Title: DMRG Studies on the Spin Liquid Ground State of the Kagome Model

Date: Feb 26, 2013 02:00 PM

URL: http://pirsa.org/13020147

Abstract: I will present a density-matrix renormalization group (DMRG) study of the S=1/2 Heisenberg antiferromagnet on the kagome lattice to identify the conjectured spin liquid ground state. Exploiting SU(2) spin symmetry, which allows us to keep up to 16,000 DMRG states, we consider cylinders with circumferences up to 17 lattice spacings and find a spin liquid ground state with an estimated per site energy of -0.4386(5), a spin gap of 0.13(1), very short-range decay in spin, dimer and chiral correlation functions and finite topological entanglement consistent with the logarithm of 2, ruling out gapless, chiral or non-topological spin liquids. All this would provide strong evidence for a gapped topological Z_2 spin liquid.

DMRG Study on the Spin Liquid Ground State of the Kagome Model

Stefan Depenbrock, LMU Munich

with

Ian McCulloch, University of Queensland
Ulrich Schollwöck, LMU Munich

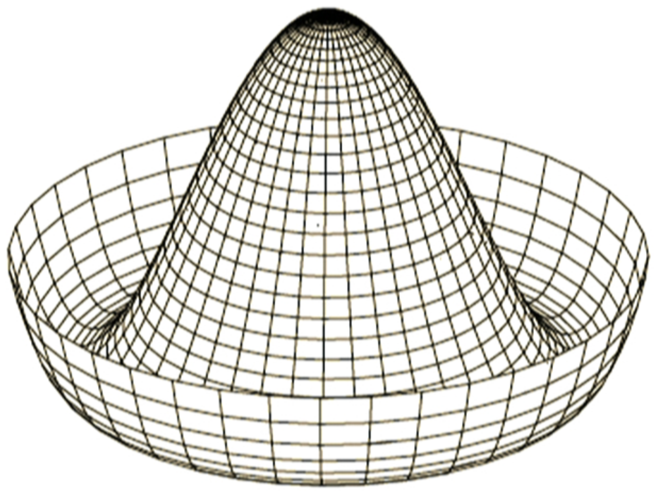
Phys. Rev. Lett. 109, 067201 (2012)

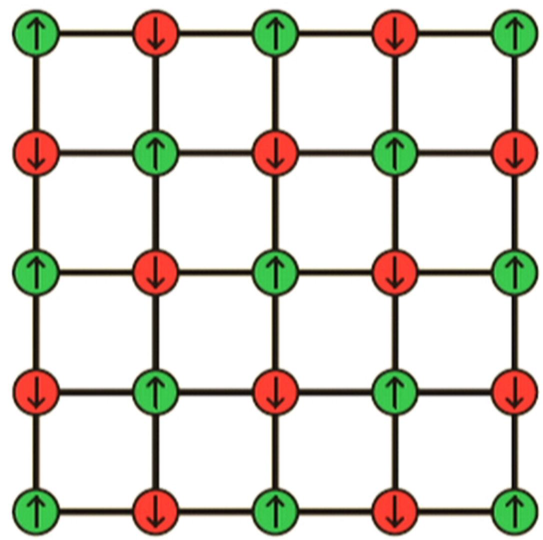
Perimeter Institute
2013-02-26

Landau Theory

Ordering of physical systems associated with spontaneous symmetry breaking.

- **Order associated with broken symmetry**
- **Local order parameter detects ordered phase**





Is there order without broken symmetries?

Groundstates of Frustrated Magnets

What happens at zero temperature?

- Disordered

- Conventional order:
  e.g. Néel ordered or coupled dimers

- Valence-bond crystals
  Full symmetry of Hamiltonian, but broken space-group symmetry

- Exotic order:
  Spin liquid
  Topological order
  . . .

Quantum Spin Liquids

- Exotic groundstates outside Landau paradigm:
  Ordered groundstate without broken symmetry
  No local order parameter
  Order related to long-range entanglement?
- Possibly connected to high temperature superconductivity
- Topologically ordered spin liquids might be useful for quantum computation

Route to Spin Liquids

Spin liquids appear as solutions in field theories for many frustrated systems

Key: Maximize quantum fluctuations

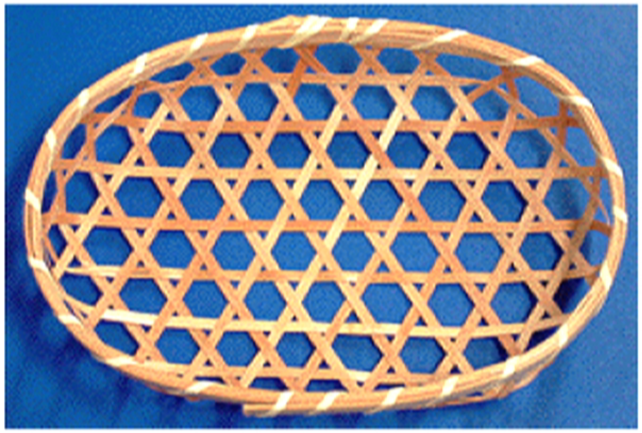
- Small spin
- Low coordination number
- Low dimension
- Strong frustration
- Many classically degenerate states

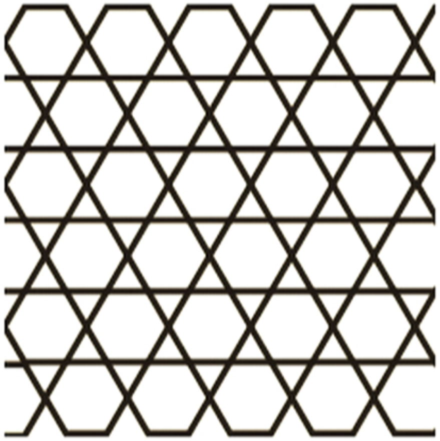
The Model

Considered here: antiferromagnetic Heisenberg model on kagome lattice

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathcal{S}_i \mathcal{S}_j$$

- First appearance as model for Helium on graphite substrate (Elser 1989)
- Occurs naturally in some compounds such as Herbertsmithite
- Promising candidate for spin liquid groundstate





