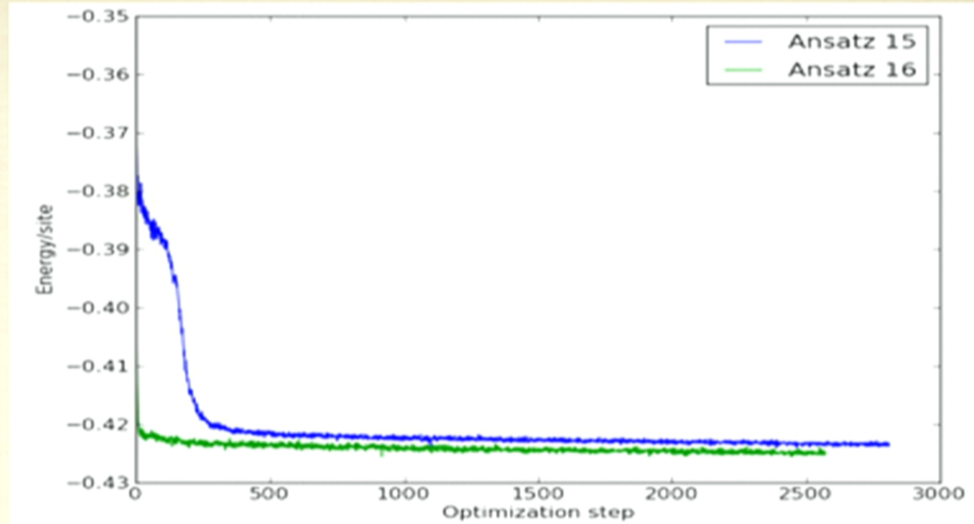
Am I a spin liquid characterized by the typical theoretical lore?

and

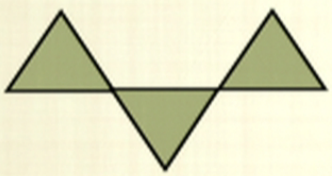
if so, which one am I?

Searching for the best PBCS

And the Winner (amongst PBCS) is ...



A spin liquid



Not a Spin Liquid (slightly)

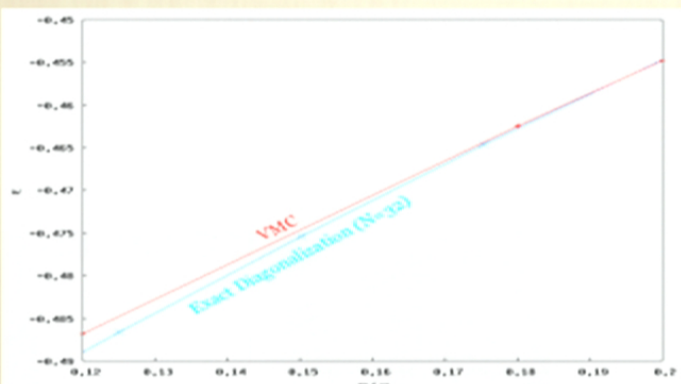
The Honeycomb

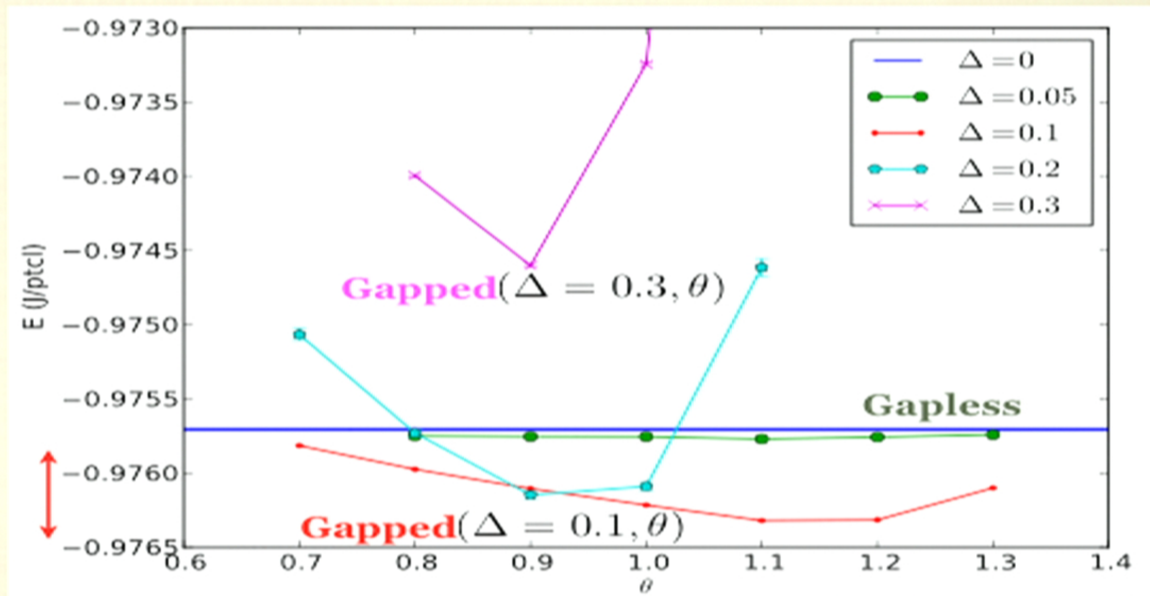
sps (Lu and Ran)

$$H_F = -t \sum_{\langle i,j \rangle, s} f^\dagger_{is} f_{js} + \sum_{\langle\langle ij \rangle\rangle} \Delta_{ij} (f^\dagger_{i\uparrow} f^\dagger_{j\downarrow} - f^\dagger_{i\downarrow} f^\dagger_{j\uparrow}) + h.c.$$

$$\Delta_{ij} = \Delta e^{i\theta} \quad i,j \in A$$

$$\Delta_{ij} = \Delta e^{-i\theta} \quad i,j \in B$$





Optimized by:

- Pairing Function Opt.
- Searching over Suggested Hamiltonians

WHY ME?

