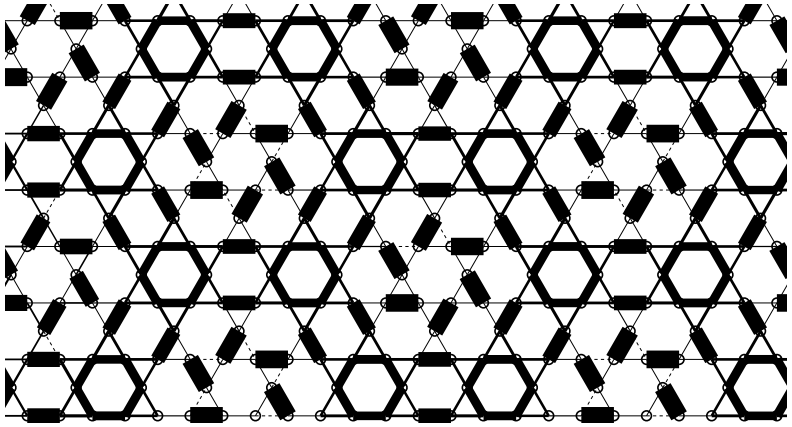
Spin Liquid Ground state of the S=1/2 Heisenberg model on the Kagome lattice

- Introduction; previous work
- DMRG techniques
- Spin Liquid versus the hexagonal valence bond crystal
- Energies
- Nature of the spin liquid
- Gaps

Collaborators: Simeng Yan and David Huse

Special thanks to Andreas Laüchli

A little history



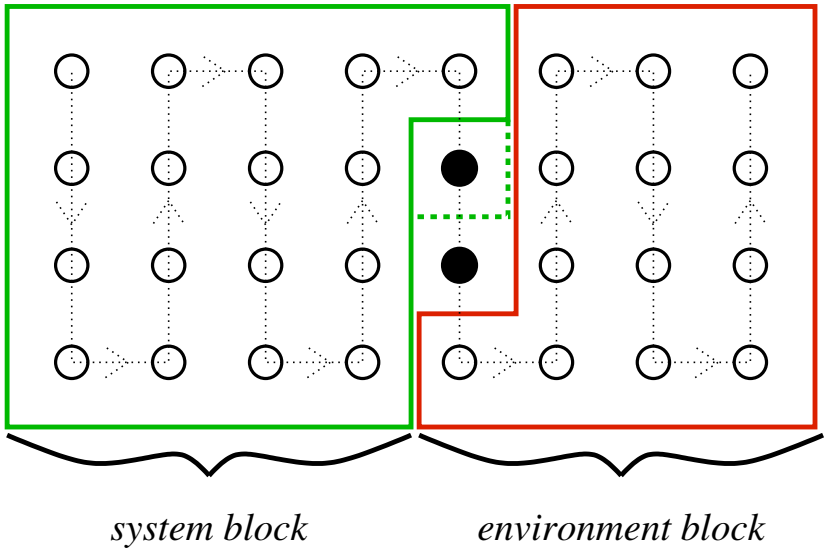
The S=1/2 Heisenberg Kagome systems has long been thought to be an ideal candidate for a spin liquid because of its high frustration. General agreement there is no magnetic order.

- Key question: is it a valence bond crystal or a spin liquid? What kind of VBC or SL?
- Three key approaches have supported a "hexagonal valence bond crystal" (HVBC) with a 36 site unit cell (Marston and Zeng)
  - Series expansions of Singh and Huse (E=-0.433(1))
  - MERA of Evenbly and Vidal (E < -0.4322 exact bound!)
    - Multiscale entanglement renormalization ansatz, a tensor product relative of DMRG capable of infinite 2D
  - Effective Dimer Model, Poilblanc et al (but SL close by)

- Favoring a spin liquid:
  - A gapless SL with a good variational energy (E = -0.429) with very few parameters was found by Hermele, Ran, Lee, and Wen.
  - A DMRG study by Jiang, Weng and Sheng found a spin liquid
    - They used fully periodic boundary conditions...
    - Largest systems had an E= -0.431
- Exact diagonalizations up to 36 sites give E ~ -0.438 on larger clusters
- Evidence overall seemed to favor the HVBC; higher energy than Lanczos attributed to finite size effects.

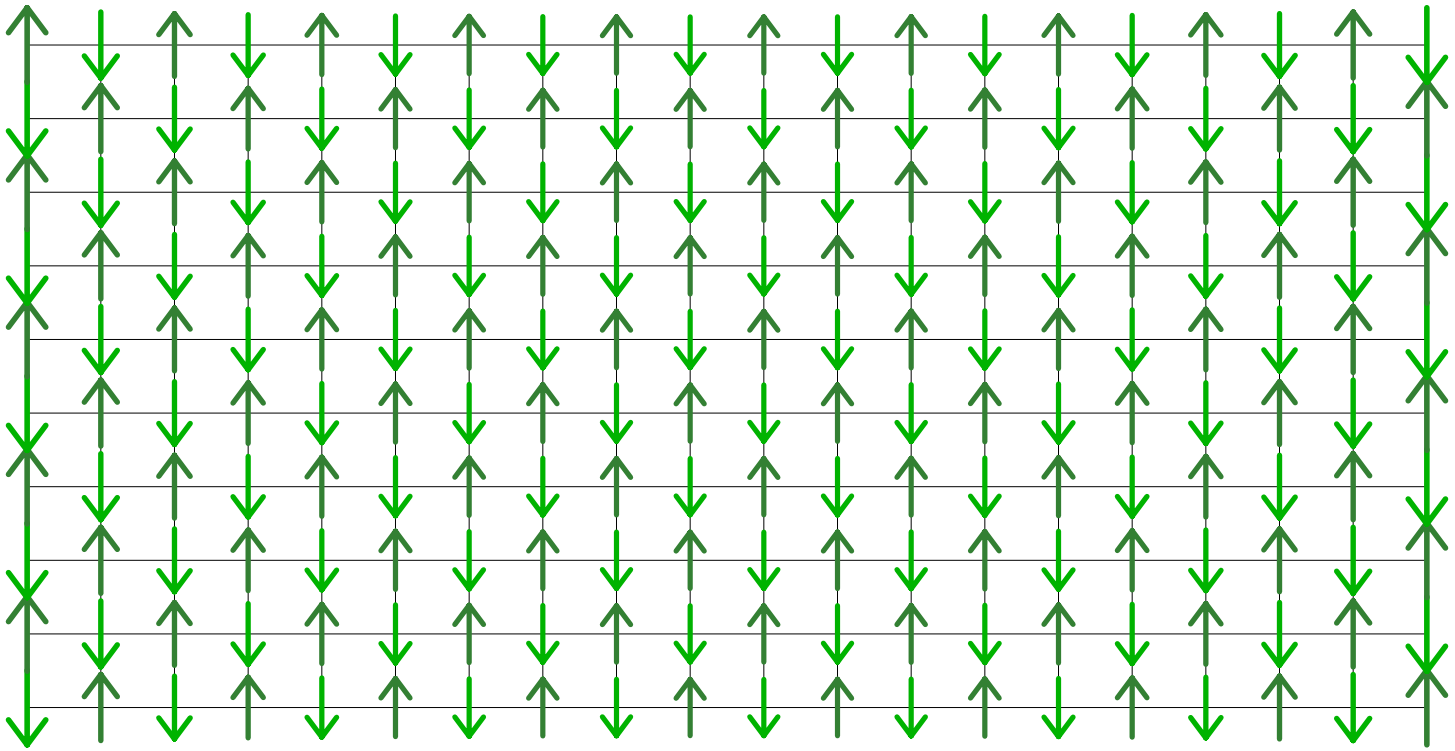
DMRG for Two dimensions

- 2D Lattice mapped onto 1D
- More sweeps needed



- Accuracy falls off exponentially with width (Liang & Pang 1994).
  - Now understood as consequence of QI "Area Law"
- Continued improvement in techniques (and computers) have allowed pretty big 2D systems...

