Title: Frustrated Magnets and Quantum Spin Liquids

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Abstract: A
quantum spin liquid is a solid whose atoms have magnetic moments but, because
of quantum fluctuations, these moments fluctuate like a liquid even at zero
temperature. Two dimensional spin liquids have been suggested as a way to
produce high temperature superconductivity, and to build quantum computers. Just as helium is the only element which is a liquid at zero temperature,
2D spin liquids have been extremely difficult to find, despite decades of
effort, raising the question, do realistic spin liquids even exist?
Recently, apparent spin liquids have been found experimentally, stimulating theoretical
work to find simple model Hamiltonians of frustrated spin systems that have
spin liquid ground states.

In this talk, I will give a broad overview of spin liquids and then focus on
our simulations of the kagome Heisenberg model, a simple, realistic model of
some of the recent experimental spin liquids, where we find a spin liquid
ground state.

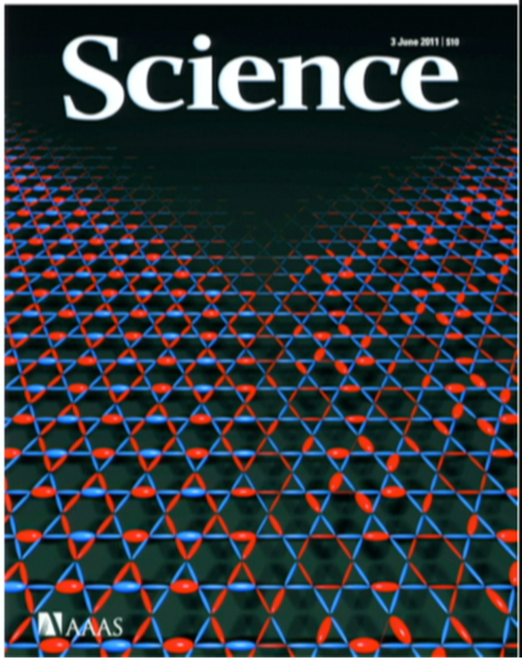
Frustrated Magnets and Quantum Spin Liquids

Steve White, UC Irvine

Collaborators:
Simeng Yan (UCI) and David Huse (Princeton)

Outline

- What is a quantum spin liquid?
- Why are they so interesting?
- The Kagome Heisenberg model--a realistic model with a spin liquid ground state



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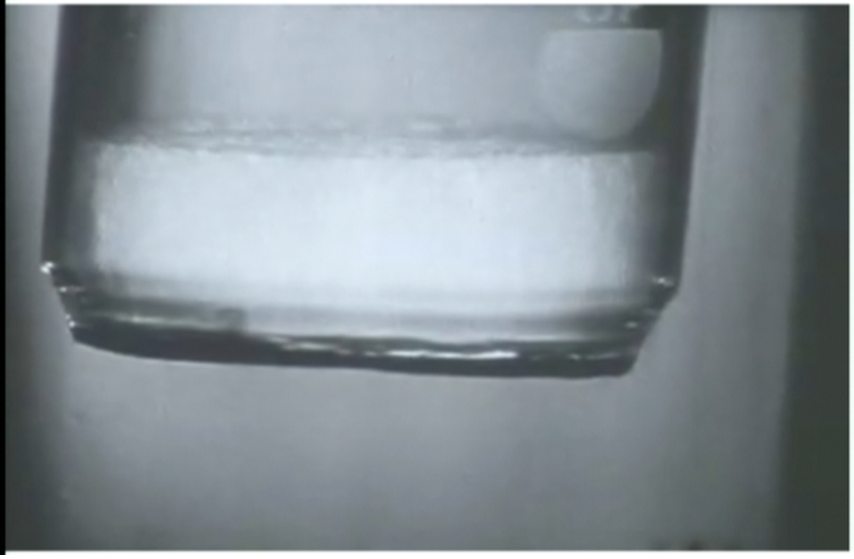
Here's a better version of this question: Is there any element or substance which does not order even at absolute zero?



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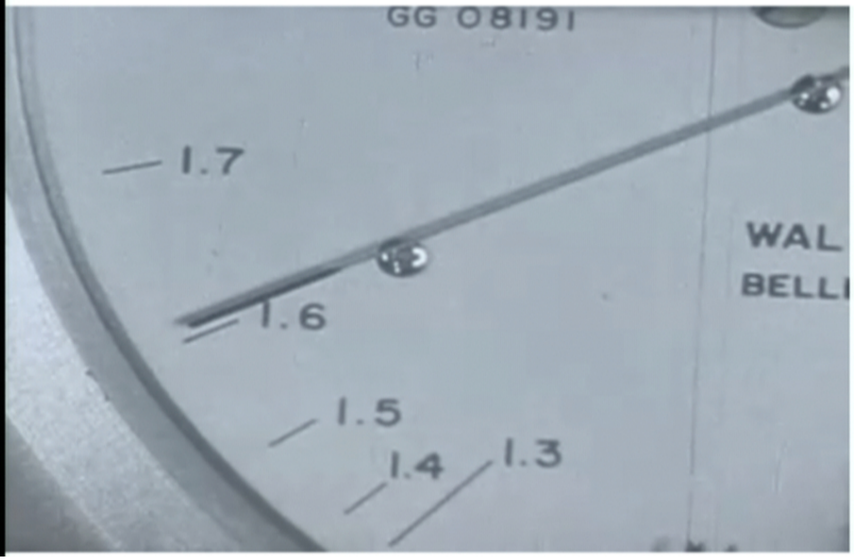

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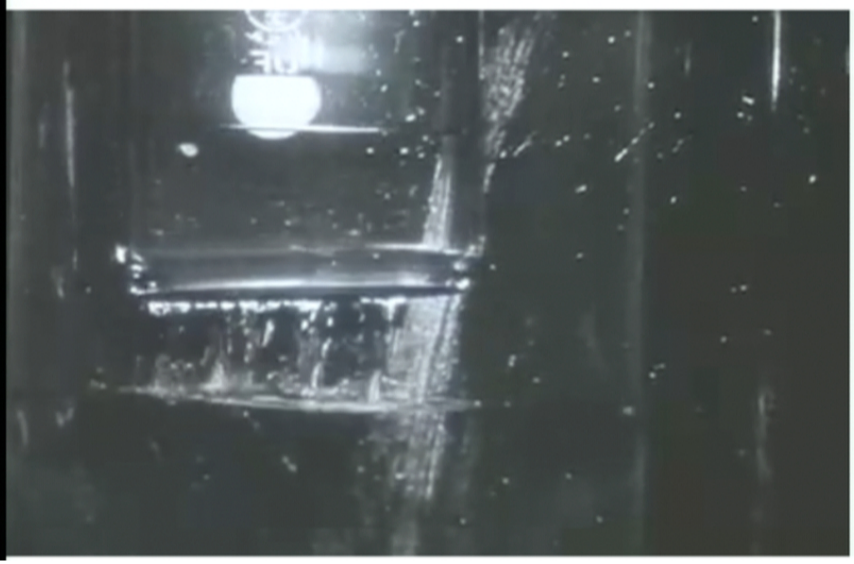