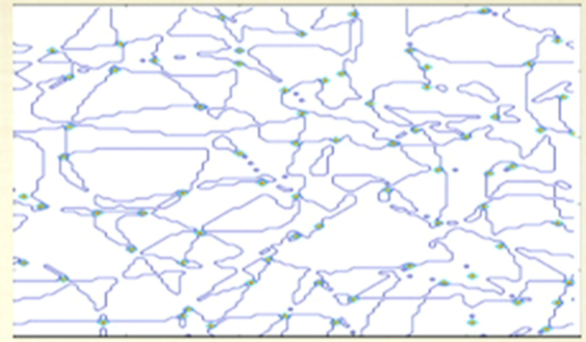
$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

J1 Nodes set by Marshall Sign Rule

Positive		Negative
$\Psi(\uparrow\downarrow\uparrow\downarrow\uparrow)$	$\longrightarrow$	$\Psi(\downarrow\uparrow\uparrow\downarrow\uparrow)$
$\Psi(\downarrow\uparrow\uparrow\uparrow\downarrow)$	$\longleftarrow$ $\longrightarrow$	$\Psi(\uparrow\downarrow\uparrow\uparrow\downarrow)$
$\Psi(\uparrow\uparrow\downarrow\uparrow\downarrow)$	$\longleftarrow$ $\longrightarrow$	$\Psi(\uparrow\uparrow\uparrow\downarrow\downarrow)$

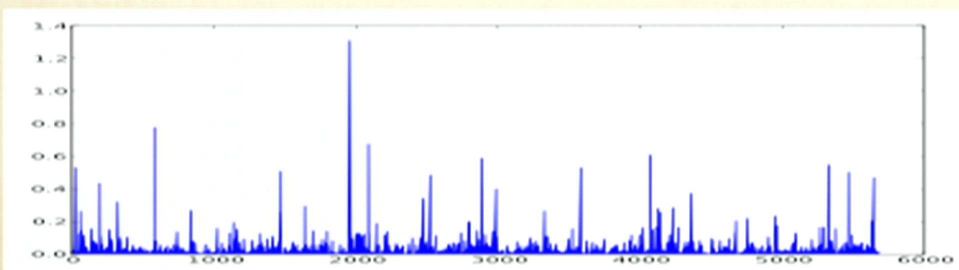
Quantify by

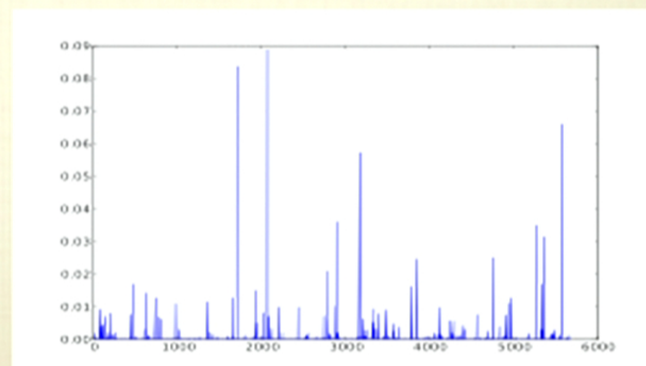
$$\sum_{\langle ij \rangle \in s} 1/2 \frac{\langle s'_{ij} | \Psi \rangle}{\langle s \, | \Psi \rangle} \text{ if } s_i \neq s_j$$



NODES MATTER!

$$\Psi(s_1, s_2, \ldots s_n) > 0$$
$$\Psi(s_1, s_2, \ldots s_n) = 0$$
$$\Psi(s_1, s_2, \ldots s_n) < 0$$





WHY ME?

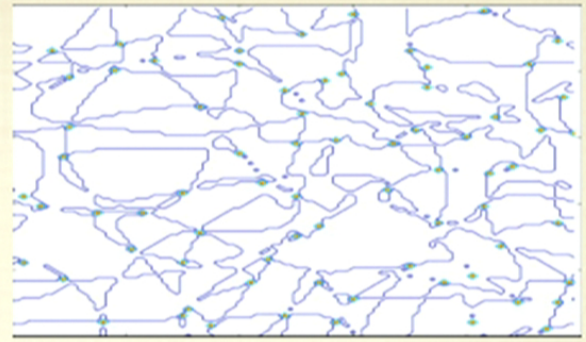
$$H = J_1 \sum_{\langle ij \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle ij \rangle\rangle} S_i \cdot S_j$$

J1 Nodes set by Marshall Sign Rule

Positive		Negative
Ψ(↑↓↑↓↑)	⟶	Ψ(↓↑↑↓↑)
Ψ(↓↑↑↑↓)	⟵ ⟶	Ψ(↑↓↑↑↓)
Ψ(↑↑↓↑↓)	⟵ ⟶	Ψ(↑↑↑↓↓)

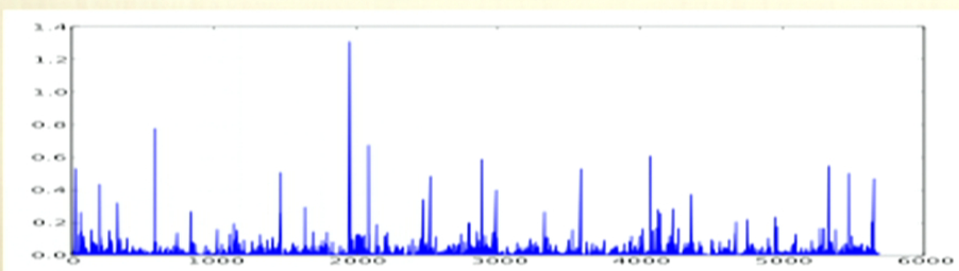
Quantify by

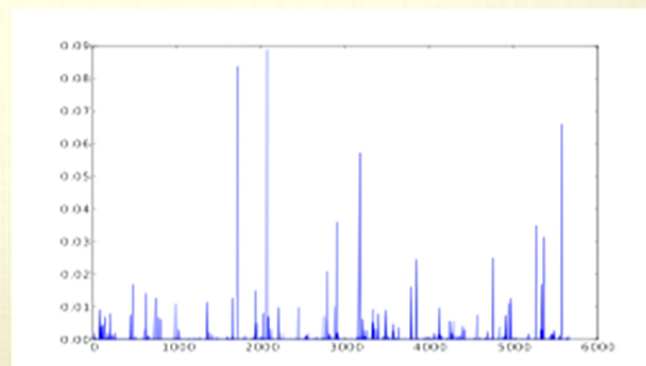
$$\sum_{\langle ij \rangle \in s} 1/2 \frac{\langle s'_{ij} | \Psi \rangle}{\langle s \, | \Psi \rangle} \text{ if } s_i \neq s_j$$



NODES MATTER!

$$\Psi(s_1, s_2, \ldots s_n) > 0$$
$$\Psi(s_1, s_2, \ldots s_n) = 0$$
$$\Psi(s_1, s_2, \ldots s_n) < 0$$





Why Me?

