

Title: Searching for Spin Liquids

Date: May 09, 2013 09:00 AM

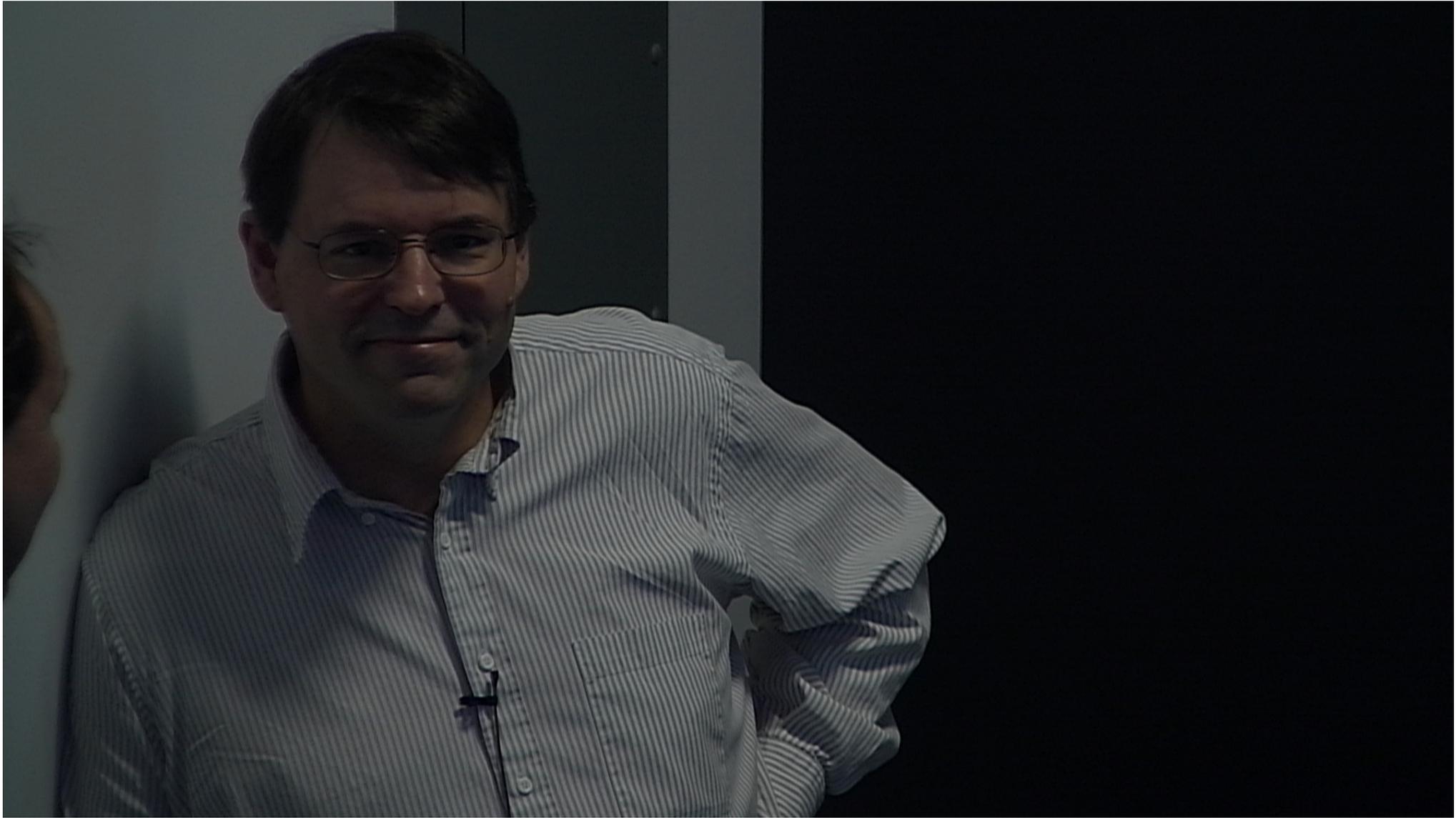
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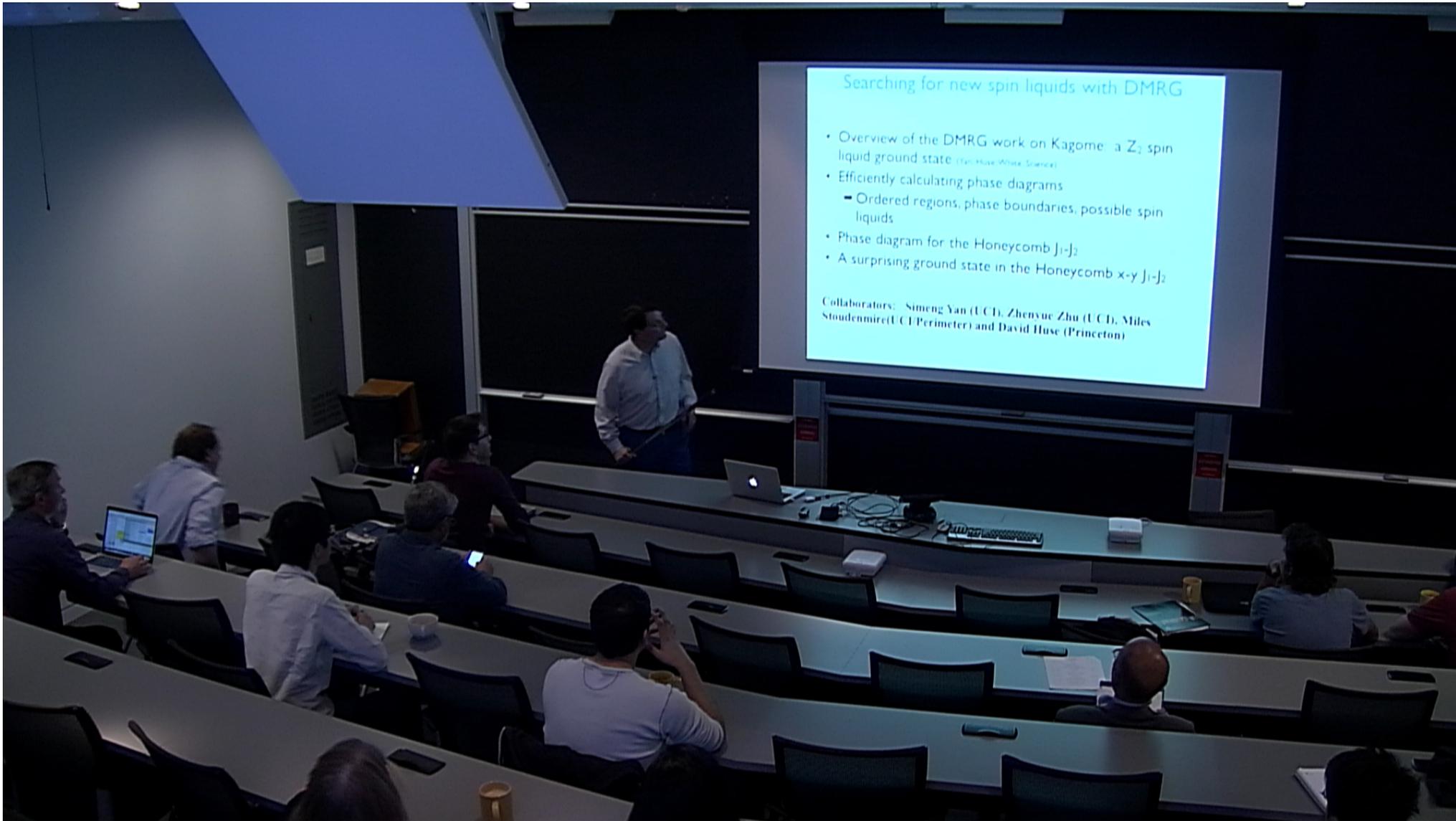
Abstract:

Searching for new spin liquids with DMRG

- Overview of the DMRG work on Kagome: a Z_2 spin liquid ground state (Yan, Huse, White, Science)
- Efficiently calculating phase diagrams
 - ➔ Ordered regions, phase boundaries, possible spin liquids
- Phase diagram for the Honeycomb J_1 - J_2
- A surprising ground state in the Honeycomb x - y J_1 - J_2

Collaborators: Simeng Yan (UCI), Zhenyue Zhu (UCI), Miles Stoudenmire(UCI/Perimeter) and David Huse (Princeton)





Searching for new spin liquids with DMRG

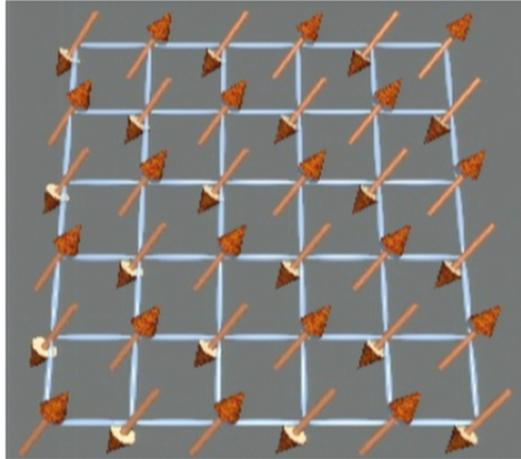
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Quantum Spin Liquids: what are they?

