Title: Gapless spin liquids in frustrated Heisenberg models

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Abstract: <span>We present our recent numerical calculations for the Heisenberg model on the square and
 Kagome lattices, showing that gapless spin liquids may be stabilized in highly-frustrated
 regimes. In particular, we start from Gutzwiller-projected fermionic states that may
 describe magnetically disordered phases,[1] and apply few Lanczos steps in order to improve
 their accuracy. Thanks to the variance extrapolation technique,[2] accurate estimations of
 the energies are possible, for both the ground state and few low-energy excitations.
 Our approach suggests that magnetically disordered phases can be described by Abrikosov
 fermions coupled to gauge fields.

 For the Kagome lattice, we find that a gapless U(1) spin liquid with Dirac cones
 is competitive with previously proposed gapped spin liquids when only the nearest-neighbor
 antiferromagnetic interaction is present.[3,4] The inclusion of a next-nearest-neighbor term
 lead to a Z_2 gapped spin liquid,[5] in agreement with density-matrix renormalization group
 calculations.[6] In the Heisenberg model on the square lattice with both nearest- and
 next-nearest-neighbor interactions, a Z_2 spin liquid with gapless spinon excitations is
 stabilized in the frustrated regime.[7] This results are (partially) in agreement with recent
 density-matrix renormalization group on large cylinders.[8]

 [1] X.-G. Wen, Phys. Rev. B {\bf 44}, 2664 (1991); Phys. Rev. B {\bf 65}, 165113 (2002).
 [2] S. Sorella, Phys. Rev. B {\bf 64}, 024512 (2001).
 [3] Y. Iqbal, F. Becca, S. Sorella, and D. Poilblanc, Phys. Rev. B 87, 060405(R) (2013).
 [4] Y. Iqbal, D. Poilblanc, and F. Becca, Phys. Rev. B 89, 020407(R) (2014).
 [5] W.-J. Hu, Y. Iqbal, F. Becca, D. Poilblanc, and D. Sheng, unpublished.
 [6] H.-C. Jiang, Z. Wang, and L. Balents, Nat. Phys. 8, 902 (2012);
 S. Yan, D. Huse, and S. White, Science 332, 1173 (2011).
 [7] W.-J. Hu, F. Becca, A. Parola, and S. Sorella, Phys. Rev. B 88, 060402(R) (2013).
 [8] S.-S. Gong, W.Z., D.N. Sheng, O.I. Motrunich, and M.P.A. Fisher, arXiv:1311.5962 (2013).

Gapless spin liquids in frustrated Heisenberg models

Federico Becca

CNR IOM-DEMOCRITOS and International School for Advanced Studies (SISSA)

Perimeter Institute for Theoretical Physics, May 2014

iom Istituto Officina dei Materiali

Y. Iqbal (ICTP, Trieste), W.-J. Hu (now CSUN)

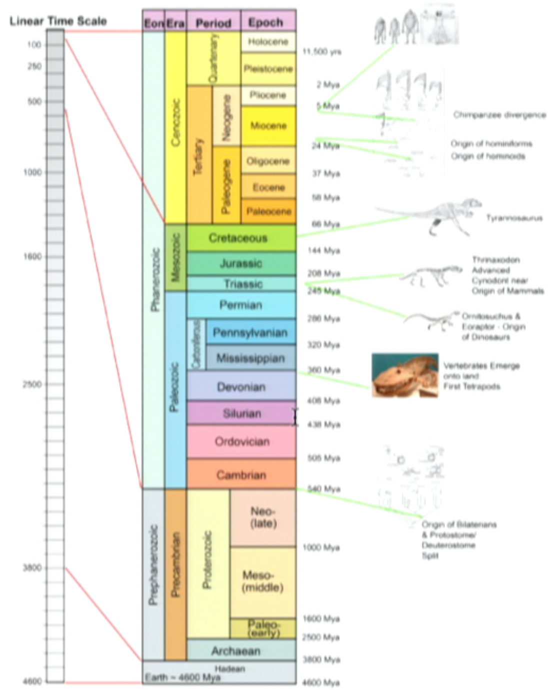
A. Parola (Como), D. Poilblanc (CNRS, Toulouse), and S. Sorella (SISSA)

1. Introduction

2. The Heisenberg model on the frustrated square lattice

3. The Heisenberg model on the Kagome lattice

The evolution of life on earth



Cenozoic:
Dinosaurs disappeared.
New forms of animals developed
(more clever than dinosaurs).
Hominoids conquered the planet.