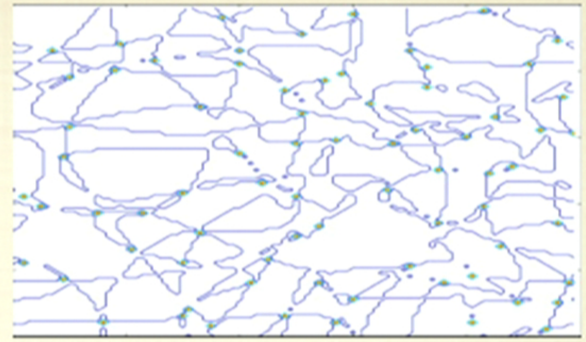
$$H = J_1 \sum_{\langle i,j \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle i,j \rangle\rangle} S_i \cdot S_j$$

J1 Nodes set by Marshall Sign Rule

Positive		Negative
$\Psi(\uparrow\downarrow\uparrow\downarrow\uparrow)$	$\longrightarrow$	$\Psi(\downarrow\uparrow\uparrow\downarrow\uparrow)$
$\Psi(\downarrow\uparrow\uparrow\uparrow\downarrow)$	$\leftrightarrows$	$\Psi(\uparrow\downarrow\uparrow\uparrow\downarrow)$
$\Psi(\uparrow\uparrow\downarrow\uparrow\downarrow)$	$\leftrightarrows$	$\Psi(\uparrow\uparrow\uparrow\downarrow\downarrow)$

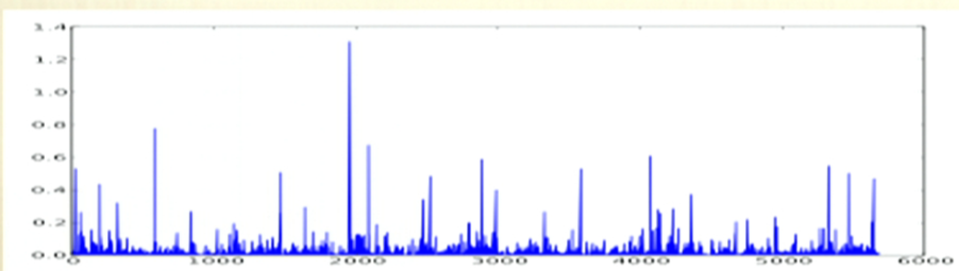
Quantify by

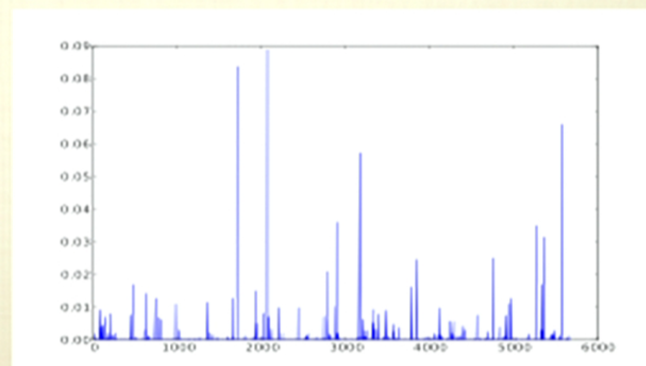
$$\sum_{\langle ij \rangle \in s} 1/2 \frac{\langle s'_{ij} | \Psi \rangle}{\langle s \, | \Psi \rangle} \text{ if } s_i \neq s_j$$



Nodes Matter!

$$\Psi(s_1, s_2, \ldots s_n) > 0$$
$$\Psi(s_1, s_2, \ldots s_n) = 0$$
$$\Psi(s_1, s_2, \ldots s_n) < 0$$





WHY ME?

$$H = J_1 \sum_{\langle ij \rangle} S_i \cdot S_j + J_2 \sum_{\langle\langle ij \rangle\rangle} S_i \cdot S_j$$

J1 Nodes set by Marshall Sign Rule

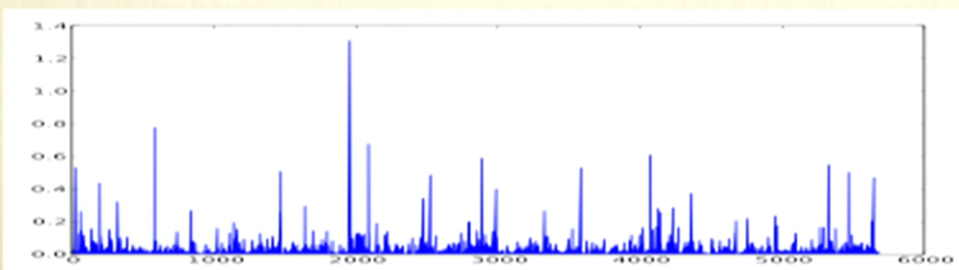
Positive		Negative
$\Psi(\uparrow\downarrow\uparrow\downarrow\uparrow)$	$\longrightarrow$	$\Psi(\downarrow\uparrow\uparrow\downarrow\uparrow)$
$\Psi(\downarrow\uparrow\uparrow\uparrow\downarrow)$	$\longrightarrow$	$\Psi(\uparrow\downarrow\uparrow\uparrow\downarrow)$
$\Psi(\uparrow\uparrow\downarrow\uparrow\downarrow)$	$\longrightarrow$	$\Psi(\uparrow\uparrow\uparrow\downarrow\downarrow)$

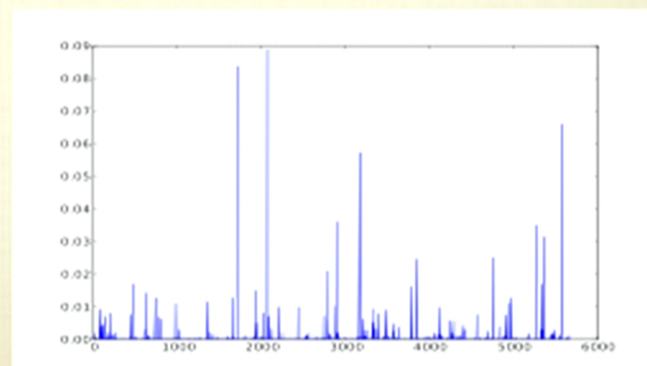
Quantify by

$$\sum_{\langle ij \rangle \in s} 1/2 \frac{\langle s'_{ij} | \Psi \rangle}{\langle s \, | \Psi \rangle} \text{ if } s_i \neq s_j$$

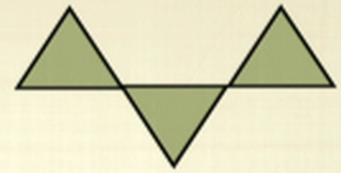
NODES MATTER!