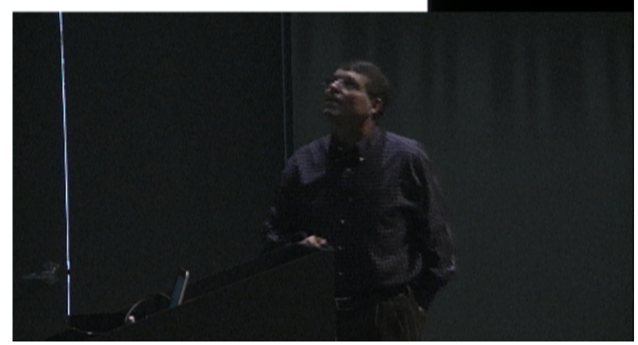

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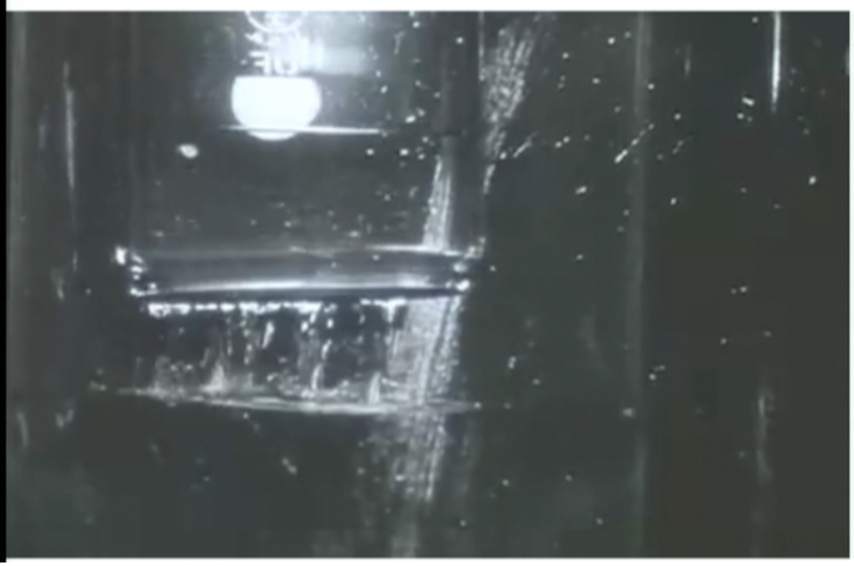
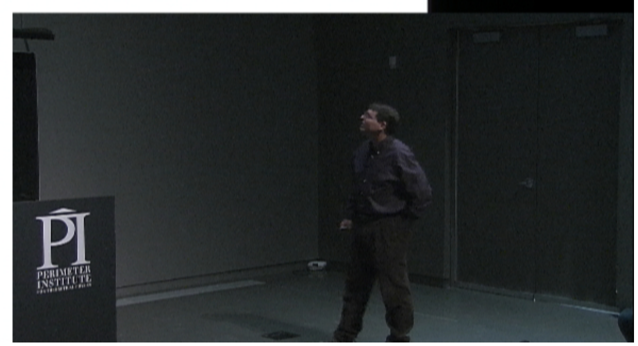
Let's change the question again for a condensed matter physicist: is there any magnetic material which does not magnetically order even at absolute zero?





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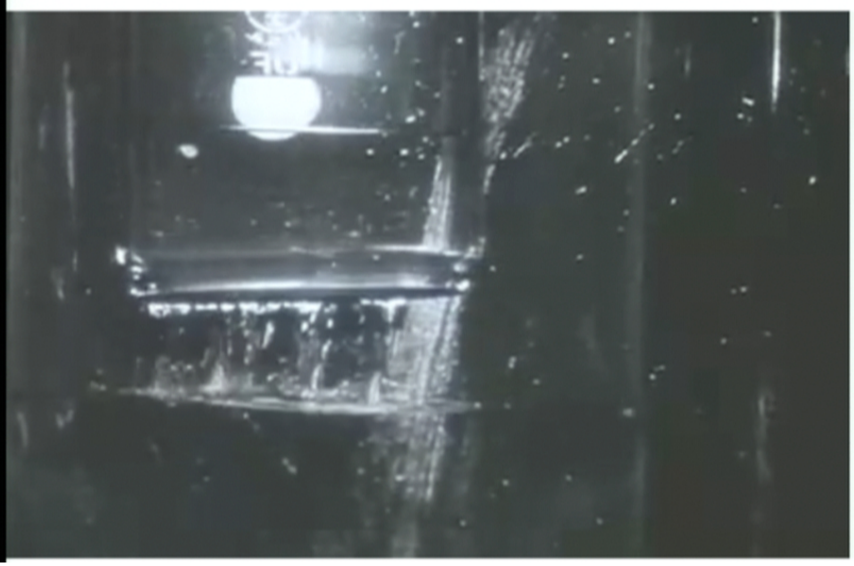
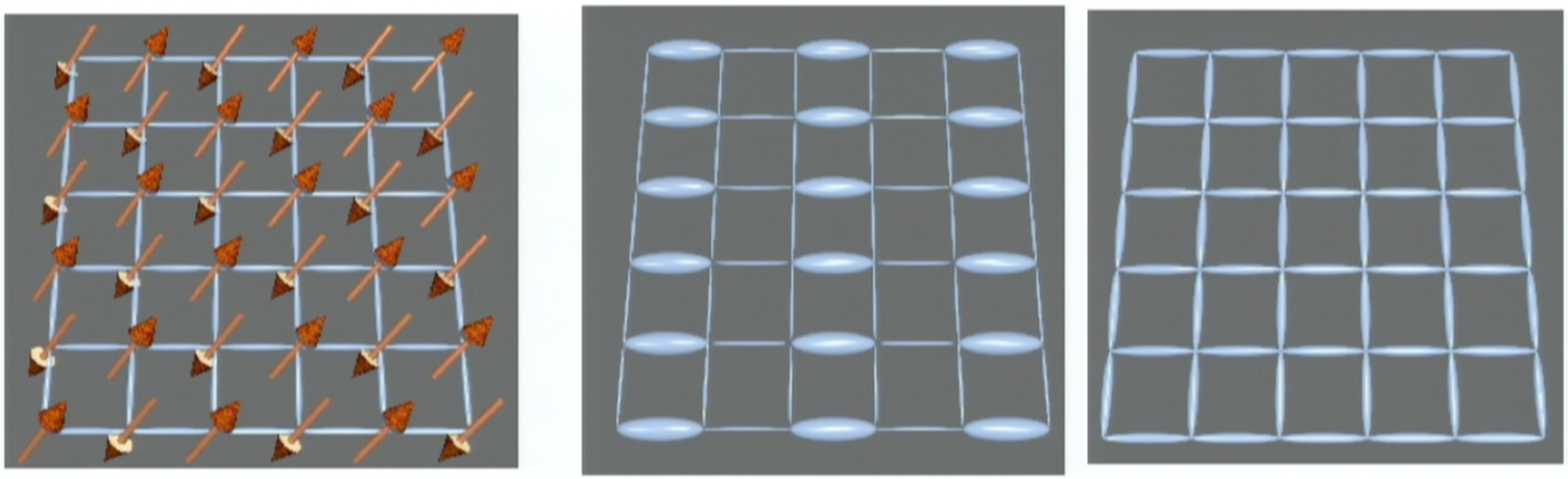


Maybe! Yes! Such a system would be called a spin liquid.

Quantum Spin Liquids: what are they?

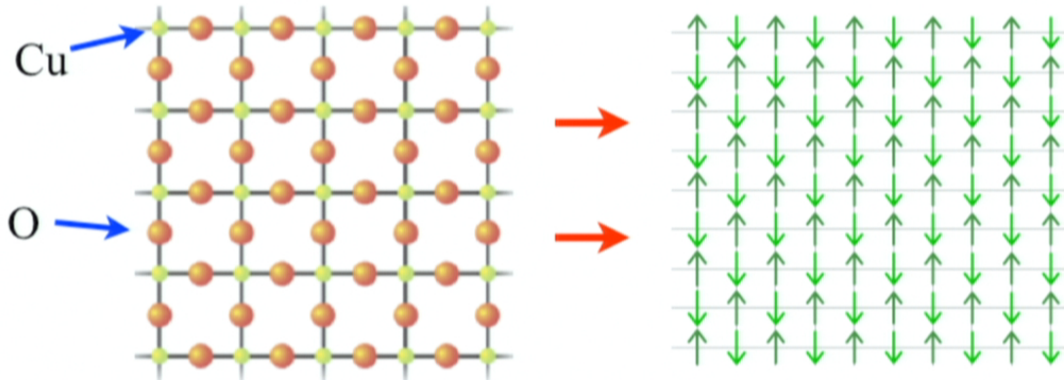
- Starting ingredient: a lattice of localized spins. ~~Metals~~ ~~Band Insulators~~
- Then (at least) three classes of possible <u>ground states.</u>



Magnetic order	Valence bond order	Spin liquid
$\langle\psi\|\vec{S}_i\|\psi\rangle \neq 0$	$\langle\psi\|\vec{S}_i \cdot \vec{S}_j\|\psi\rangle \neq const$ $VB = \frac{1}{\sqrt{2}}(\|\uparrow\downarrow> - \|\downarrow\uparrow>)$	No broken symmetries

- A spin liquid has no order at T=0 because quantum fluctuations overcome all tendencies for order.