Short History of the Kagome Model: Theory

Plethora of groundstates proposed:

- Valence Bond Crystal
  - Marston & Zeng 1991
  - Singh & Huse 2007
- Z(2) spin liquid
  - Sachdev 1992
  - Wang & Vishwanath 2006
- Chiral spin liquid
  - Wen, Wilczek, Zee 1989
  - Yang, Warman, Girvin 1993
- Gapless spin liquid
  - Hermele, Ran, Lee, Wen 2008

Short History of the Kagome Model: Theory

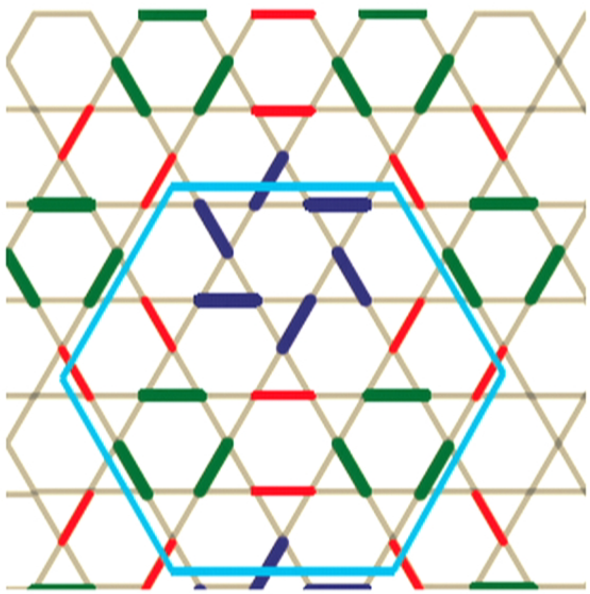
Plethora of groundstates proposed:

- Valence Bond Crystal
  - Marston & Zeng 1991
  - Singh & Huse 2007
- Z(2) spin liquid
  - Sachdev 1992
  - Wang & Vishwanath 2006
- Chiral spin liquid
  - Wen, Wilczek, Zee 1989
  - Yang, Warman, Girvin 1993
- Gapless spin liquid
  - Hermele, Ran, Lee, Wen 2008

The Kagome Puzzle: Valence Bond Crystals

Various proposals in literature

Series expansion gives lowest energy for 36-site VBC



The Kagome Puzzle: Spin Liquids

Spin liquid: no broken symmetry

Classification can be done via projective symmetry groups

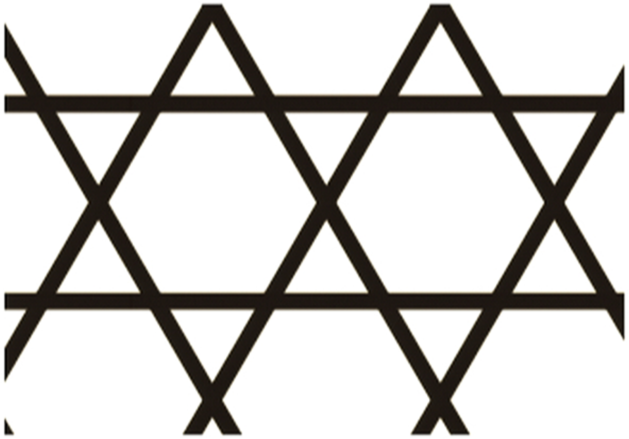
(X.-G. Wen: PRB 76, 165113)

Relevant here:

• gapless spin liquid

• gapped chiral spin liquid

• gapped spin liquid without chiral ordering



The Kagome Puzzle: Early Numerics

- Exact diagonalization of small samples with inconclusive results:
  Disordered groundstate (Leung & Elser 1993)
  Maybe some chiral contributions (Waldtmann *et al* 1998)
  Scaling of gaps hard to predict (Sindzingre & Lhuillier 2009)
  Correlations without clear structure (Läuchli & Lhuillier 2009)

- Diagonalization in valence bond basis (Zeng & Elser 1995)

- Contractor renormalization (Budnik & Auerbach 2004)

- Monte Carlo methods (*e.g.* Iqbal 2011)

- Quantum dimer models (Poilblanc, Mambrini, Schwandt 2010)

- Series expansion (Singh & Huse 2007)

Increasing Interest: More numerics

Advanced numerical techniques: Renewed interest

- DMRG on torus systems finds spin liquid
  Jiang, Weng, Sheng 2008
- Tensor network method MERA find VBC
  Evenbly, Vidal 2009
- Gutzwiller-projected Monte Carlo finds gapless spin liquid
  Poilblanc, Iqbal 2011
- DMRG on large cylinders finds strong evidence for spin liquid
  Yan, Huse, and White, Science 332, 1173 (2011)