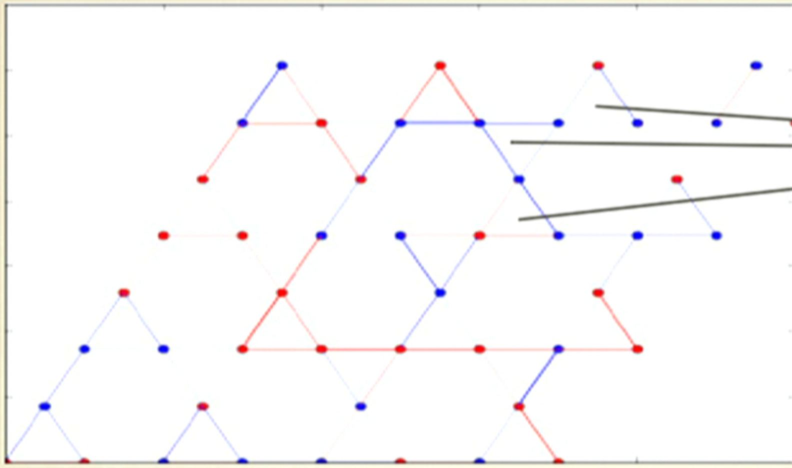
$$\Psi(s_1, s_2, \ldots s_n) > 0$$
$$\Psi(s_1, s_2, \ldots s_n) = 0$$
$$\Psi(s_1, s_2, \ldots s_n) < 0$$



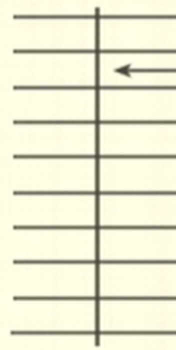


The Kagome





Fluxes "like" Dirac Spin Liquid



$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$

Site Asymmetry: 0.03

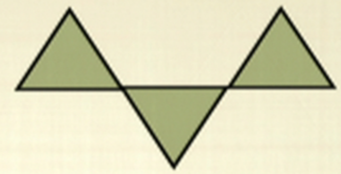
Bond Asymmetry: 0.012

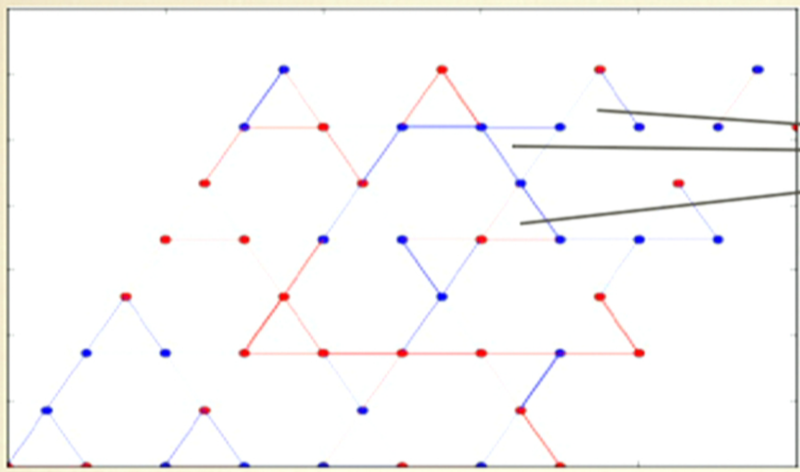
Very Tiny Asymmetry

Optimized By:

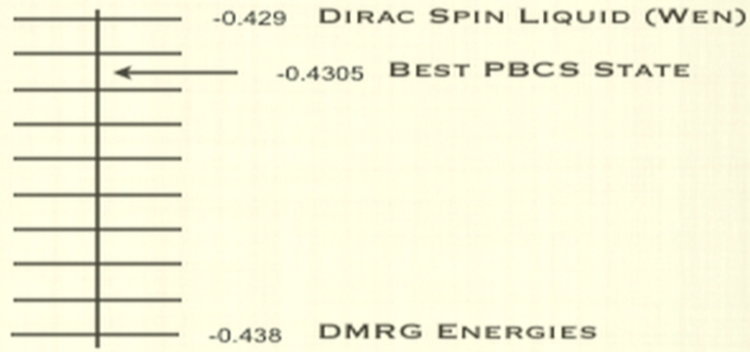
- Pairing Function Opt.
- Starting from Each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

The Kagome





Fluxes "like" Dirac Spin Liquid



$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$

Site Asymmetry: 0.03

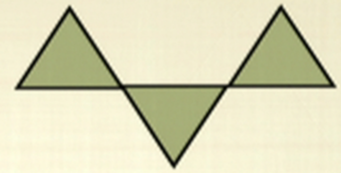
Bond Asymmetry: 0.012

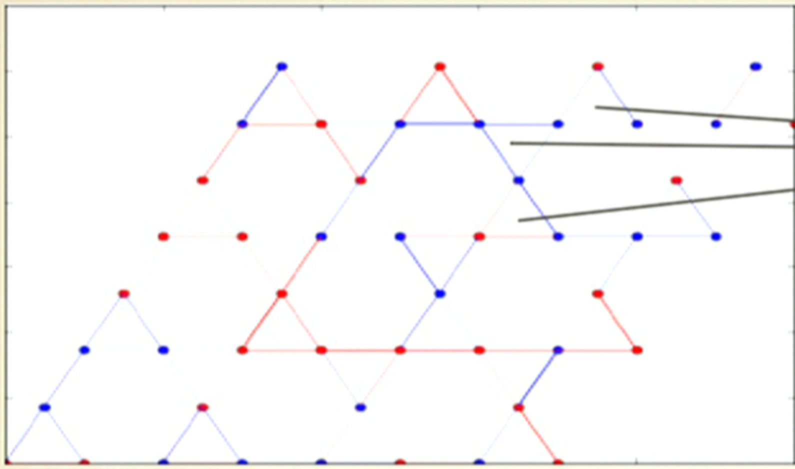
Very Tiny Asymmetry

Optimized by:

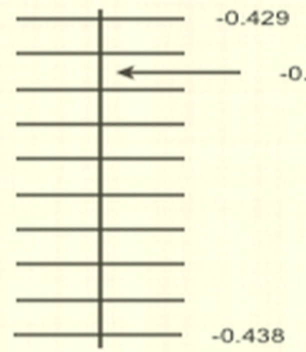
- Pairing Function Opt.
- Starting from Each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