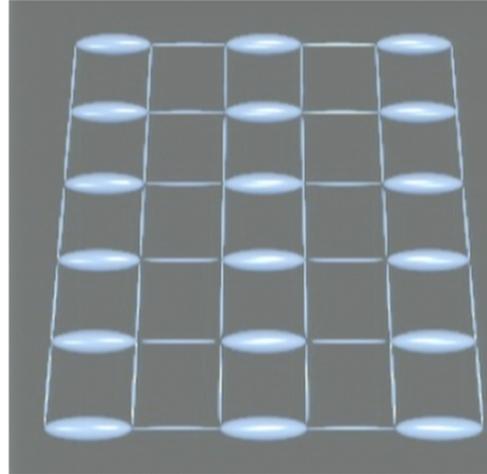
- Starting ingredient: a lattice of localized spins. ~~Metals~~
- Then (at least) three classes of possible ground states.

~~Band
Insulators~~



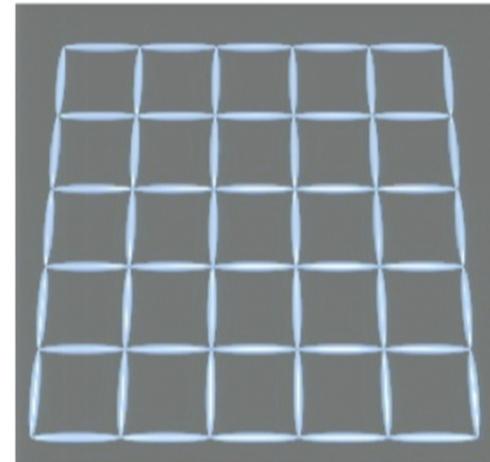
Magnetic order

$$\langle \psi | \vec{S}_i | \psi \rangle \neq 0$$



Valence bond order

$$\langle \psi | \vec{S}_i \cdot \vec{S}_j | \psi \rangle \neq \text{const}$$



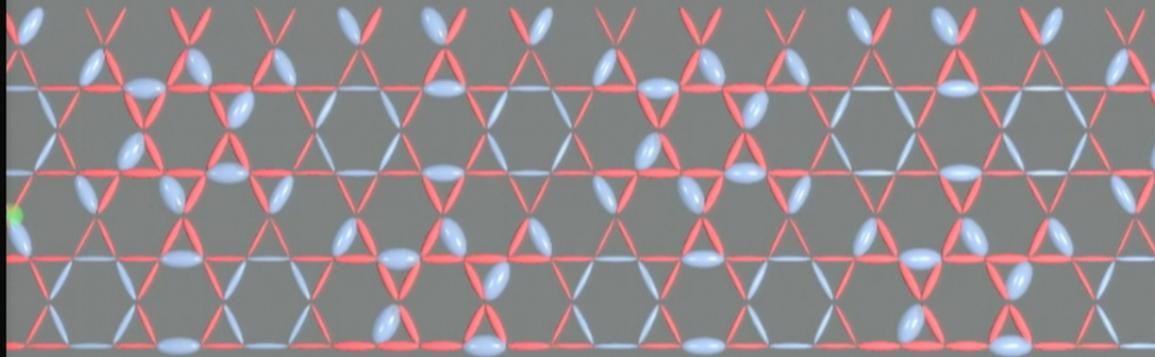
Spin liquid

No broken symmetries

- This talk will not emphasize topological order; several talks after me will.

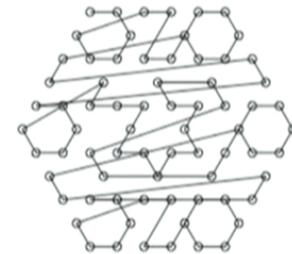
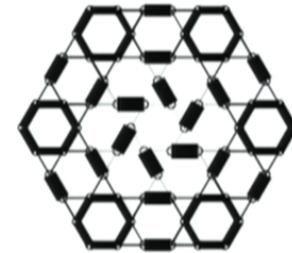
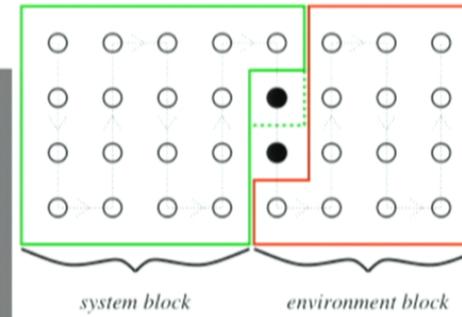
Sample DMRG simulation on Kagome

XC8 cylinder, biased to HVBC



$swp=3, m=120, E=-89.8440$

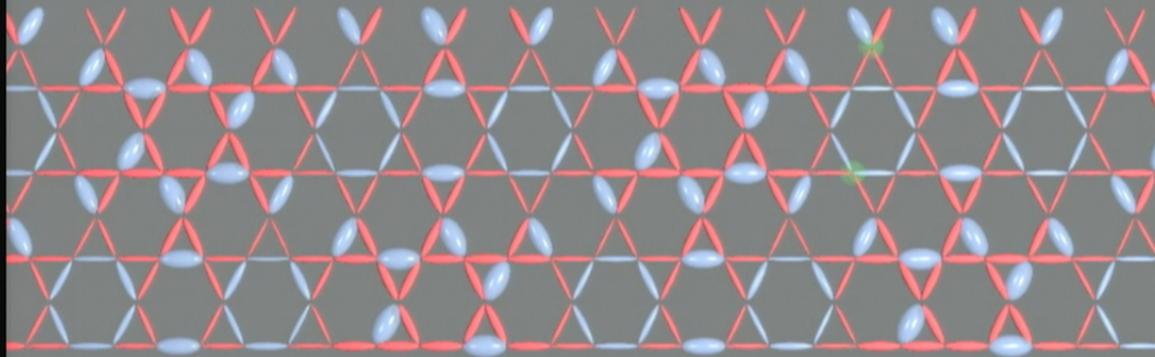
Density matrix renormalization group = energy minimization method over matrix product states



Highly biased path

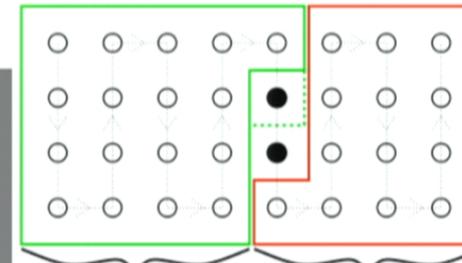
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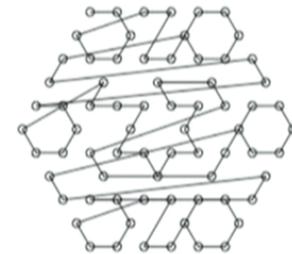
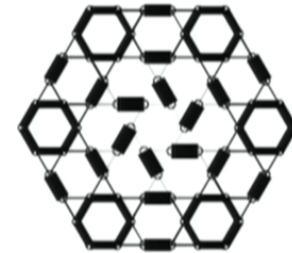
$swp=3, m=120, E=-89.8023$

Density matrix renormalization group = energy minimization method over matrix product states



system block

environment block



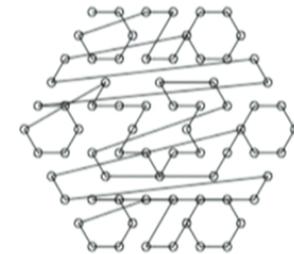
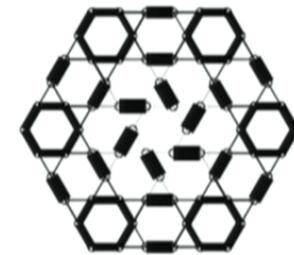
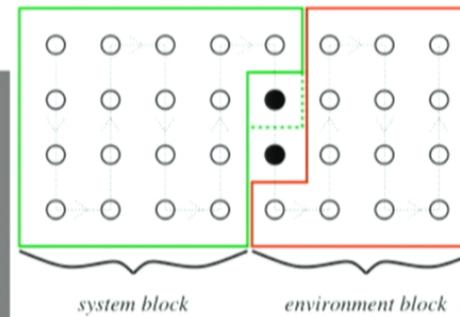
Highly biased path