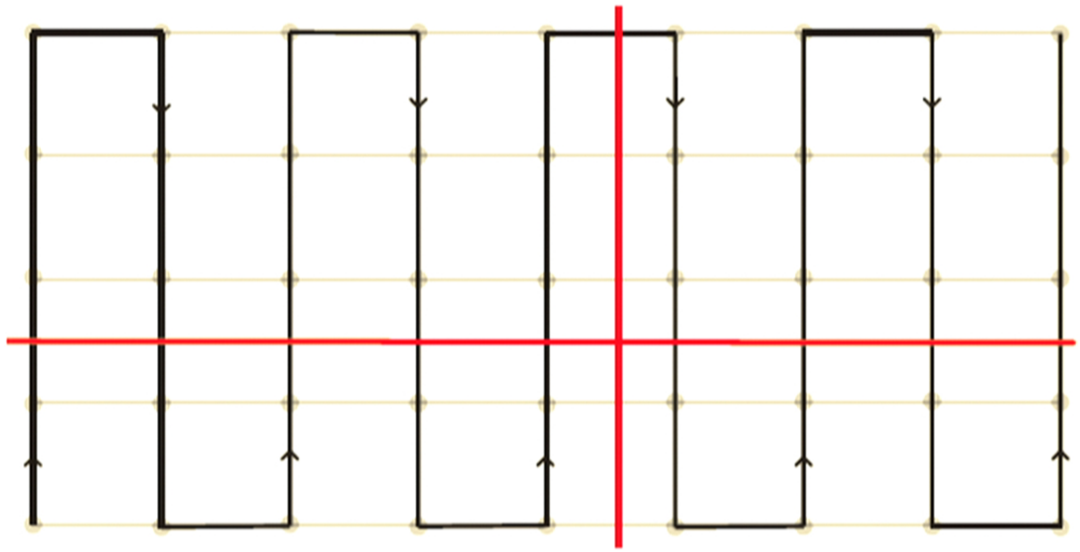
This Talk

Inspired by White′s results: Performed new DMRG study with main goals

- Make use of non-abelian symmetries to reach larger systems
- SU(2) Symmetry enables higher precision
- Conclusively calculate the spin gap: unbiased calculation possible
- Additional calculations possible due to lower error
- Employ new tools from quantum information theory
- Determine type of spin liquid

DMRG: More Than One Dimension

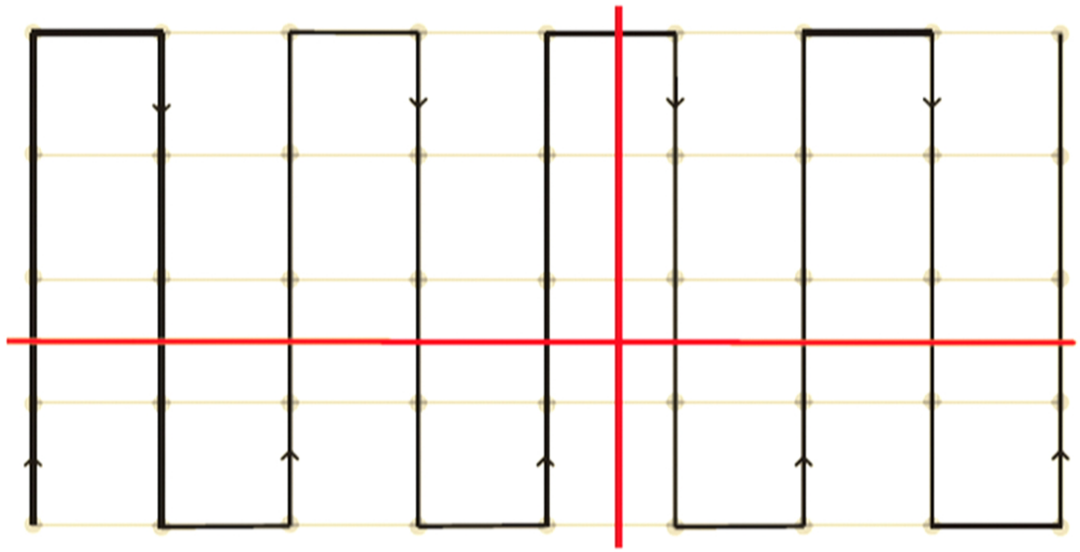
- Good scaling with matrix dimension allows treatment of finite 2D systems
- Mapping of two-dimensional system to a chain:
  Introduces long-range interactions in the Hamiltonian!



Key: Don't use doubly periodic boundary conditions

DMRG: More Than One Dimension

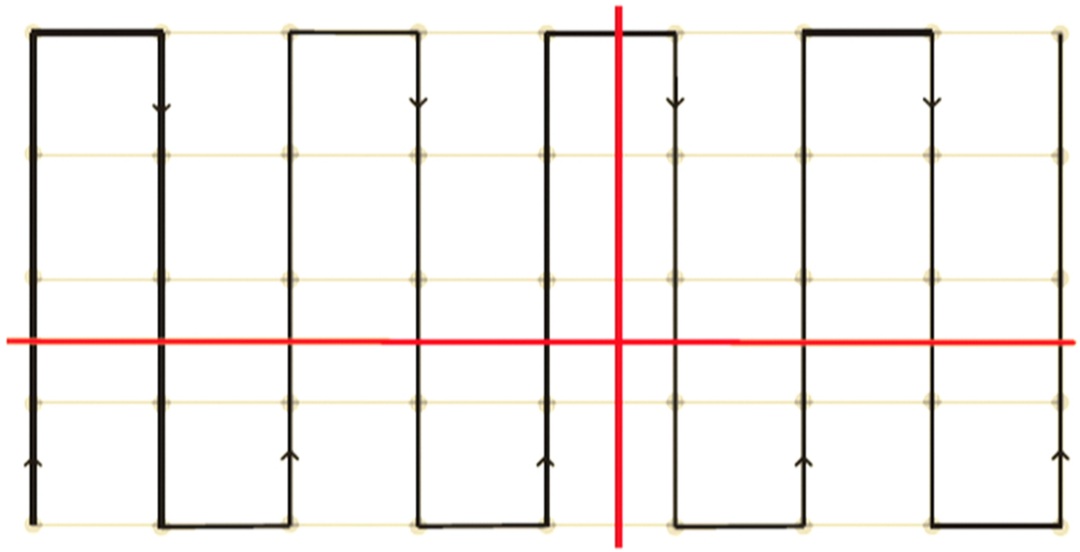
- Good scaling with matrix dimension allows treatment of finite 2D systems
- Mapping of two-dimensional system to a chain:
  Introduces long-range interactions in the Hamiltonian!