The Kagome





Fluxes "like" Dirac Spin Liquid



$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$

Site Asymmetry: 0.03

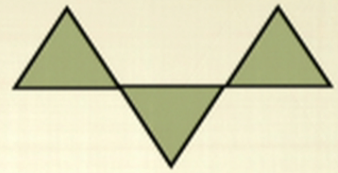
Bond Asymmetry: 0.012

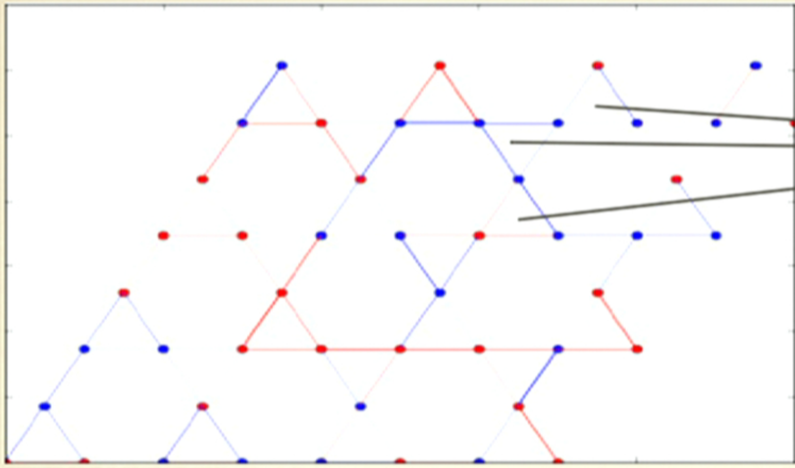
Very Tiny Asymmetry

Optimized by:

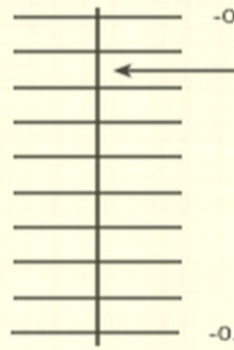
- Pairing Function Opt.
- Starting from Each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

The Kagome





Fluxes "like" Dirac Spin Liquid



$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$

Site Asymmetry: 0.03

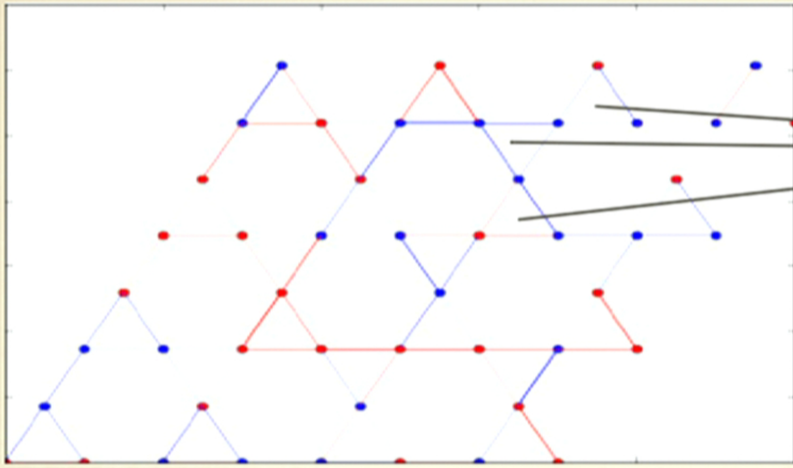
Bond Asymmetry: 0.012

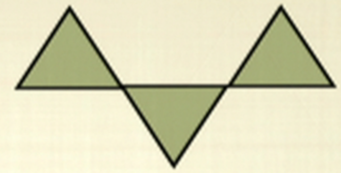
Very Tiny Asymmetry

Optimized by:

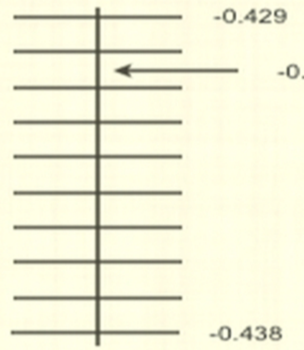
- Pairing Function Opt.
- Starting from each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

The Kagome





Fluxes "like" Dirac Spin Liquid



$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$

Site Asymmetry: 0.03

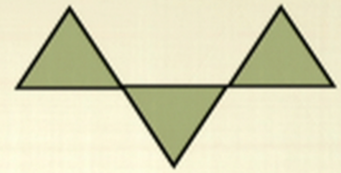
Bond Asymmetry: 0.012

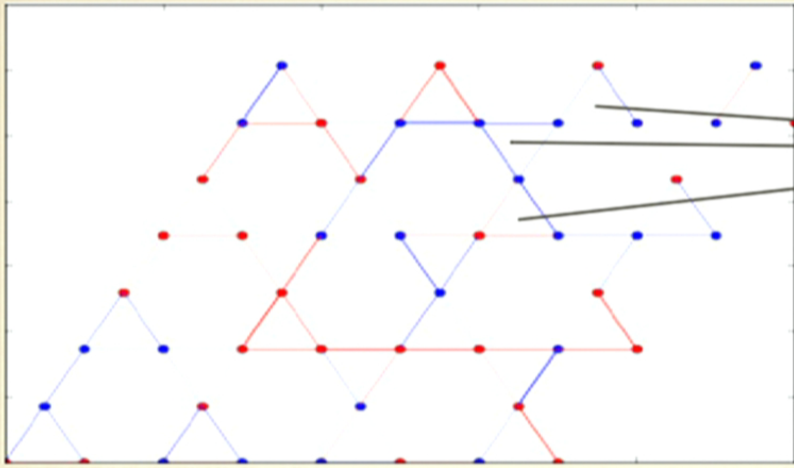
Very Tiny Asymmetry

Optimized By:

- Pairing Function Opt.
- Starting from each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