Square lattice: benchmark against QMC



20 x 10

- Cylindrical BCs: periodic in y, open in x
- 21 sweeps, up to m=3200 states, 80 hours
- See White&Chernyshev, PRL 99, 127004 (2007)

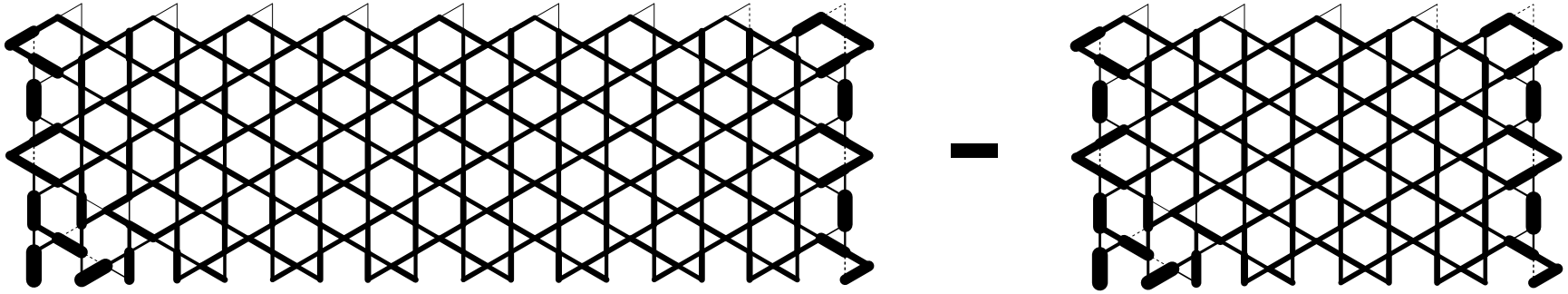
Energy, extrapolated to thermo limit using series of cylinders
-0.669444(5)

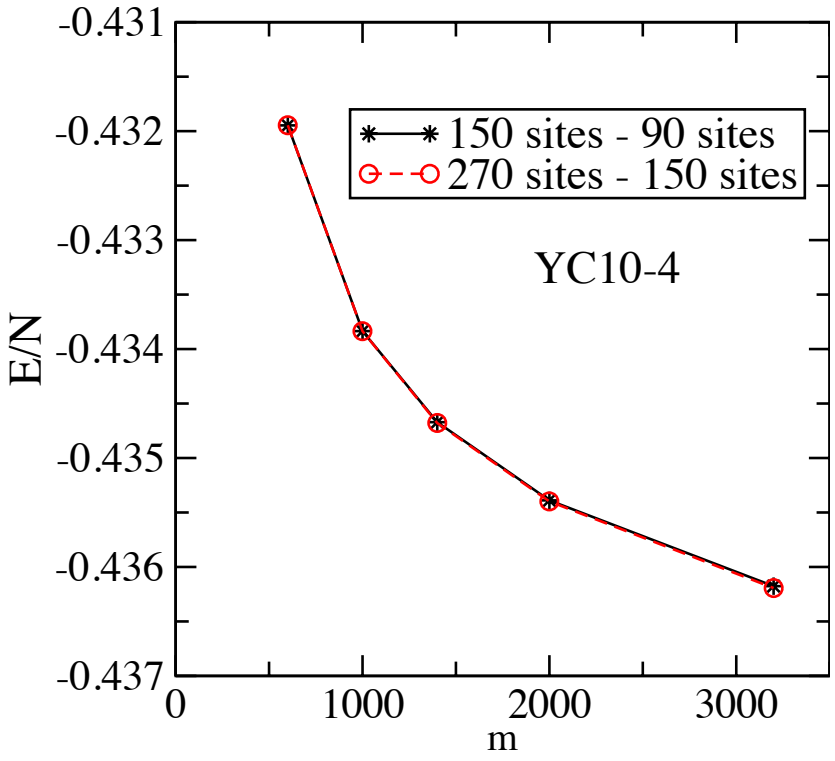
Sandvik, QMC (1997):
-0.669437(5)

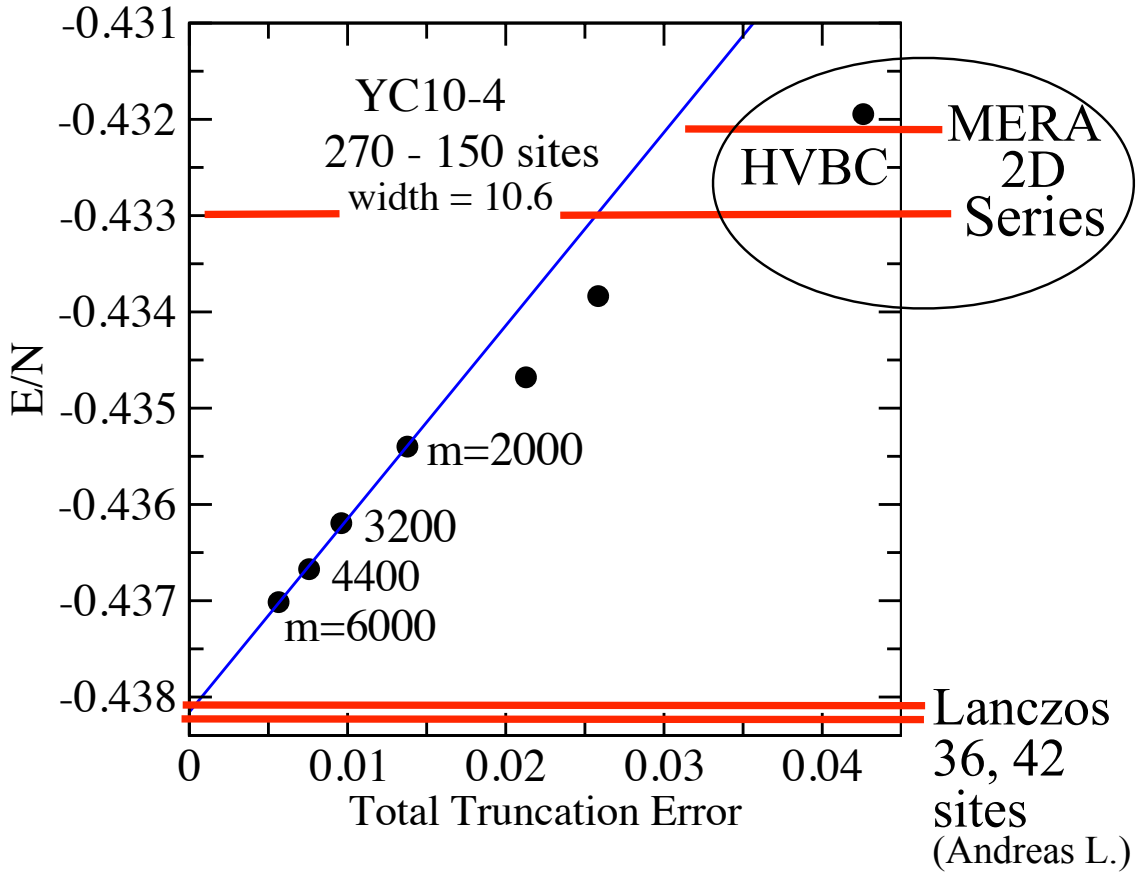
Practical Issues for Kagome

1. Metastability: getting stuck in a higher energy state (usually an issue only on wider cylinders)
   - Need to understand system and find a simple state close to the ground state to initialize DMRG
2. Strong dependence on width (and shift) of cylinders
   - Need to do many cylinders and understand patterns of behavior
3. Open edges--obtaining bulk cylinder behavior
   - This is a minor problem for this system
   - Open ends useful for pinning, selecting different topological sectors...

