

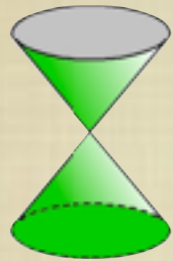
FROM THE HONEYCOMB TO THE KAGOME:
WHAT CAN WAVE-FUNCTIONS TEACH US
ABOUT SPIN LIQUIDS AND HOW TO GO BEYOND
THEM?

BRYAN CLARK, PRINCETON CENTER FOR
THEORETICAL SCIENCE

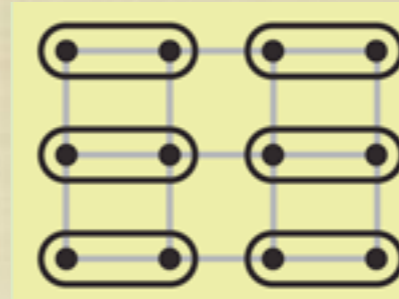
COLLABORATORS: DIMA ABANIN, SHIVAJI SONDHI, JESSE KINDER, ERIC NEUSCAMMAN,
MICHAEL LAWLER, GARNET CHAN

PERIMETER: DEC. 12, 2011

BORING PHASES*



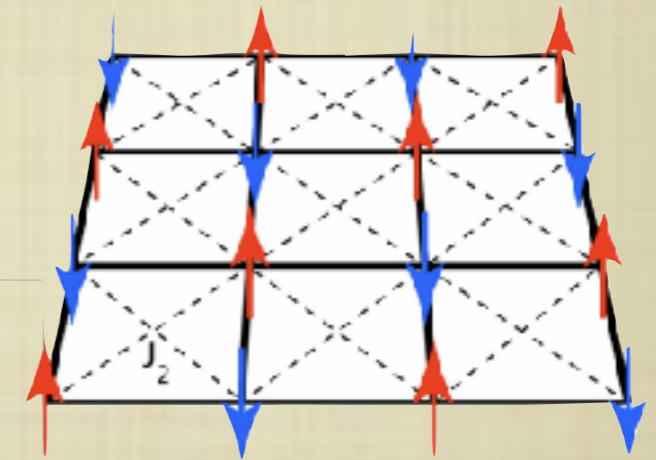
Semi-metal



Valence Bond Crystal



Spin liquid



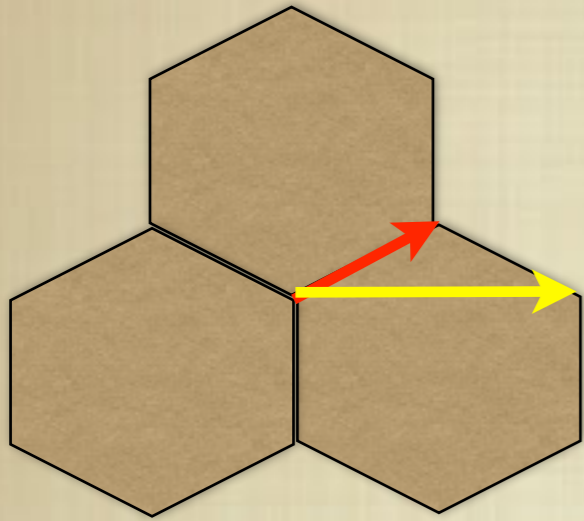
Neel State

* TECHNICAL TERM FOR PHASES WE THINK WE UNDERSTAND

THE TALE OF 3 SPIN LIQUIDS...

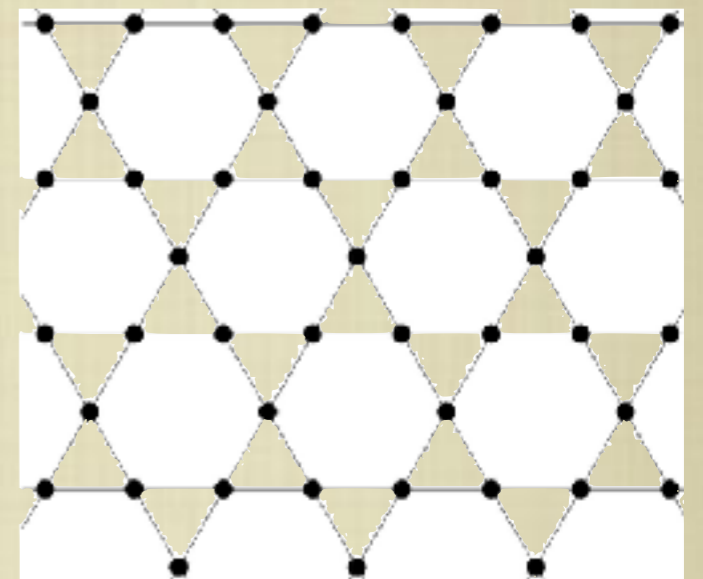
HEISENBERG MODEL:

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



HONEYCOMB

KAGOME



YAN, WHITE, HUSE

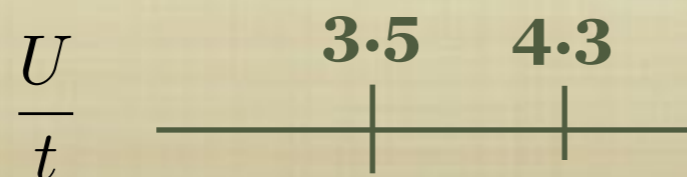
START HERE



HUBBARD MODEL:

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

MENG, ET. AL



WHY STUDY SPIN LIQUIDS

Recent experimental evidence.

herbertsmithite

volborthite

vesignieite

$\text{Na}_4\text{Ir}_3\text{O}_8$

$\text{EtMe}_3\text{Sb}[\text{Pd}(\text{dmit})_2]_2$

Possible ground state of simple model.

Relevance to high T_c

Topological Order

Not described by Fermi Liquid Theory nor Landau Theory for Phase Transitions.

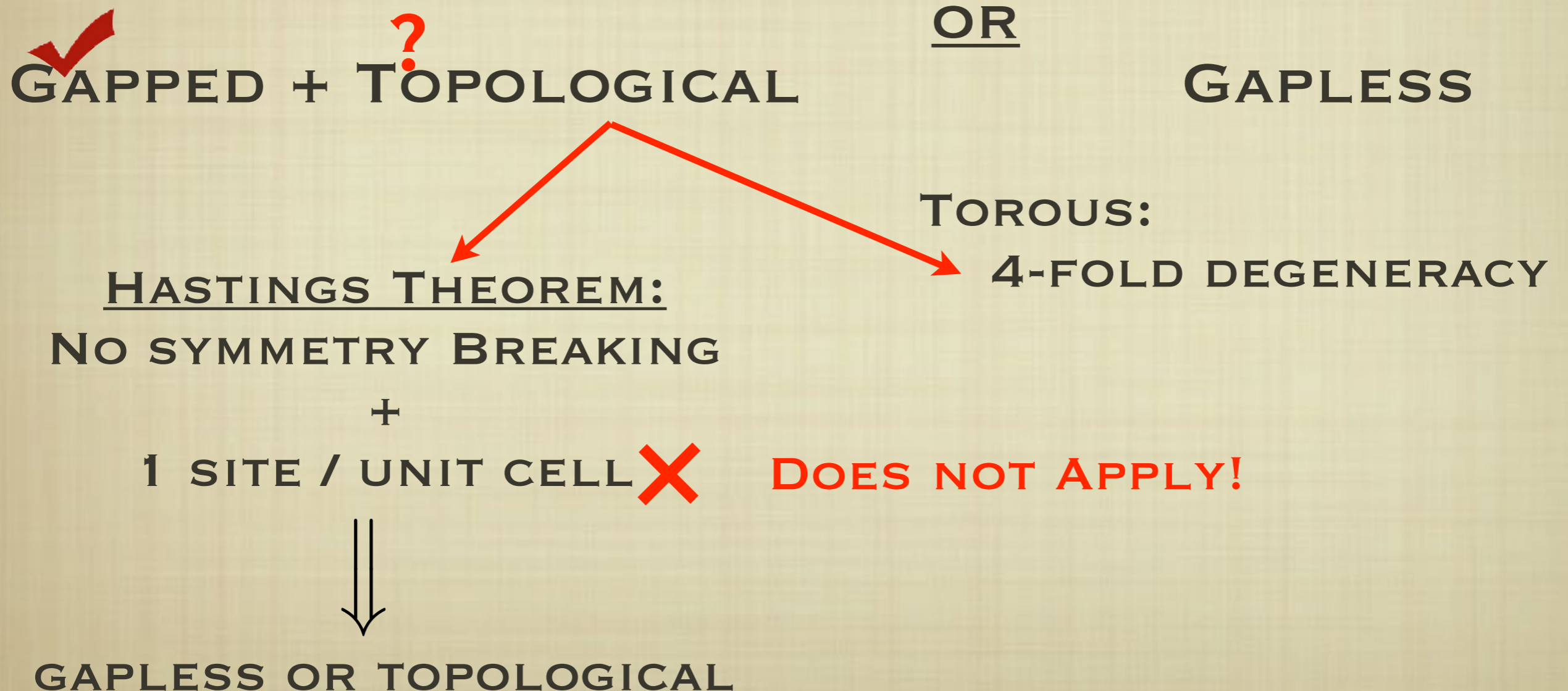
SPIN LIQUIDS

~~BLACK HOLES~~ HAVE NO HAIR



- NO MAGNETIC ORDER
- NO LOCAL ORDER PARAMETERS
- NO SYMMETRY BREAKING

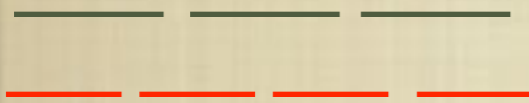
MAKES IT HARD TO IDENTIFY AND LEARN ANYTHING ABOUT.



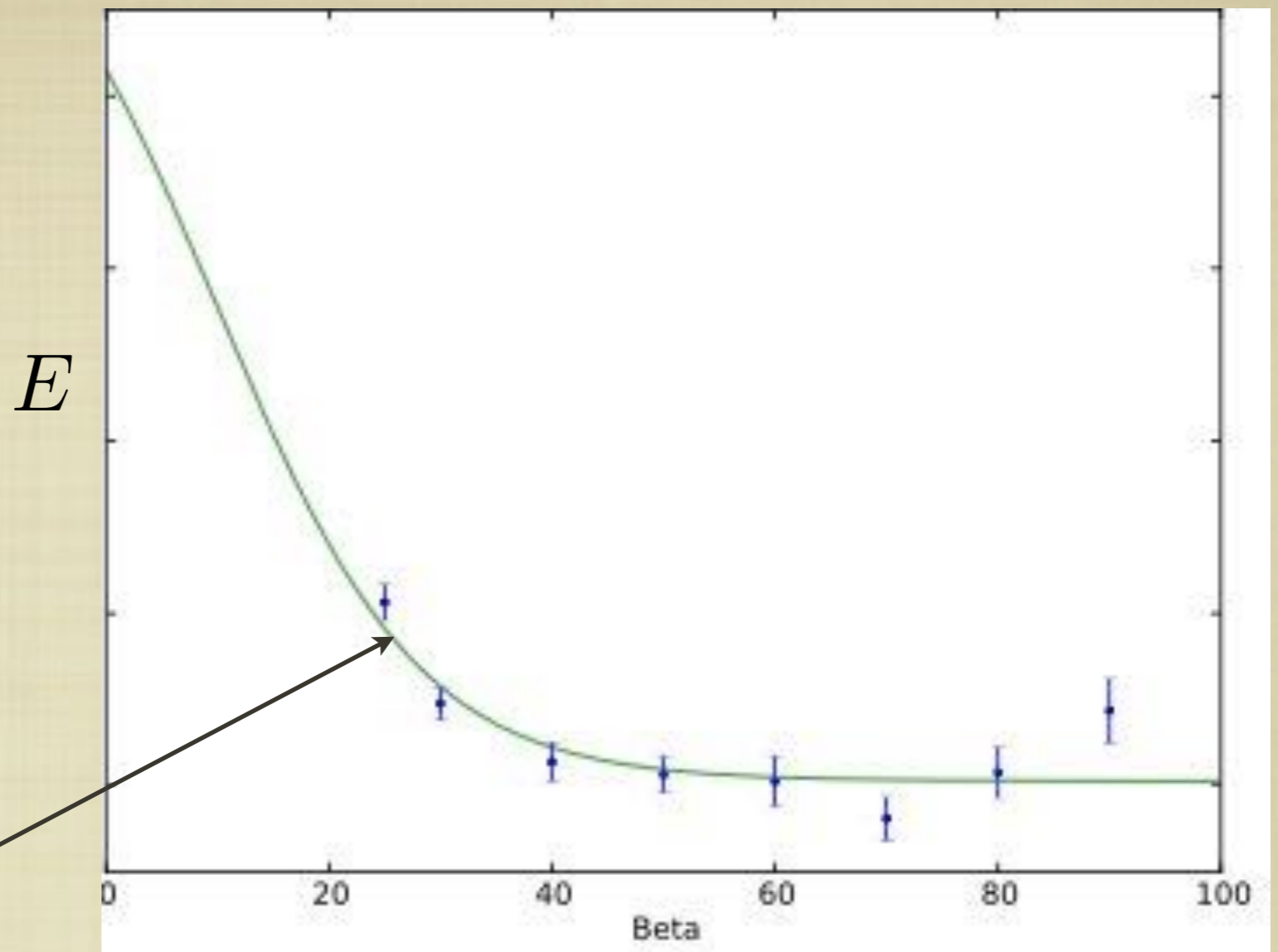
WE'LL ALWAYS HAVE QMC

Spectra:

$$N = \infty$$



$N = \text{'large'}$



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:

$$N = \infty$$

—

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

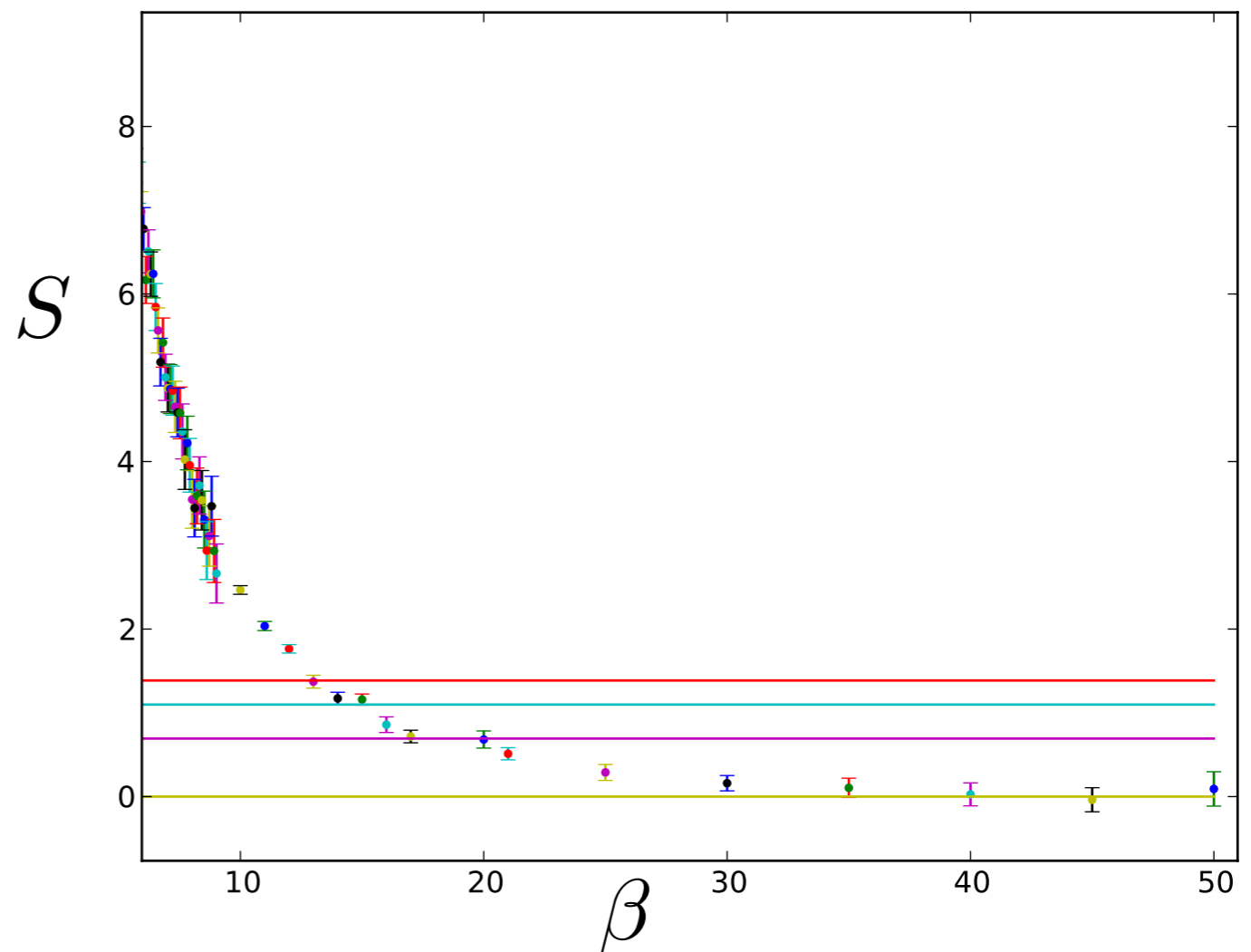
$$N = \text{'large'}$$

—

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

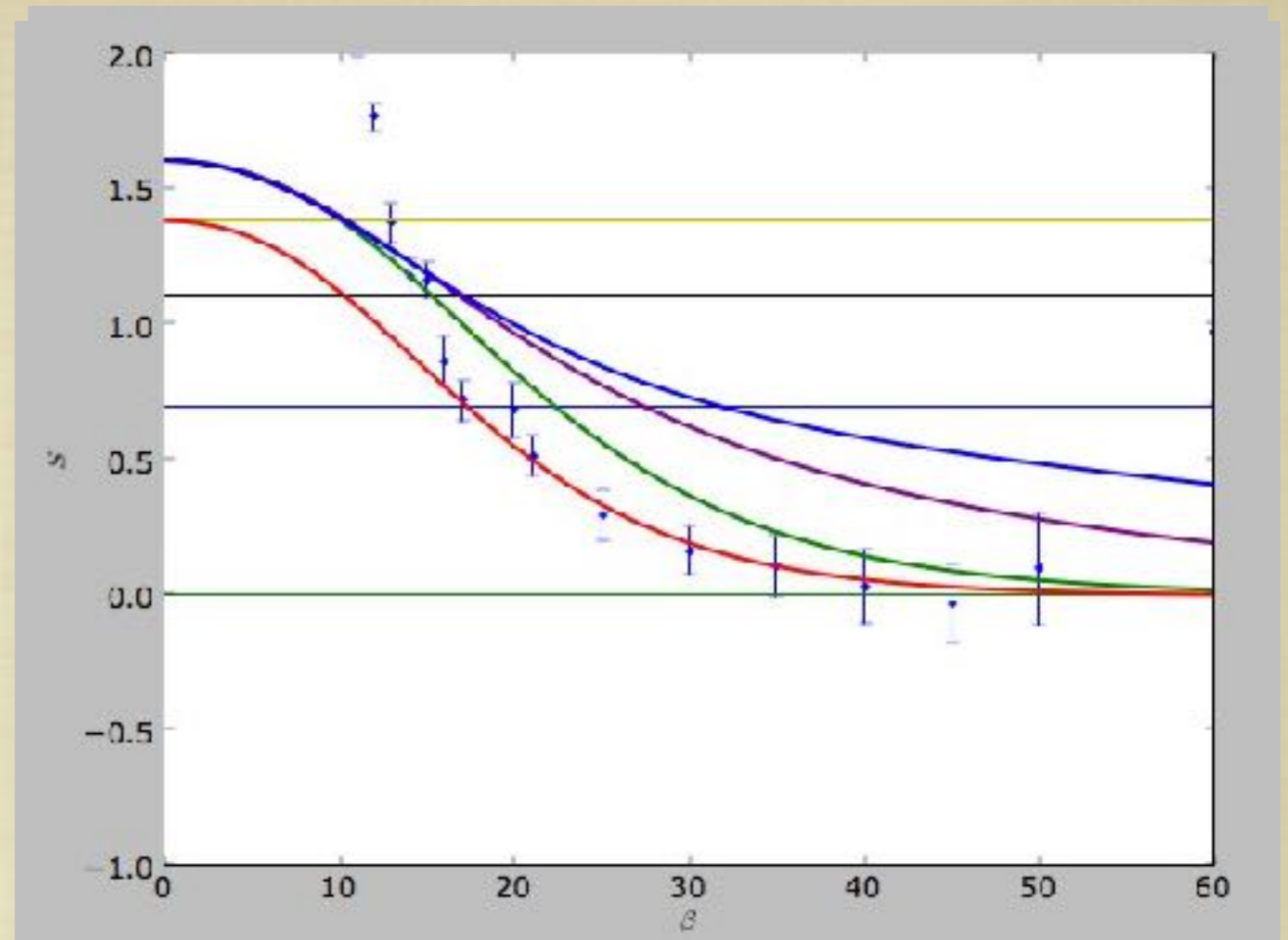
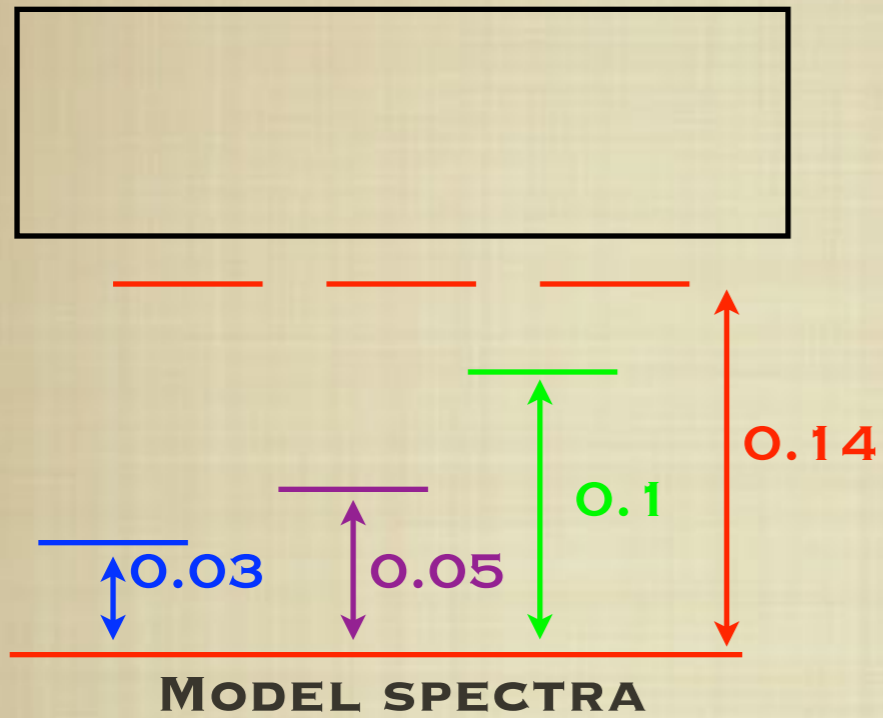
≡≡≡

$$S(0) = 0$$



CAN WE QUANTIFY THIS?

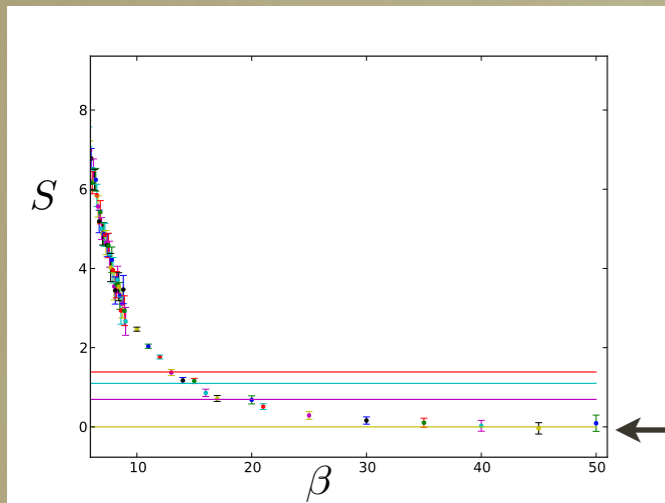
QUANTIFICATION



6x6 SYSTEM

■ NO WAY TO FIX THIS SPECTRA!

YOUR QMC IS MISSING A STATE!



I.

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 $\text{LOG}(2)$ FOR ANY T !

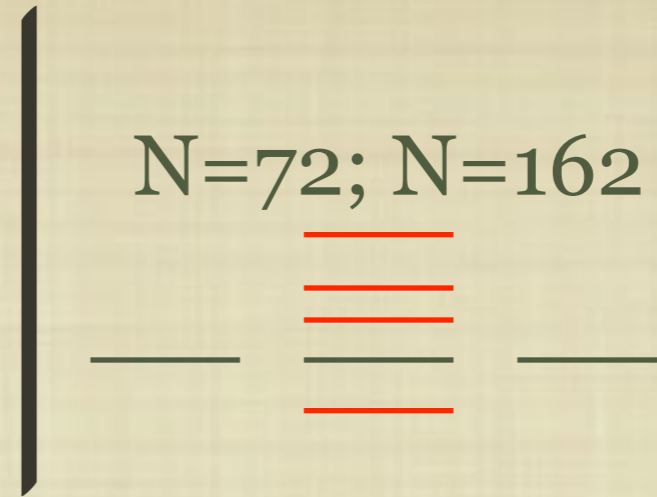
WHAT ABOUT MY SPIN LIQUID?

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.



OTHER

SOME GAP IS OFF?

THE EXOTIC POSSIBILITY:

THIS ISN'T A SPIN LIQUID!

BUT ... THERE IS NO SYMMETRY BREAKING

A NE 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

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

“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

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

LEARN THINGS BY PROBING CORRELATIONS:

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

RVB

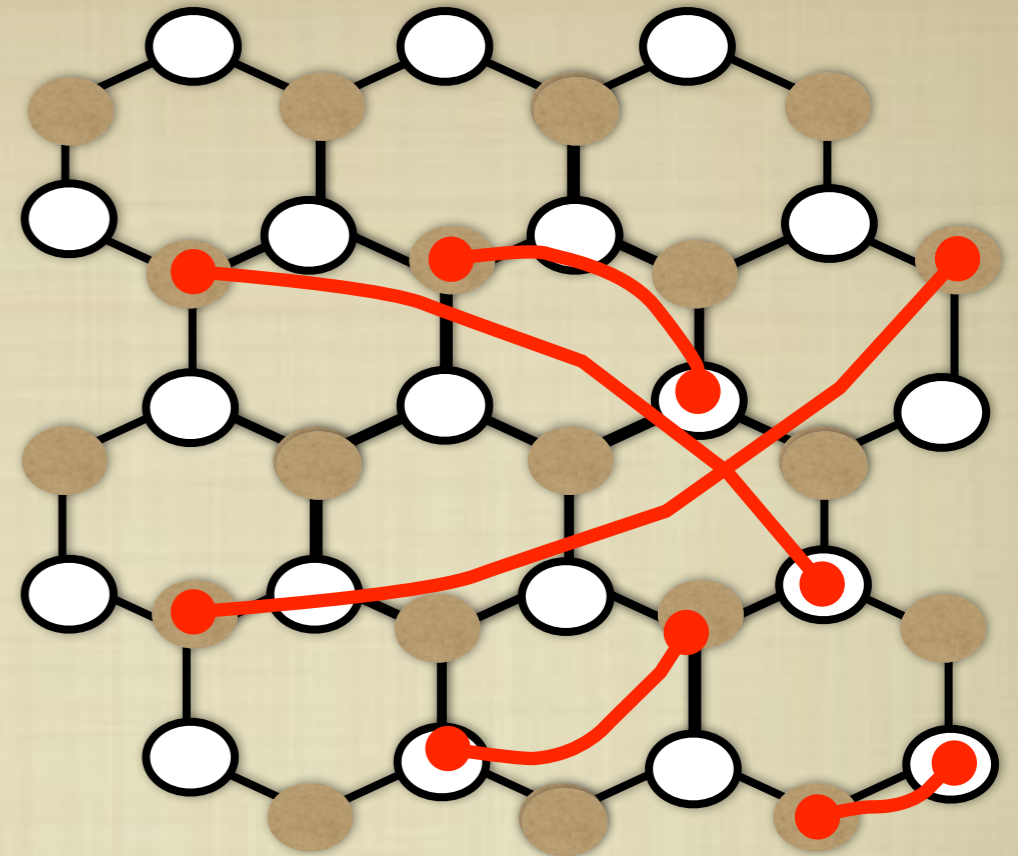
RVB wave functions

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

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.

Note: Only showing some of the dimers



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 $S_i = \frac{1}{2} f_{i\alpha} \vec{\sigma}_{\alpha\beta} f_{i\beta}$ $f_{i\alpha}^\dagger f_{i\alpha} = 1$ $f_{i\alpha} f_{i\beta} \epsilon_{\alpha\beta} = 0$

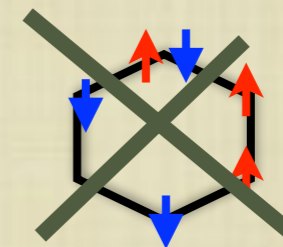
$$H_F = -t \sum_{\langle i,j \rangle, s} f_{is}^\dagger f_{js} + \sum_{ij} \Delta_{ij} (f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger) + h.c.$$

Solve mean field Hamiltonian and implement constraint by projection.

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

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

Project out double and zero occupancy.



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

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.