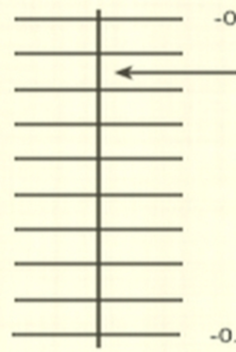
The Kagome





Fluxes "like" Dirac Spin Liquid

$$|\rho_{ij}| = \sqrt{\det \rho_{ij}}$$



Site Asymmetry: 0.03

Bond Asymmetry: 0.012

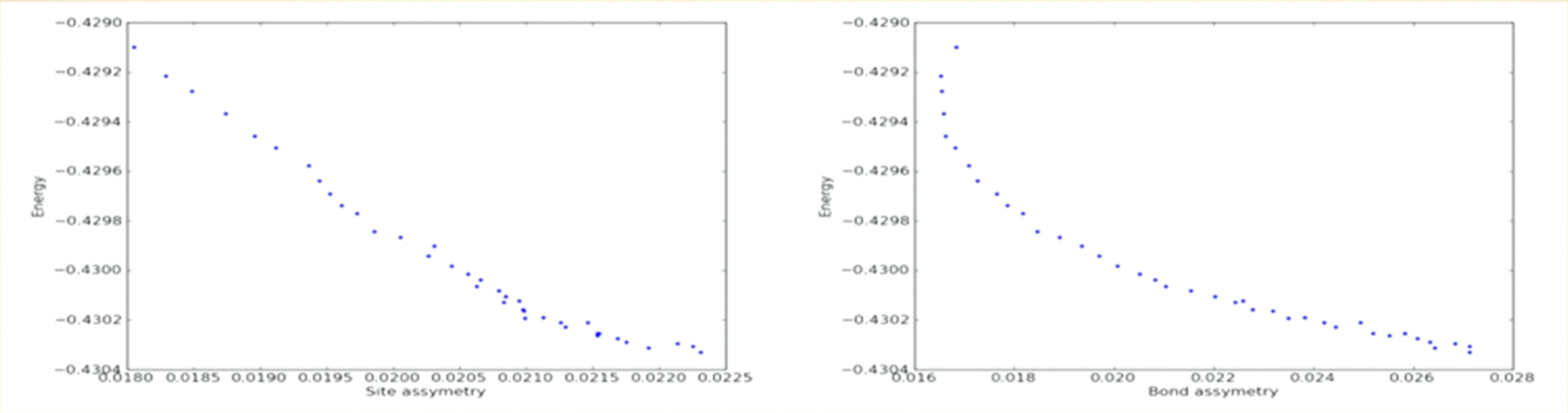
Very Tiny Asymmetry

Optimized by:

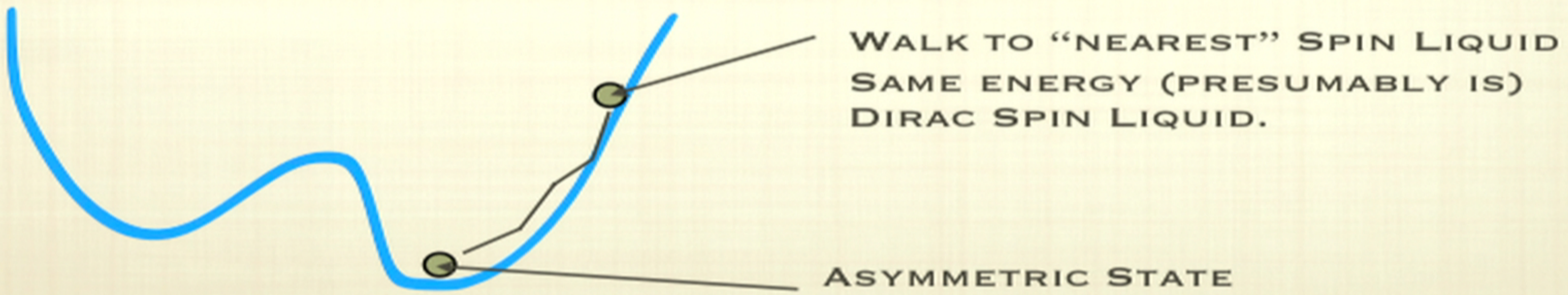
- Pairing Function Opt.
- Starting from each PSG
- With Stochastic Opt and Stochastic Reconfiguration.

Does the asymmetry really help?

I.

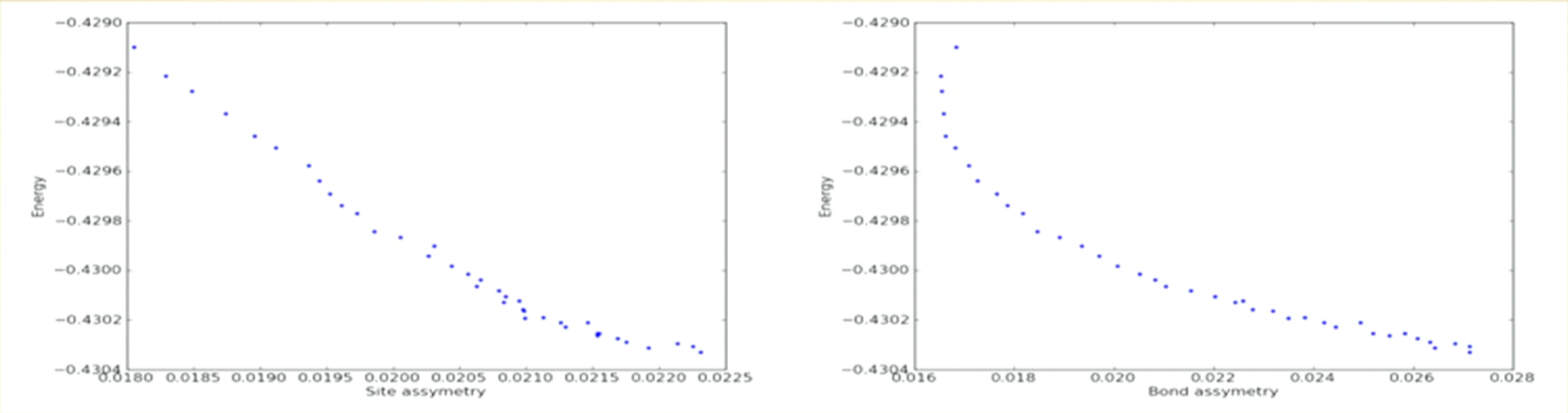


II.

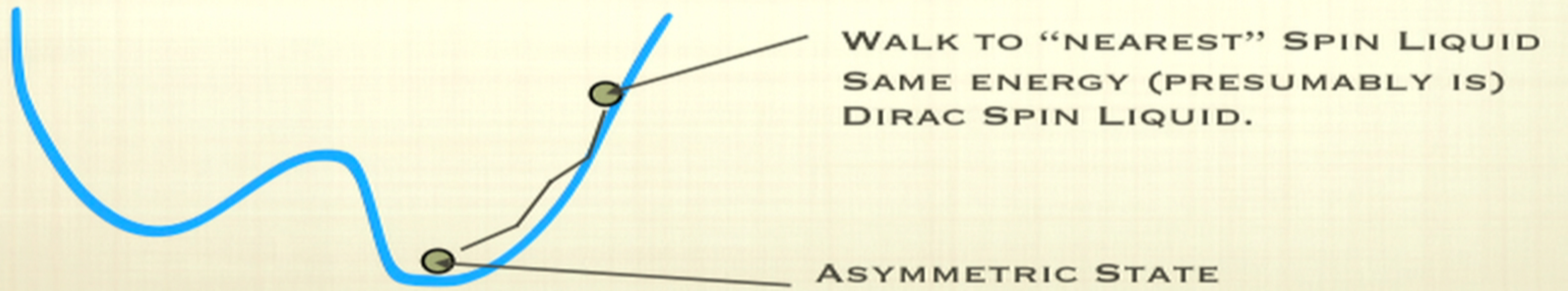


Does the asymmetry really help?