Ground state energies per site

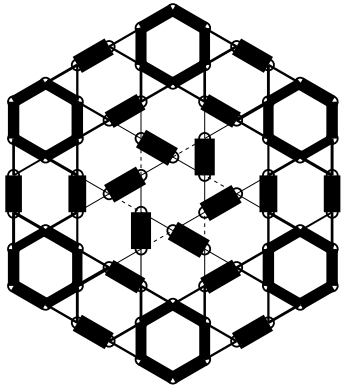


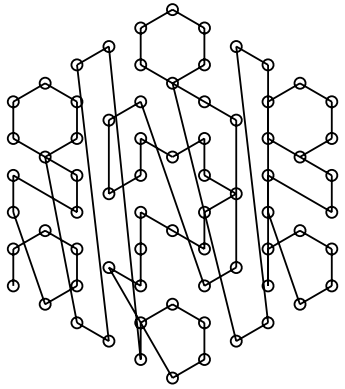




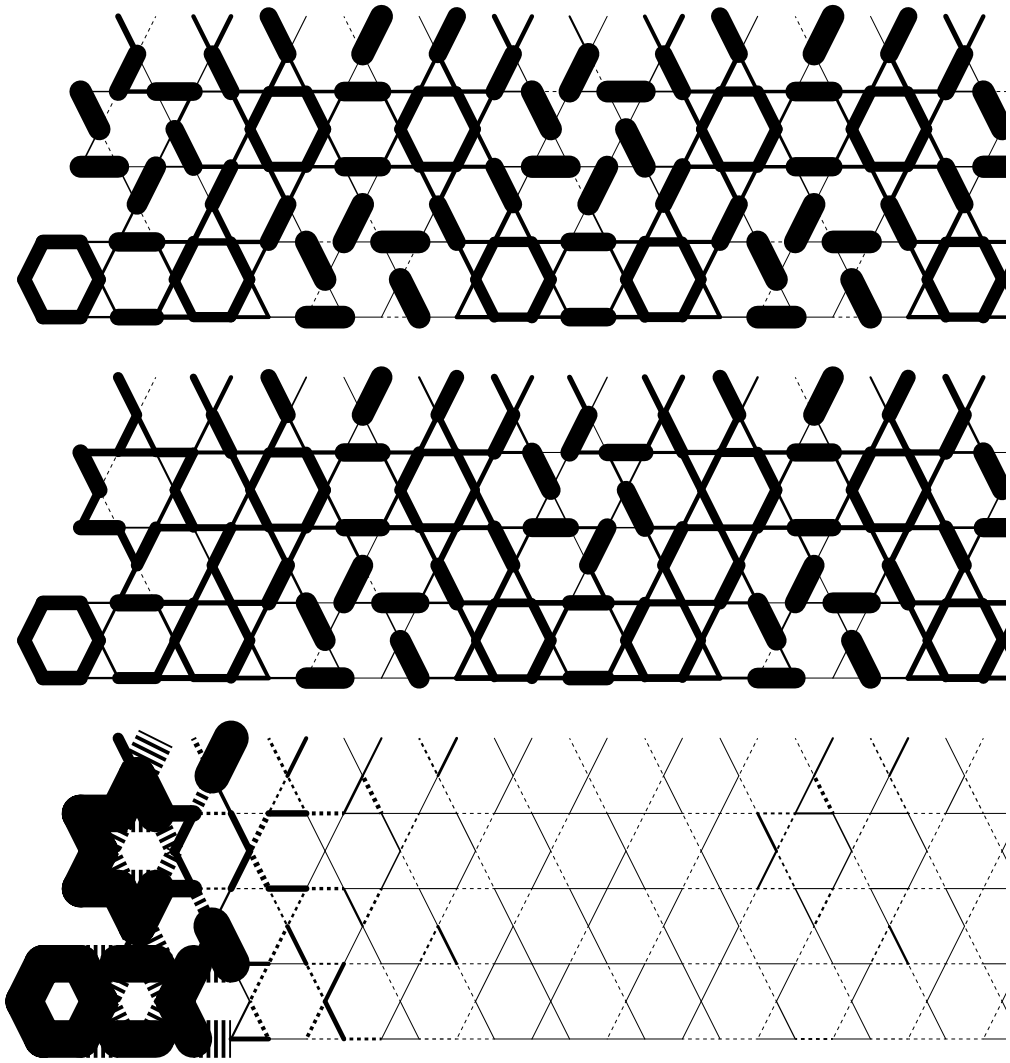
Direct comparison of HVBC and SL

- Given metastability, and possible biases, how can you rule out the HVBC?
  - Make all the biases favor the HVBC. Then, if it's unstable, you have strong evidence.
  - To make a strong bias: make the DMRG mapping to 1D follow the HVBC state!





    - Nonresonating HVBC stable at m=2
  - Other ways to promote HVBC: initial state (pinning "fields" = strong J's); edge shaped to match HVBC



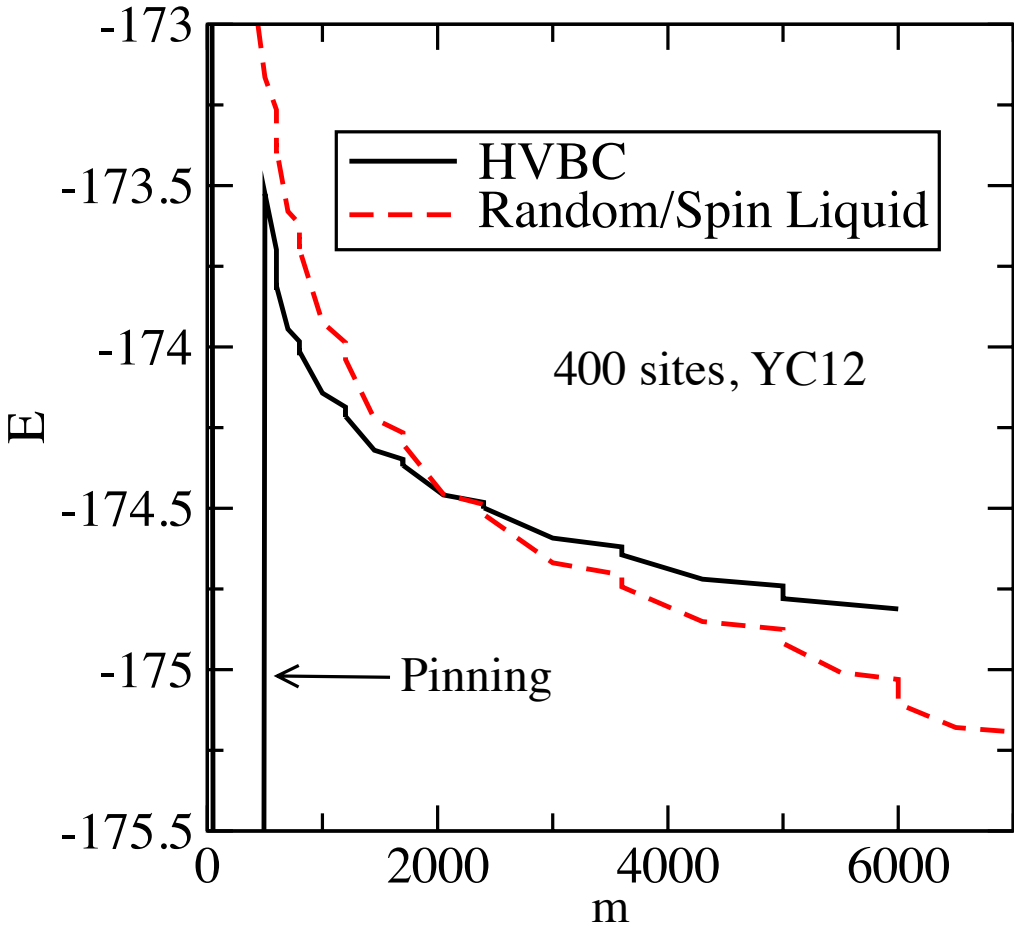
This run had special path and edges tuned to favor HVBC.

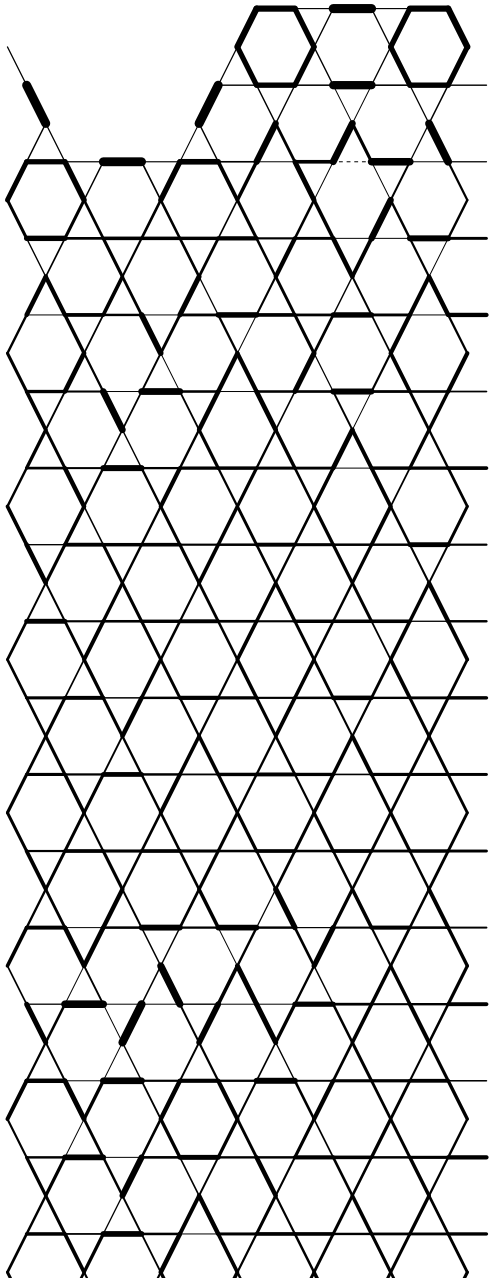
HVBC is metastable for small m, but for m ~ 2400 it transitions to the spin liquid