Mesozoic:
Great extinction.
Dinosaurs prevailed over others
(very simple-minded animals).

Paleozoic:
Sudden appearance of many invertebrates
but also the first vertebrates.
Evolution into sophisticated amphibians.

Precambrian:
Only few multicellular life forms
(life was very simple and boring).

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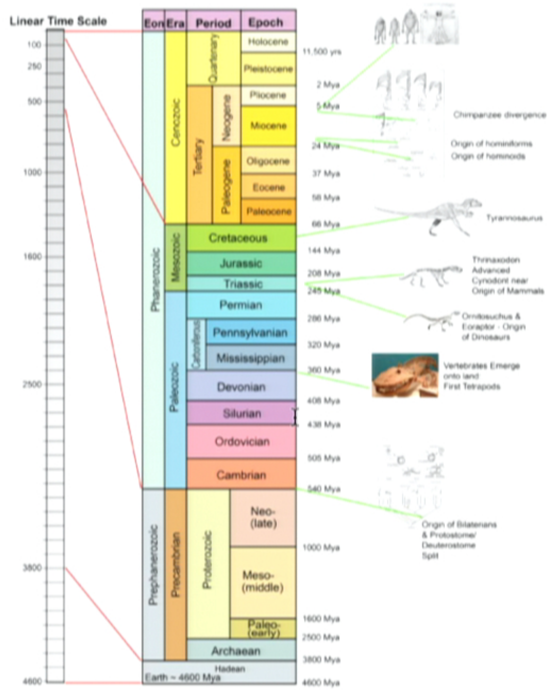

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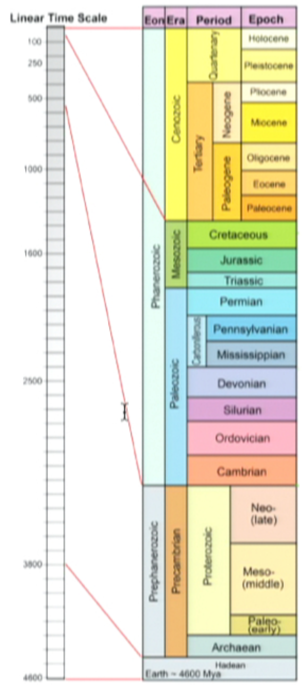
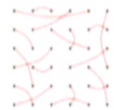
The evolution of magnetic systems



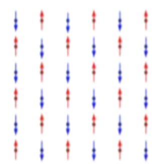


Today: New era of long-range spin liquids?

~2001: First examples of short-range (gapped) RVB

~1987~2001: Dimers prevailed

1973: Anderson suggested disordered RVB states



Ordered states are the only possible ones

Different kinds of spin liquids



 *

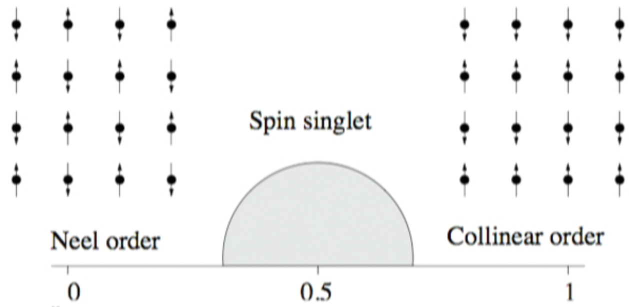
Folklore in the community working on frustrated magnets:

- DMRG always produces excellent spin liquids
- Other numerical methods produce no good liquids

* This is not a classification of spin liquids

The Heisenberg model on the frustrated square lattice

$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



- For $J_2/J_1 \ll 1$: Antiferromagnetic order at $\mathbf{Q} = (\pi, \pi)$
- For $J_2/J_1 \gg 1$: Antiferromagnetic order at $\mathbf{Q} = (\pi, 0)$ and $\mathbf{Q} = (0, \pi)$
- For $J_2/J_1 \sim 0.5$: Disordered phase (RVB liquid, dimer order or more exotic?)