Key: Don't use doubly periodic boundary conditions

DMRG: More Than One Dimension

- Good scaling with matrix dimension allows treatment of finite 2D systems
- Mapping of two-dimensional system to a chain:
  Introduces long-range interactions in the Hamiltonian!



Key: Don't use doubly periodic boundary conditions

Here:

- SU(2) symmetric implementation

  Previously: U(1) symmetry

- Single-site algorithm

- Up to 5000 SU(2) states (equivalent to 20000 U(1) states)

  White: up to 8000 states

  Jiang: up to 6000 states

- Up to 700 sites

  White: up to 600 sites

  Jiang: up to 120 sites

- Kagome lattice on cylindrical systems with width up to 17

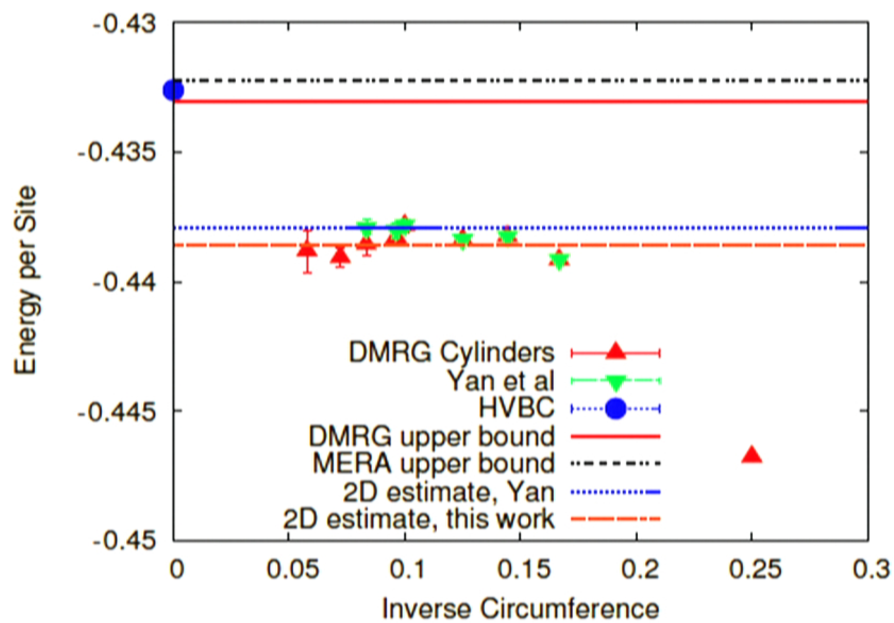
  White: cylinders up to width 12

  Jiang: tori up to width 5

Groundstate Energies

Obtain ground state energy for given system:

1. Increase number of states while sweeping until convergence
2. Extrapolate in truncation error to obtain estimate
3. Use subtraction method to obtain estimates for bulk energy per site

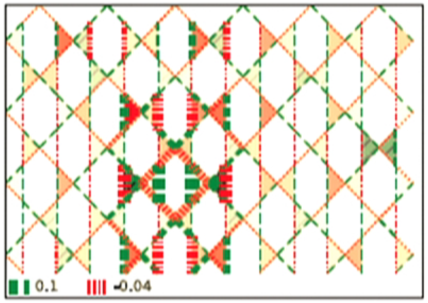


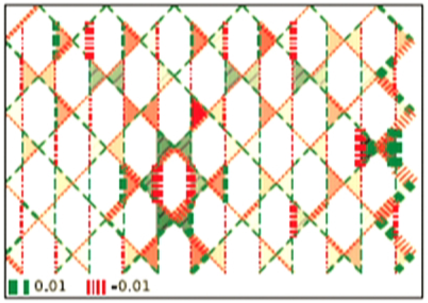
Details: Phys. Rev. Lett. 109, 067201 (2012)

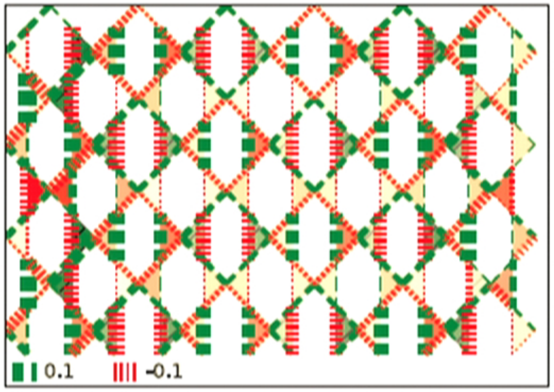
Groundstate Properties: Resonances

Energies agree with earlier studies - but is it the same groundstate?

- **Check resonance patterns**







Spin Liquid Theories: What can DMRG tell us?

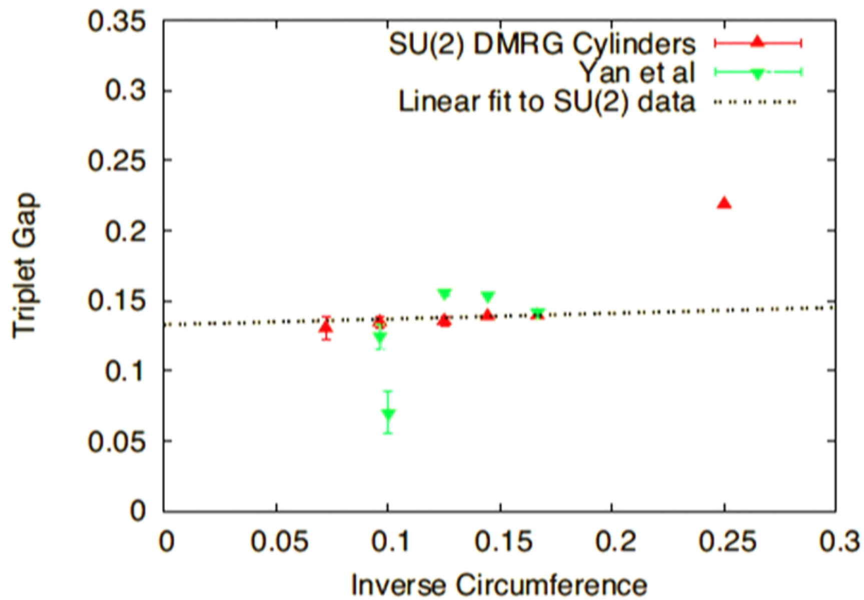
	Z(2)	U(1)	Chiral QSL
Gap	yes	no	yes
Structure Factor	no clear signature	$\vec{q}=0$ or $\sqrt{3}\times\sqrt{3}$	no clear signature
Spin-Spin Correlations	exponential	power-law	exponential
Dimer-Dimer Correlations	exponential	power-law	exponential
Chiral Correlations	exponential	?	slow decay
Topological Entanglement Entropy	$\mathcal{S}_{topo} = \log_2(2) = 1$	$\mathcal{S}_{topo} = 0$	$\mathcal{S}_{topo} = \log_2(\sqrt{2}) = \frac{1}{2}$