With standard path HVBC is immediately unstable, m ~ 100

SL energy for this cylinder, bulk:
-0.43824(2) XC8

Ruling out an HVBC on a width 12 cylinder





Comparison with HVBC Series expansion

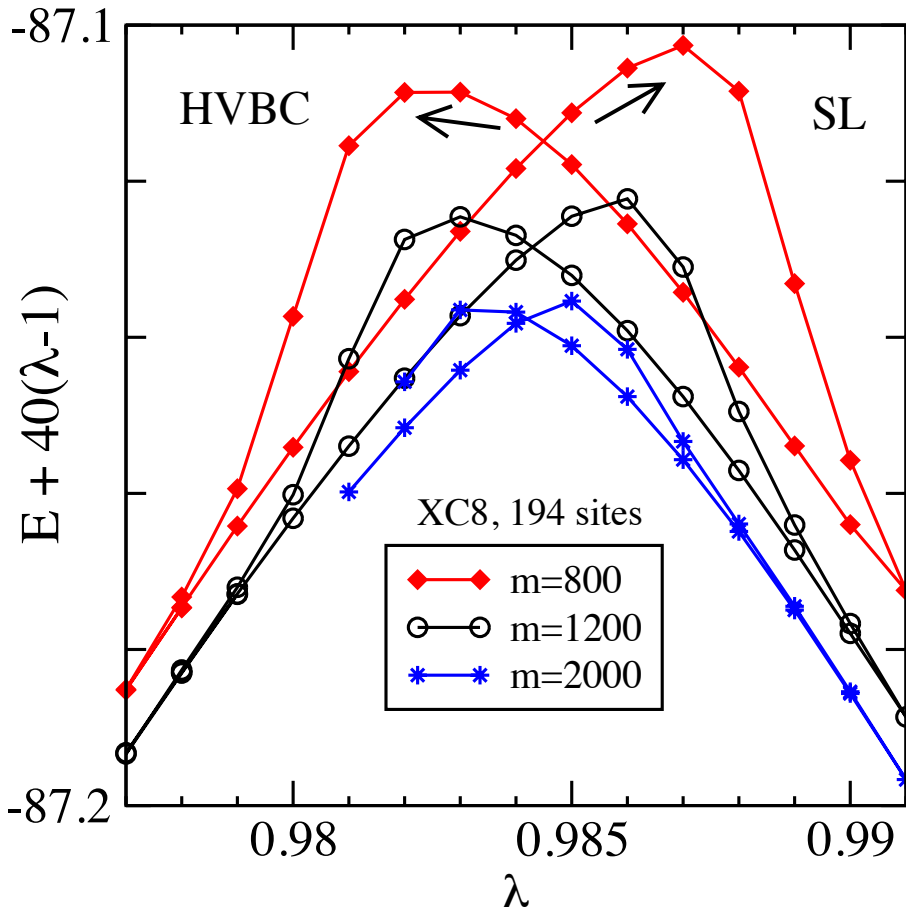
Series Expansion Hamiltonian:

$$H(\lambda) = \sum_{\text{strong bonds}} \vec{S}_i \cdot \vec{S}_j + \lambda \sum_{\text{weak bonds}} \vec{S}_i \cdot \vec{S}_j$$

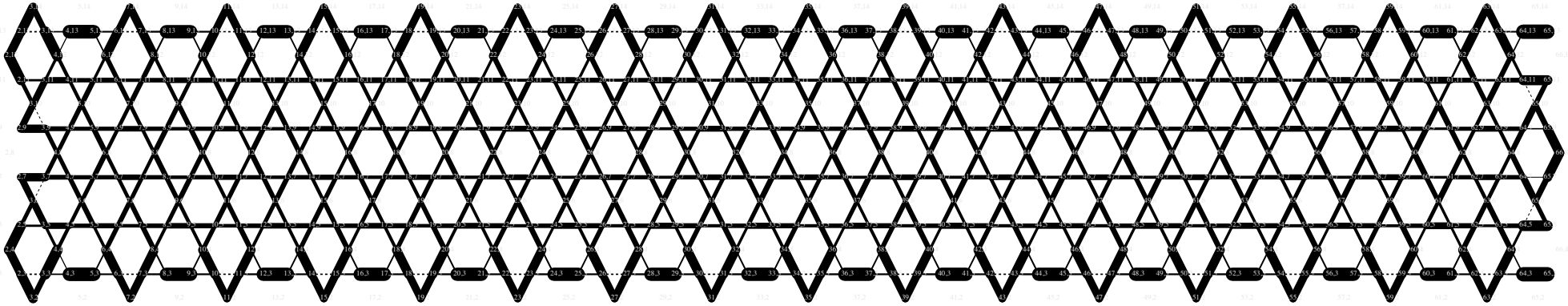
We can simulate H(λ) vs λ to look for a transition.
A "hysteresis plot" shows evidence for a first order transition separating the HVBC and SL at λ_c=0.984

For $\lambda < \lambda_c$, the series works fine: at λ=0.98 series gives E=-0.431(1), DMRG gives E=-0.4324.

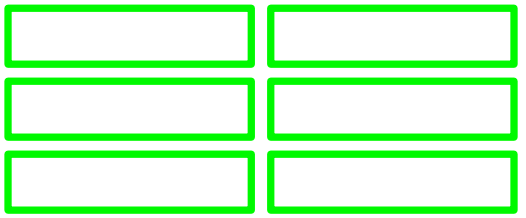
Thus the series estimate for 2D is probably good for the HVBC: -0.433(1)