Undoped cuprates (high T_c superconductors): local magnetic moments but not a spin liquid



Planar cuprate

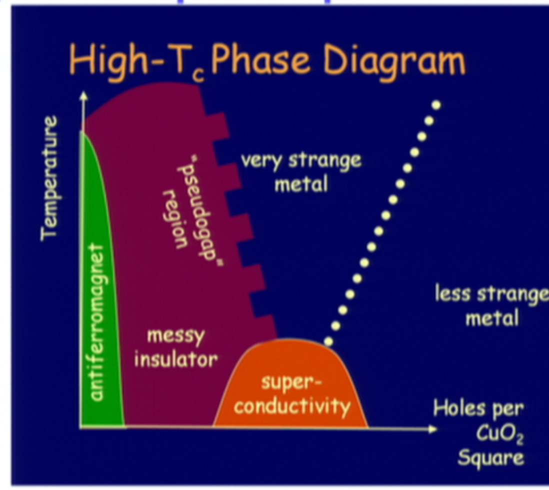
2D square lattice S=1/2 Heisenberg model

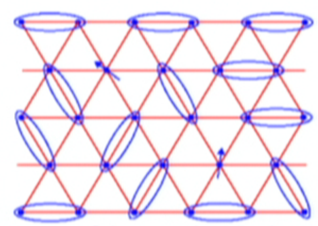
$$\mathcal{H} = J \sum_{<i,j>} \mathbf{S}_i \mathbf{S}_j$$

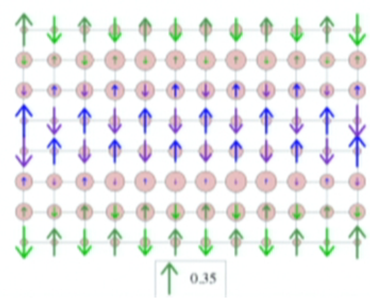
- This model has no exact solution--but it is well-understood through the combination:
  - Approximate analytic theory (esp. NLσM, Chakravarty, Halperin, & Nelson)
  - Numerical simulations (esp quantum Monte Carlo)
  - Experiments
- Key property: antiferromagnetic order: $|\langle \vec{S}_i \rangle| \approx 0.307 \neq \frac{1}{2}$

High temperature superconductivity and spin liquids

- Undoped: |S| reduced by 40%: proximity to a spin liquid?
- Phil Anderson: doping could induce a spin liquid with the singlet pairs already there!
  - Superconductivity arises naturally.
- "resonating valence bonds" (RVB), an idea dating back to Linus Pauling.
- This led to a big surge in interest in spin liquids.
- Eventually, interest waned...
  - 2D systems with spin liquid ground states were very hard to find
  - Competing ideas arose to explain the disappearance of AF order, including "stripes"







White & Scalapino

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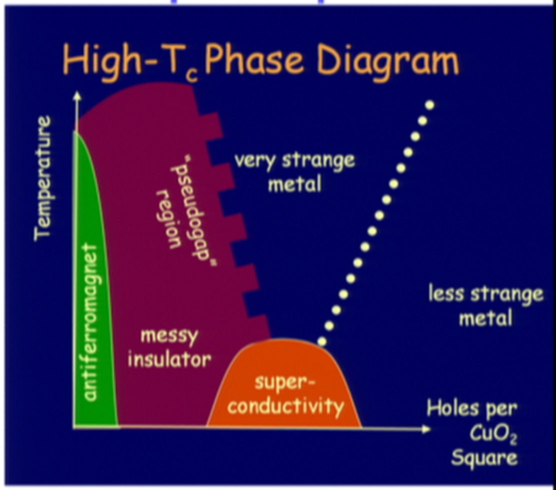
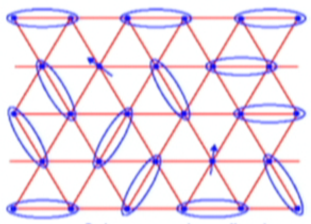
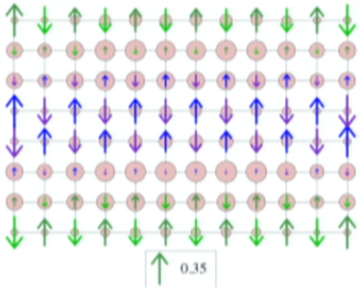






White & Scalapino

Spin liquids, the next generation

Recently there has been a new upsurge in interest in spin liquids. A few of the reasons:

- New materials, new theories
- Topological order (Wen) and possible topological quantum computing (Kitaev)
- Exotic fractional excitations--anyons

Xiao-Gang Wen

Even more recently:

- Integration of entanglement and other ideas from quantum information into condensed matter
    - Characterize exotic states
    - Identify hidden transitions
    - New methods to numerically simulate quantum states
    - Positive identification of spin liquids through numerical simulation!

Alexei Kitaev

Kagome systems: funny names

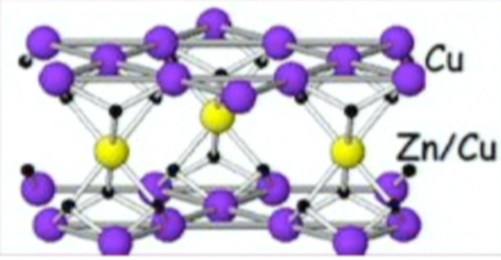
Kagome: Is it the name of a Japanese physicist?

No! It's a Japanese basket!

$ZnCu_3(OH)_6Cl_2$: the most interesting current Kagome material. Is it named after a person?

Yes, with both first and last names!

Herbertsmithite!



- No magnetic order down to fractions of 1K; it appears to be a spin liquid
- Complications: high concentration of impurities?

What is the right model?

How do you make a spin liquid?

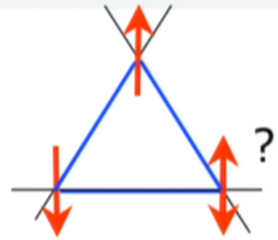
- Suppose you didn't know about superfluid He: how would you know where to look for a quantum liquid?
  - KE vs PE
  - So you have two "knobs" to turn: low mass, weak interactions
    - He is the natural candidate
- Can we turn a knob for spins to increase the KE, decrease the PE?

$$\vec{S}_i \cdot \vec{S}_j = \underbrace{S_i^z S_j^z}_{\text{"PE"}} + \frac{1}{2}\underbrace{(S_i^+ S_j^- + S_i^- S_j^+)}_{\text{"KE (spin flips)"}}$$

  - The knob for KE/PE is usually "stuck". And, if you turn up the KE x-y knob, the order rotates to that direction and it is the new PE.
  - Other knobs:
    - Few neighbors/1D
    - Frustration

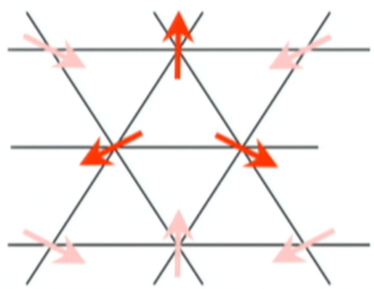
Frustration

Frustration: triangular lattice structure prevents satisfying all bonds



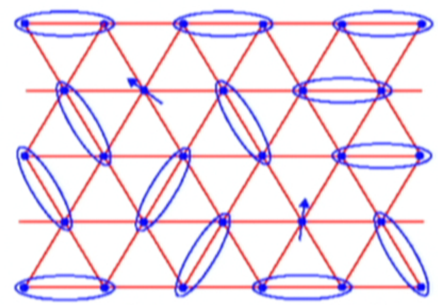
Example: the triangular lattice:

Classical Spins →



120° order

Anderson's original RVB proposal was for the triangular lattice



RVB state $= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

P.W.Anderson, *Mat. Res. Bul.* **8**, 153 (1973).
P.Fazekas and P.W.Anderson, *Phil Mag* **30**, 23 (1974).