Sample DMRG simulation on Kagome

XC8 cylinder, biased to HVBC

$swp=34, m=8000, E=-90.7421$

Density matrix renormalization group = energy minimization method over matrix product states



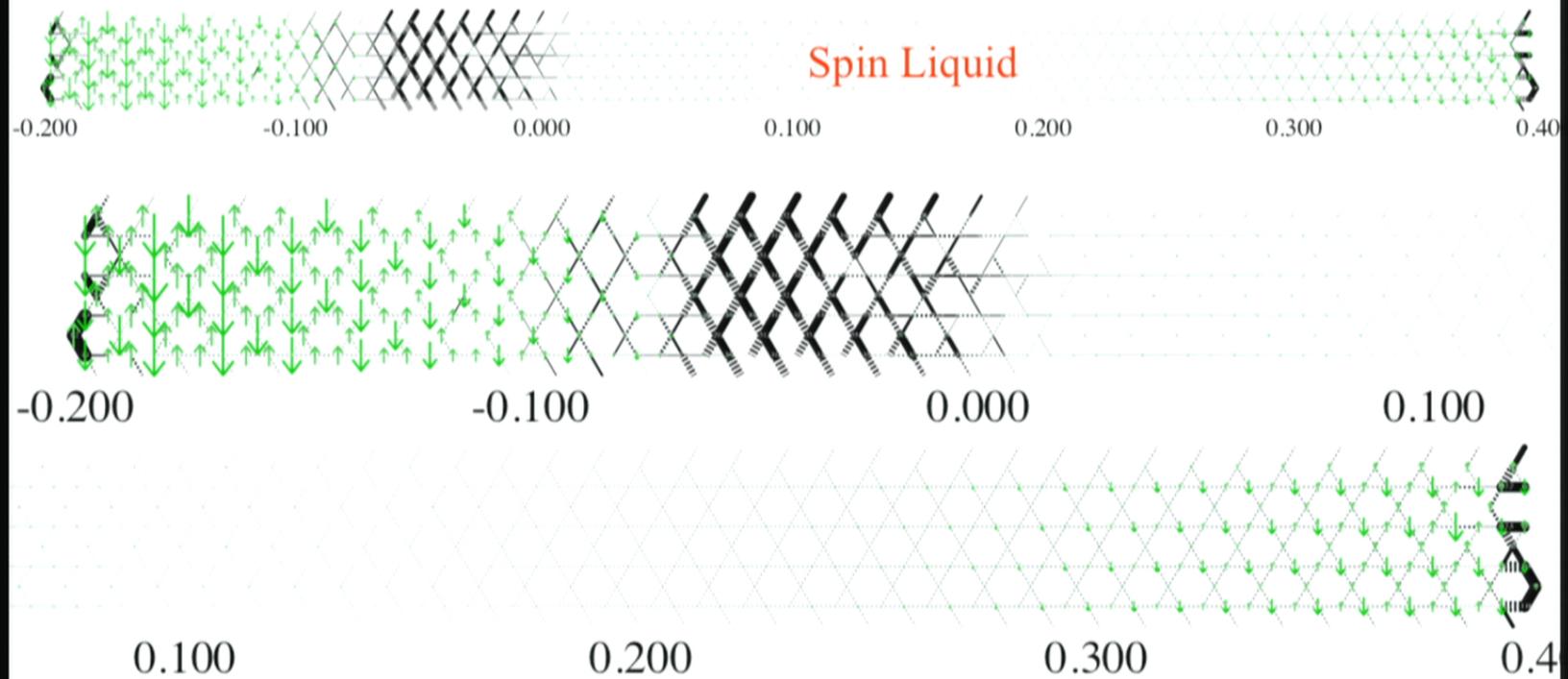
Highly biased path



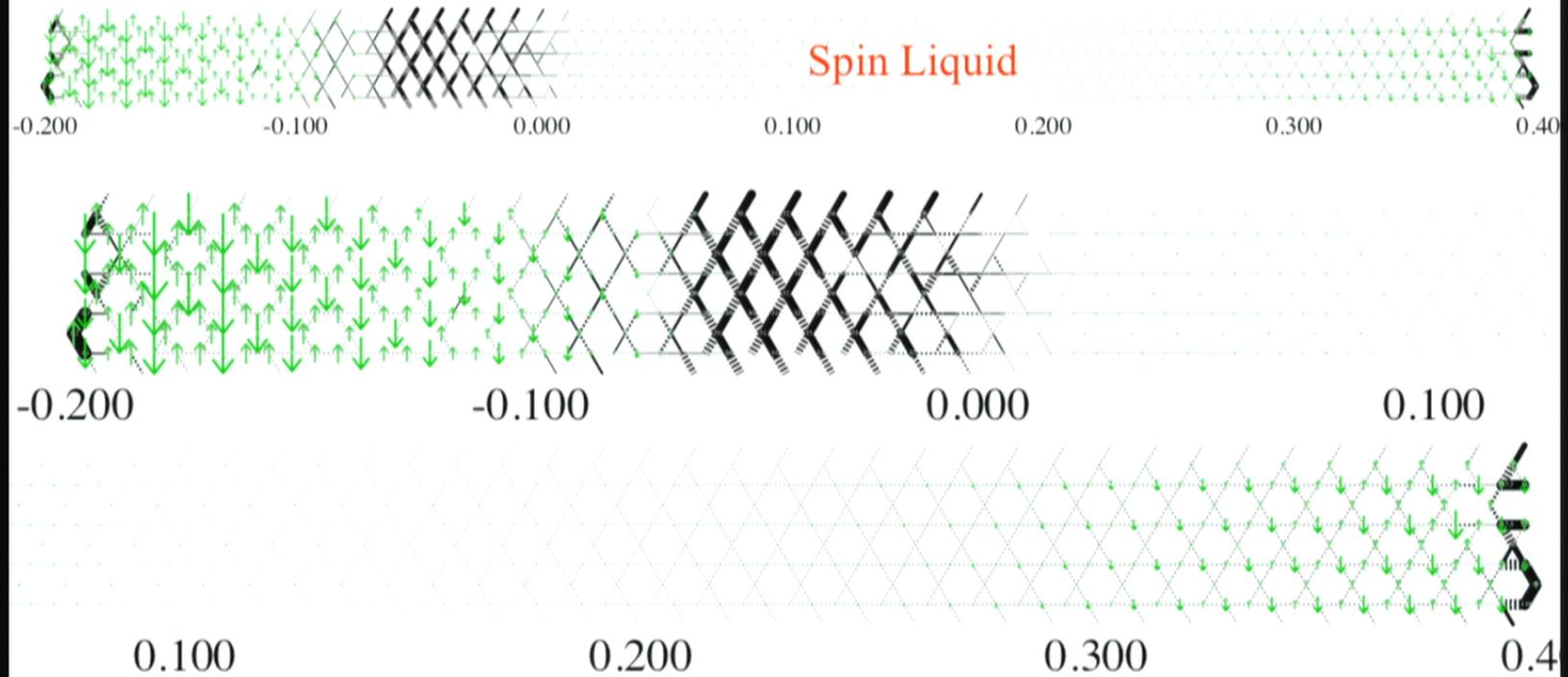
Making the case for the spin liquid

1. Energy: “much” lower than HVBC compared to finite size effects; matches exact diagonalization
2. Even when biases are manipulated to favor HVBC, still get SL
3. New best exact 2D upper bound on energy from SL
4. Detected first order transition on path from HVBC to SL
5. Very short correlation lengths (all types); wide range of cylinder widths give same SL behavior
6. When nnn parameter J_2 added, shows large SL phase with bigger gaps. ED shows same behavior
7. New VBC (diamond pattern) shows why HVBC was the wrong starting point; 8-site resonances dominant