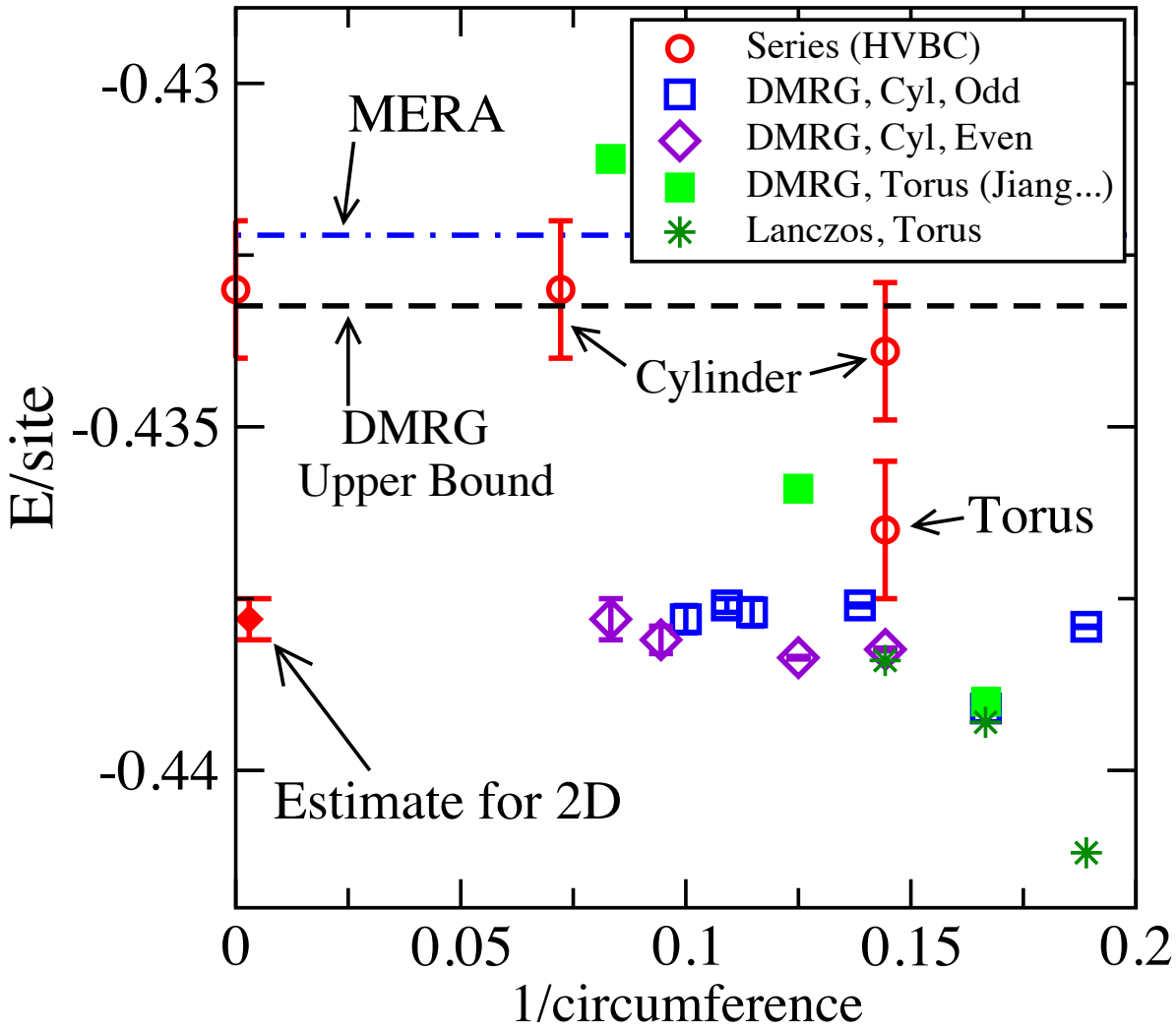
A Rigorous Upper Bound on the 2D energy



- A variational calculation like DMRG for an open cluster can provide a rigorous upper bound on the 2D energy.
- Given an open cluster of N sites, N even, which tiles 2D, then a product state of the cluster state over all tiles has energy E/N
- This is crude, with convergence as the inverse width.
- Previous best rigorous bound was from MERA, E/N = -0.43221. The spin liquid is so much lower than the HVBC we get a new best upper bound with N = 576, E/N = -0.433238.



Energies of various cylinders and methods

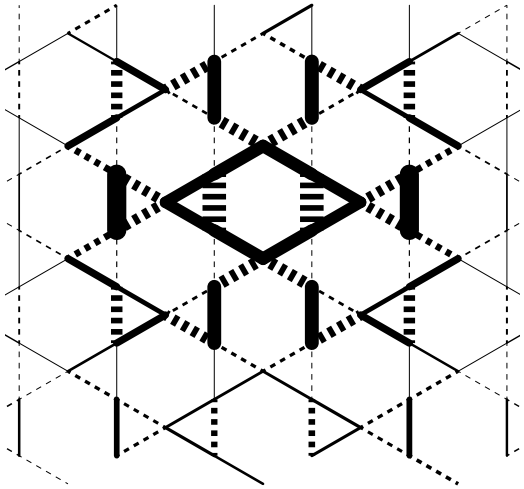


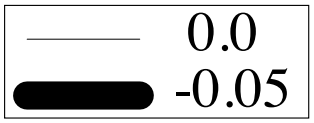
Nature of the Spin Liquid

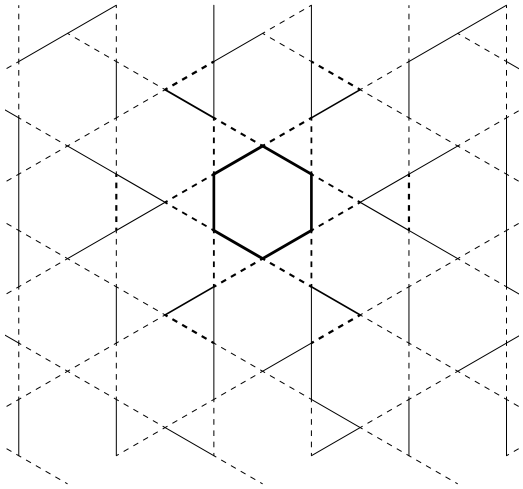
- A natural starting point is a nearest neighbor RVB state.
- The resonance of short loops significantly lowers the energy. The shortest loop that can resonate in the kagome is the hexagon, and much theoretical work has started with the perfect hexagons.
- However, we find that the 8 site loops are dominant in the spin liquid!

Response to small bond perturbations

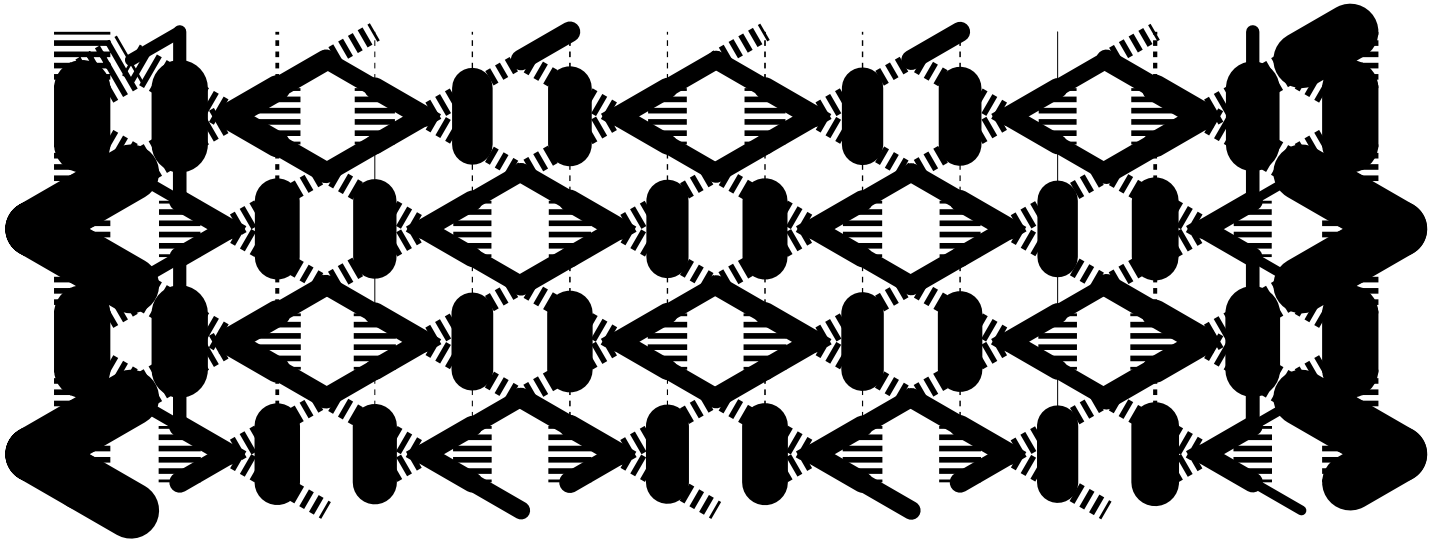
Response to 1% increase in J on one diamond





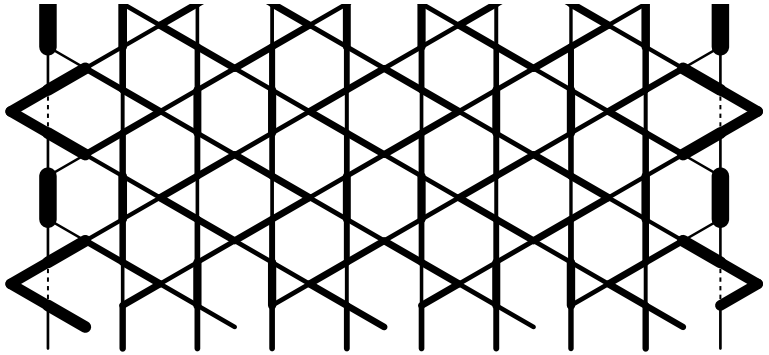


Response to 1% increase in J on one hexagon

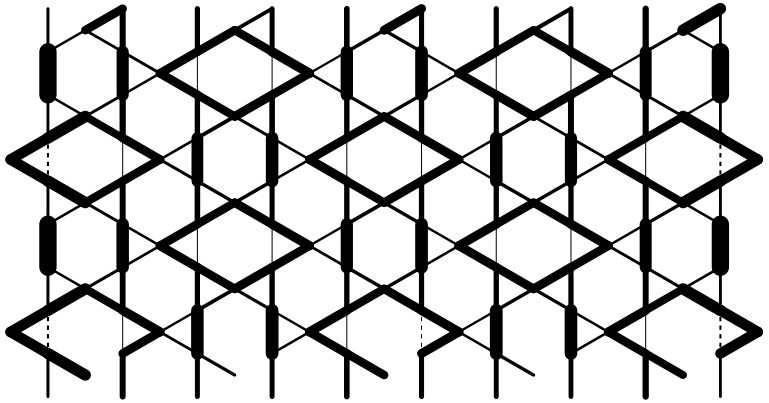


Response to 0.5% increase/decrease in J on fat vertical bonds: the "diamond pattern", which fits only on the even cylinders