Unfortunately, the triangular lattice has 120° magnetic order.

Numerical approaches

- Exact diagonalization of small clusters (Lanczos method, sparse techniques exploiting symmetries)
  - Exponential growth in Hilbert space limits sizes, $N_{state} \sim 2^N$
- Quantum Monte Carlo: frustration ⇒ sign problem

Fermions:

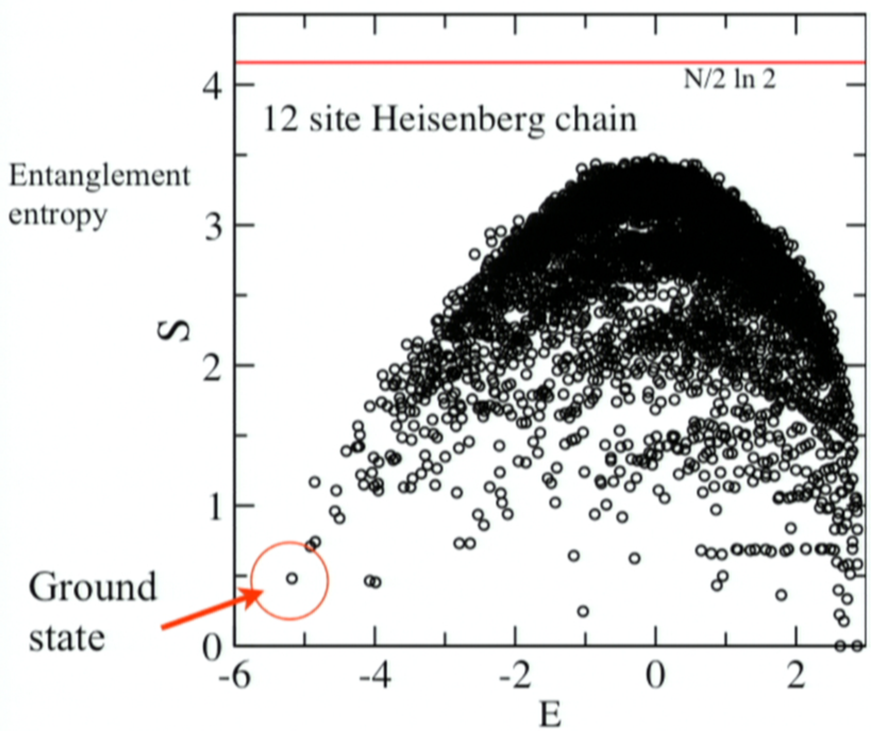
$\psi \rightarrow -\psi$

Negative Probabilities

- Low Entanglement methods (DMRG, PEPs, MERA)
  - Density Matrix Renormalization Group: originally based or RG ideas, not entanglement
  - Now understood as the natural low entanglement approach for 1D

Ground states have low entanglement!

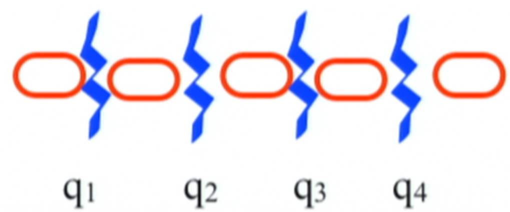
(compared to the horribly high entanglement they could have)



Von Neumann Entanglement entropy S for every eigenstate

Why? <u>The short answer:</u> high entanglement doesn't help reduce the energy!

Low entanglement ⇒ few quantum fluctuations across a cut ⇒ representation with a few states ⇒ efficient "matrix product state" representation of the ground state

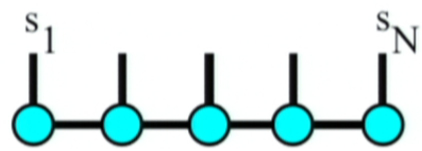


Matrix Product States = DMRG

$$\Psi(s_1,s_2,..s_N) \approx A^1[s_1]\, A^2[s_2]\, \ldots\, A^N[s_N]$$

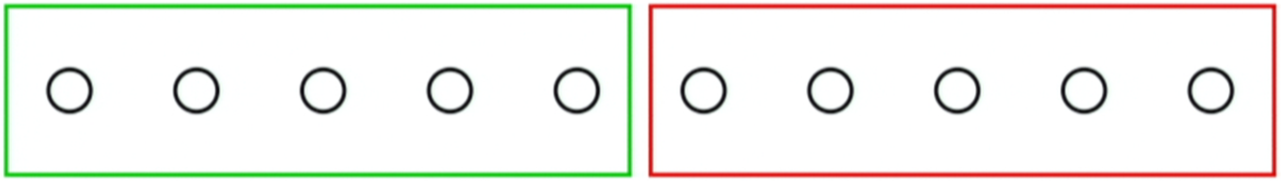
Exp'ly large

2^N



Highly compressed

$N\, m^2$



Sweeping

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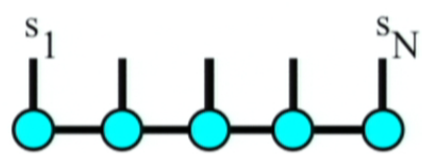

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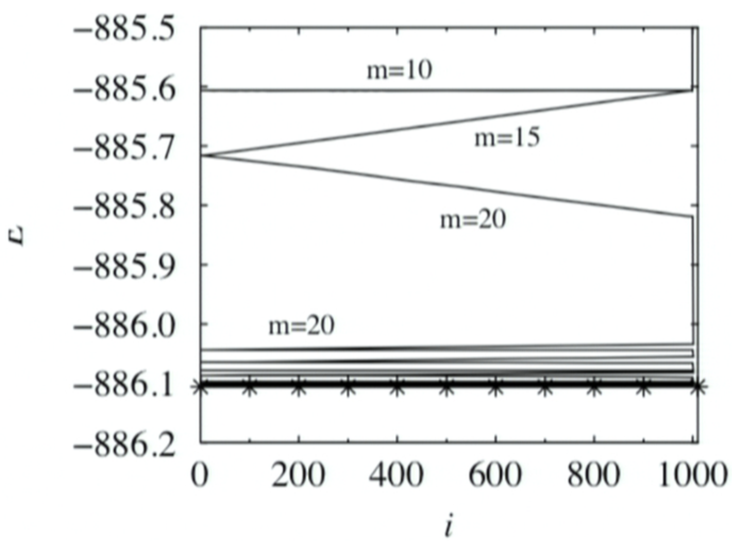
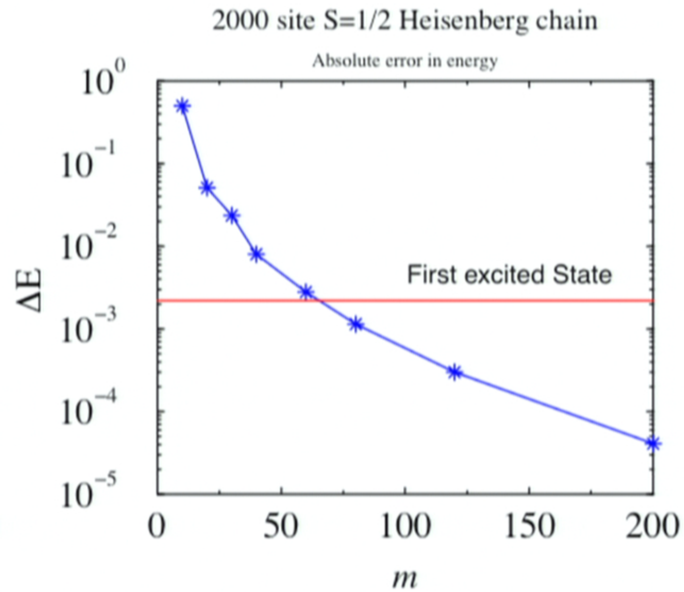
Sweeping