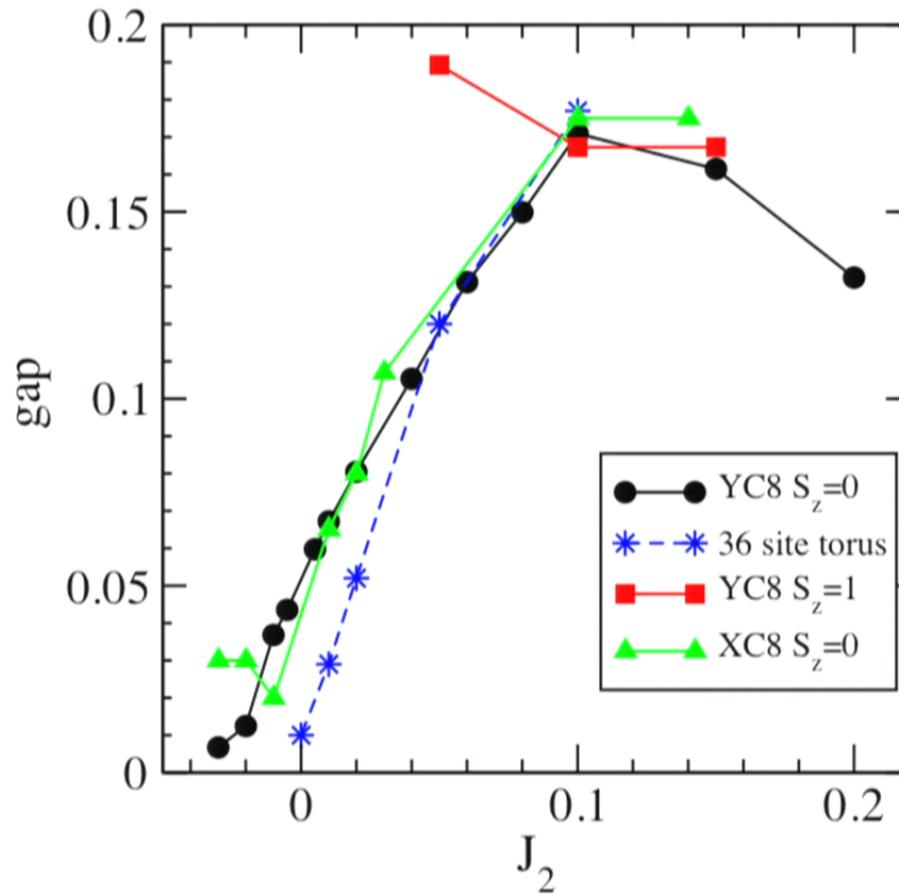
Varying J_2 with x coordinate



Varying J_2 with x coordinate



Next nearest neighbor J_2

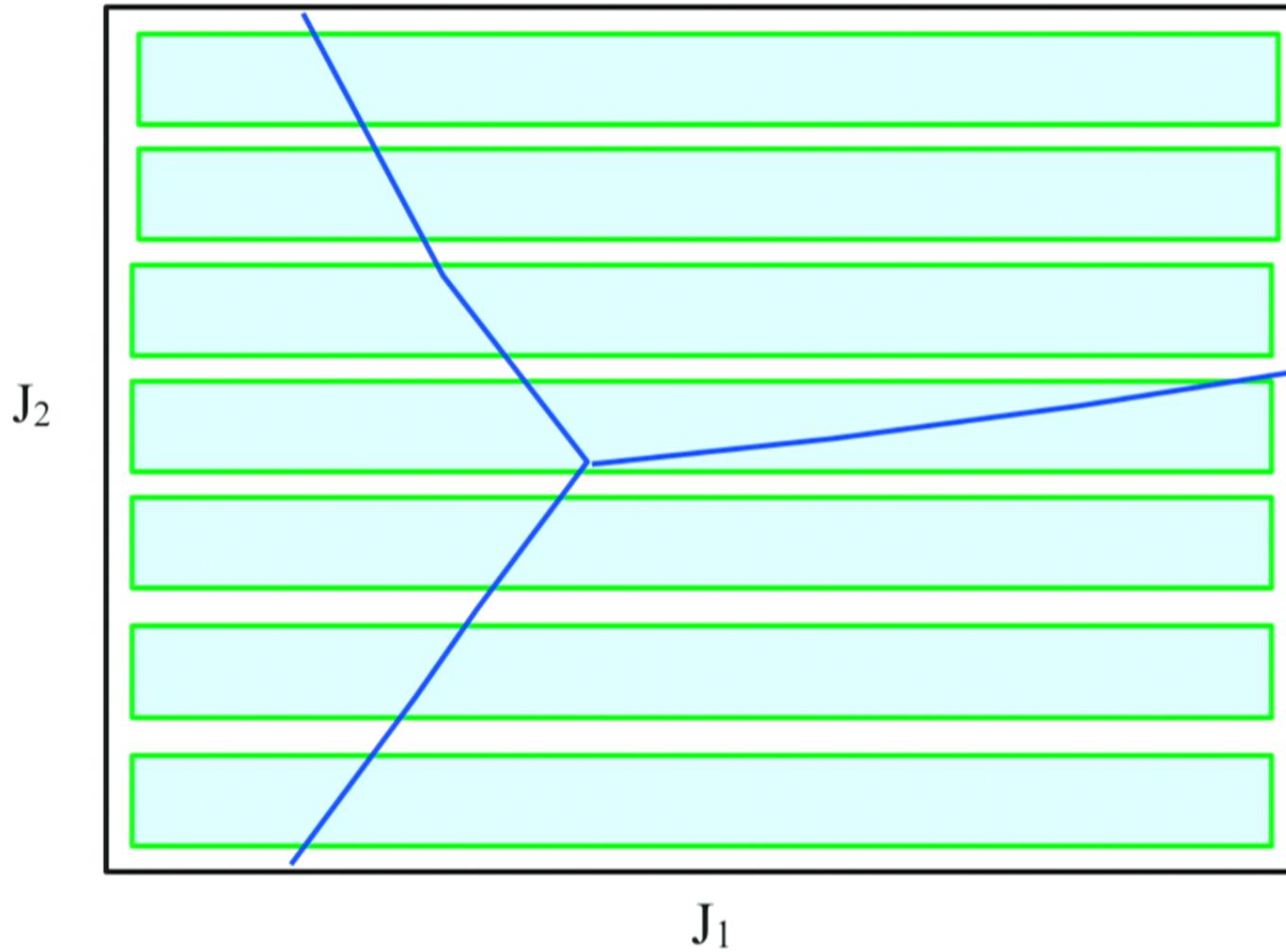


36 site exact
diagonalization:
Sindzingre and
Lhuillier

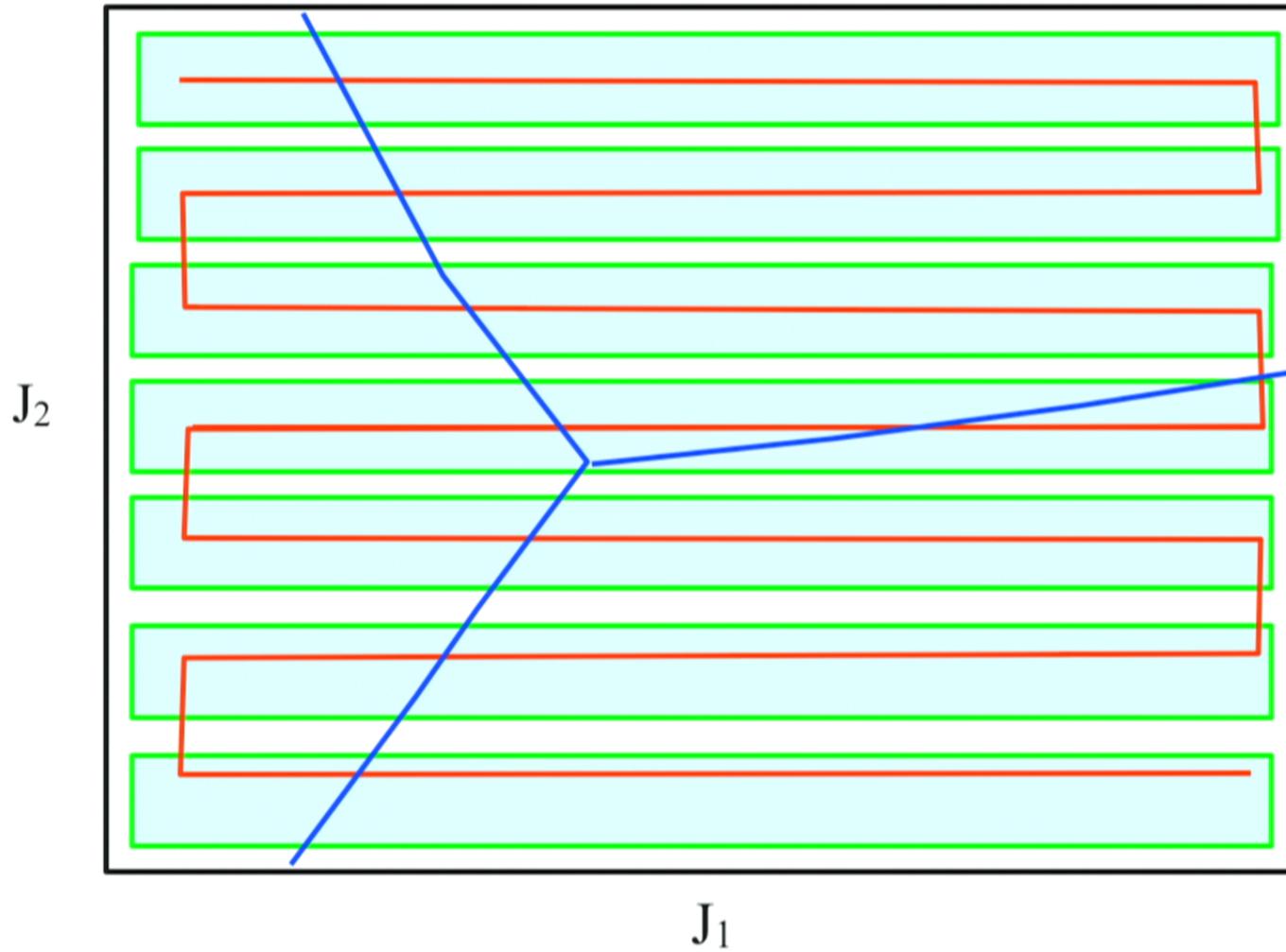
The finite size shift of
the phase boundary
explains the many low
lying states in ED.