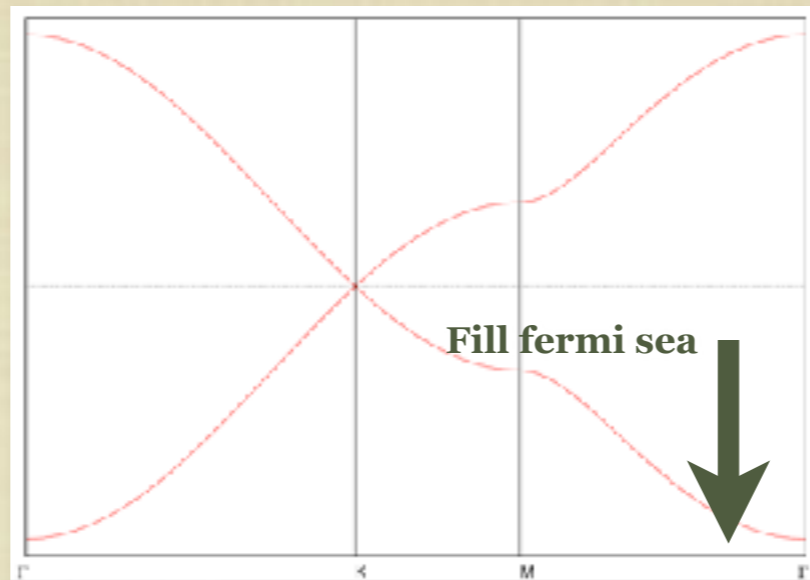
$$H_F = -t \sum_{\langle i,j \rangle, s} f_{is}^\dagger f_{js}$$

Solve mean field and project.

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

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

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



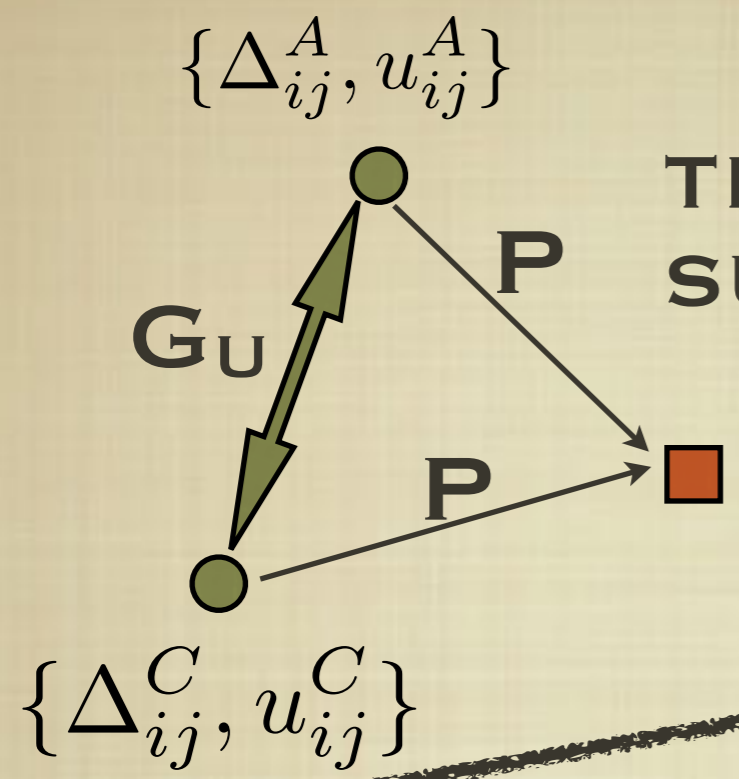
Projected Gutzwiller: $P \Psi_{\text{gutz}}$

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

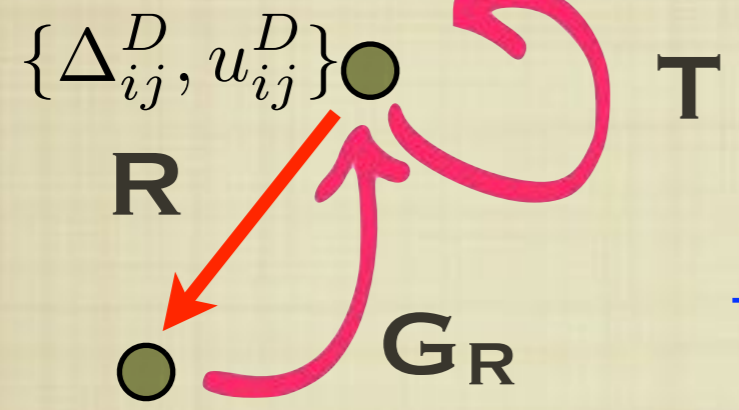
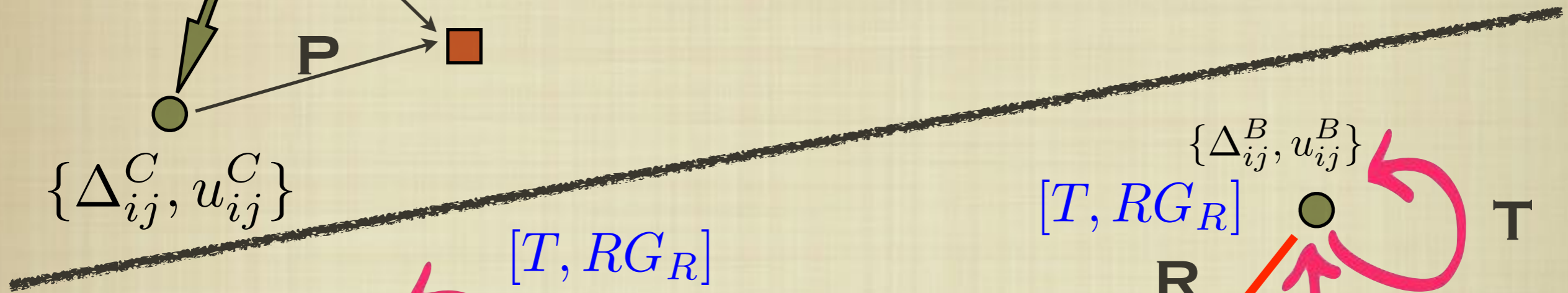
Zero parameter wave function!

FACT I: 2 MEAN FIELD \rightarrow 1 SPIN WF

PSG



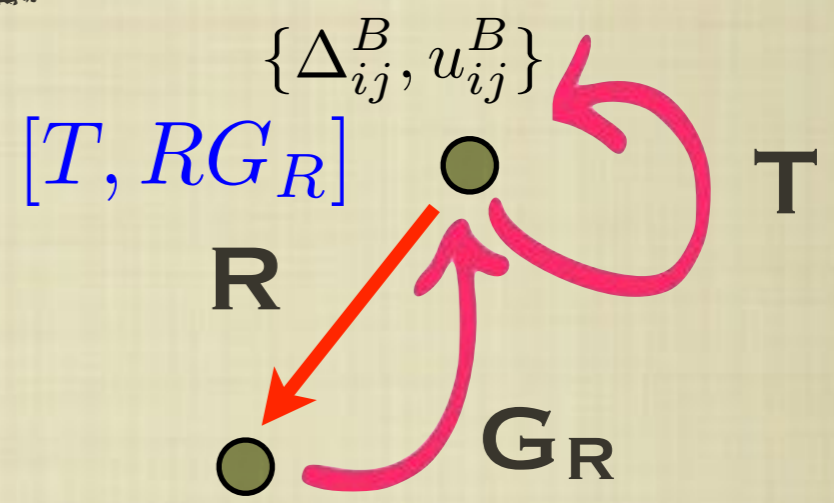
THESE 2 STATES RELATED BY LOCAL SU(2) GAUGE TRANSFORMATION



$[T, RG_R]$

[T, RG_R] PHASE

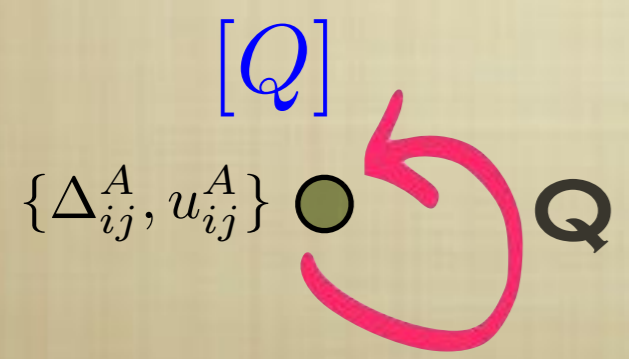
$$\begin{aligned} &\{\Delta_{ij}^D, u_{ij}^D\} \\ &\{\Delta_{ij}^B, u_{ij}^B\} \end{aligned}$$



$[T, RG_R]$

[Q] PHASE

$$\{\Delta_{ij}^A, u_{ij}^A\}$$



$[Q]$

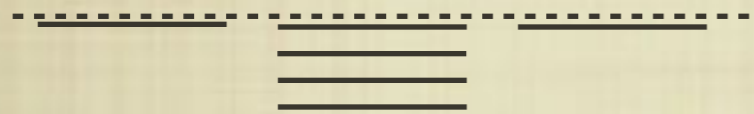
DEGENERACY AT THE MEAN FIELD

(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 FERM SEA?

PARTICULARLY BAD IN THE KAGOME WHERE SOMETIMES YOU HAVE MACROSCOPIC DEGENERACY!

TYPICAL SOLUTION: GIVE UP!

SOLUTION:

INSTEAD OF OPTIMIZING THE MEAN FIELD PARAMETERS OF H,
OPTIMIZE $\Phi(R, R')$ DIRECTLY

$\sim N^2$ PARAMETERS

$$\frac{\partial E}{\partial \phi} = \dots$$

SOLUTIONS BEGAT PROBLEMS

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

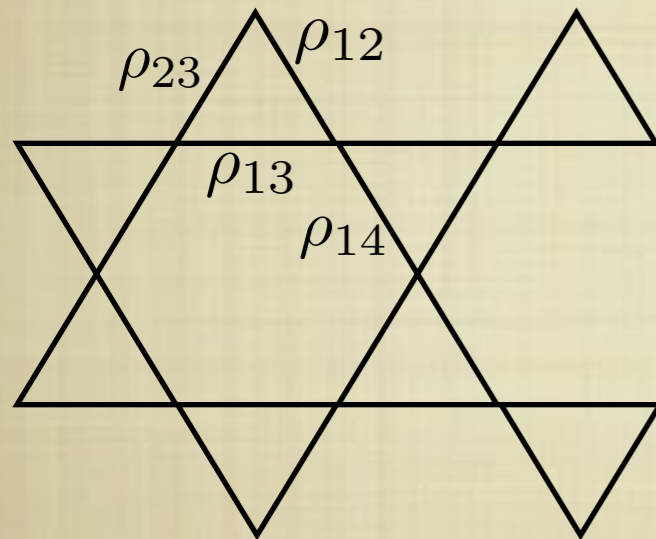
$$\Phi[i, j] = \begin{bmatrix} 0.2 & 0.2 & 1.4 \\ 0.2 & 4.2 & 3.3 \\ 1.4 & 3.3 & 0.3 \end{bmatrix}$$

AM I A SPIN LIQUID?

WHICH ONE?

ANOMALOUS DENSITY MATRIX

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



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

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

IF A SPIN LIQUID, ALL BONDS ARE IDENTICAL

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

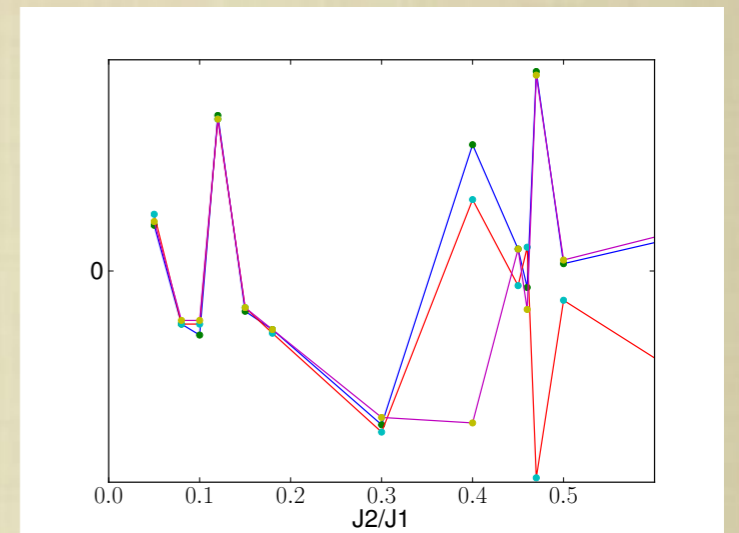
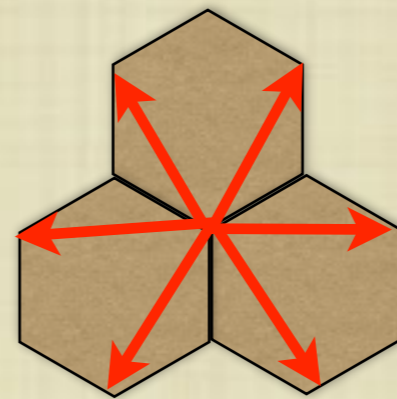
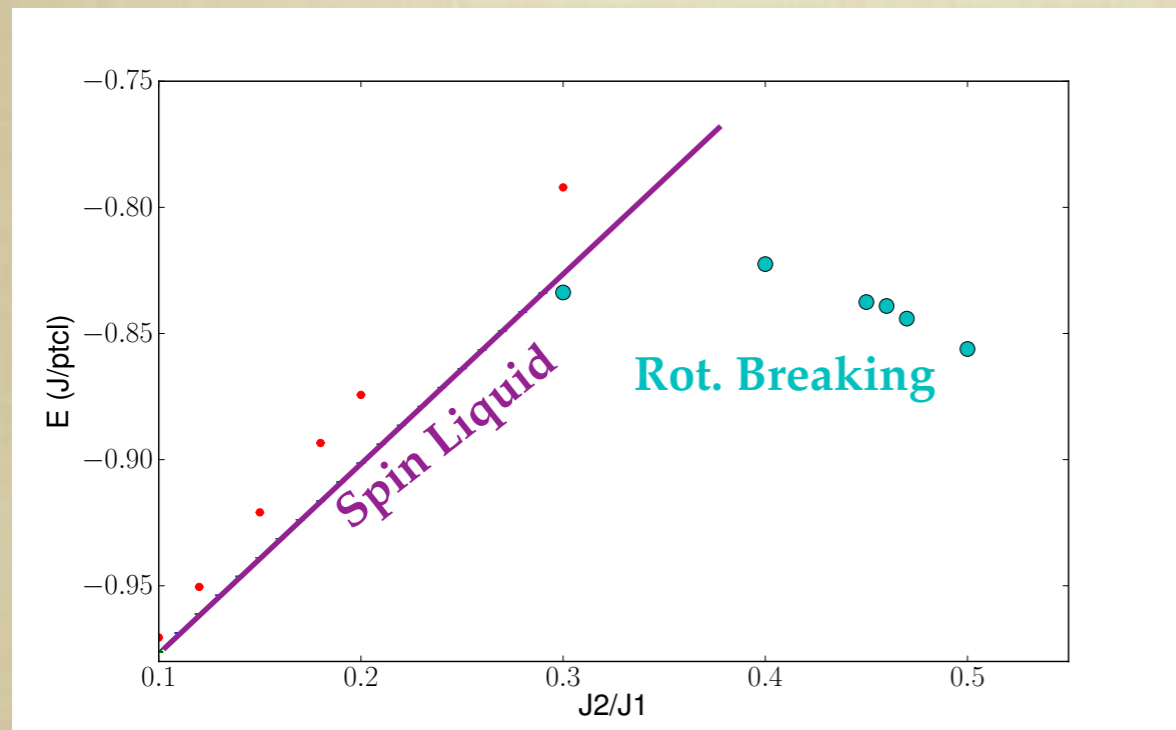
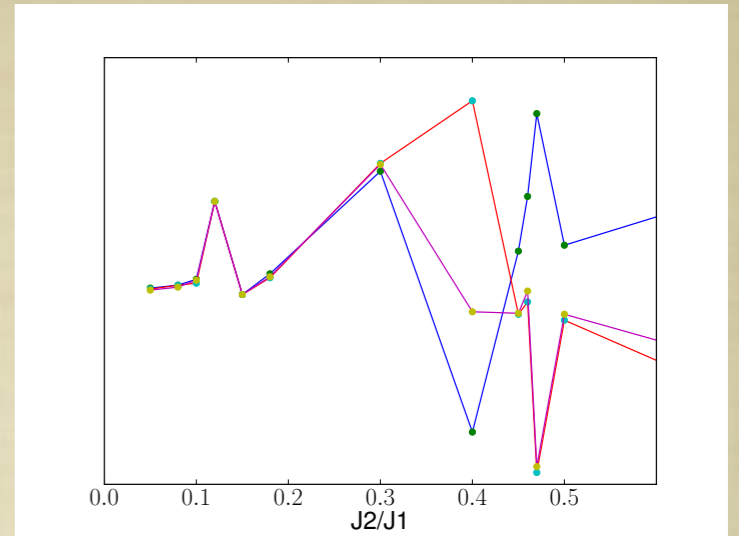
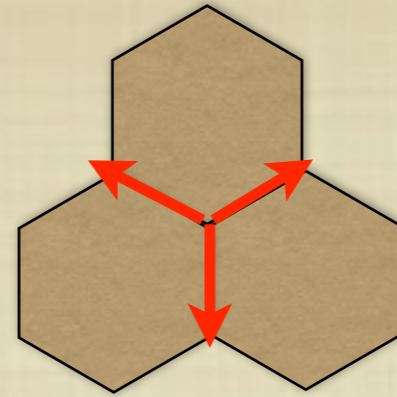
$$\phi_{ijk\dots l} = i^{N_{\text{loop}}} W_{ij} \cdot W_{jk} \cdot \dots \cdot W_{li}$$