DMRG Convergence in 1D

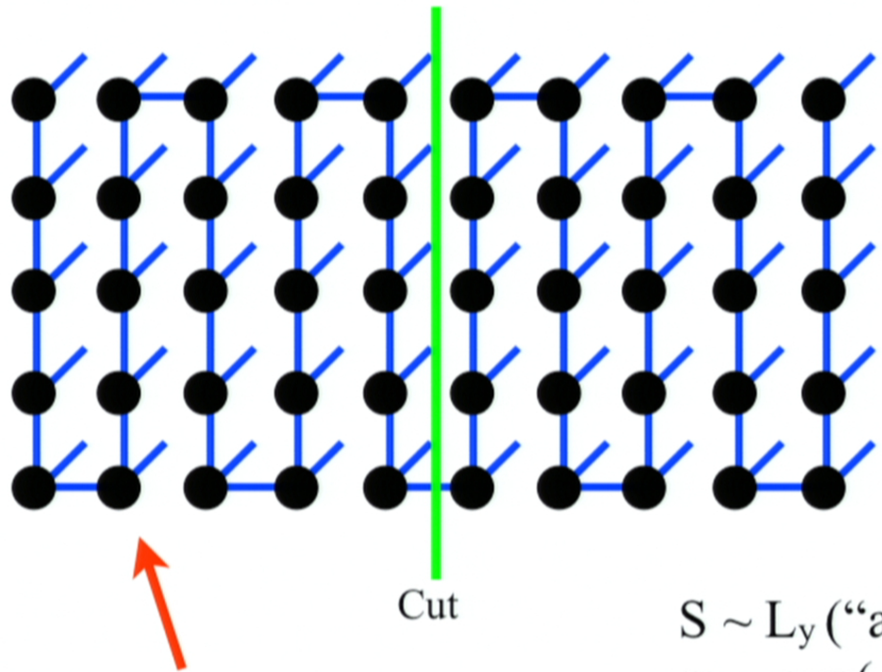




Comparison with Bethe Ansatz

2D algorithms

- Traditional DMRG method (MPS state)



$S \sim L_y$ ("area law")

$m \sim \exp(a\ L_y)$

Calc time: $L_x L_y^2 m^3$; allows $m \sim 10000$, $L_y \sim 10\text{-}12$

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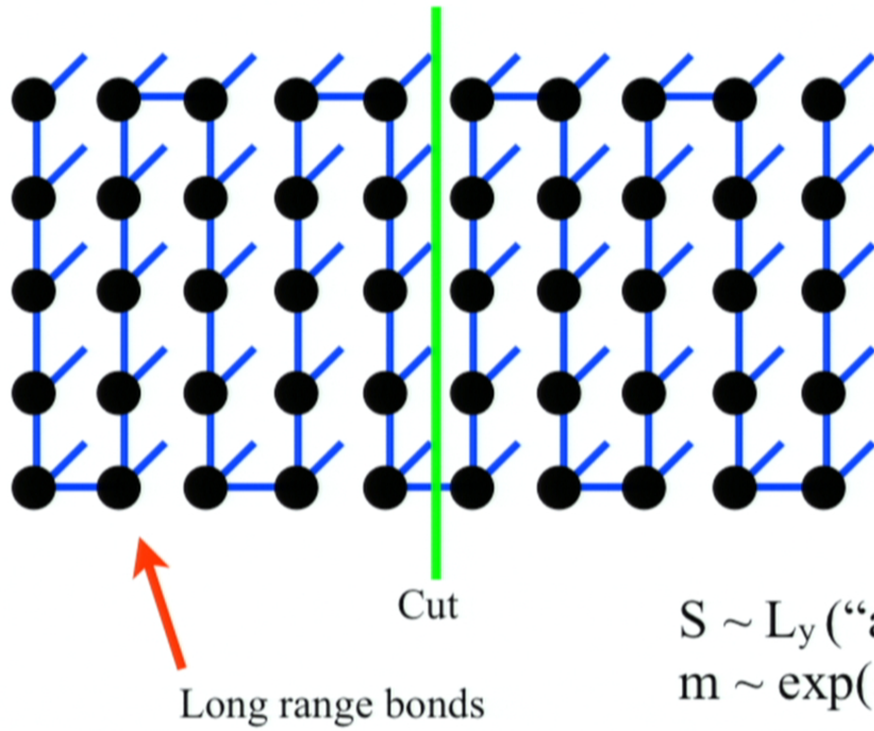

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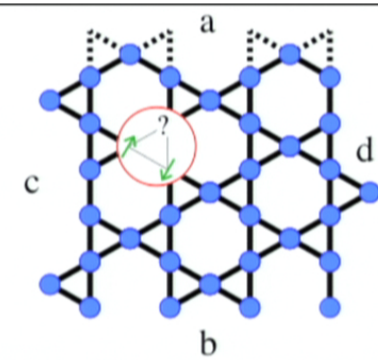
Kagome Basics



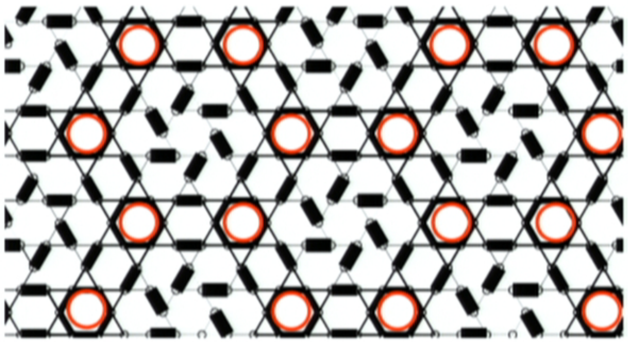
- The Heisenberg model on the kagome lattice is one of the most frustrated systems
  - Without frustration, magnetic order
  - Much more frustrated than the triangular lattice
- The kagome lattice has a small coordination z=4

- It has an exponentially large number of degenerate VB configurations
- Resonance of the VBs breaks the degeneracies

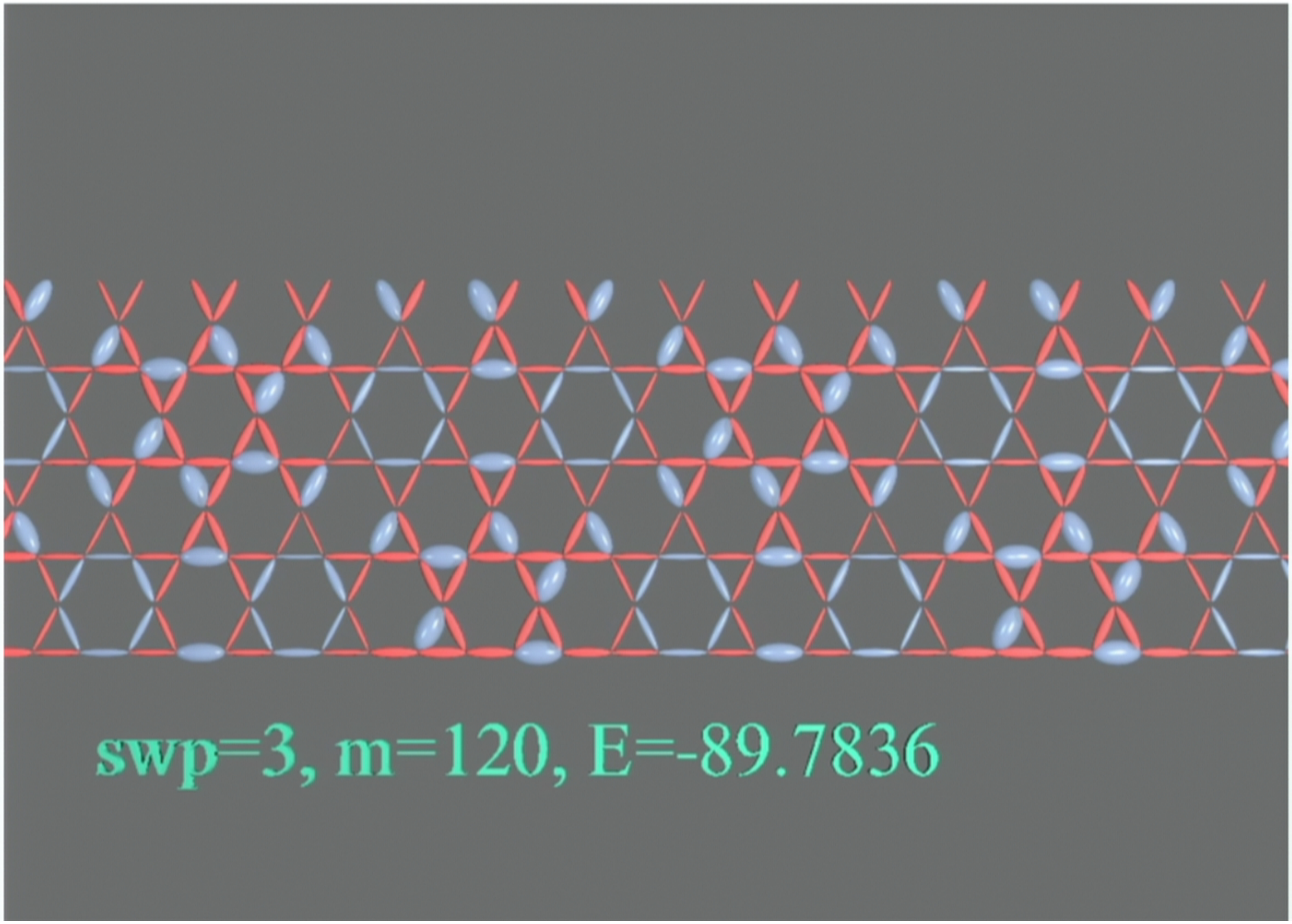
All these features make the kagome Heisenberg model an <u>excellent</u> candidate for an RVB ground state, a <u>spin liquid</u>. But, it could also be a <u>valence bond crystal</u>.