Note: no sign of 4-fold
degeneracy for torus

Varying parameters of H along the cylinder



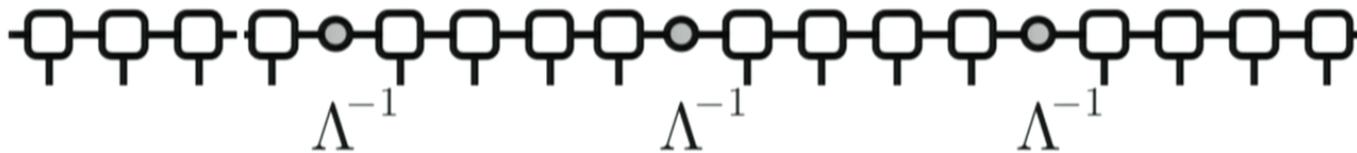
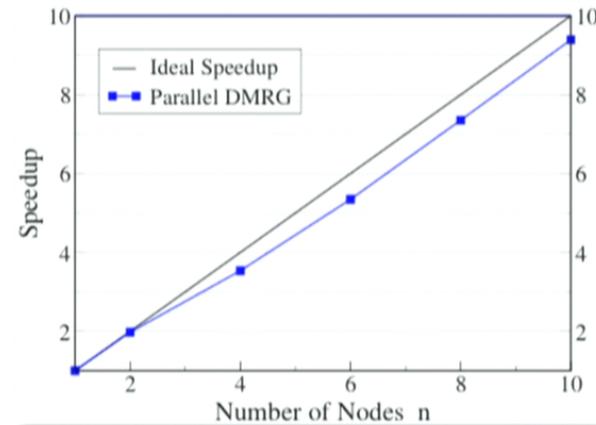
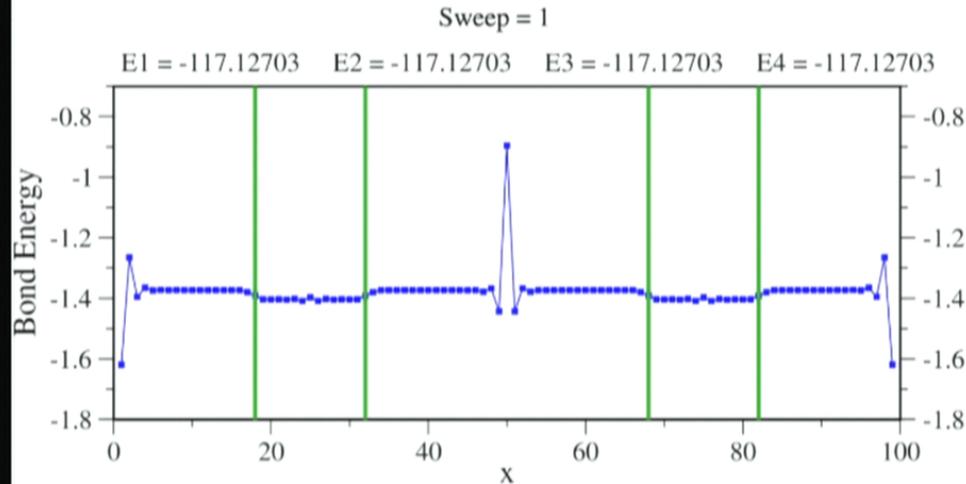
Varying parameters of H along the cylinder



Parallel DMRG

Stoudenmire & White, PRB **87**, 155137 (2013)

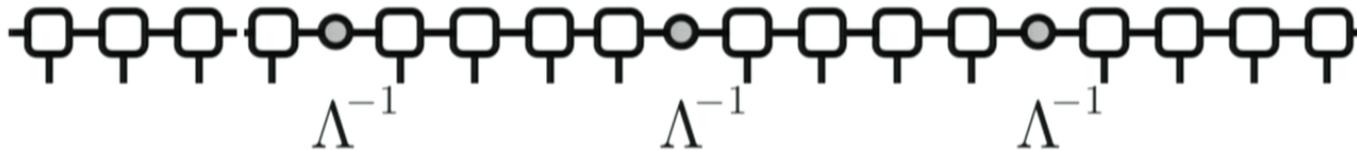
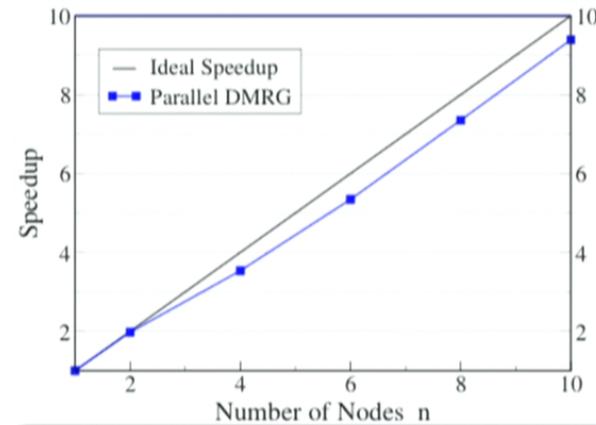
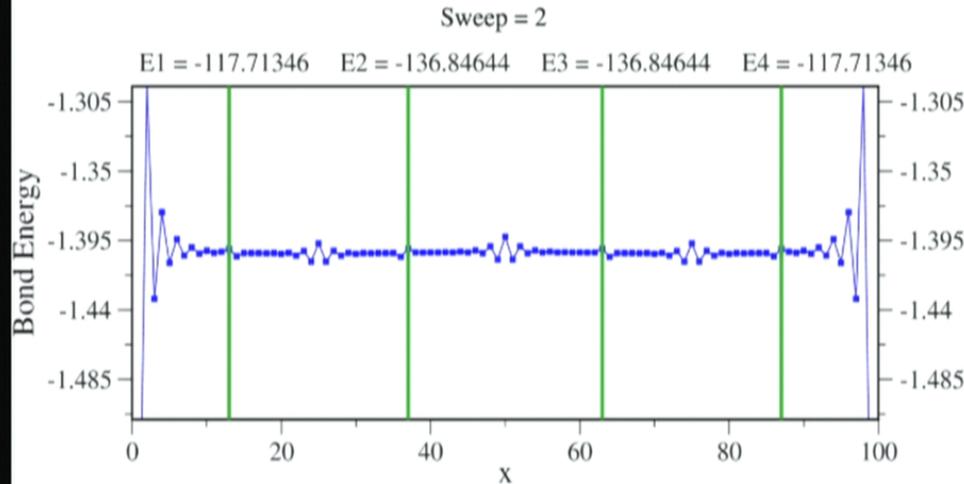
- Parallelize single DMRG calculation across **real space** blocks
- Nearly ideal speedup
- Key step: MPS gauge transformation at block boundaries, each block has orthogonal environment