Experimental realization in Li_2VOSiO_4 ($J_2 \gtrsim J_1$) and $VOMoO_4$ ($J_2 < 0.5 J_1$)

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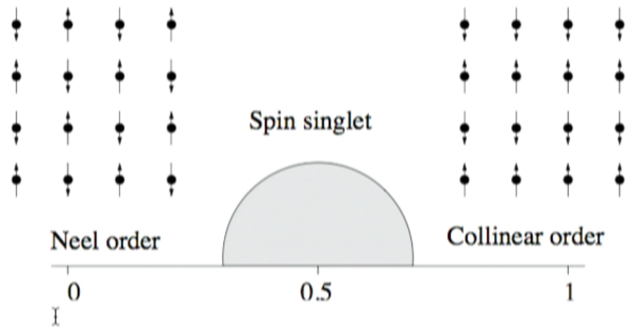

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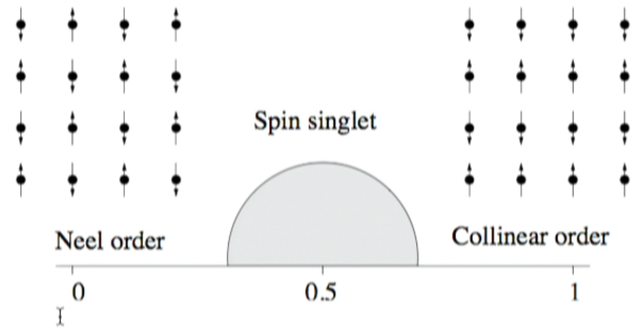

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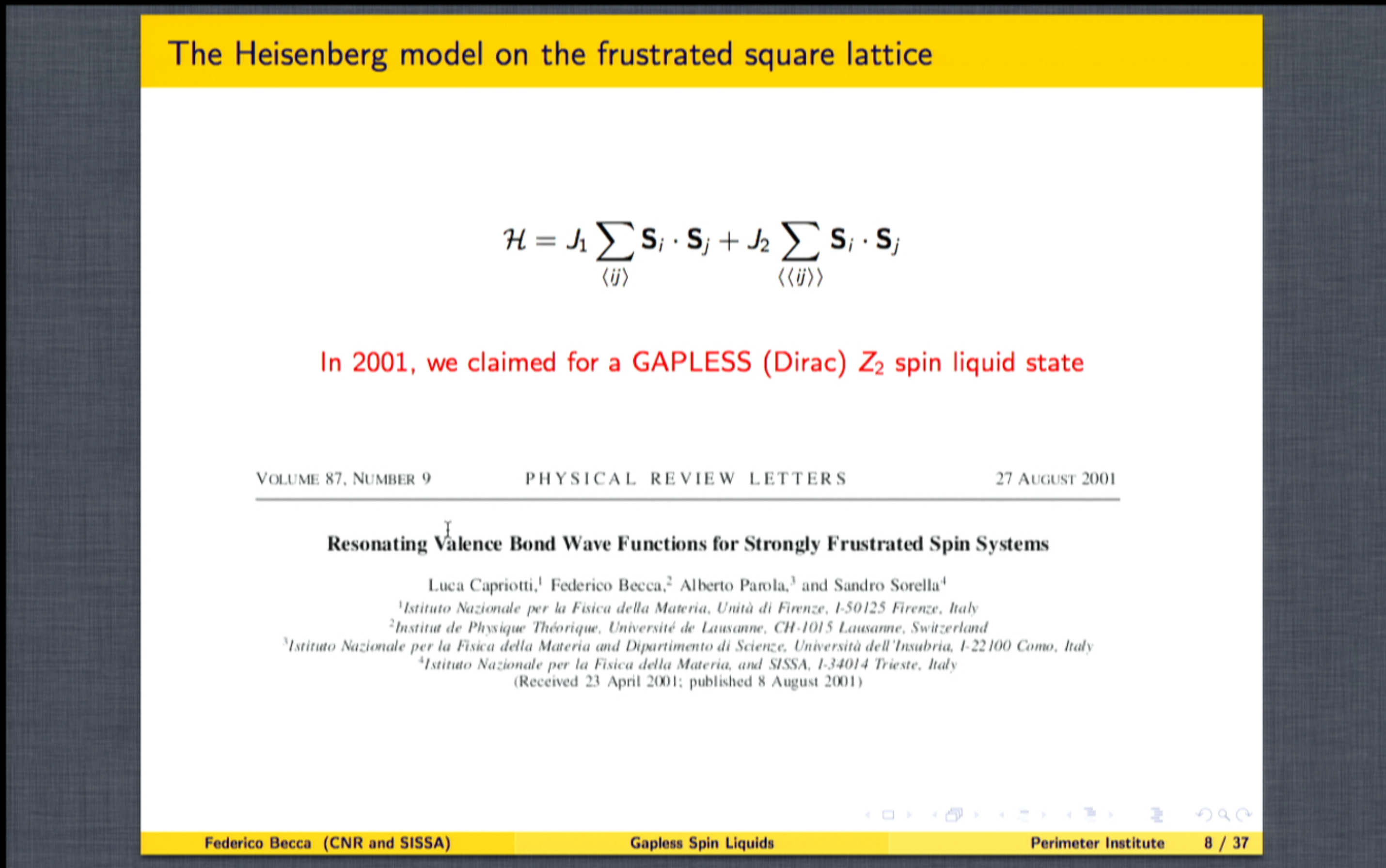
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VOLUME 87, NUMBER 9
PHYSICAL REVIEW LETTERS
27 AUGUST 2001
Resonating Valence Bond Wave Functions for Strongly Frustrated Spin Systems
Luca Capriotti,[1] Federico Becca,[2] Alberto Parola,[3] and Sandro Sorella[4]
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[4]Istituto Nazionale per la Fisica della Materia, and SISSA, I-34014 Trieste, Italy
(Received 23 April 2001; published 8 August 2001)
Federico Becca (CNR and SISSA)
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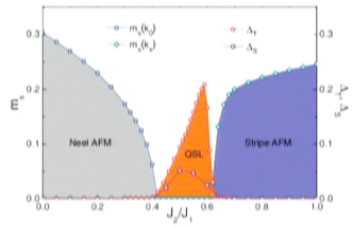
Recent DMRG calculations