Valence bond crystal versus spin liquid

- Early field theory treatments gave a Z_2 spin liquid as a possible ground state (Sachdev, ...)
- Other approximate treatments pointed to a complicated 36 site unit cell VBC, the honeycomb VBC. Why?
  - ➡ Resonance only occurs in loops
  - ➡ Shortest loop is 6 site hexagon
  - ➡ Close pack the hexagons w/o touching
  - ➡ Use higher order flucs to break ties
  - ➡ The resulting HVBC appears (meta)stable: it doesn't melt into a spin liquid!

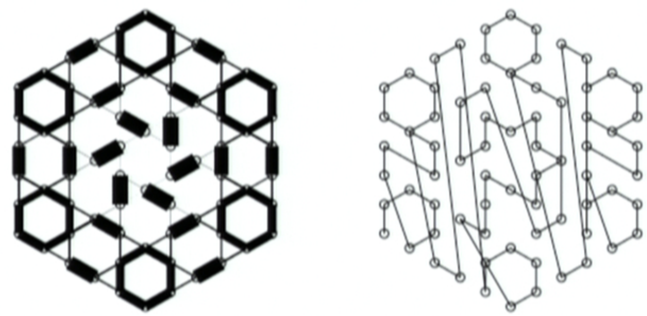


XC8 cylinder, biased to HVBC



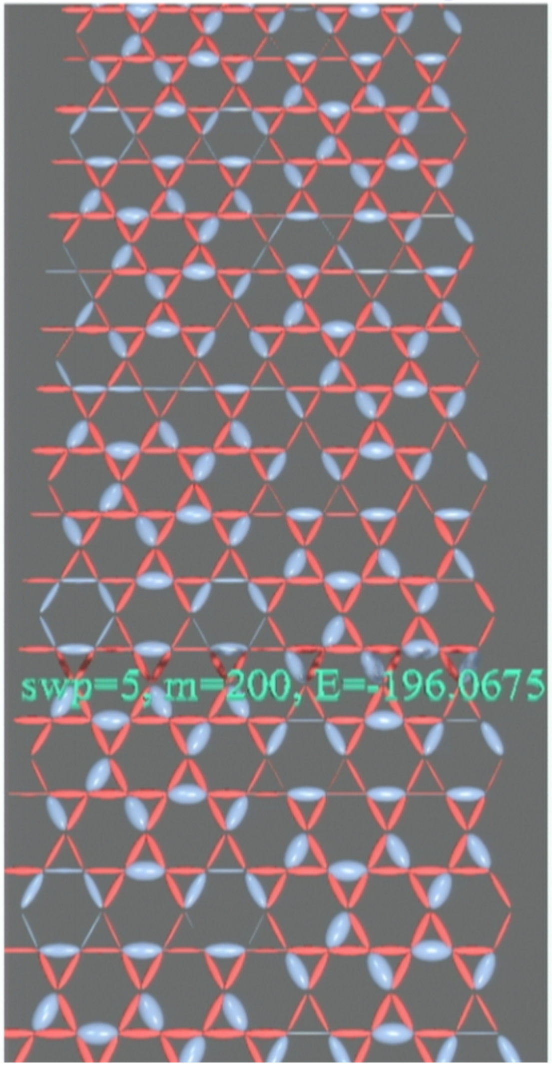
Direct comparison of HVBC and SL

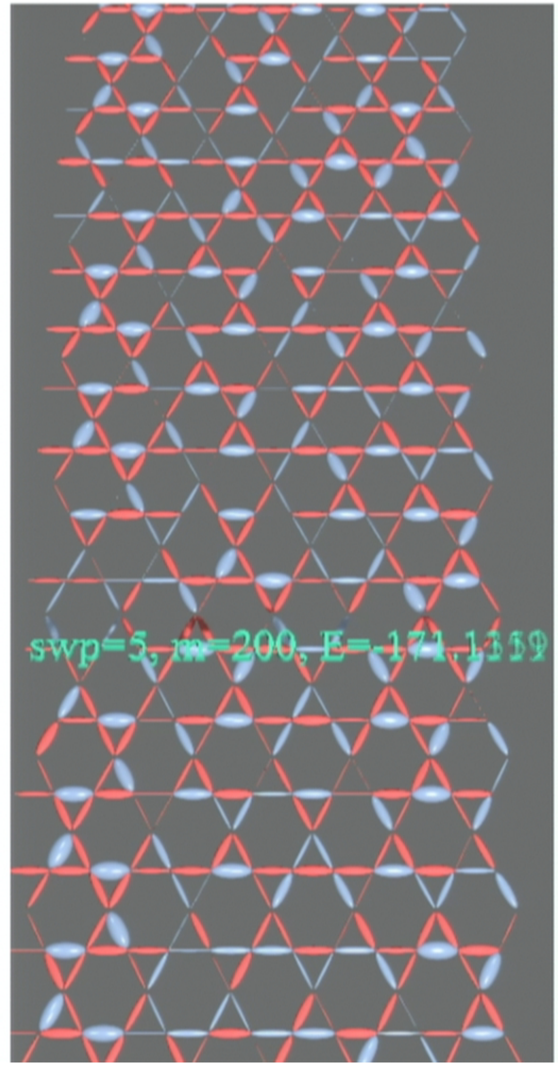
- Given metastability, and possible biases, how can you rule out the HVBC?
  - Make all the biases favor the HVBC. Then, if it's unstable, you have strong evidence.
  - To make a strong bias: make the DMRG mapping to 1D follow the HVBC state!



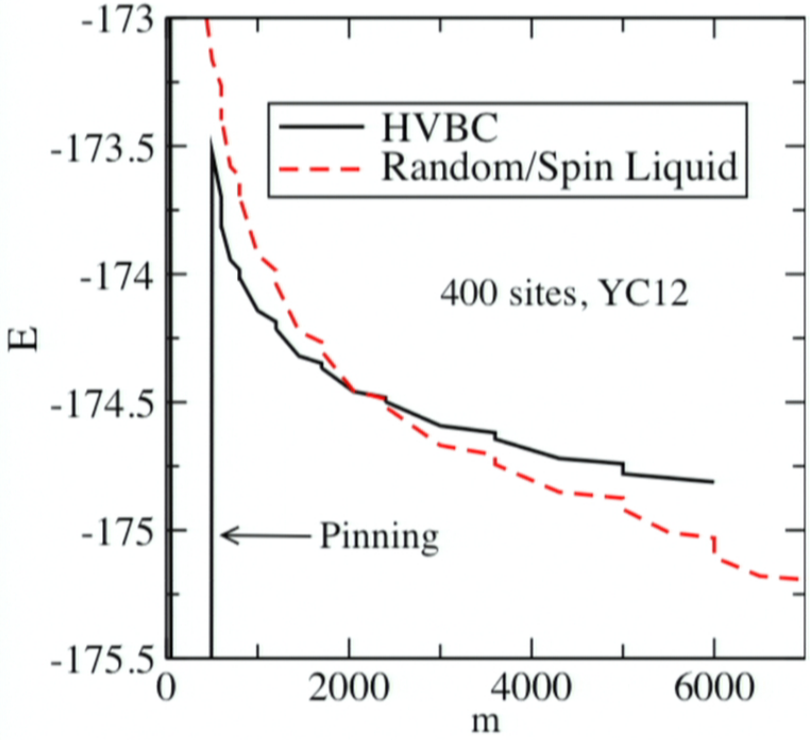
    - Nonresonating HVBC stable at m=2
  - Other ways to promote HVBC: initial state (pinning "fields" = strong J's); edge shaped to match HVBC