$$\theta = 2\arccos((\text{Tr}\Phi_{ijk\dots l})/2)$$

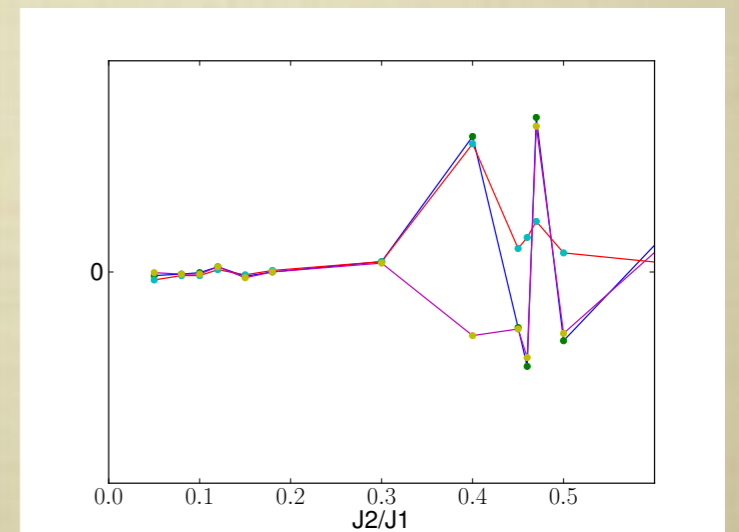
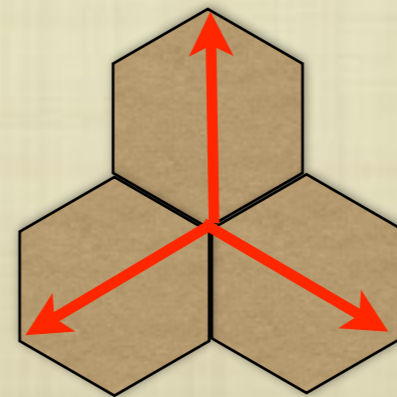
DIFFERENT SPIN LIQUIDS
HAVE DIFFERENT FLUXES

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:

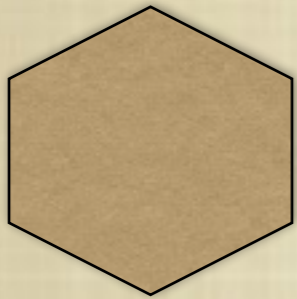
Am I a spin liquid characterized by the typical theoretical lore?

and

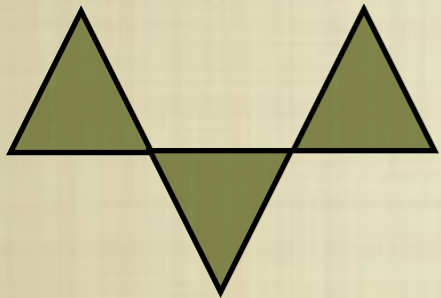
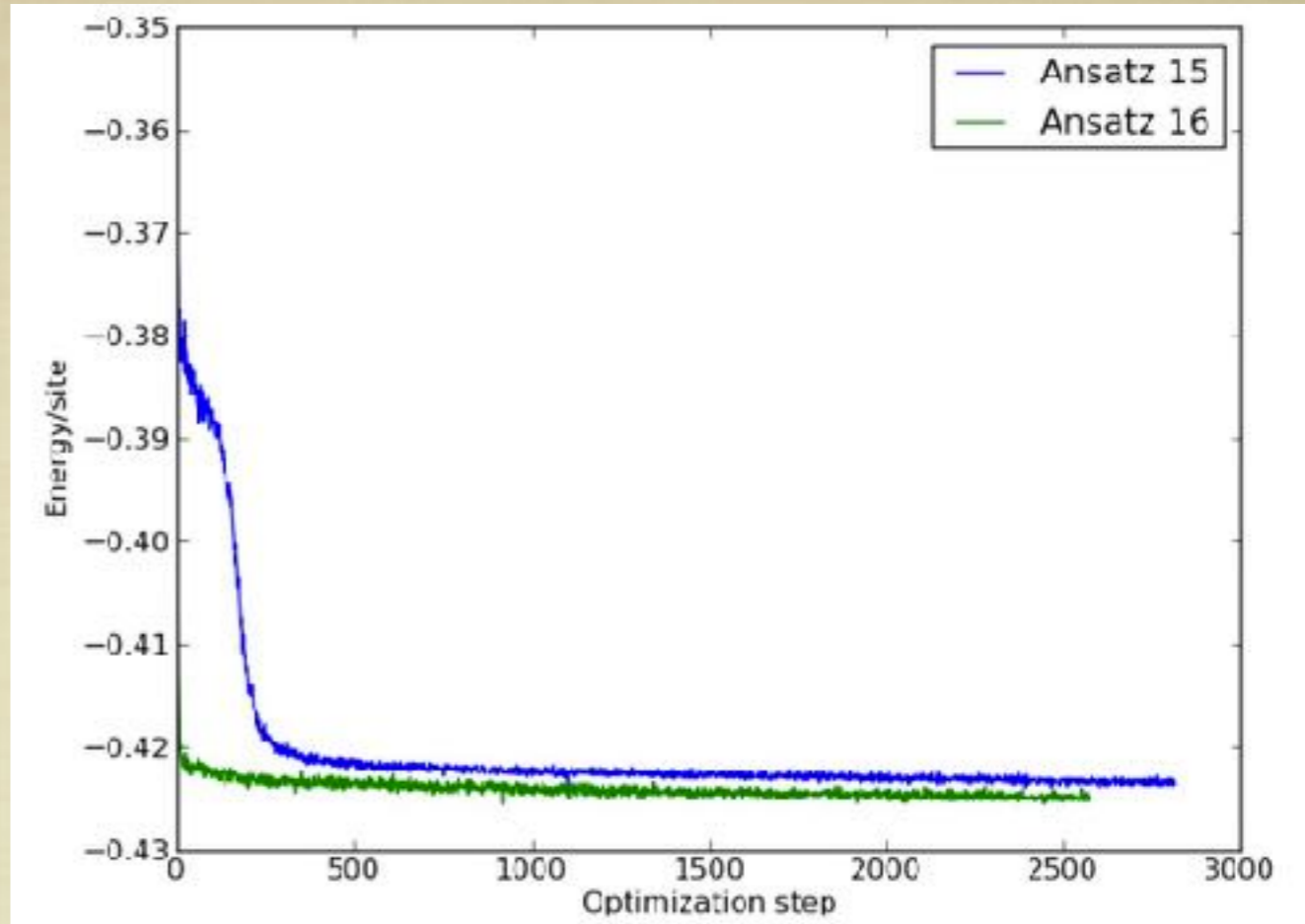
if so, which one am I?

SEARCHING FOR THE BEST PBCS

AND THE WINNER
(AMONGST PBCS) IS ...

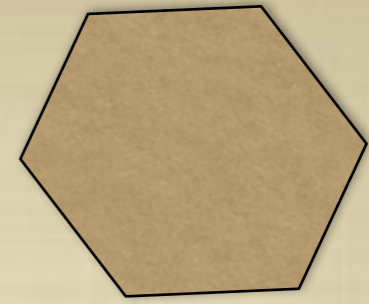


A SPIN LIQUID



NOT A SPIN LIQUID (SLIGHTLY)

THE HONEYCOMB

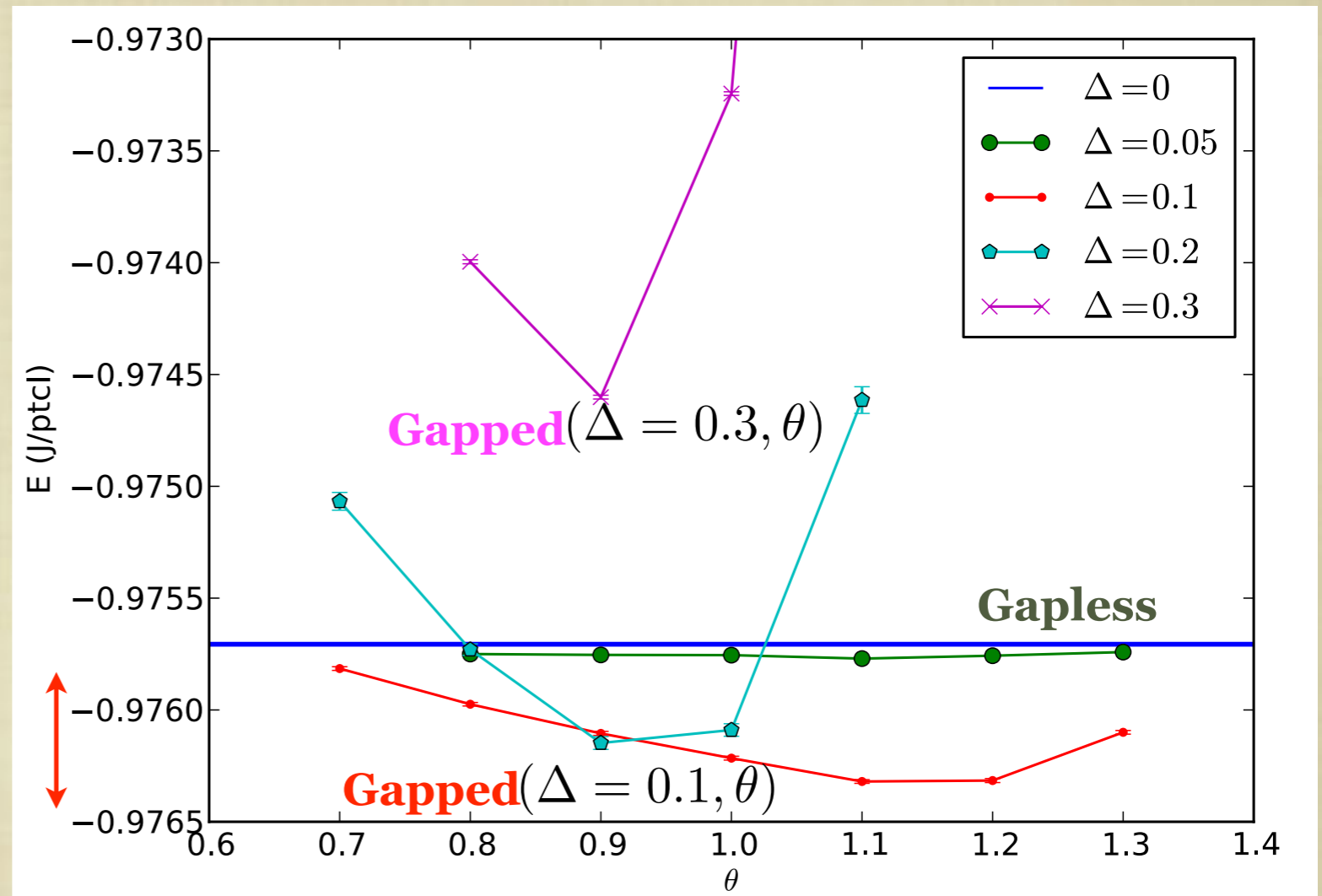
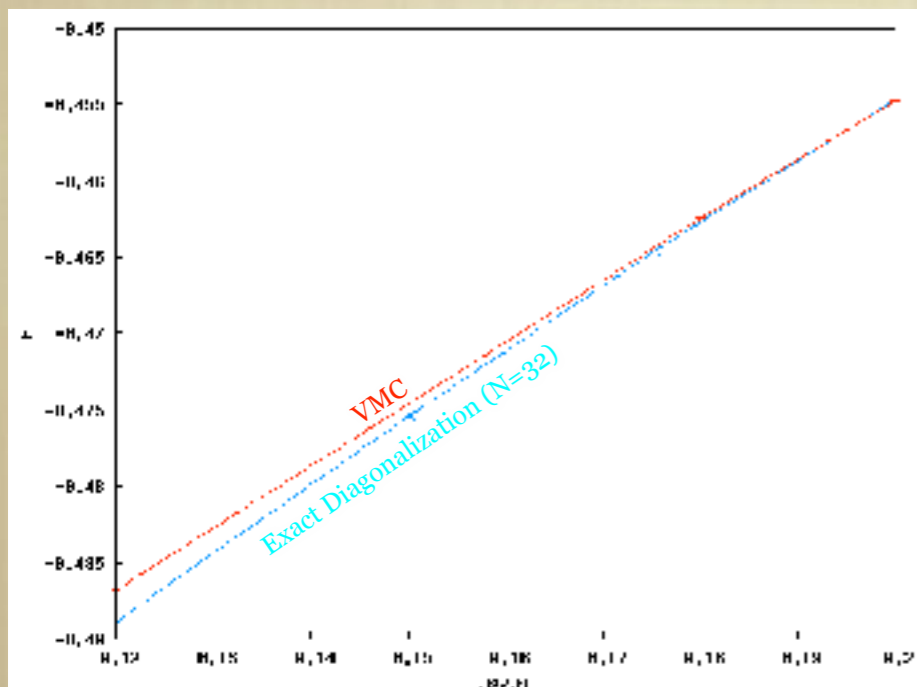


sps (Lu and Ran)