Triplet Gap

SU(2) Symmetry allows direct access to groundstate in spin S=1 sector.

Unbiased calculation of spin gap possible!

1. Calculate ground state in spin S=0 and S=1 sectors
2. Extrapolate to vanishing truncation error



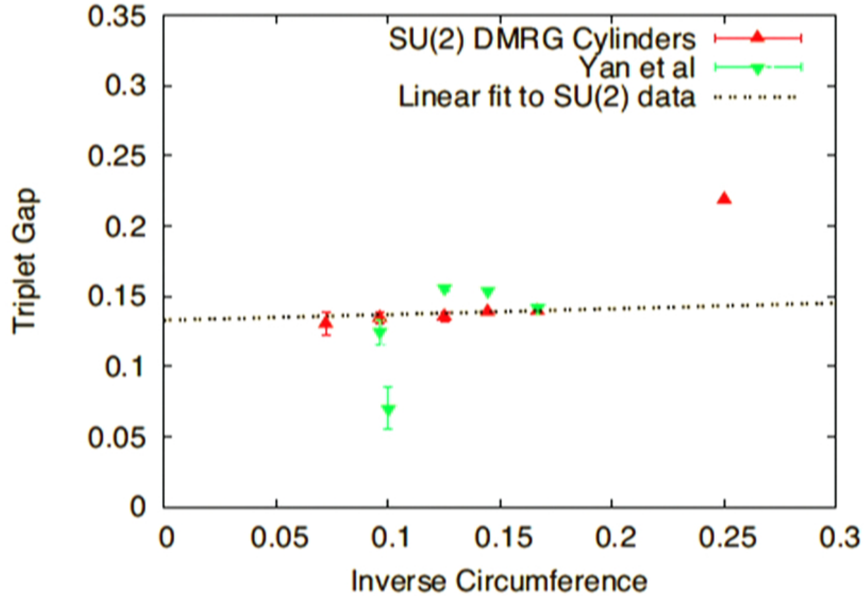
Details: Phys. Rev. Lett. 109, 067201 (2012)

Triplet Gap

SU(2) Symmetry allows direct access to groundstate in spin S=1 sector.

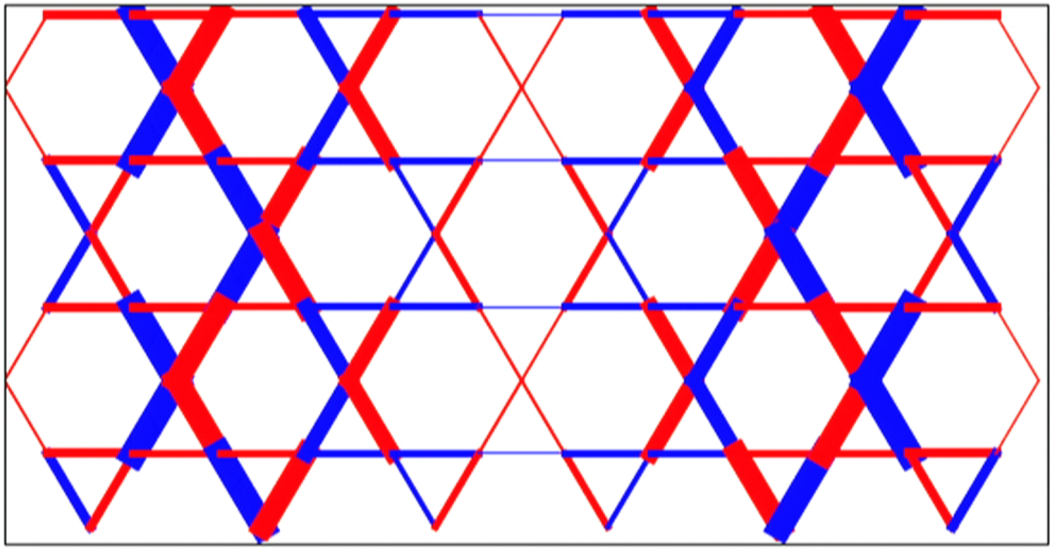
Unbiased calculation of spin gap possible!