Parallel DMRG

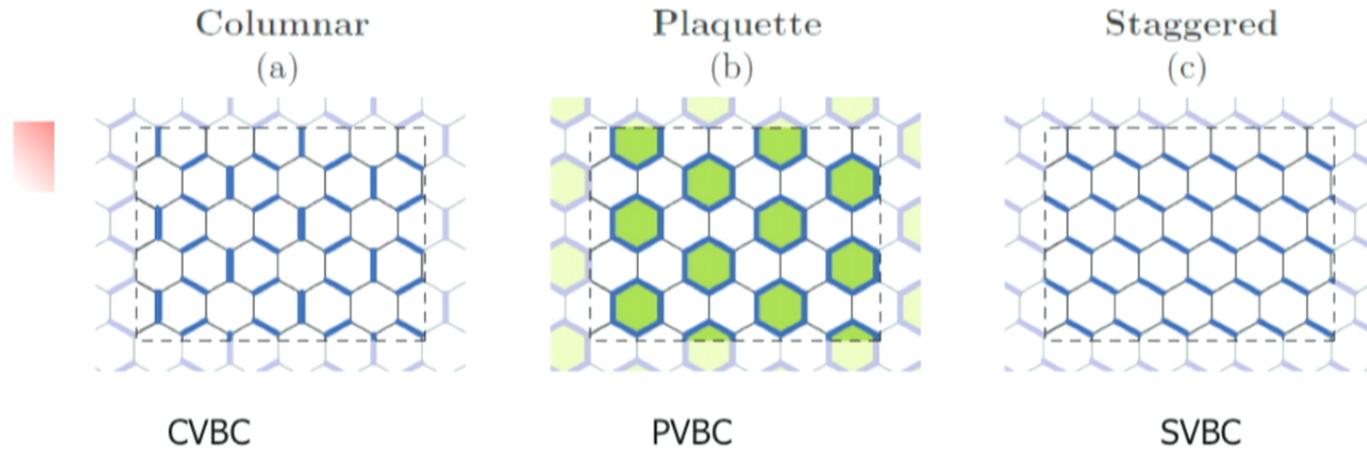
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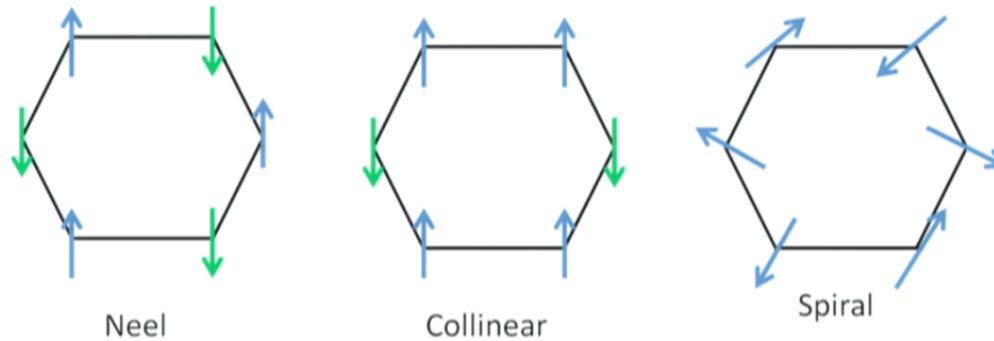
Honeycomb J1-J2 model: is there a spin liquid phase?

Zhu, Huse, and White, PRL 2013



(A. F. Albuquerque, et al. PRB 2011)

Some possible magnetic ordered states on honeycomb lattice.

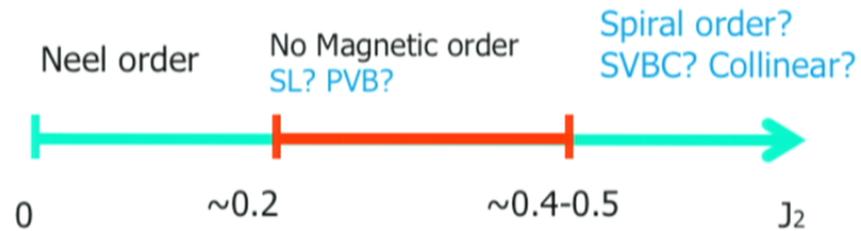


Honeycomb J1-J2 model



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

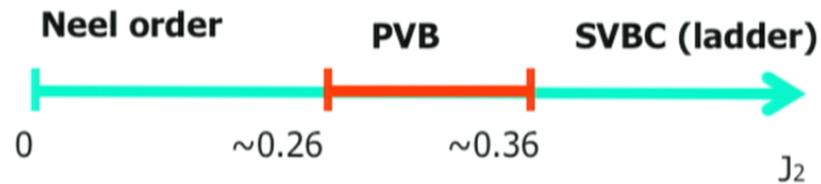
Previous studies



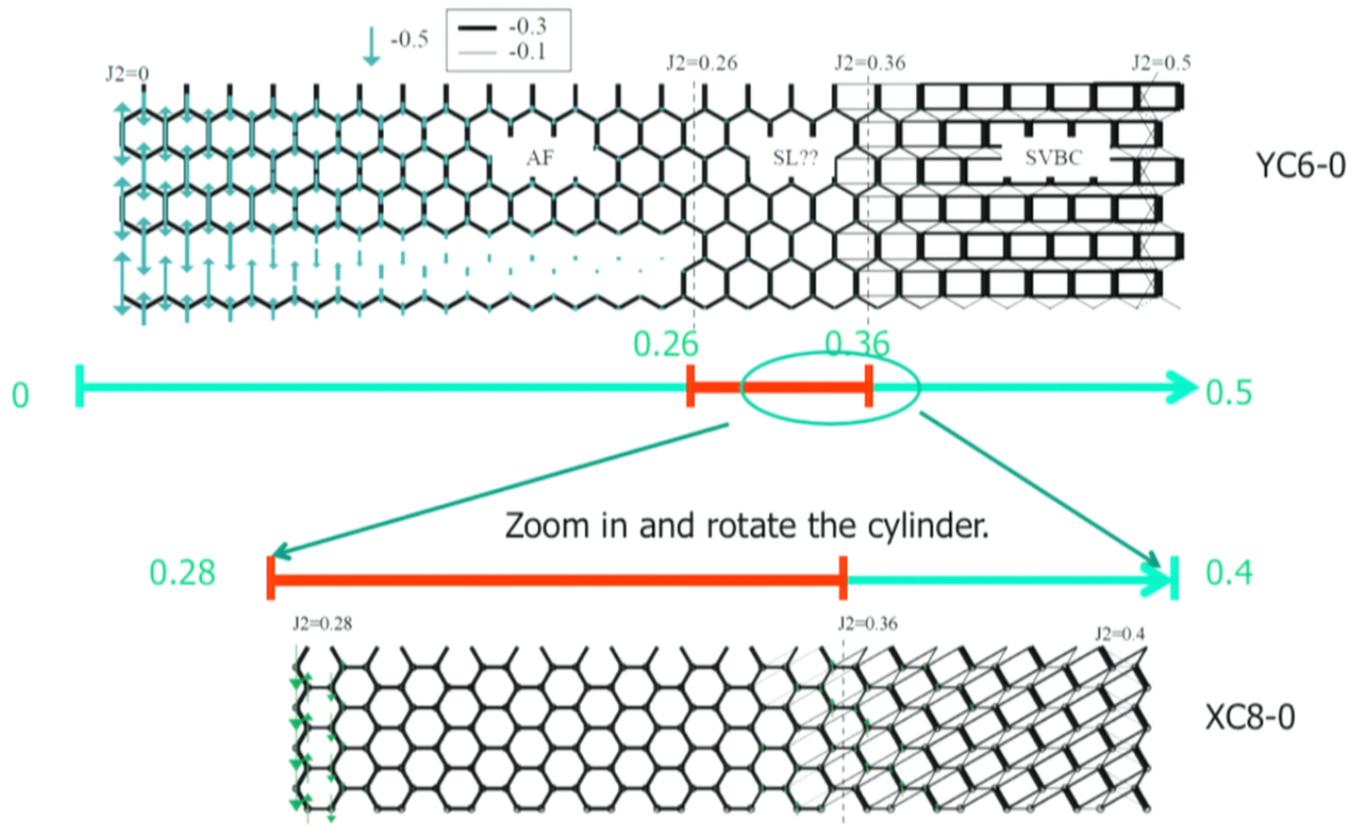
Spin liquid (SL) by VMC.
(B. K. Clark, et al. PRL 2011)
(F. Mezzacapo, et al. PRB 2012)

PVB order by exact diagonalization etc.
(H. Mosadeq, et al, JPC 2011)
(A. F. Albuquerque, et al. PRB 2011)
(P. H. Y. Li, et al. JPC 2012)

Our results



Position-dependent J_2 scans



Determining order parameters via a pinned cylinder with an optimal aspect ratio.



Too tall



Just right!