Jiang, Yao, and Balents, PRB **86**, 024424 (2012)

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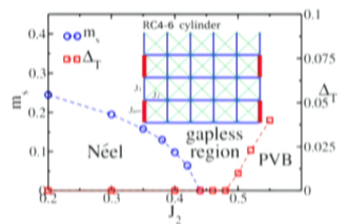

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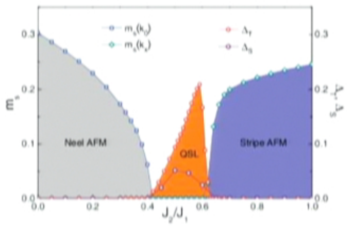

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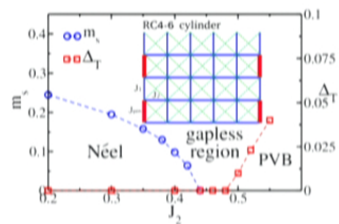

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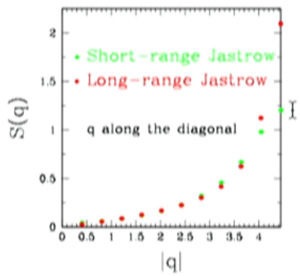
Describing magnetic phases

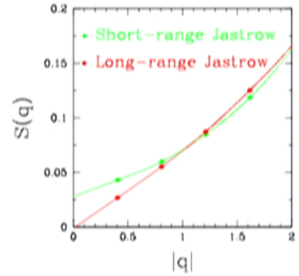
$$|\Psi_{AF}\rangle = \mathcal{P}_{(S_z=0)} \exp[\frac{1}{2}\sum_q v_q S^z_q S^z_{-q}]|0\rangle \qquad |0\rangle = \prod_i (-1)^{R_i} | \rightarrow\rangle_i$$

From a spin-wave calculation:

- Long-range spin-spin Jastrow factor $v_q \sim 1/|q|$
- Fluctuations (i.e., Jastrow) orthogonal to the classical order (i.e., $|0\rangle$)

Manousakis, RMP **63**, 1 (1991)





$$|\Psi_q\rangle = S^z_q|\Psi_0\rangle \qquad E_q - E_0 \sim \frac{\langle -K\rangle q^2}{S(q)} \sim c\,|q|$$