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

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

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



OPTIMIZED BY:

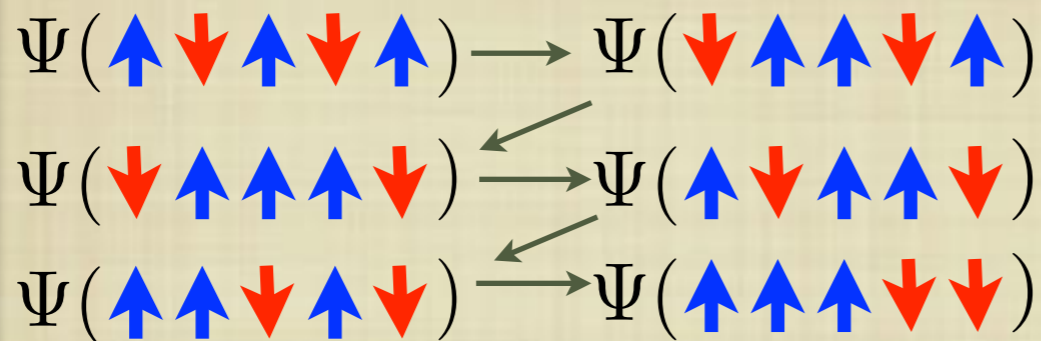
- PAIRING FUNCTION OPT.
- SEARCHING OVER SUGGESTED HAMILTONIANS

WHY ME?

J1 Nodes set by Marshall Sign Rule

Positive

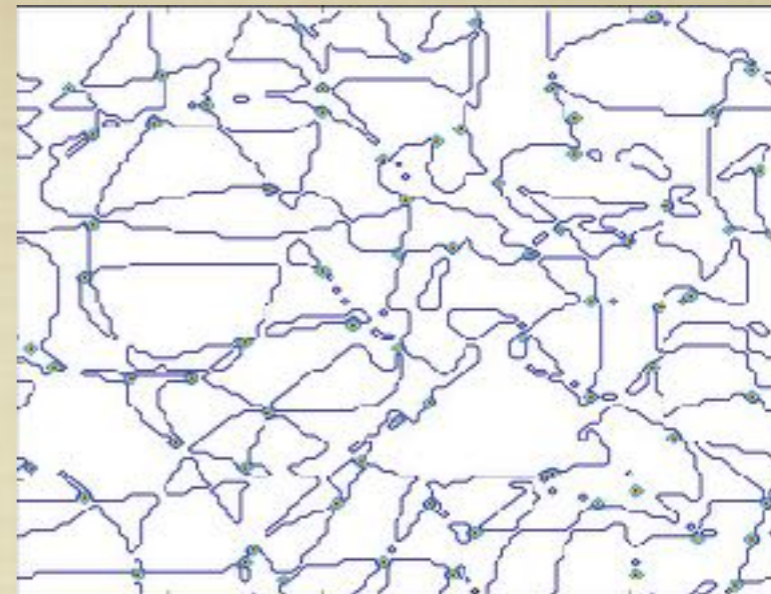
Negative



Quantify by

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

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

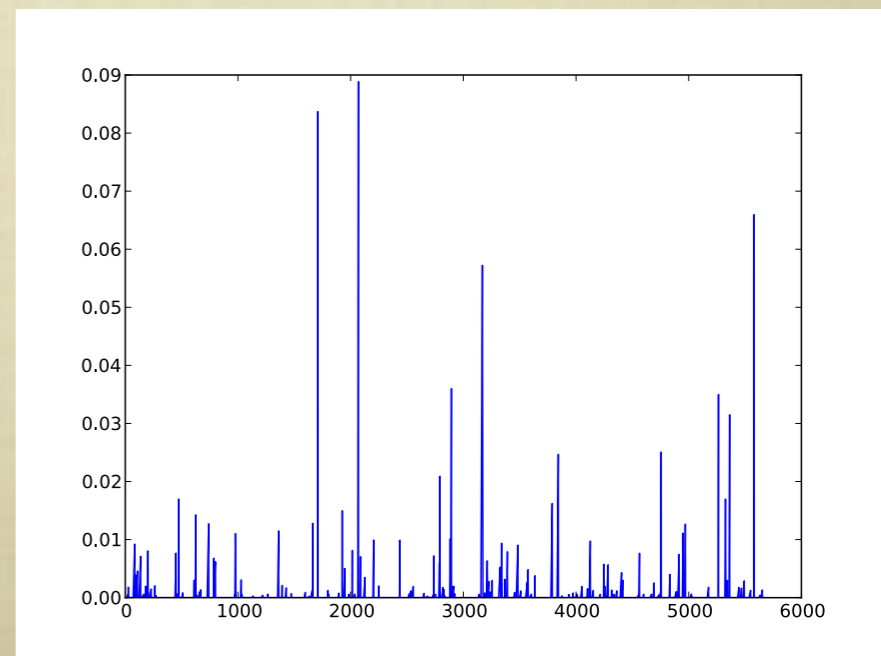
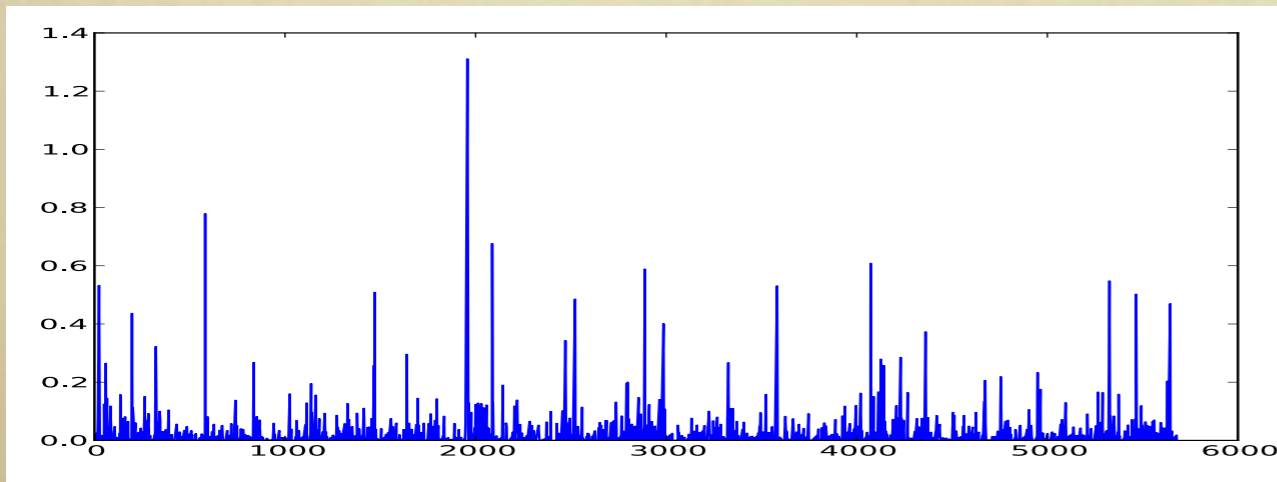


NODES MATTER!

$$\Psi(s_1, s_2, \dots, s_n) > 0$$

$$\Psi(s_1, s_2, \dots, s_n) = 0$$

$$\Psi(s_1, s_2, \dots, s_n) < 0$$

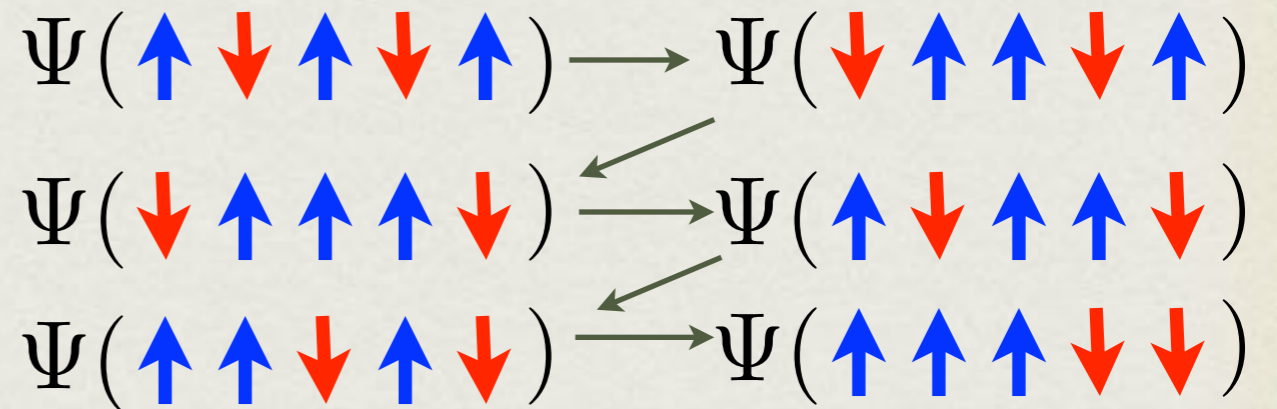


Marshall Sign

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

Positive sign

Negative sign



Any wf that minimizes the ground state energy of H (on a bipartite lattice), has the sign structure as above.

$$\langle E \rangle = \langle \Psi | H | \Psi \rangle = \sum_s \langle \Psi | s \rangle \langle s | H | \Psi \rangle = \sum_s |\langle \Psi | s \rangle|^2 \frac{\langle s | H | \Psi \rangle}{\langle s | \Psi \rangle}$$

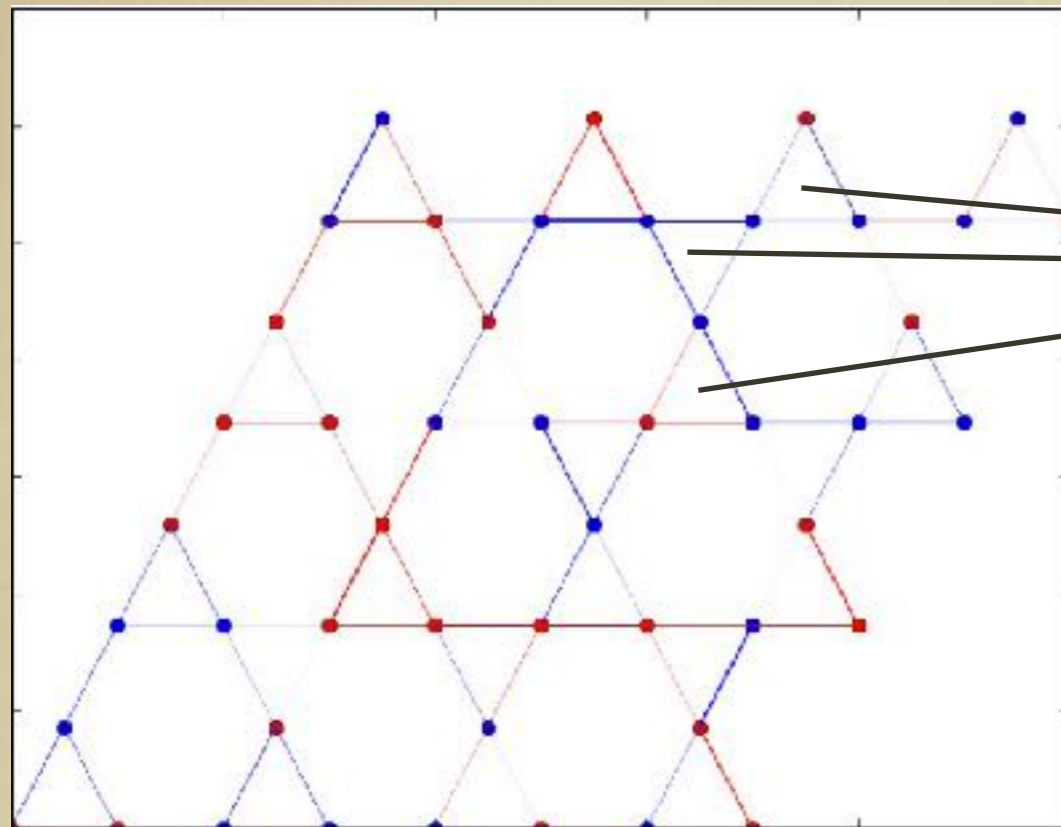
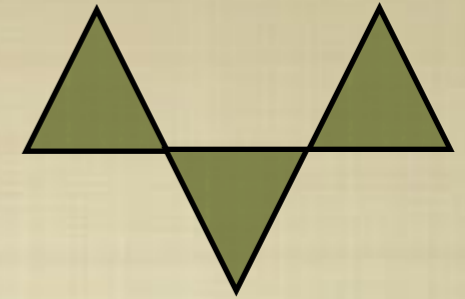
Let s'_{ij} be s with spins i and j flipped.

$$\frac{\langle s | H | \Psi \rangle}{\langle s | \Psi \rangle} = \sum_{\langle ij \rangle \in s} \begin{cases} 1/4 & \text{if } s_i = s_j \\ -1/4 + 1/2 \frac{\langle s'_{ij} | \Psi \rangle}{\langle s | \Psi \rangle} & \text{if } s_i \neq s_j \end{cases}$$

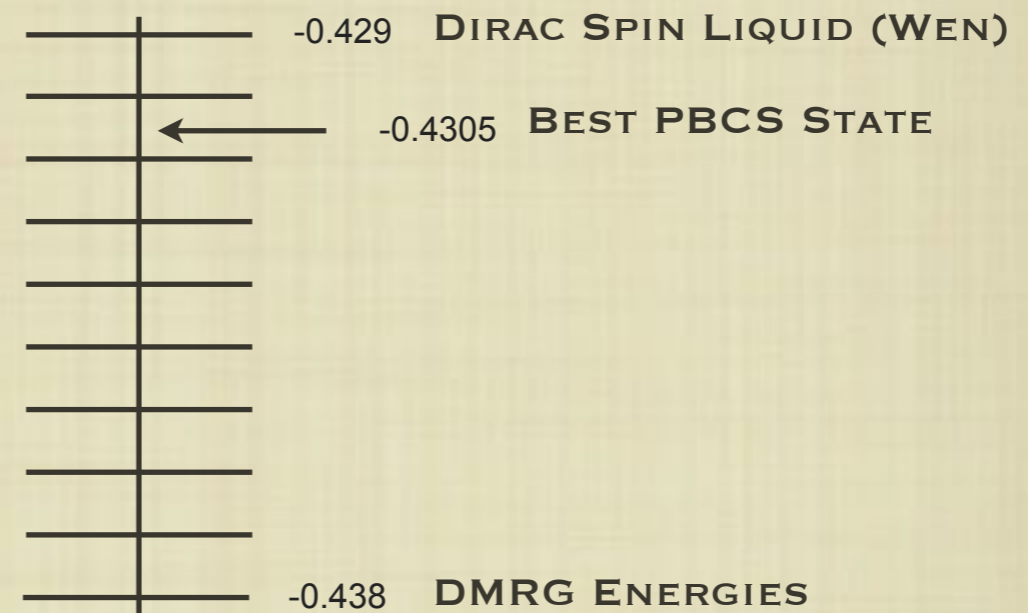
If we can choose the sign of Ψ so this is always negative, this is the best we can do.