I.



II.

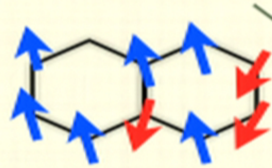
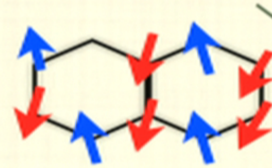


Right Long Wavelength Physics?

Energy is high because short range tension?

$$\Psi \equiv \Psi_{\mathrm{HE}}\Psi_{\mathrm{PBCS}}$$

Huse-Elser (EPS or CPS)

$$|\Psi\rangle = \alpha_1 \Big|$$

$$\Big\rangle + \alpha_2 \Big|$$

$$\Big\rangle$$

$$|\Psi\rangle = \sum_{n_1 n_2 \ldots n_k} \alpha^{n_1 n_2 \ldots n_k} |n_1 n_2 \ldots n_k\rangle$$

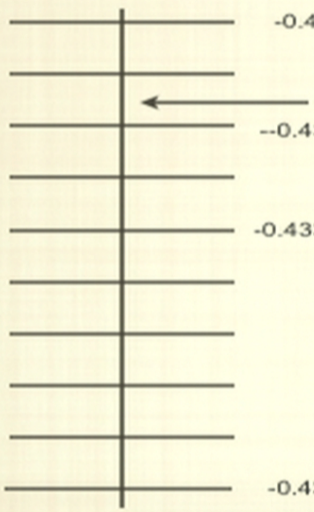
$$\alpha^{n_1 n_2 \ldots n_k} = \alpha^{n_1 n_2} \alpha^{n_1 n_3} \ldots \alpha^{n_2 n_k} \ldots \alpha^{n_{k-1} n_k}$$

$$\alpha^{n_i n_j} = \underline{f(\vec{r}_i - \vec{r}_j)}$$

These are the parameters. Optimize this.

Right Long Wavelength Physics?

Maybe if you just use the PBCS for the nodal structure?



A Theoretical Disconnect

MPS ⟷ PBCS

How do we Bridge this Disconnect?

<u>One idea:</u>

$$\Psi = \sum_k \alpha_k \det M_k$$

$$M_k^{ij} = \phi_{j[k]}(r_i)$$

A Complete Fermionic Basis

A Theoretical Disconnect

MPS ⟷ PBCS

How do we bridge this disconnect?

One idea:

$$\Psi = \sum_k \alpha_k \det M_k$$

$$M_k^{ij} = \phi_{j[k]}(r_i)$$

A Complete Fermionic Basis

The story so far...

The "canonical wave-functions" seem reasonable for the honeycomb but not the kagome. Something is missing theoretically.

Next: How would you approach this if you didn't want simple wave-functions?

FNDMC: Project out Excitations

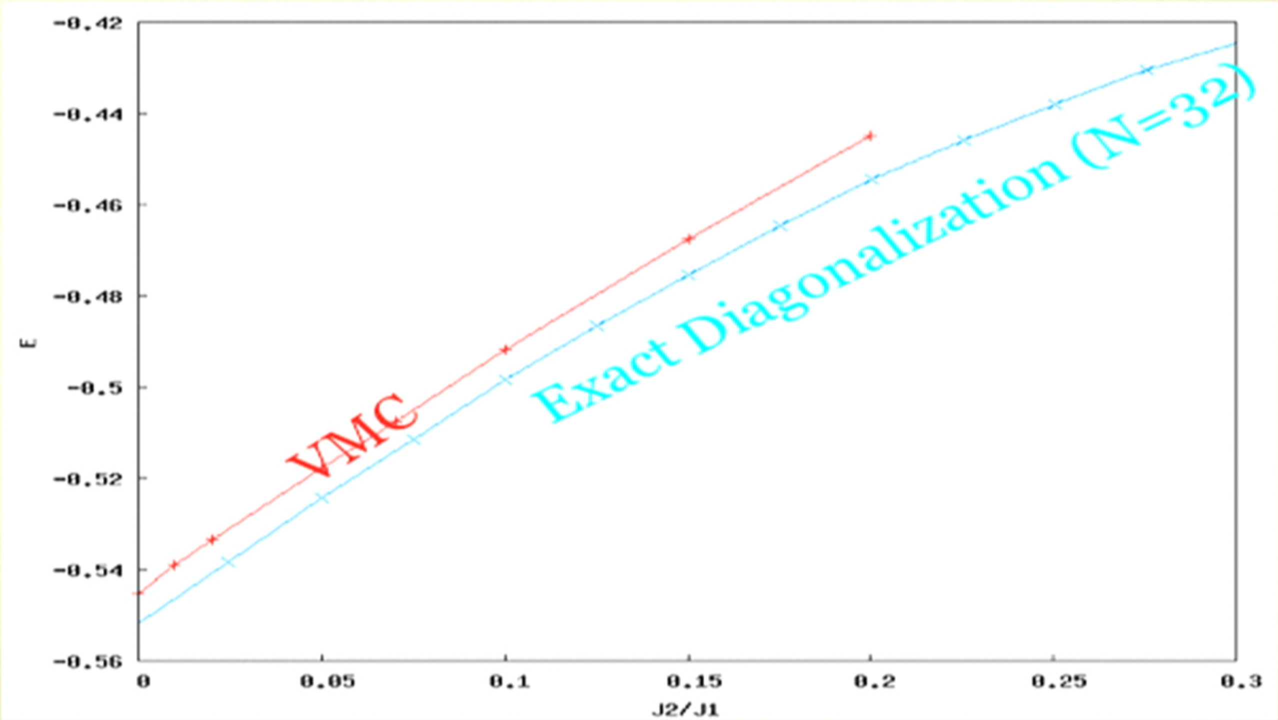
Let's compare against exact diagonalization (for small systems)

This example: H-E with pairs

$|\Psi_{\mathrm{HE}}\rangle$

Use a good variational guess to set the nodes.