1. Calculate ground state in spin S=0 and S=1 sectors
2. Extrapolate to vanishing truncation error

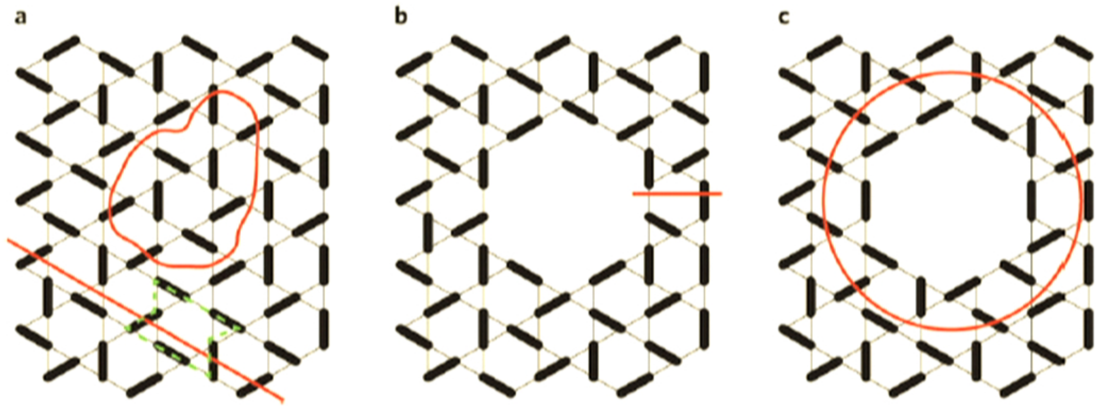


Details: Phys. Rev. Lett. 109, 067201 (2012)

Excitation Properties



Entanglement Entropy: Loops and Topology

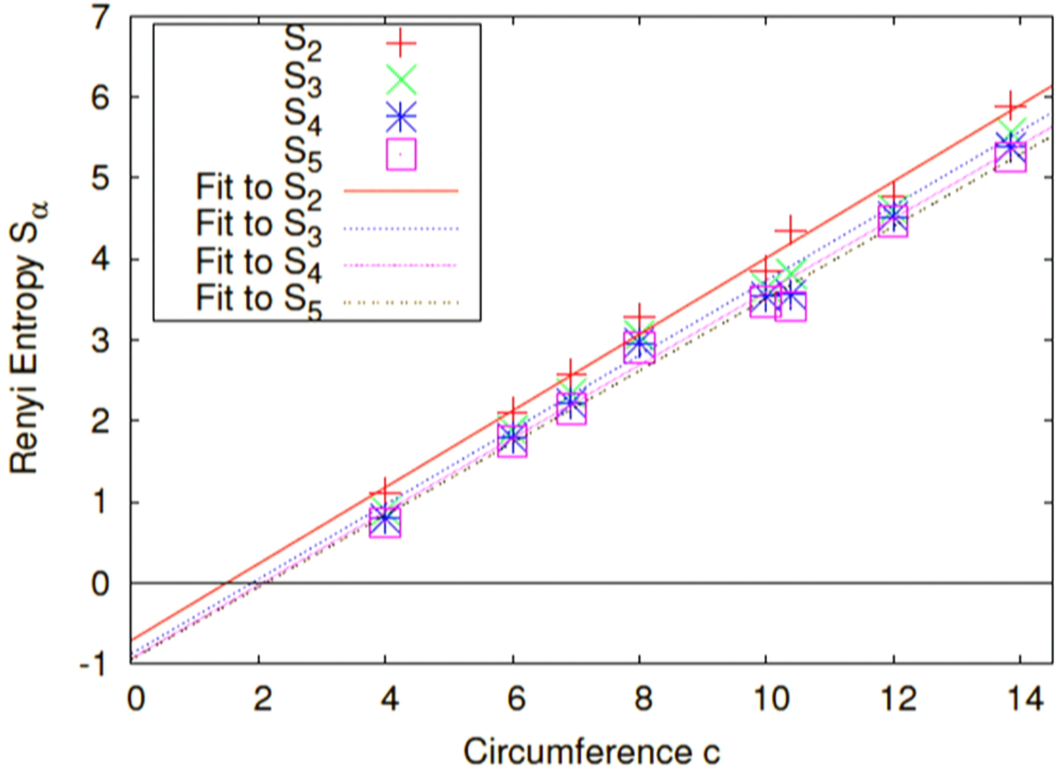


Idea:
Distinguish topological states by counting number of cut valence bonds

Plot: S. White, Nature Physics 2012

Entanglement Entropy

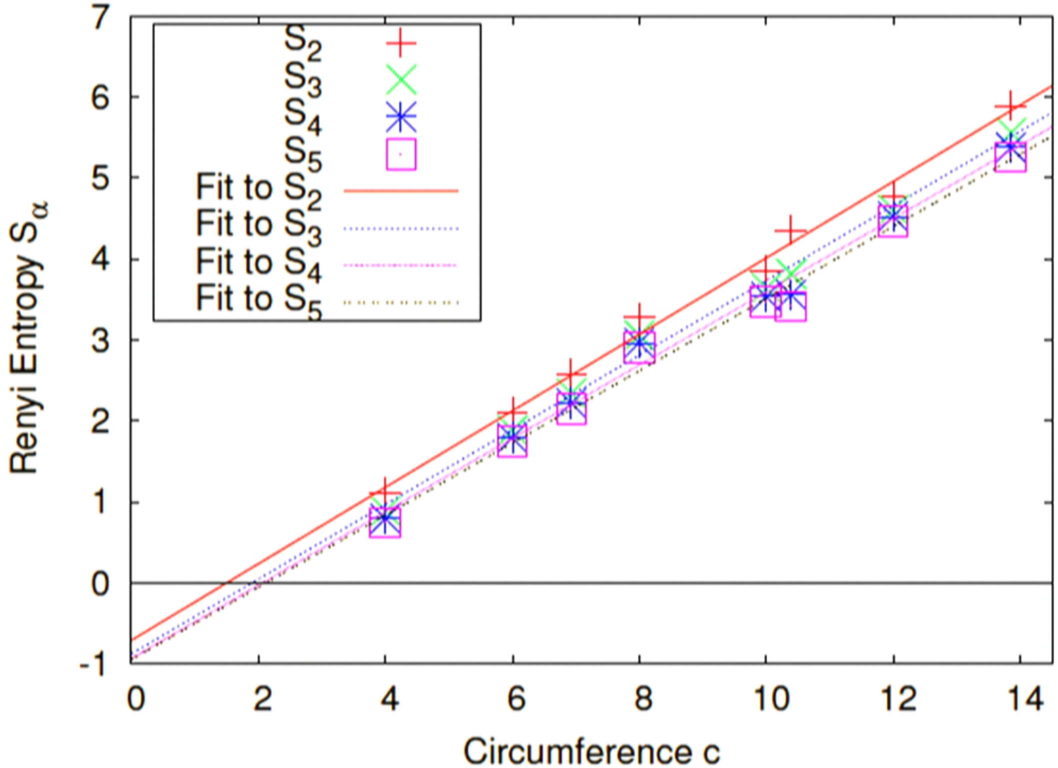
- Extrapolation in circumference via linear fit
- Exact value of topological entanglement entropy hard to determine, but definitely finite