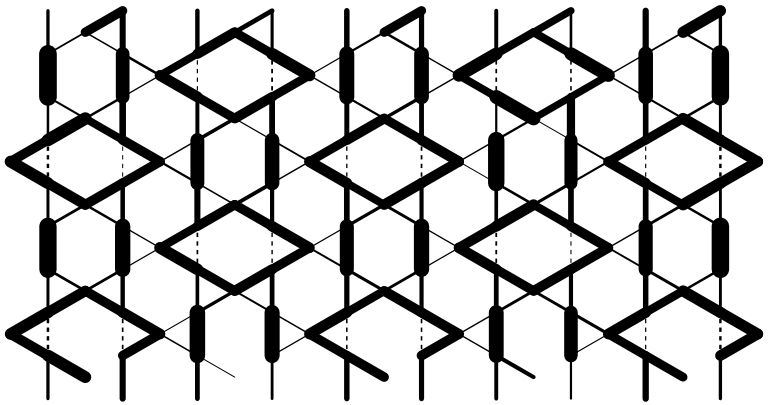
The diamond pattern provides the ideal DMRG initial state for the spin liquid



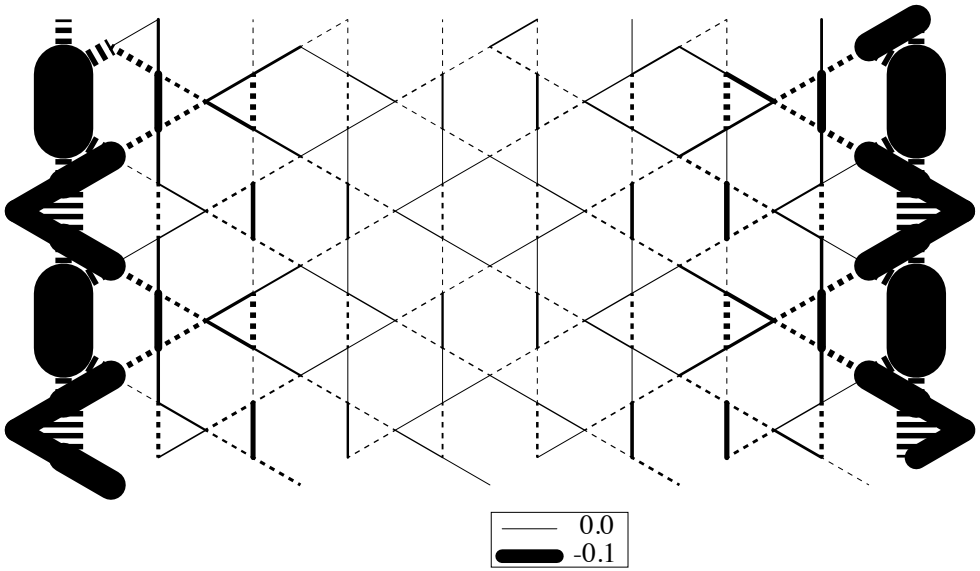
m=400
pinning
off



m=300
pinning field
still on

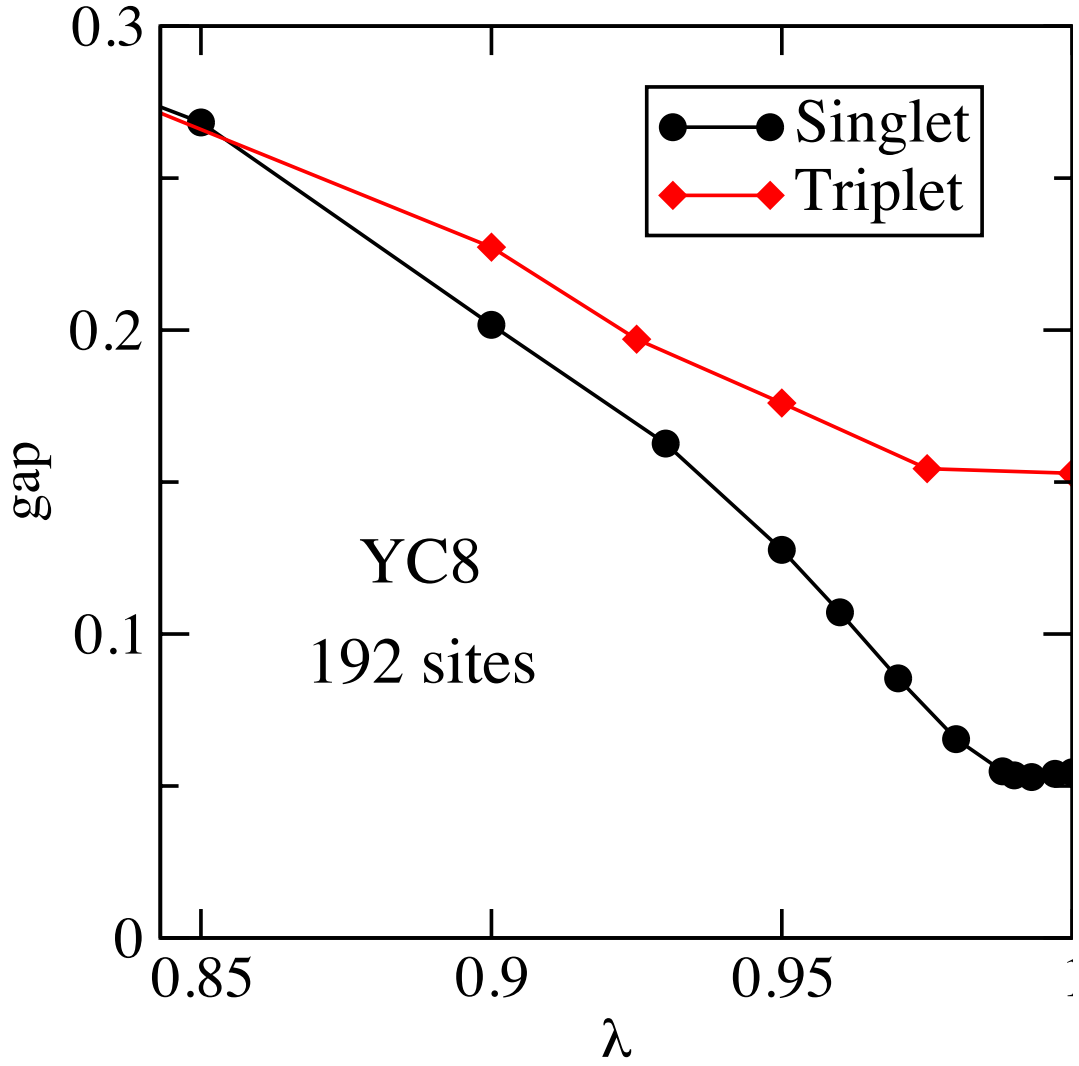


m=200
pinning field
on, 0.05



m=600

The diamond pattern VBC is continuously connected to the spin liquid with open gaps