Describing magnetically disordered phases

$$S_i^\mu = \frac{1}{2} c_{i,\alpha}^\dagger \sigma_{\alpha,\beta}^\mu c_{i,\beta}$$

$$\mathcal{H} = -\frac{1}{2} \sum_{i,j,\alpha,\beta} J_{ij} \left(c_{i,\alpha}^\dagger c_{j,\alpha} c_{j,\beta}^\dagger c_{i,\beta} + \frac{1}{2} c_{i,\alpha}^\dagger c_{i,\alpha} c_{j,\beta}^\dagger c_{j,\beta} \right)$$

$$c_{i,\alpha}^\dagger c_{i,\alpha} = 1 \quad c_{i,\alpha} c_{i,\beta} \epsilon_{\alpha\beta} = 0$$

- At the mean-field level:

$$\mathcal{H}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu\delta_{ij}) c_{i,\alpha}^\dagger c_{j,\alpha} + \sum_{i,j} (\eta_{ij} + \zeta\delta_{ij})(c_{i,\uparrow}^\dagger c_{j,\downarrow}^\dagger + c_{j,\uparrow}^\dagger c_{i,\downarrow}^\dagger) + h.c.$$

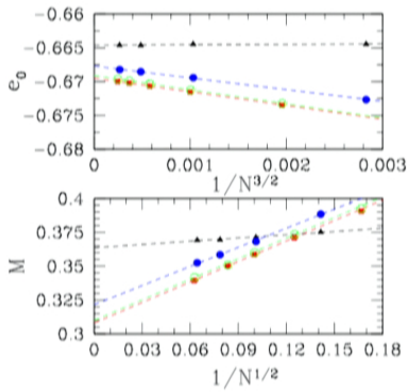
$$\langle c_{i,\alpha}^\dagger c_{i,\alpha} \rangle = 1 \quad \langle c_{i,\alpha} c_{i,\beta} \rangle \epsilon_{\alpha\beta} = 0$$

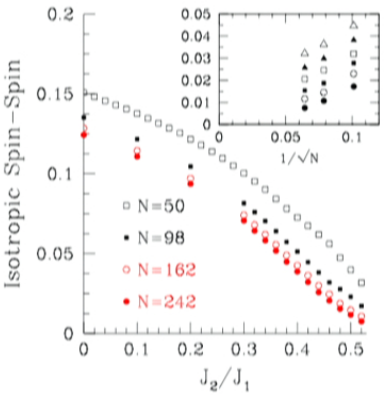
- Then, we reintroduce the constraint of one-fermion per site:

$$|\Phi(\chi_{ij}, \eta_{ij}, \mu, \zeta)\rangle = \mathcal{P}_G |\Phi_{\mathrm{MF}}(\chi_{ij}, \eta_{ij}, \mu, \zeta)\rangle$$

$$\mathcal{P}_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$$

Few results for the weakly-frustrated regime





- Correct slope in the finite-size scaling at $J_2 = 0$

  $E(L) = E_0 + \frac{\beta c}{L^3} + \dots$

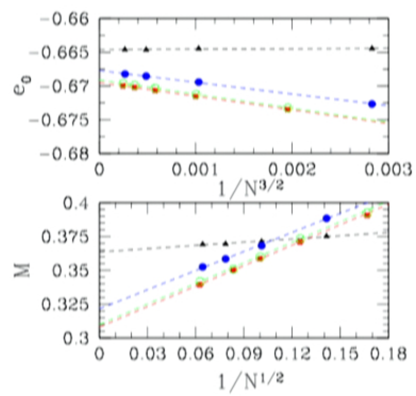
  $M^2(L) = M^2 + \frac{\alpha M^2}{c \chi_\perp L} + \dots$

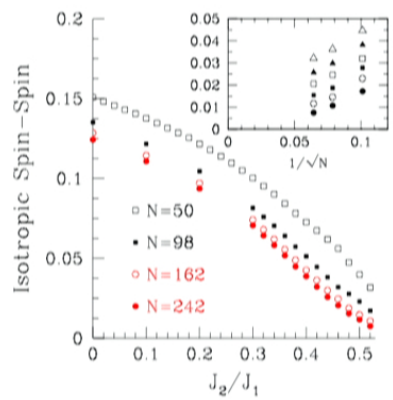
  (where L is the linear size $N = L \times L$)

- The magnetization M vanishes for $J_2/J_1 \simeq 0.48$

  (together with the variational parameter Δ_{AF})