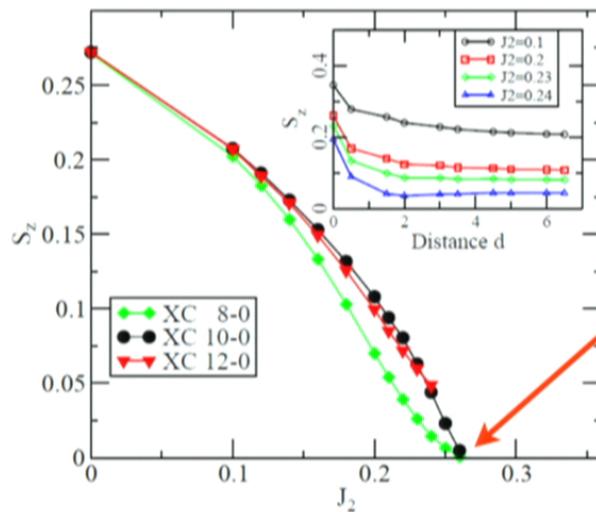


Too long

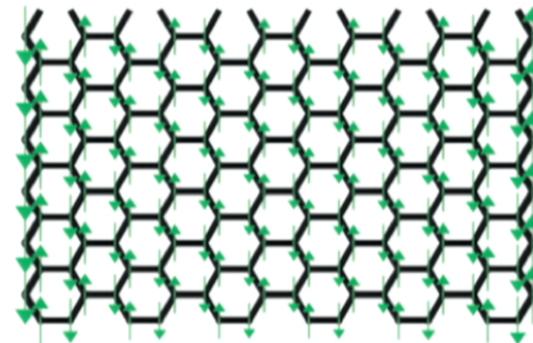
(1) Apply pinning field on both ends to favor Neel order.

(2) Aspect ratio=1.73, close to 2 have smaller finite size effect.

(White and Chernyshev PRL, 2007)



Deconfined quantum critical point!
-Ganesh, et. al.
arXiv: 1304.6340

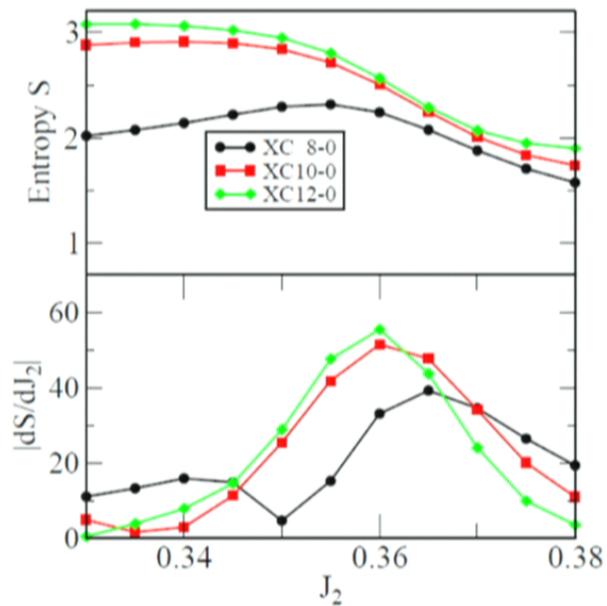


$J_2=0.1$

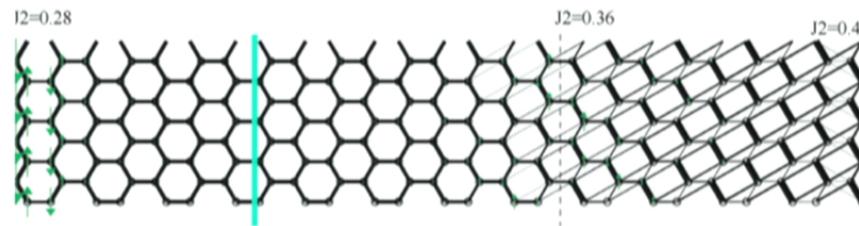
$J_2=0$, $\langle S_z \rangle = 0.272$. Magnetization close to series expansion 0.266(9) (J. Oitmaa, et al. PRB, 1992) and QMC value 0.2677 (E.V. Castro, et al. PRB, 2006).

This approach recently applied to the Hubbard honeycomb model; now clear there is no spin liquid (Assaad & Herbut, arXiv:1304.6340)

Determining phase transitions using the entanglement entropy.



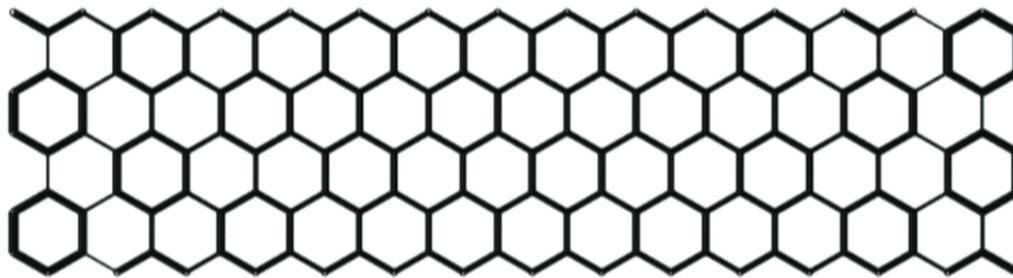
$$S_{von} = -Tr[\rho_A \log \rho_A] = -\sum_i \rho_i \log(\rho_i)$$



Use discontinuity in entanglement entropy or its derivative to determine the phase transition. (O. Legeza, et al. PRL, 2006)

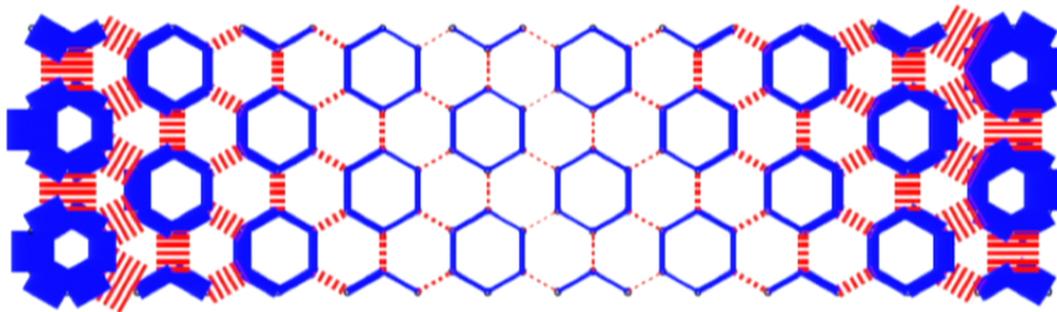
Measure the entanglement entropy on a long cylinder with J_2 varying along the cylinder.

PVB versus SL on XC and YC cylinders for $J_2=0.3$



YC5-3

Before subtracting average,
looks like SL.

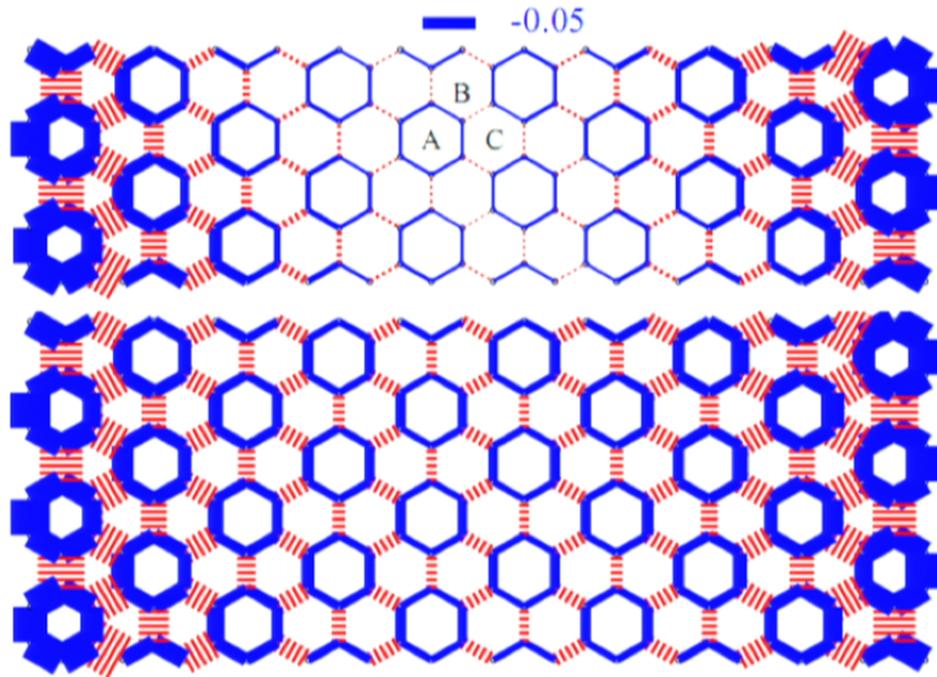


YC5-3

after subtracting
average -0.32, PVB
order appears.
Not SL!