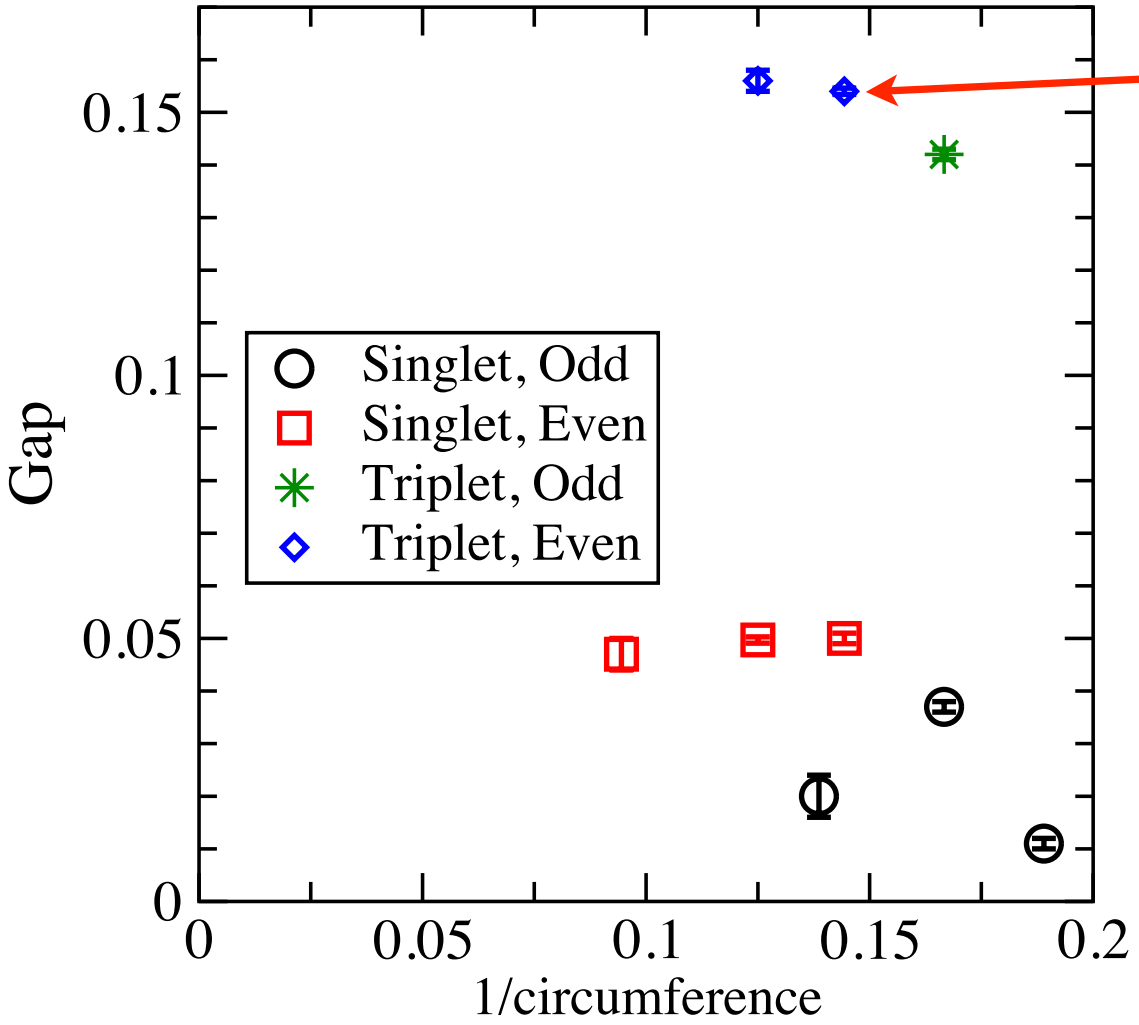


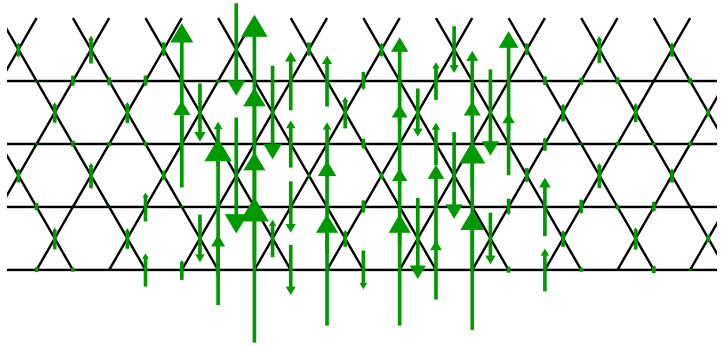
This utilizes an H(λ) that turns off all weak bonds in the diamond pattern.

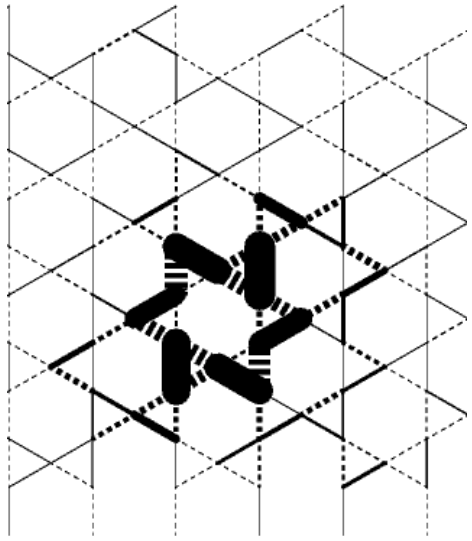
Gaps are O(1) near λ=0, and smallest near λ=1.

The diamond pattern at λ=0 is a product state, trivial topologically. What does this tell us about the spin liquid?

Singlet and Triplet Gaps

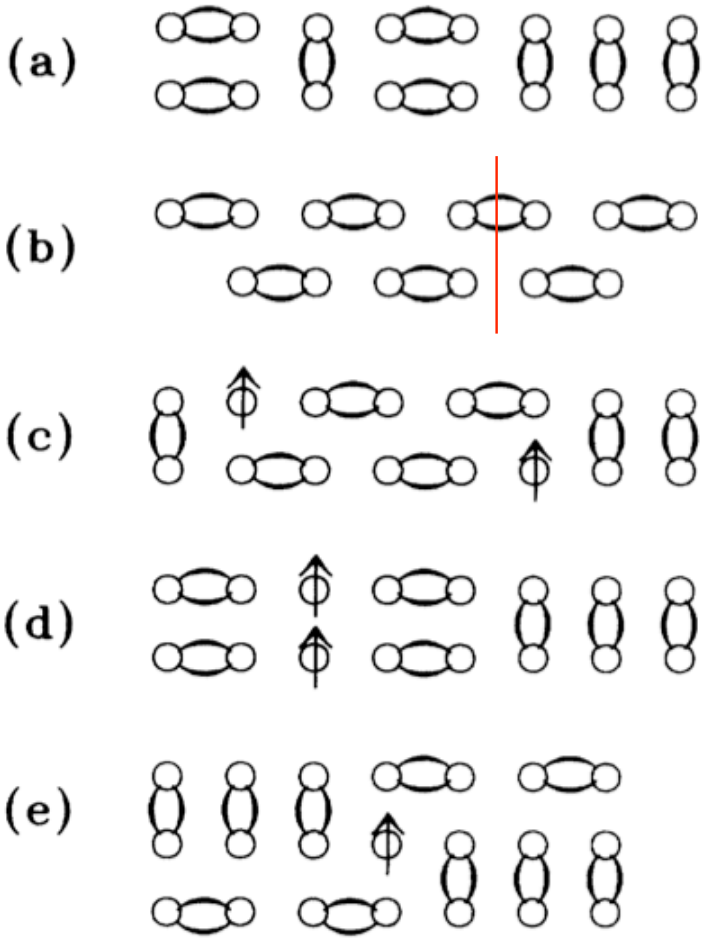






Singlet excitation
before delocalization

Odd vs Even Ladders/Cylinders



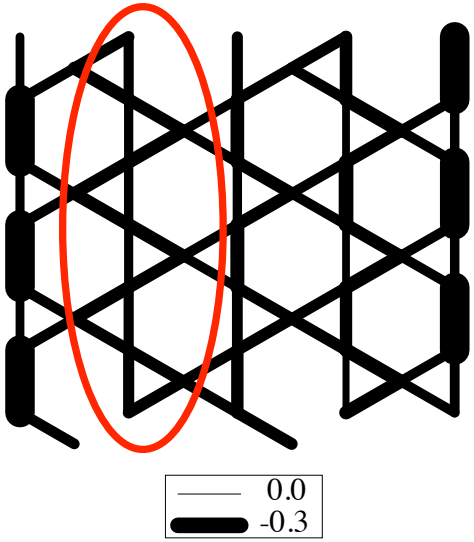
Ground state of an even ladder

Topologically odd state of an even ladder--the "staggered phase"