Few results for the weakly-frustrated regime





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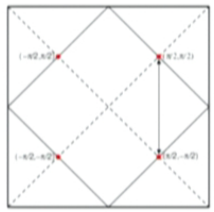
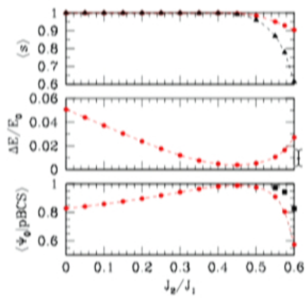
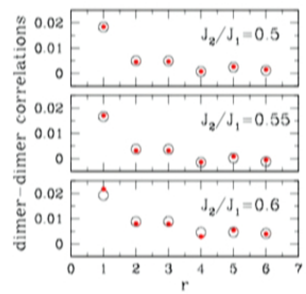
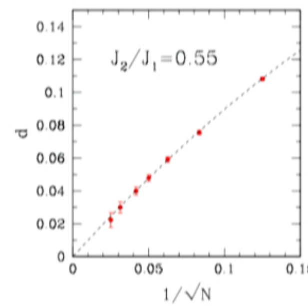
Inside the magnetically disordered phase



In 2001, we guessed:
$t_k = 2t(\cos k_x + \cos k_y)$
$\Delta_k = \Delta_{x^2-y^2}(\cos k_x - \cos k_y) + \Delta_{xy}(\sin 2k_x \sin 2k_y)$
After Wen, called Z2Azz13



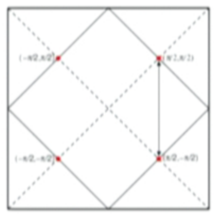




$$\langle s \rangle = \sum_x |\langle x|\Phi\rangle|^2 \mathrm{sign}\left\{\langle x|\Phi\rangle\langle x|\Psi_{\rm ex}\rangle\right\}$$

After the Wen's classification, it is the best projected fermionic state

Inside the magnetically disordered phase



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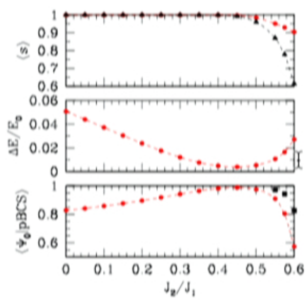

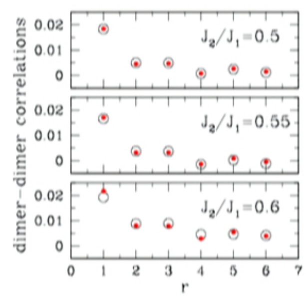

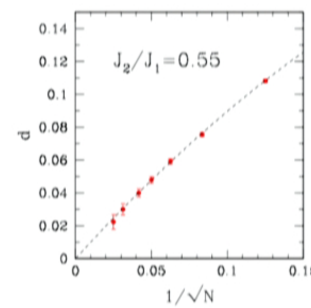

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Towards the exact ground state