Even with J_2 , this minimizes the J_1 energy.

THE KAGOME



FLUXES "LIKE" DIRAC SPIN LIQUID



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

SITE ASYMMETRY: 0.03

BOND ASYMMETRY: 0.012

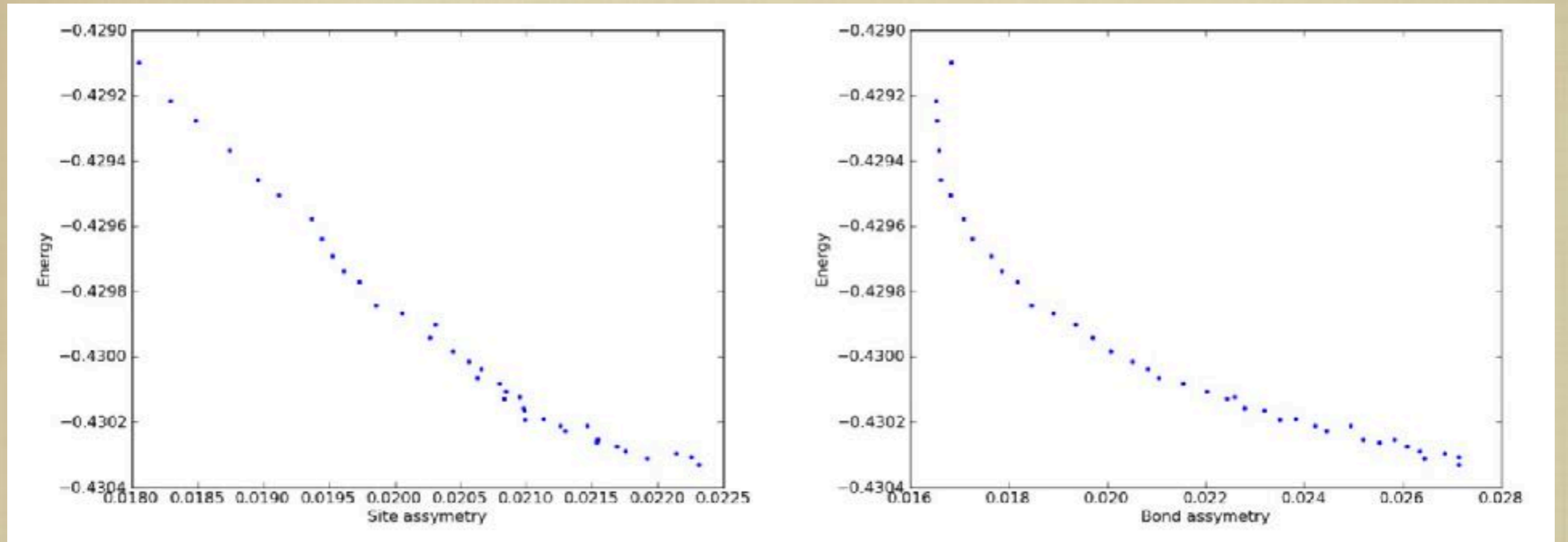
OPTIMIZED BY:

- PAIRING FUNCTION OPT.
- STARTING FROM EACH PSG
- WITH STOCHASTIC OPT AND STOCHASTIC RECONFIGURATION.

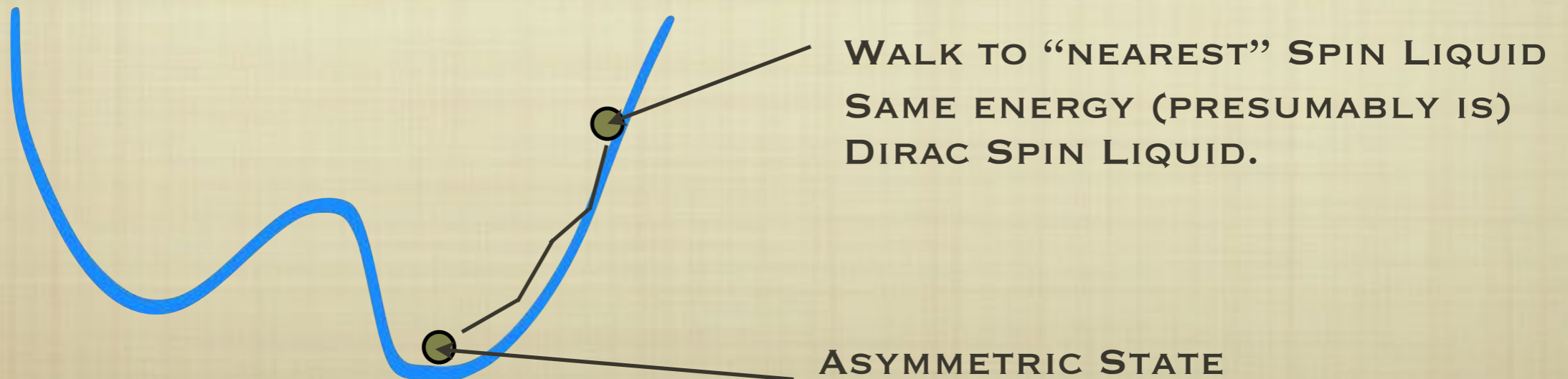
VERY TINY ASYMMETRY

DOES THE ASYMMETRY REALLY HELP?

I.



II.

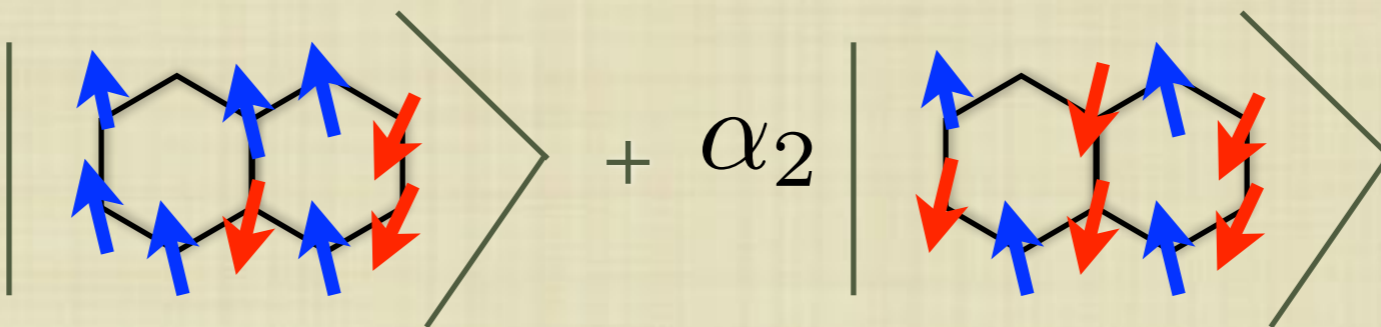


RIGHT LONG WAVELENGTH PHYSICS?

ENERGY IS HIGH BECAUSE SHORT RANGE TENSION?

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

HUSE-ELSER (EPS OR CPS)

$$|\Psi\rangle = \alpha_1 \left| \begin{array}{c} \text{Diagram 1} \end{array} \right\rangle + \alpha_2 \left| \begin{array}{c} \text{Diagram 2} \end{array} \right\rangle$$
The diagram shows two hexagonal lattices, each enclosed in a large right-pointing arrow. The first lattice has blue arrows on the left and top edges and red arrows on the right and bottom edges. The second lattice has red arrows on the left and top edges and blue arrows on the right and bottom edges.

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

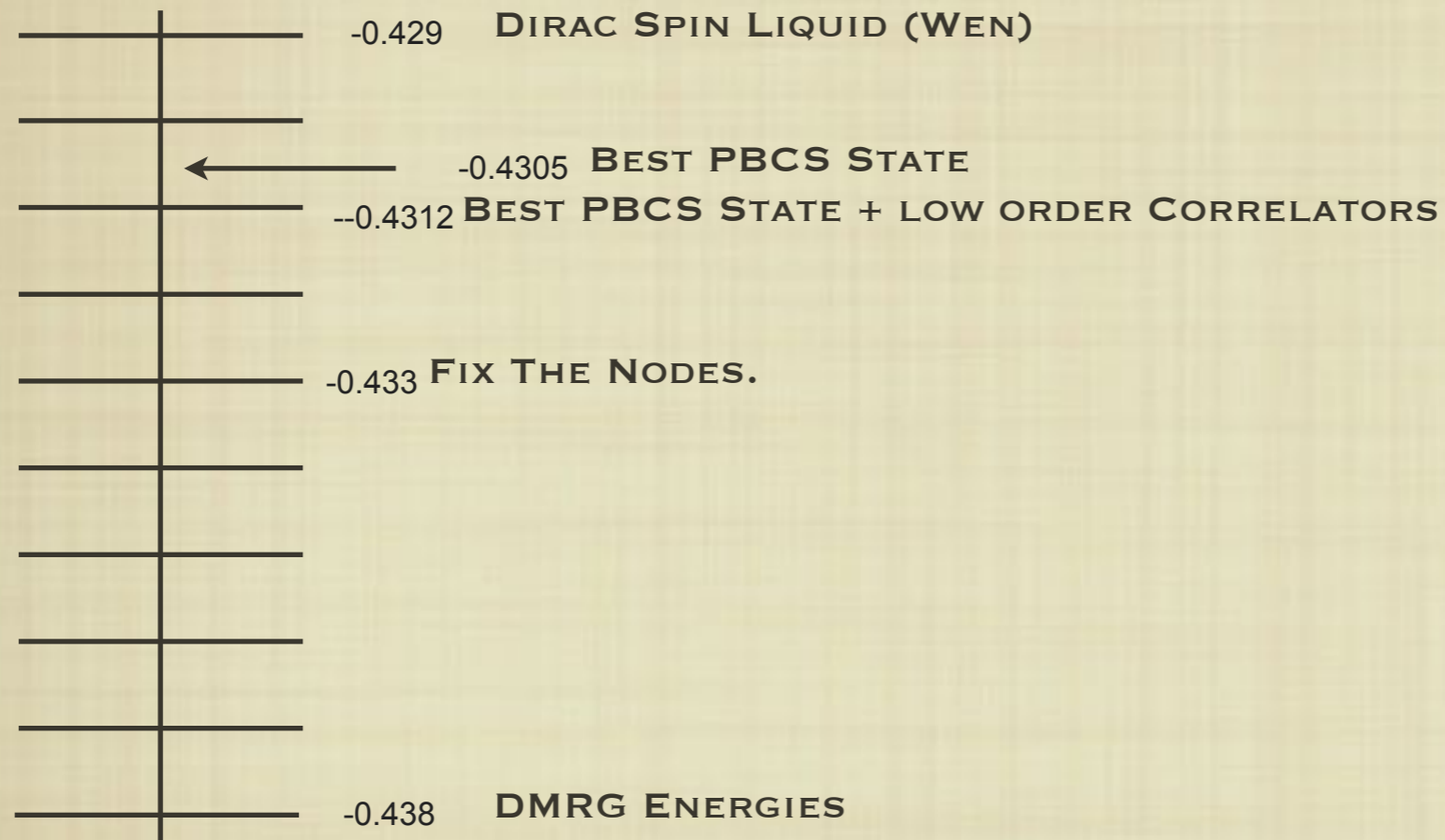
$$\alpha^{n_1 n_2 \dots n_k} = \alpha^{n_1 n_2} \alpha^{n_1 n_3} \dots \alpha^{n_2 n_k} \dots \alpha^{n_{k-1} n_k}$$

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

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?

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)

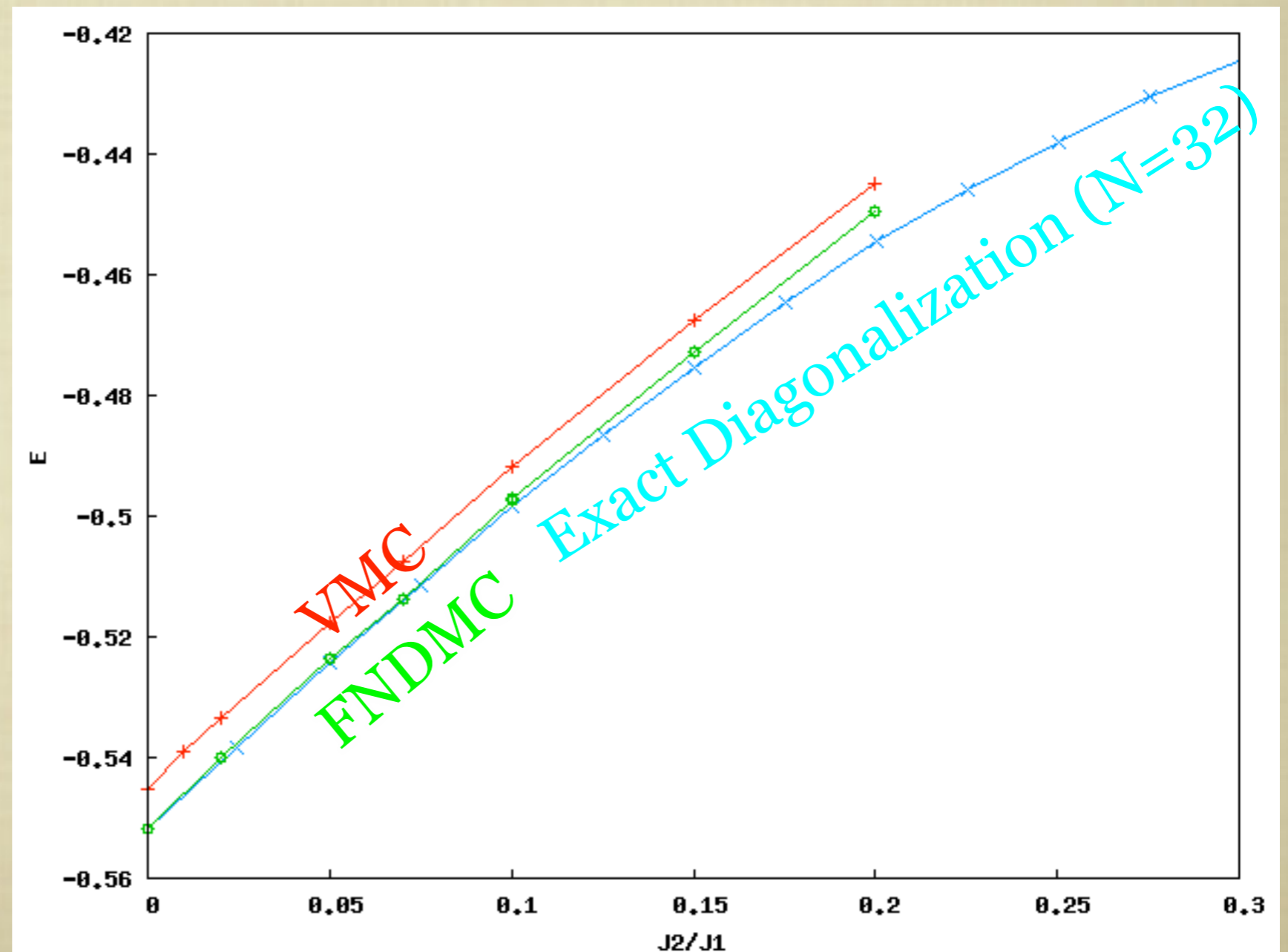
$$|\Psi_{HE}\rangle$$



USE A GOOD VARIATIONAL GUESS TO SET
THE NODES.