Two spinons

Bound spinons

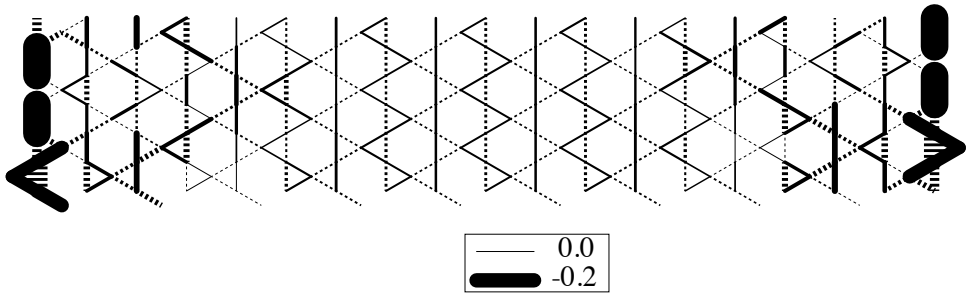
Odd ladder



Exchange Energy

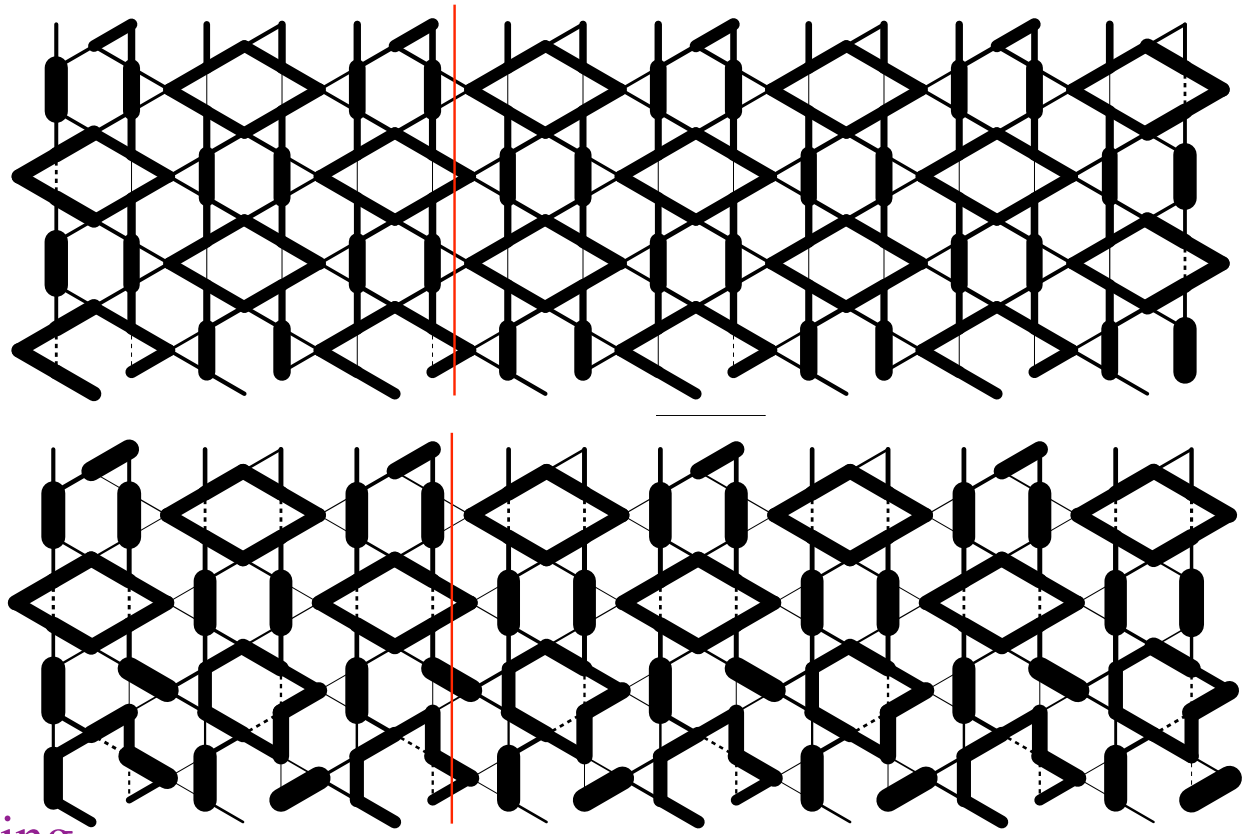
YC6: an odd cylinder

White, Noack, Scalapino, PRL 73, 886 (1994). Also similar: AKLT states



"Valence Bond Density Wave"

An odd topological state can be created by adding or subtracting sites from the open ends



Red path crosses two bonds (choose a dimer cover for each diamond)

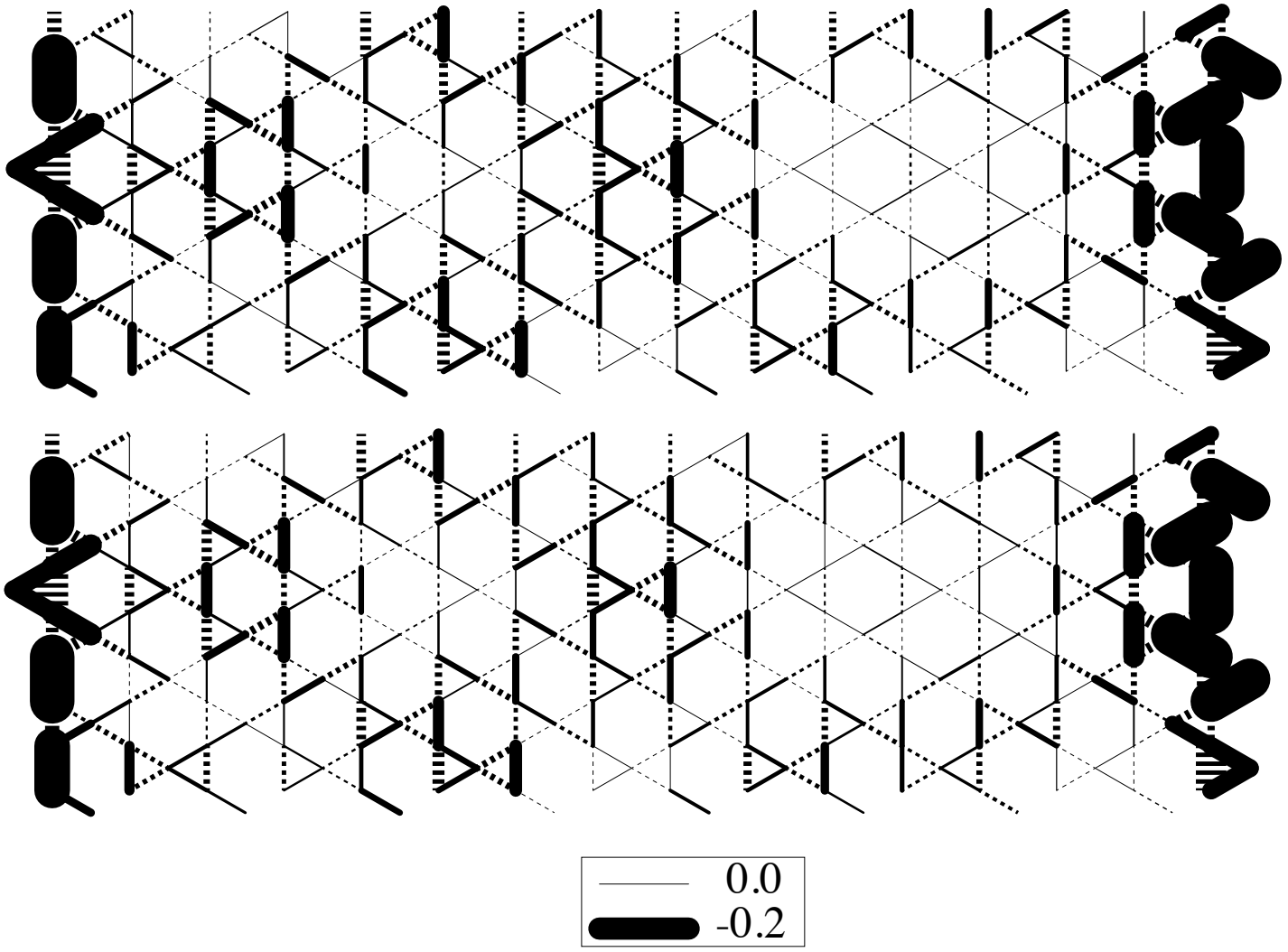
Red path crosses three bonds

Extra site

Missing site

These show initial pinning patterns.

The odd topological state on YC8



Two completely different runs, different initial states, but the same system, up to m=5000: identical irregular pattern!

This odd topo state has an excess energy of 0.00069(3) per site.
This "spinon string" also seems to have excited states, with energies ~0.01 above it for this length. Note: a torus has both topo states!

Summary

- We have presented strong evidence that the ground state of the Kagome system is a spin liquid with an energy comparable to that of exact diagonalization on small clusters.
- A first order phase transition appears to separate the HVBC from the spin liquid.
- The spin liquid is a short ranged RVB with strongly weighted 8 site resonant loops, underweighted 6 site loops.
- Singlet gap ~0.05; triplet gap 0.15 on width 8 cyl.
- It has interesting topological structure and excitations which are just beginning to be understood.