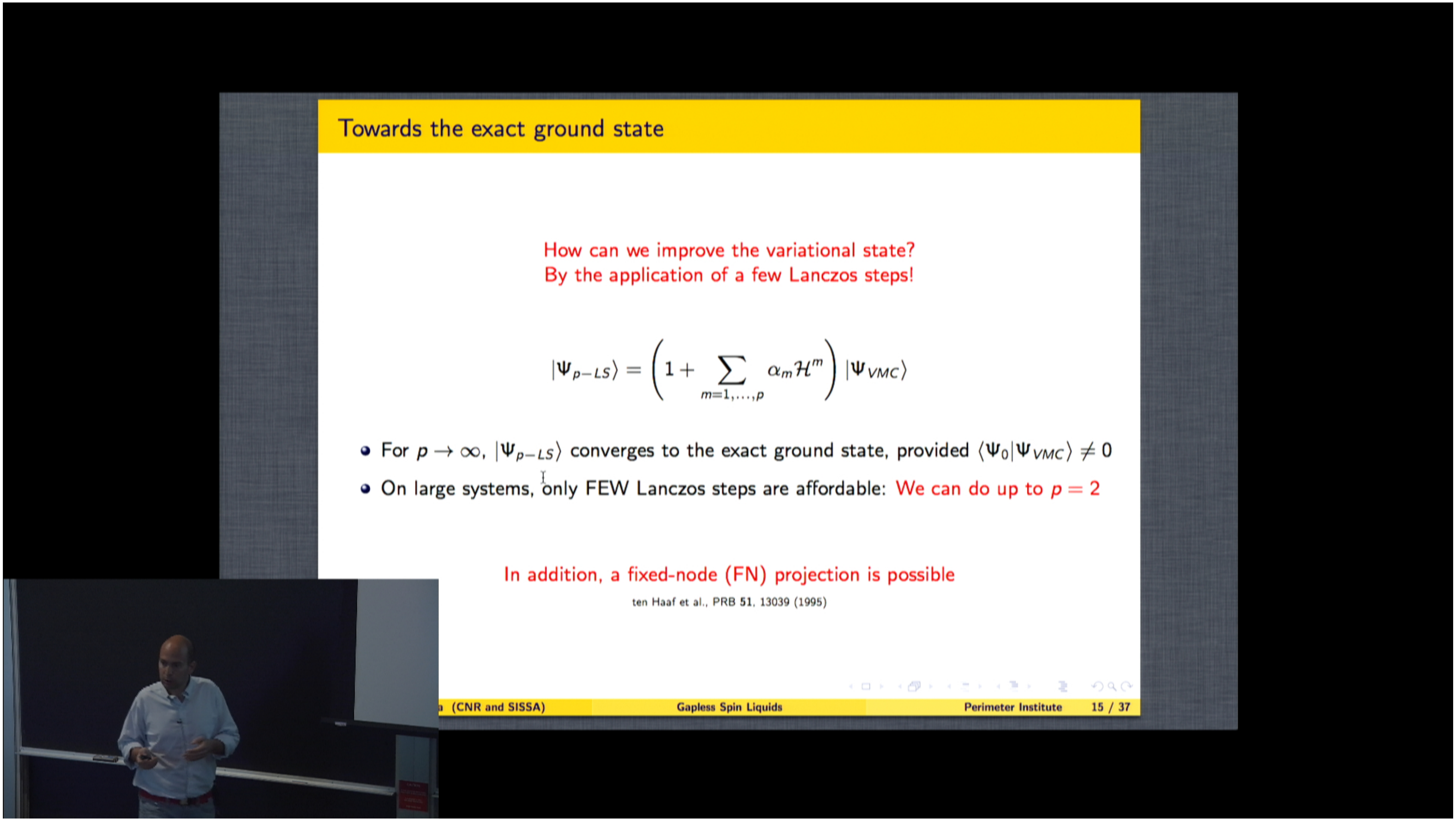
How can we improve the variational state?
By the application of a few Lanczos steps!

$$|\Psi_{p-LS}\rangle = \left(1 + \sum_{m=1,\ldots,p} \alpha_m \mathcal{H}^m\right) |\Psi_{VMC}\rangle$$

- For $p \to \infty$, $|\Psi_{p-LS}\rangle$ converges to the exact ground state, provided $\langle\Psi_0|\Psi_{VMC}\rangle \neq 0$
- On large systems, only FEW Lanczos steps are affordable: We can do up to $p = 2$

In addition, a fixed-node (FN) projection is possible

ten Haaf et al., PRB **51**, 13039 (1995)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The variance extrapolation

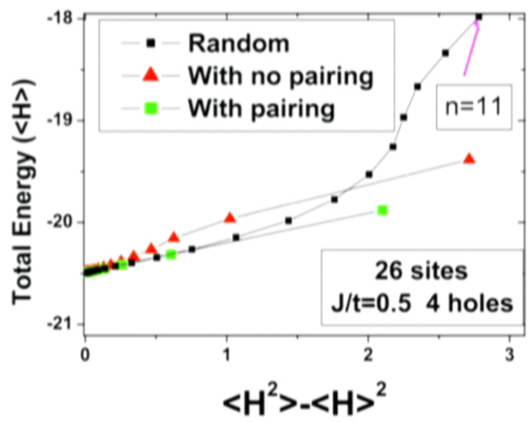
- A zero-variance extrapolation can be done

Whenever $|\Psi_{VMC}\rangle$ is sufficiently close to the ground state:

$$E \simeq E_0 + \text{const} \times \sigma^2$$

$$E = \langle \mathcal{H} \rangle / N$$
$$\sigma^2 = (\langle \mathcal{H}^2 \rangle - E^2)/N$$