NODES OF NEEL STATE
ENTIRELY CONTROLLED BY
ONE AND TWO BODY
CORRELATORS

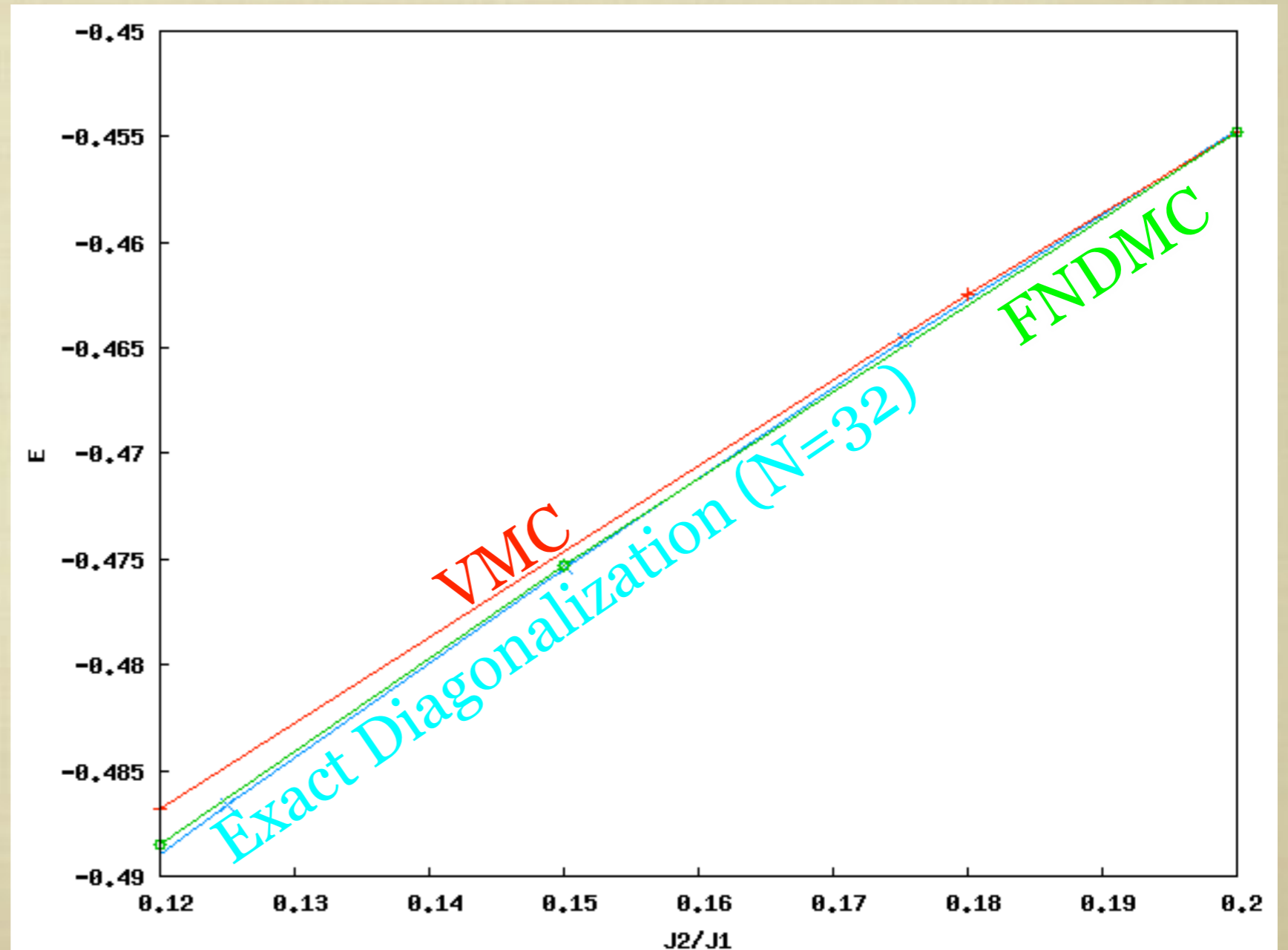
THIS EXAMPLE:
H-E WITH PAIRS



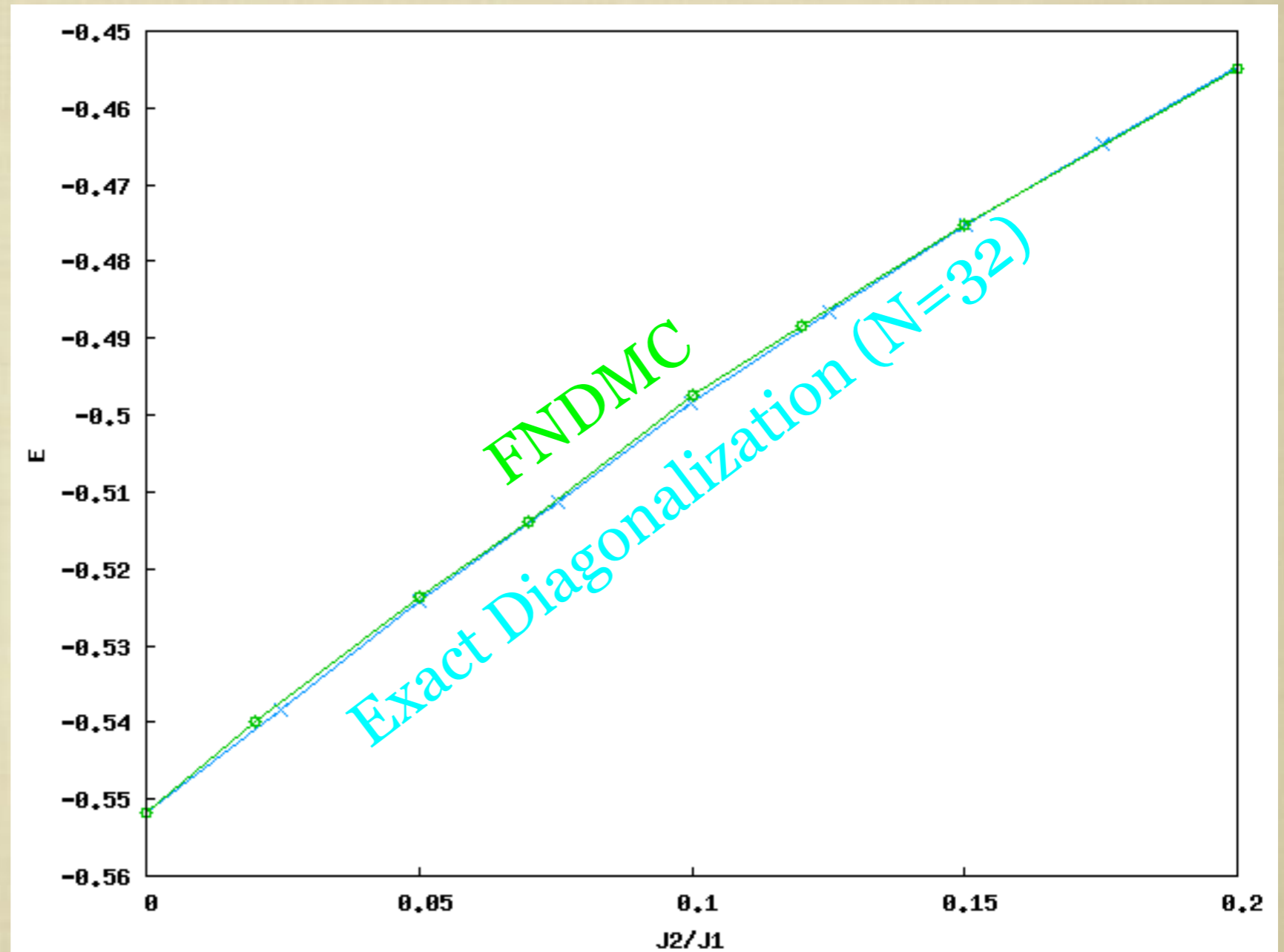
CLEANING UP LARGER J_2/J_1

AROUND $J_2/J_1 \sim 0.12$ THE PROJECTION OF THE HE VARIATIONAL ANSATZ GETS INACCURATE. NEED TO PROJECT WITH MORE SOPHISTICATED ANSATZ.

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



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!

Conclusions

Topological degeneracy of the Hubbard honeycomb is either not there or hard to get.

Honeycomb heisenberg has PBCS spin liquids competitive in energy and their nodal structure is controlled by J_1

Kagome heisenberg has PBCS that is (slightly) not a spin liquid, and is not competitive in energy with the right answer (even when you fix the short range or nodes)