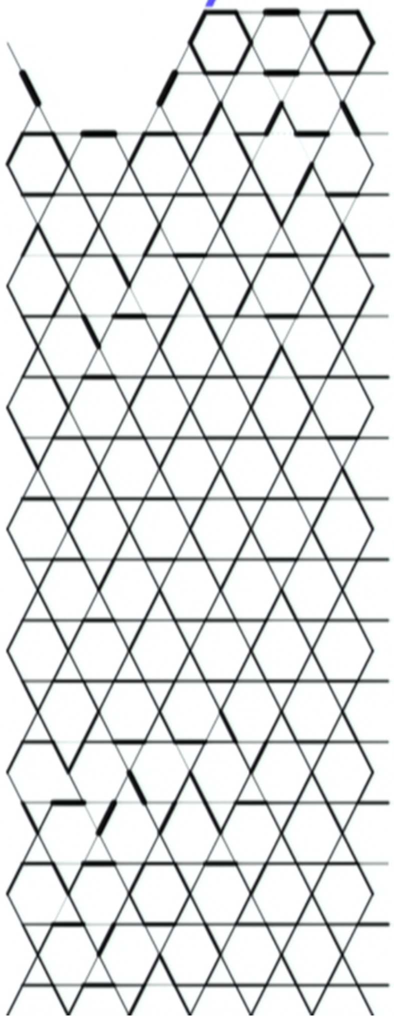
YC12 cylinder, one started in HVBC



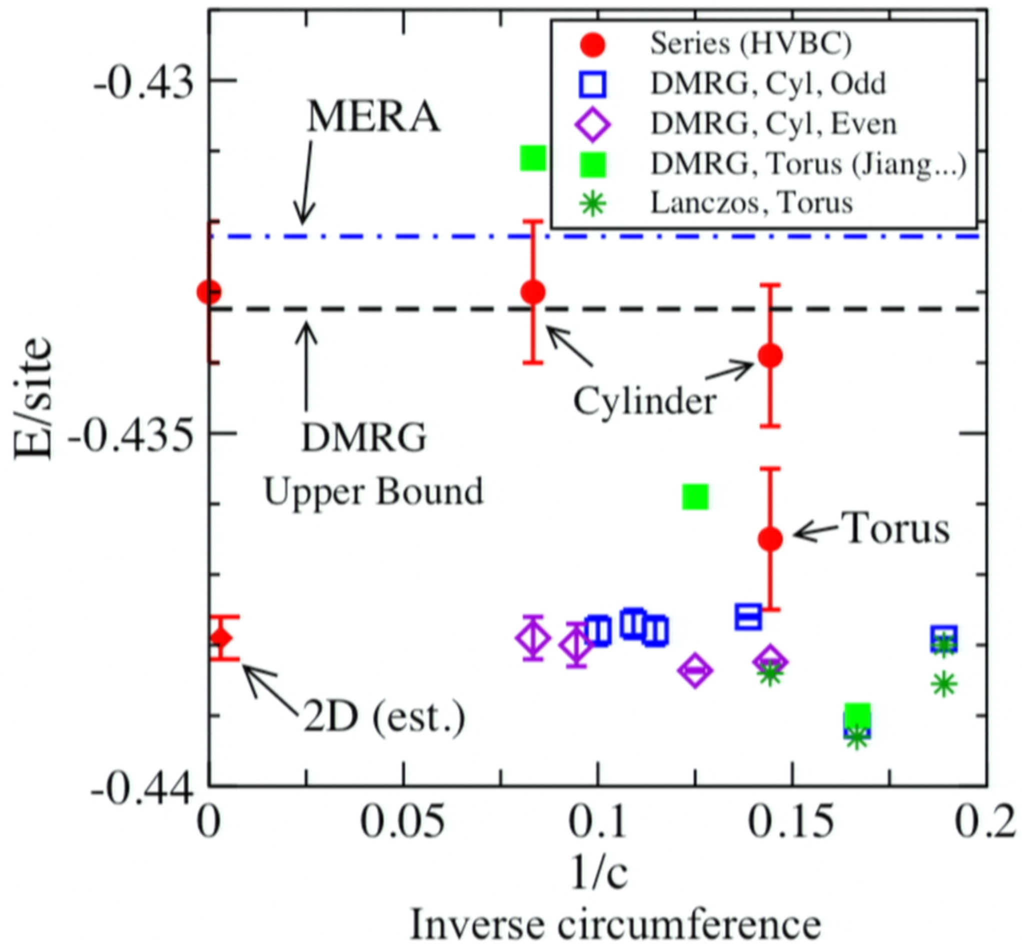


Ruling out an HVBC on a width 12 cylinder



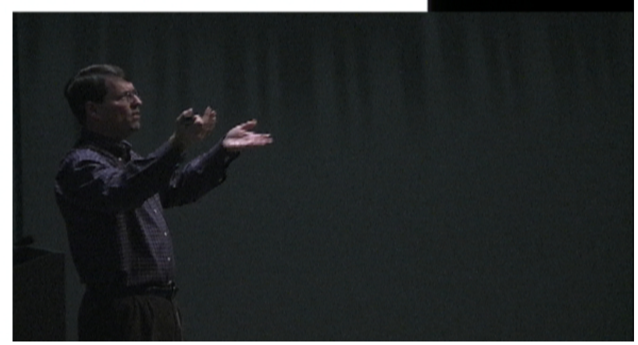


Energies of various cylinders and methods



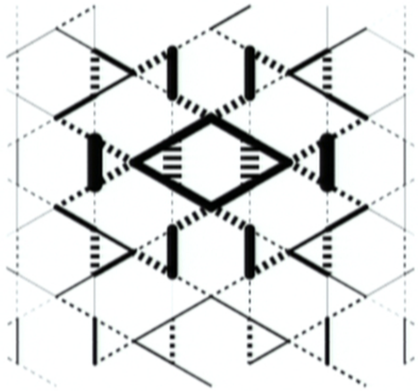
How can we understand the nature of the spin liquid?

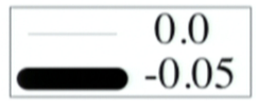
- Is it closely connected to a nearby VBC? (a "melted" VBC)
- In an RVB description, what are the key resonances?
- What do we measure to answer these questions?