Details: Phys. Rev. Lett. 109, 067201 (2012)

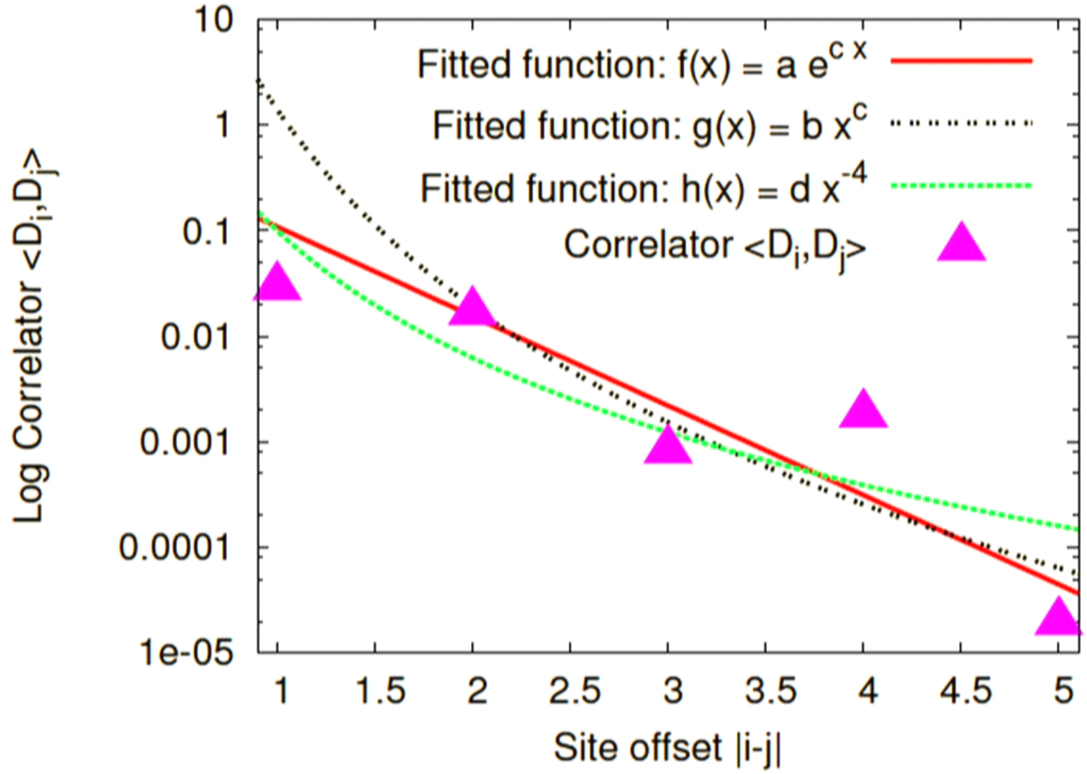
Entanglement Entropy

- Extrapolation in circumference via linear fit
- Exact value of topological entanglement entropy hard to determine, but definitely finite



Details: Phys. Rev. Lett. 109, 067201 (2012)

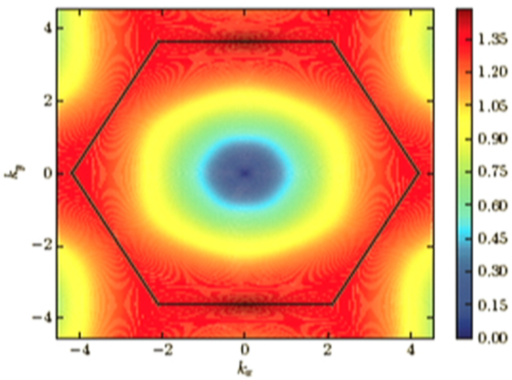
Correlation Functions: Dimer-Dimer



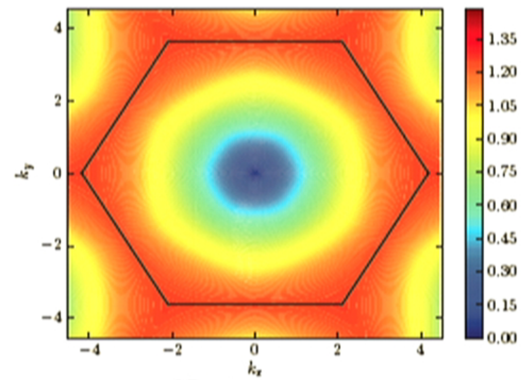
Structure Factors

What type of quantum spin liquid constitutes the ground state?