**AN ASIDE: ARE THERE REALLY SPIN
LIQUIDS HERE?**

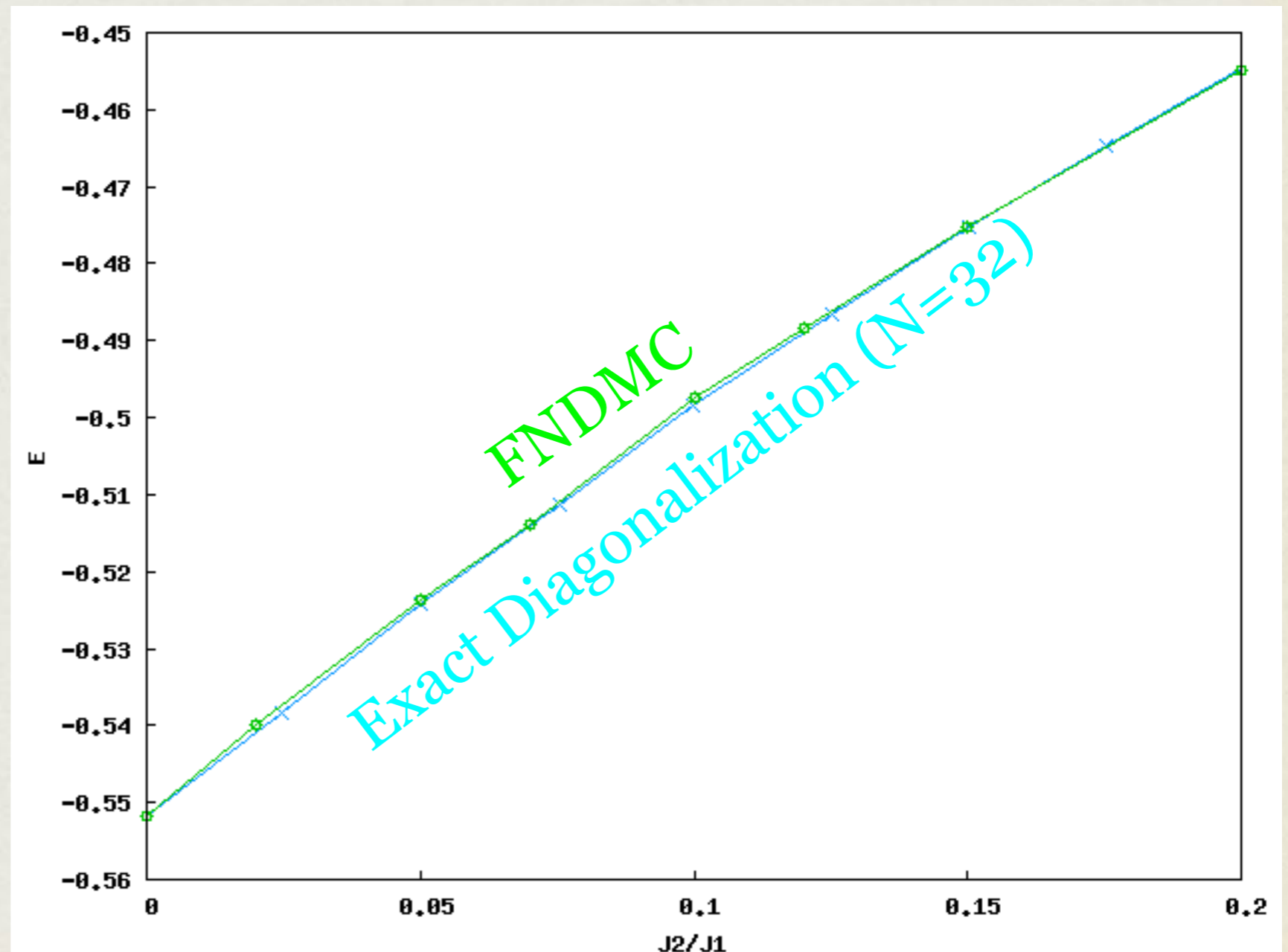
HUBBARD HONEYCOMB: PROBABLY

**HEISENBERG HONEYCOMB: PROBABLY
WITH ENOUGH HIGH ORDER TERMS**

HEISENBERG KAGOME: PROBABLY

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

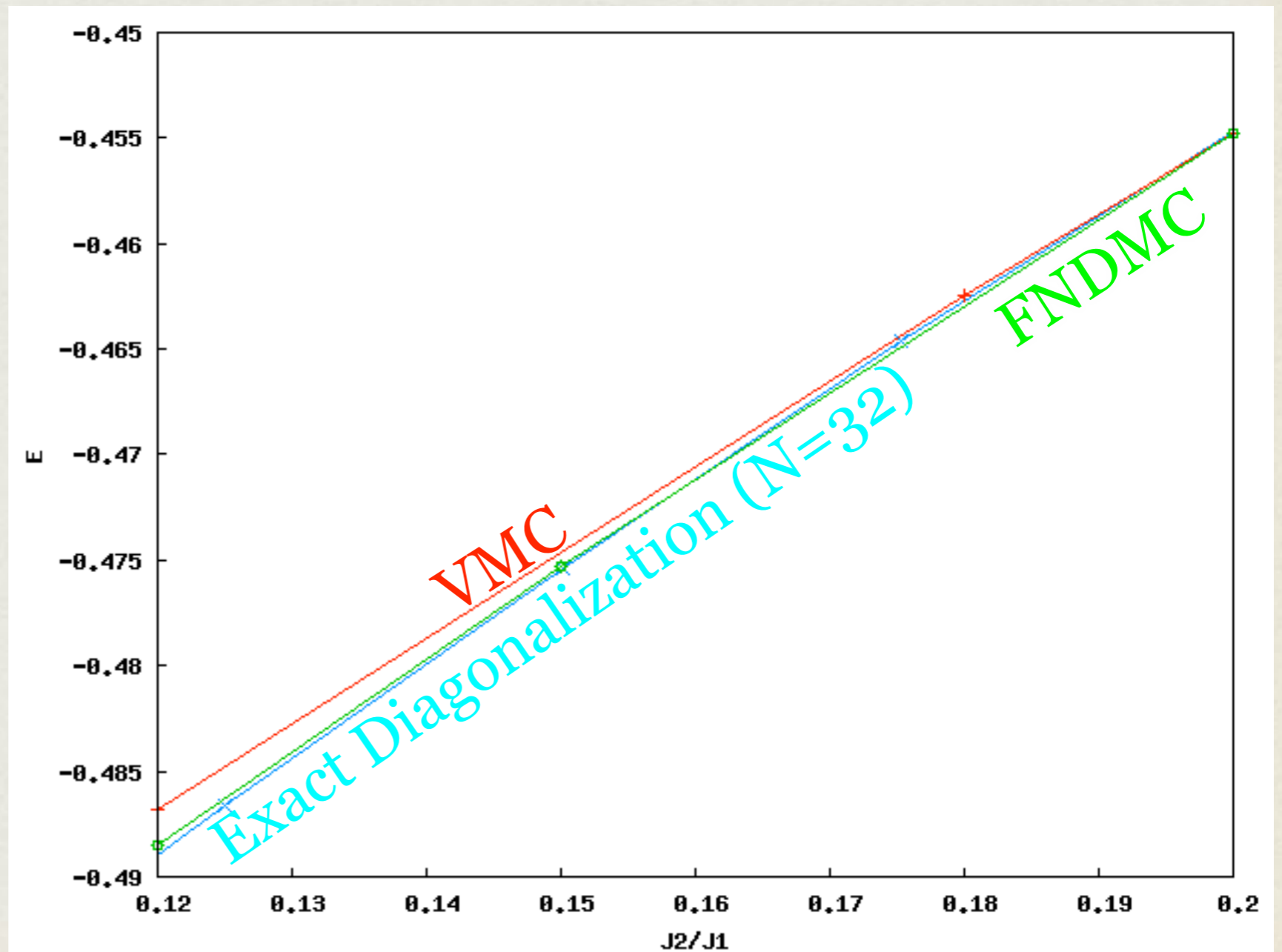
Next step (coming soon): Compute correlators such as staggered magnetization, etc. for large systems to better resolve at a quantitative level where the spin liquid state is supported.



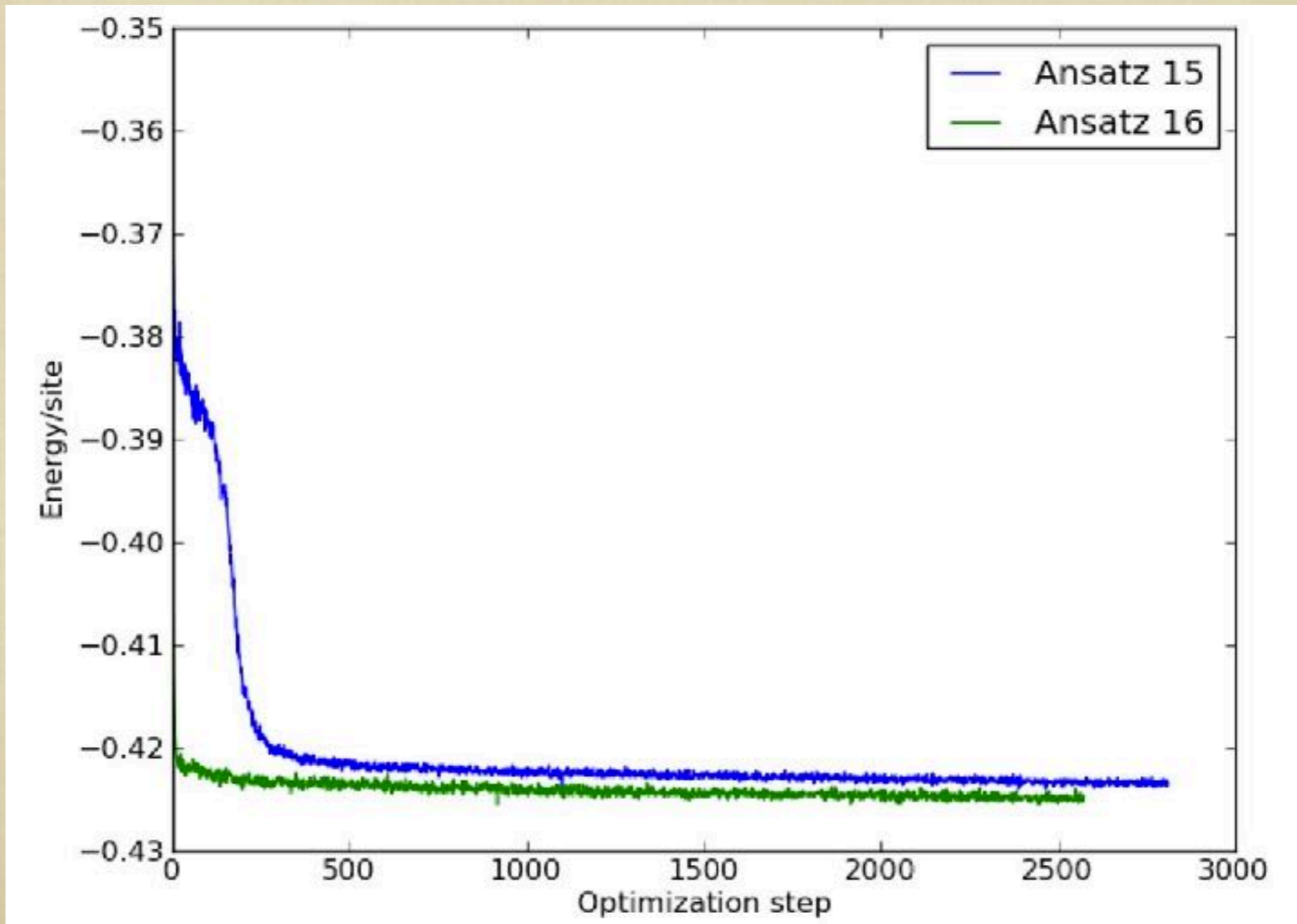
Cleaning up larger J_2/J_1

Around $J_2/J_1 \sim 0.12$ the projection of the Neel variational ansatz gets very inaccurate. Need to project more sophisticated ansatz:

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



■ ASDF



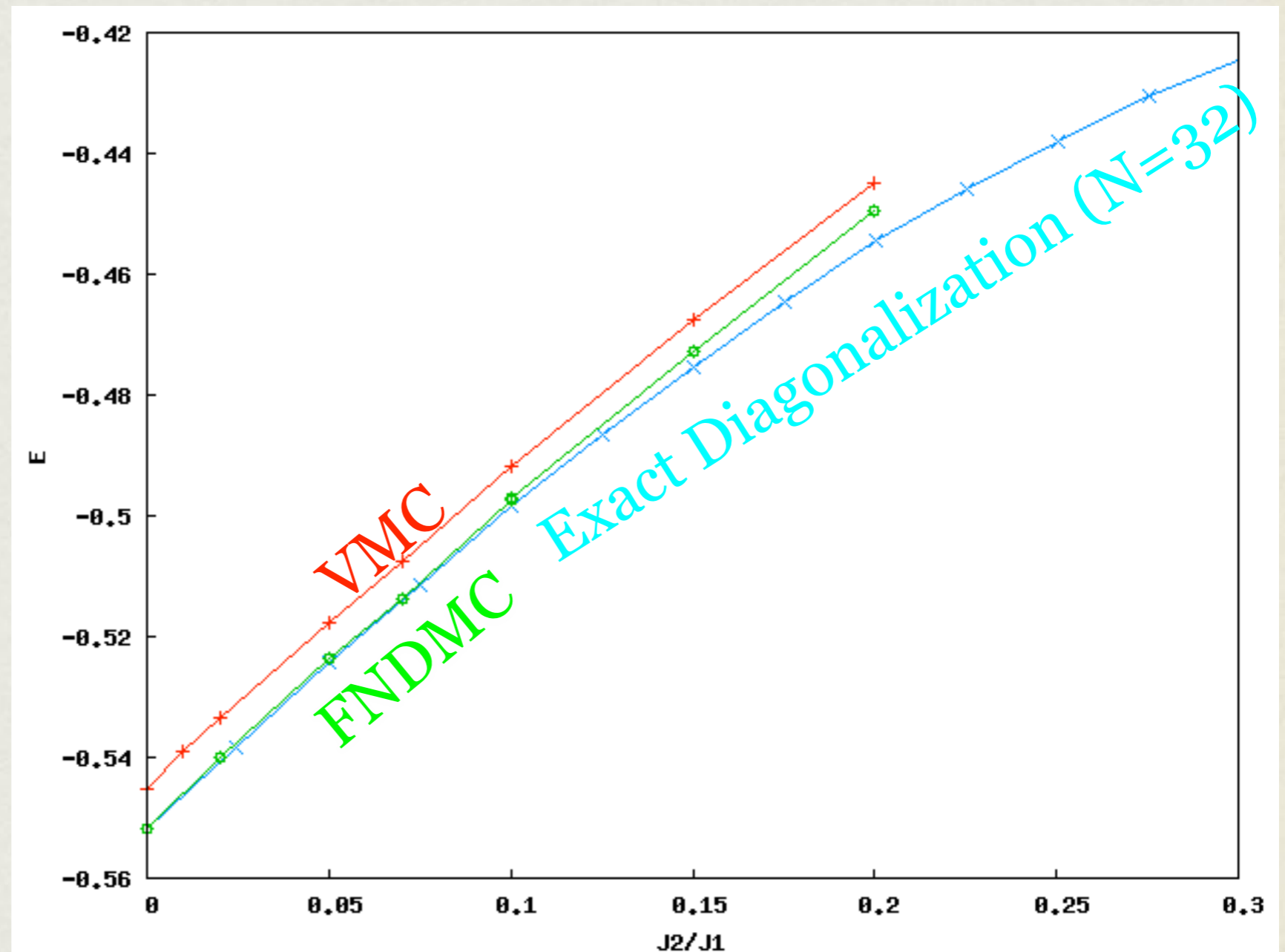
FNDMC: Project out excitations

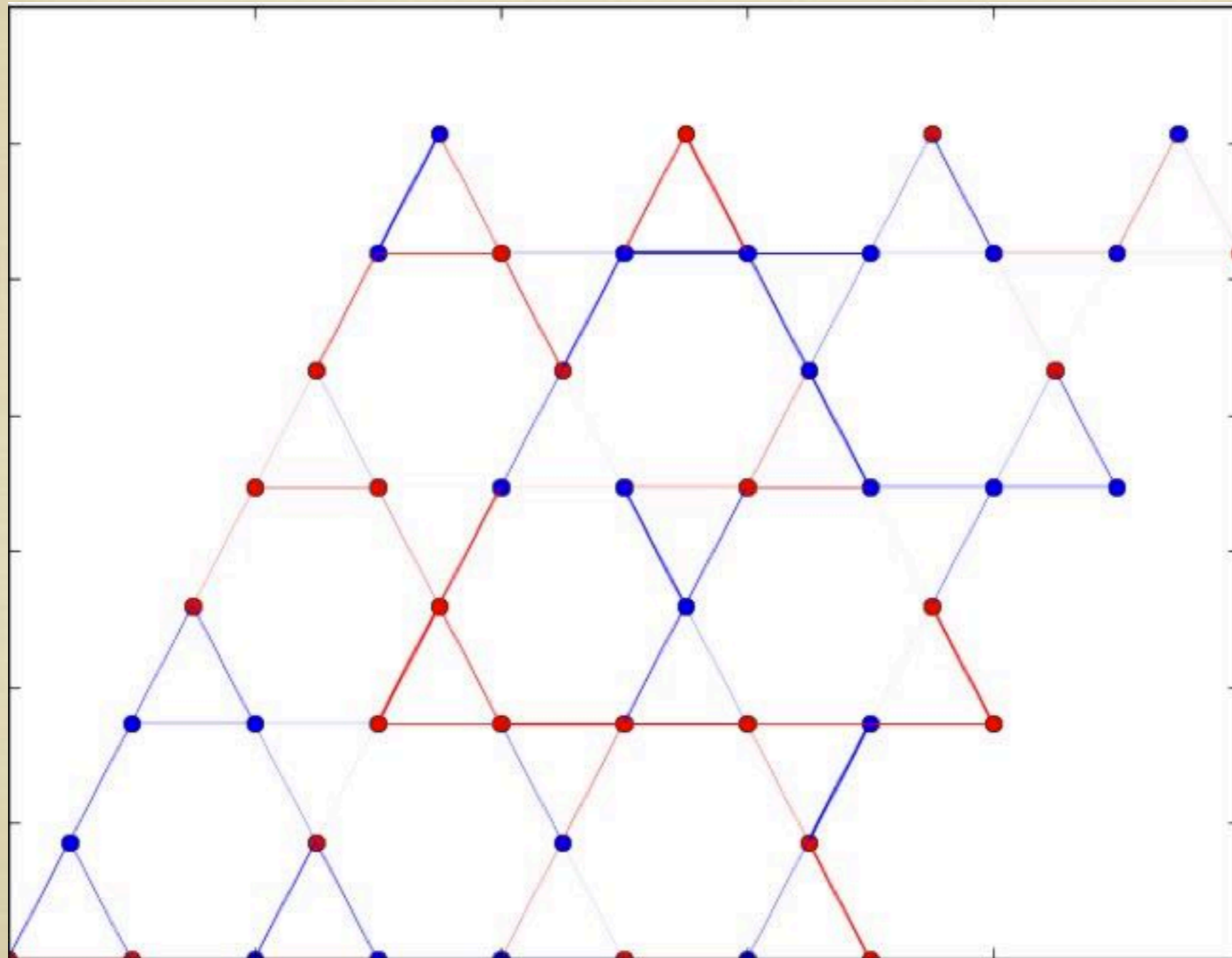
Let's compare against exact diagonalization (for small systems)

$$|\Psi_{\text{Neel}}\rangle$$

Use our best variational guess to set the nodes.

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





QUANTUM RAMPS

$$H(t) = -J \sum_{j=1}^L ([1 - \lambda(t)] s_j^x + s_j^z s_{j+1}^z)$$