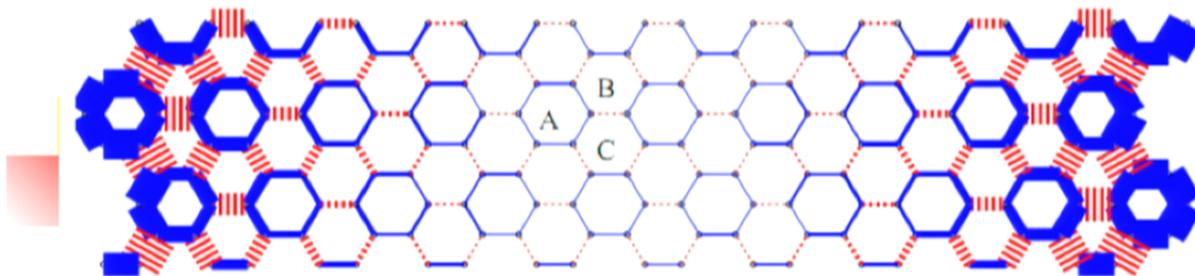
— -0.05
- - - 0.05

XC6-0, XC9-1, XC12-0 and YC5-3, YC7-3, YCN-0 cylinders can accommodate PVB order with proper length and edge.

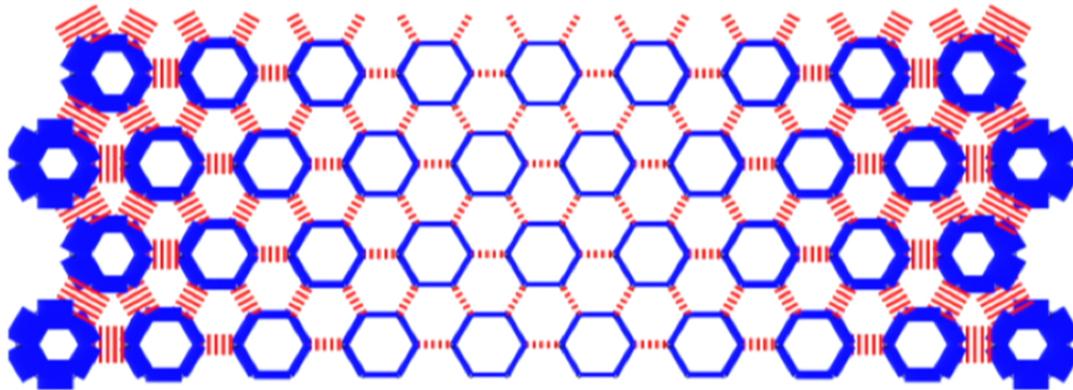


YC5-3

YC7-3



XC9-1



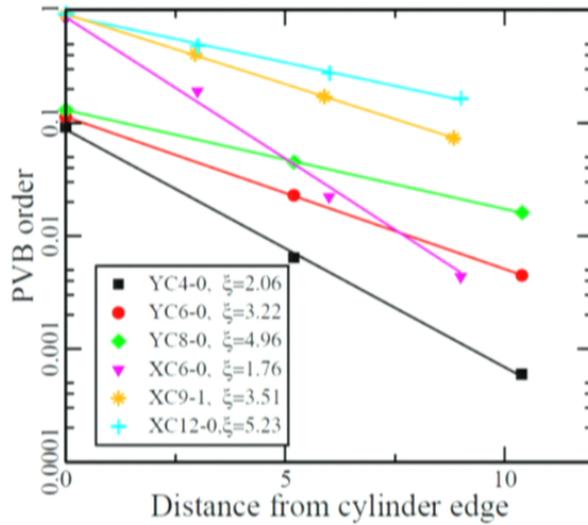
XC12-0

Wider cylinders have stronger PVB order than narrow ones.

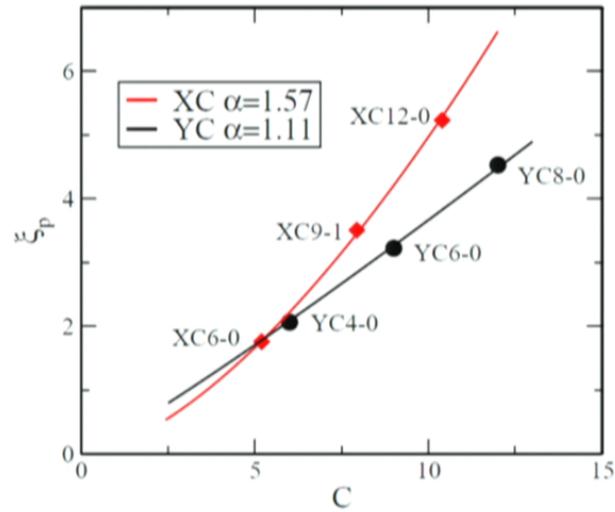
Define a complex PVB order parameter

$$P_A = E_A + E_B \exp\left(\frac{2\pi}{3}i\right) + E_C \exp\left(\frac{4\pi}{3}i\right)$$

E_A is the sum of six bonds around hexagon A. For SL phase, $P_A=0$.



Decay of PVB order from the cylinder Edge to center.

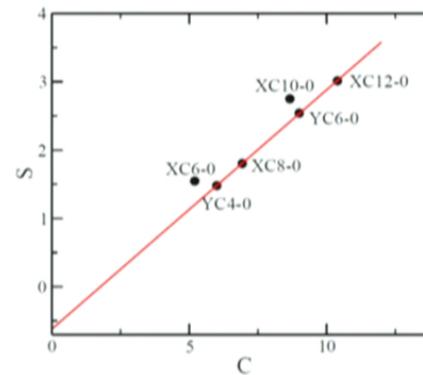


PVB order correlation length versus Cylinder width.

$$\xi_p \sim C^\alpha$$

Since $\alpha > 1$, it appears that PVB correlation length increase faster than the cylinder width. Indicate **long range PVB order** in the 2D limit.

Result holds for the entire intermediate phase.



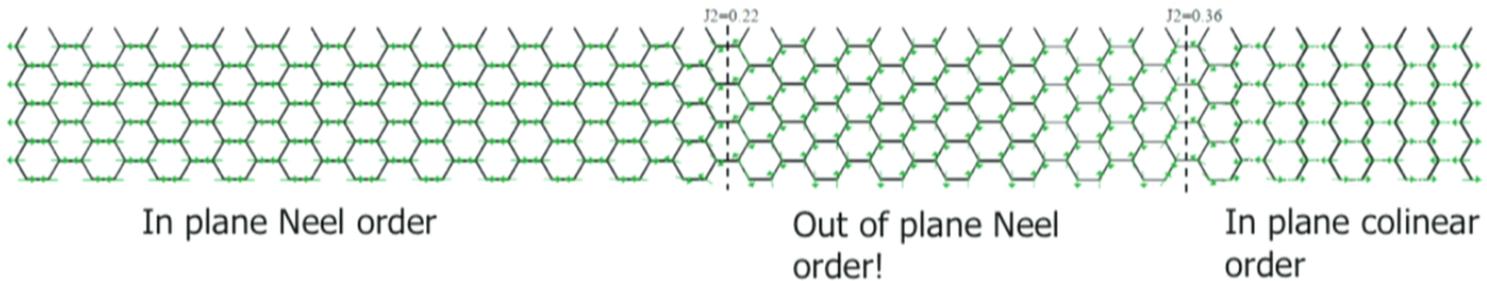
Entanglement entropy intercept = 0.619, close to $\ln(2)=0.693$.

But, since PVB correlation length is comparable to the cylinder width, it does **NOT** indicate a Z2 spin liquid.

The most interesting honeycomb phase we've found

J_1 - J_2 XY -- no z-direction terms in H

Varney, et. al, PRL 2011: Bose metal phase!

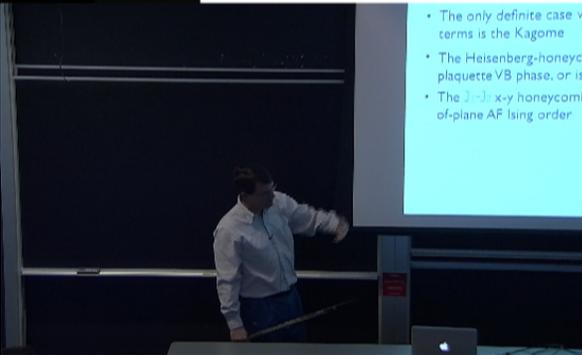


In the hard-core boson representation, the out of plane order is a CDW.
But: no n-n terms in H, which usually drive CDW! $|\langle S_z \rangle| \sim 0.14$

In simple mean field treatment, $E=0$. Is there a simple argument that this phase should occur?

Conclusions

- With DMRG, we are now able to map out rough phase diagrams quickly for some frustrated spin models.
- The only definite case we have found with J_1, J_2, J_3 terms is the Kagome
- The Heisenberg-honeycomb J_1 - J_2 model has a weak plaquette VB phase, or is nearly critical
- The J_1 - J_2 x-y honeycomb model has a surprising out-of-plane AF Ising order



- The only definite case w terms is the Kagome
- The Heisenberg-honeycomb plaquette VB phase, or is
- The J_1 - J_2 x-y honeycomb of-plane AF Ising order