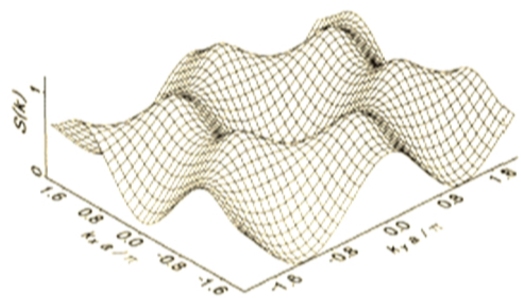
- **First hint: Structure factors** $S(\vec{q}) = \frac{1}{N}\sum_{i,j} e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}\langle \vec{S}_i \cdot \vec{S}_j \rangle$



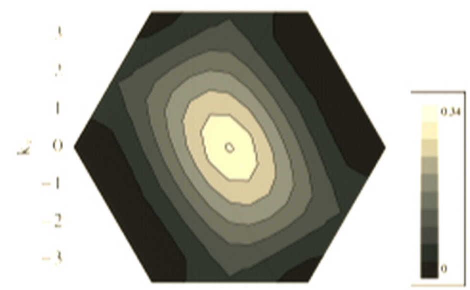
196-site YC system



27-site torus system



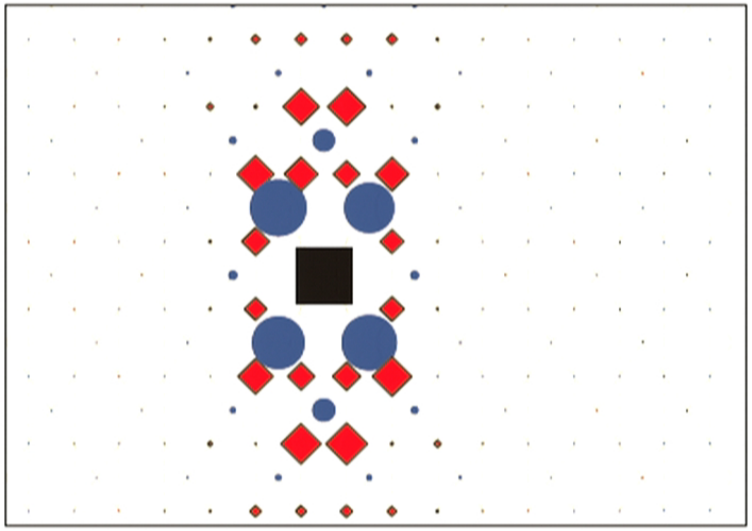
Z(2) QSL (PRB 45, 12377 (1992)):

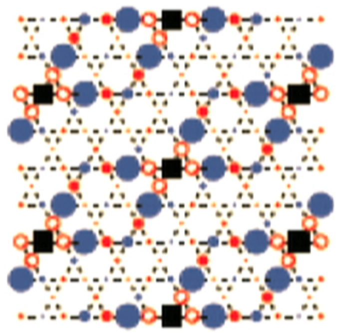


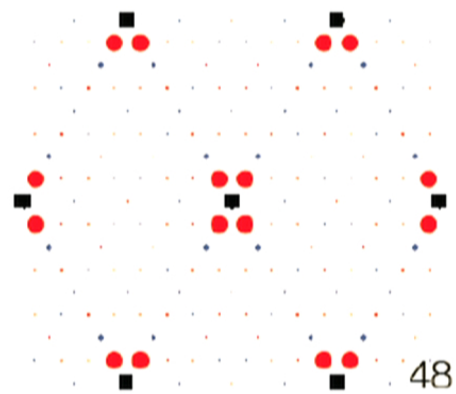
U(1) QSL (PRB 77, 224413 (2008))

Open Questions:

- **Real space correlation: What does this structure mean?**



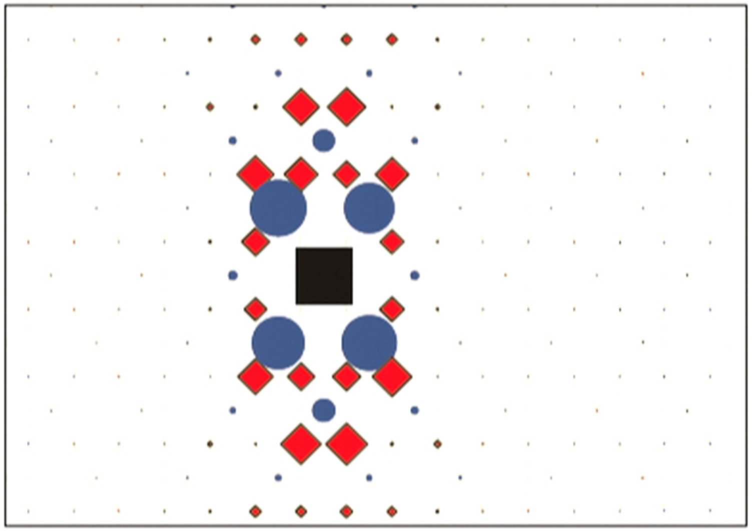


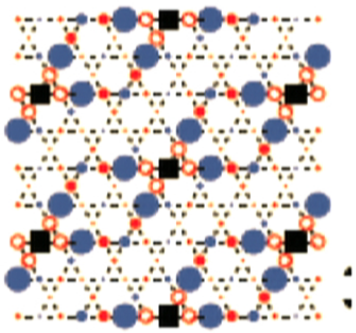


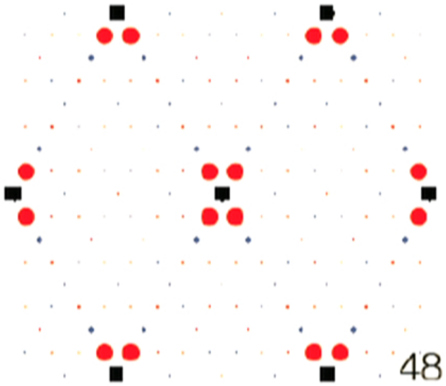
ED: Läuchli *et al*

Open Questions:

- Real space correlation: What does this structure mean?







ED: Läuchli *et al*

Open Questions

- What happens at finite J_2?
- What is the underlying theory of the spin liquid?
- Can we determine the topological statistics?
- Does DMRG always yield a Z(2) liquid?
- Do the results hold for infinite systems or even infinite cylinders?

Thank you!