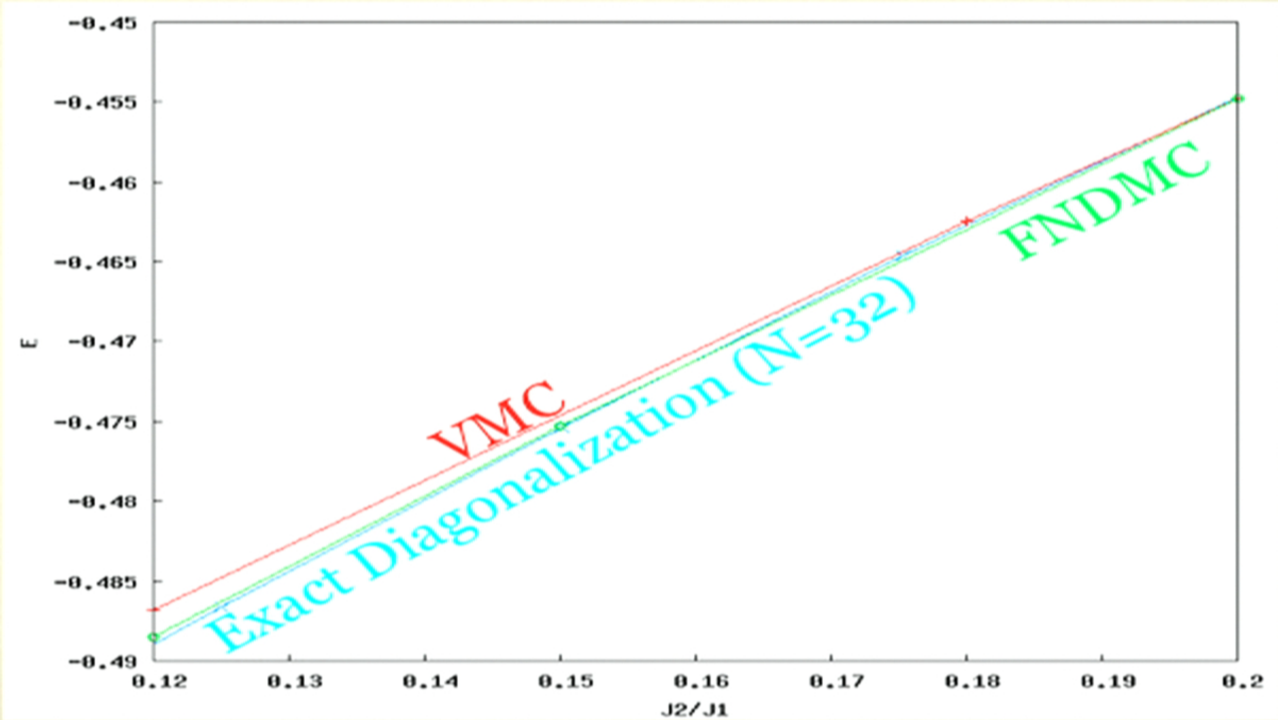
Nodes of Neel state entirely controlled by one and two body correlators



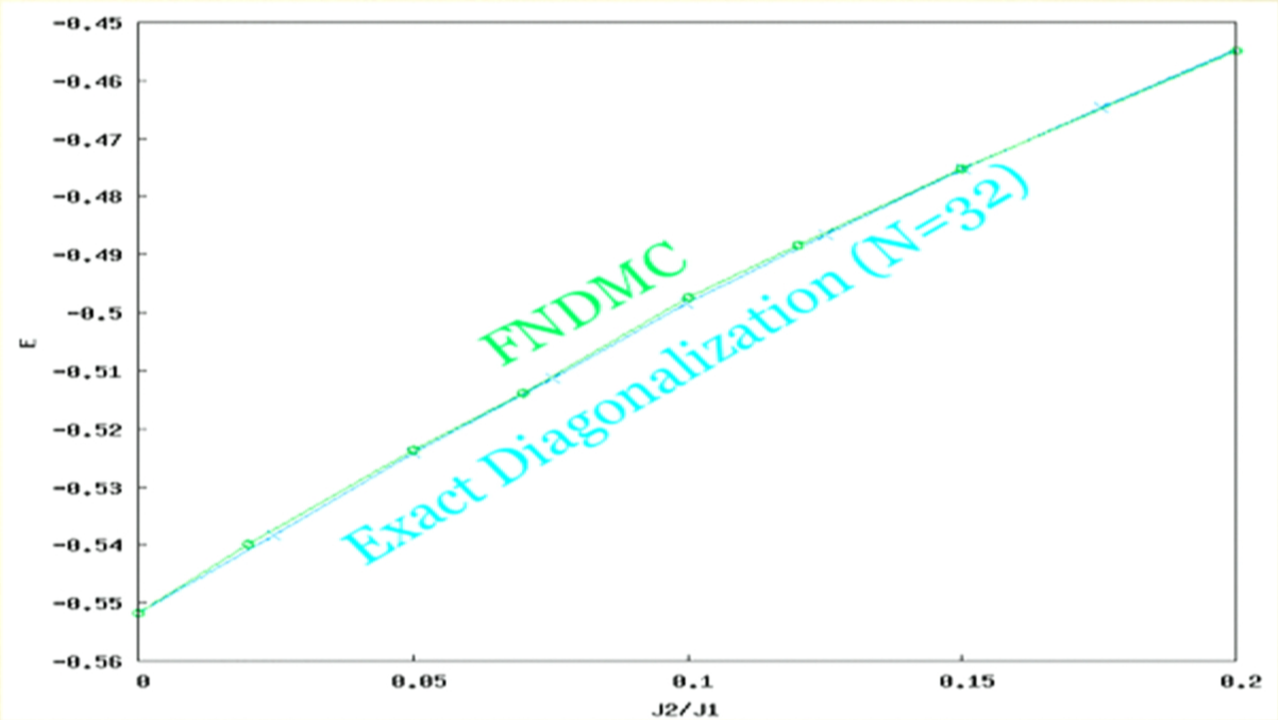
Cleaning up Larger J2/J1

AROUND J2/J1~0.12 THE PROJECTION OF THE HE VARIATIONAL ANSATZ GETS INACCURATE. NEED TO PROJECT WITH MORE SOPHISTICATED ANSATZ.

$$|\Psi_{\mathrm{PBCS}}\rangle|\Psi_{\mathrm{Neel}}\rangle$$



We are able to get quantitative accuracy close to exact diagonalization with a method whose cost scales polynomial in system size!



Other Work (A monte Carlo sampling)

- Supersolids + Superglasses
- Mesoscopic Phases
- Dynamics
  - Quantum Critical Exponents
  - Thermalization
- Method Development
  - Sign cancellation
  - O(N) Methods
  - PArticle-Hole Expansions

Conclusions

- Hubbard Honeycomb:
  - Topological Degenerate? No! (for small systems)
- Heisenberg Honeycomb:
  - Which spin liquid and why? "SPS" and because of nodes!
- Heisenberg Kagome:
  - Does the typical theoretical framework hold? Not really: In the analytically suggested variational subspace it's not even a spin liquid!