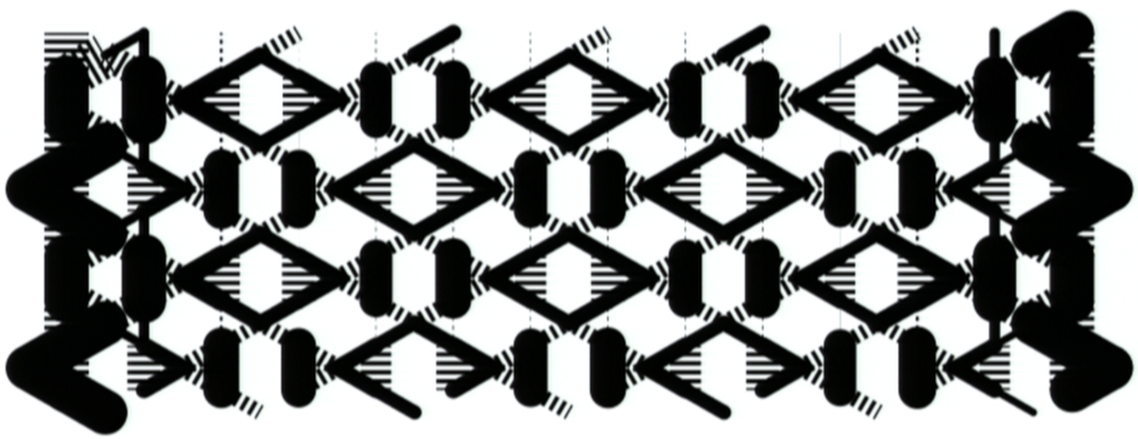
Response to small bond perturbations

Response to 1% increase in J on one diamond



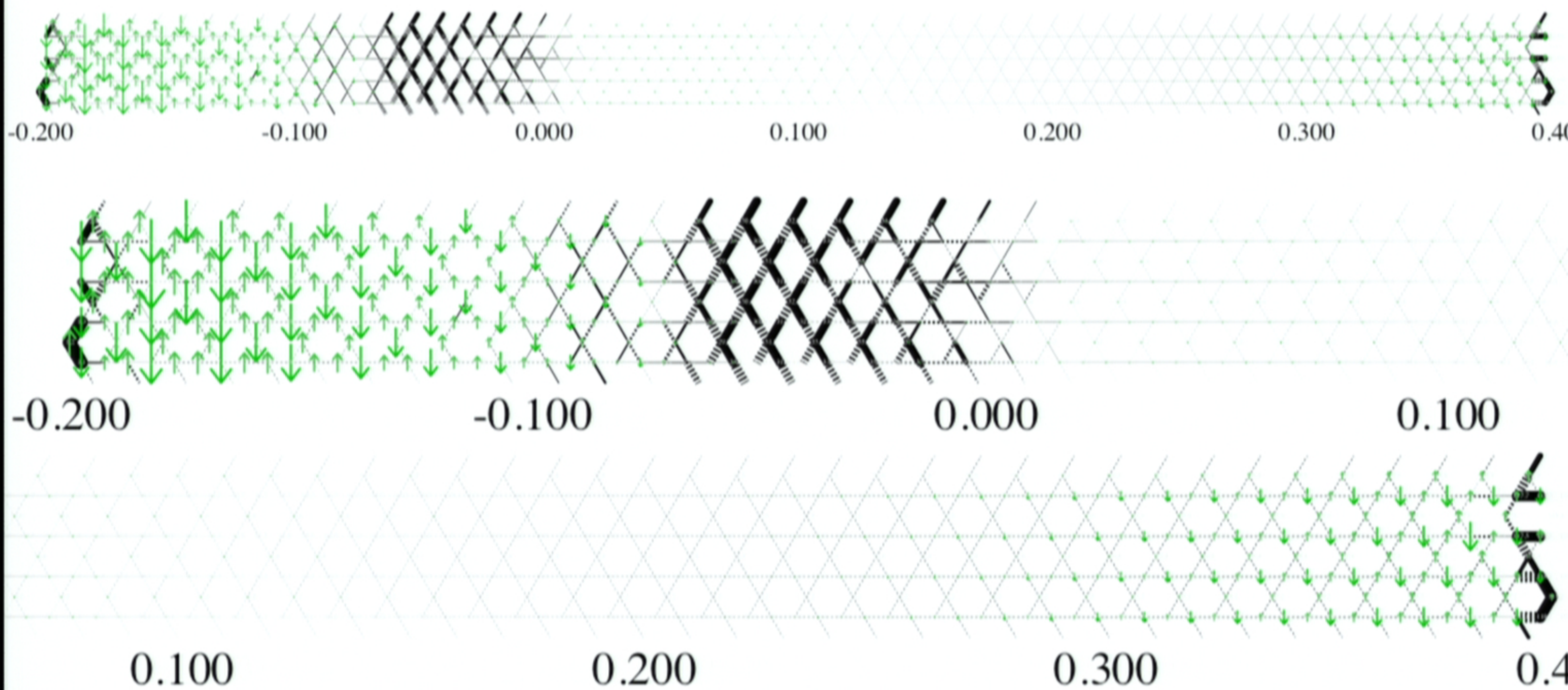


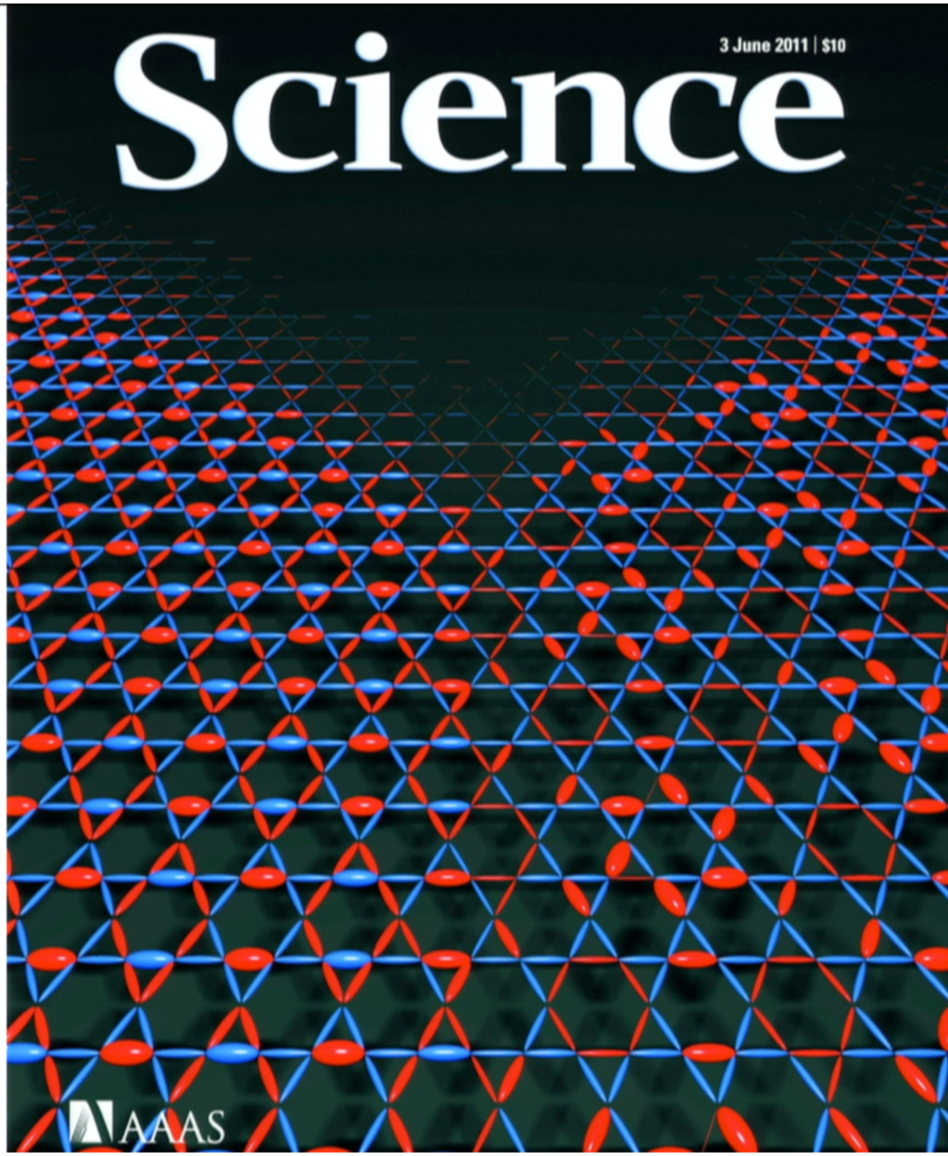
Response to 1% increase in J on one hexagon



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

Varying J_2 with x coordinate





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Conclusions

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- The spin liquid has very short correlation lengths of all types, and a gap to all spin excitations.
- The internal structure of the SL/RVB favors 8 site resonant loops, not 6 site. Close to a "diamond pattern" VBC.
- New results: next nearest neighbor J_2
  - The spin liquid phase extends to substantial $J_2>0$; but $J_2=0$ is close to the left edge of the phase.
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