How does it work?
Example: the $t-J$ model



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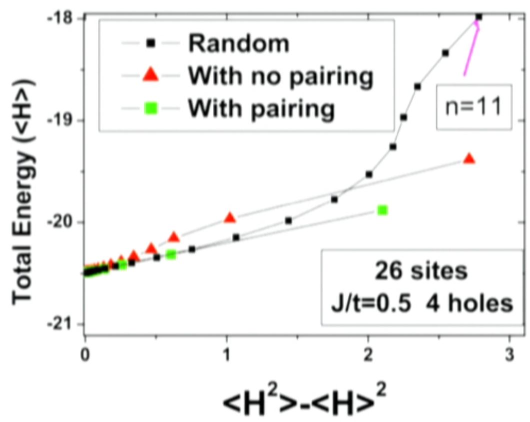


Going to the excitation spectrum

If a variational approach works also low-energy excitations must be described

$$\mathcal{H}_{\rm MF} = \sum_{i,j,\alpha} (\chi_{ij} + \mu\delta_{ij}) c^\dagger_{i,\alpha} c_{j,\alpha} + \sum_{i,j} (\eta_{ij} + \zeta\delta_{ij}) (c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + c^\dagger_{j,\uparrow} c^\dagger_{i,\downarrow}) + h.c.$$

After a Bogoliubov transformation:

$$\mathcal{H}_{\rm MF} = \sum_k (E_k \psi^\dagger_k \psi_k - E_k \phi^\dagger_k \phi_k)$$

The ground state is:

$$|\Phi^0_{\rm MF}\rangle = \prod_k \phi^\dagger_k |0\rangle$$

Excited states are obtained by:

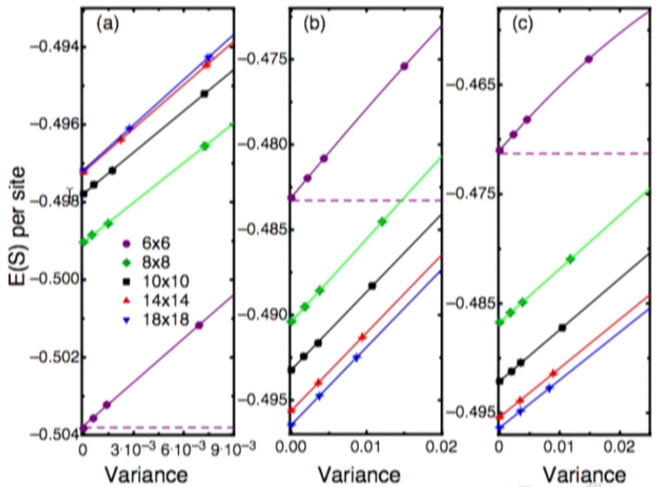
$$\phi_{q_1} \dots \phi_{q_n} \psi^\dagger_{p_1} \dots \psi^\dagger_{p_m} |\Phi^0_{\rm MF}\rangle$$

Spin excitations

Considering excited states that can be described by a SINGLE determinant, we have:

- The S=0 ground state
- The S=2 with momentum $k = (0, 0)$
- The S=1 with momentum $k = (\pi, 0)$ or $k = (0, \pi)$

Test case: $J_2/J_1 = 0.5$ and 6×6 cluster



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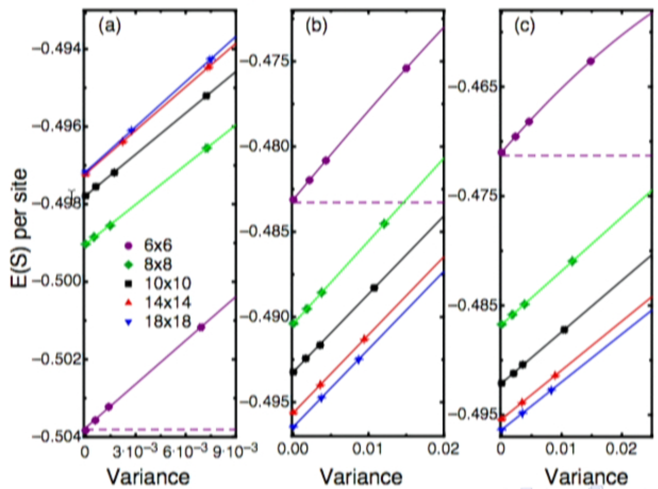
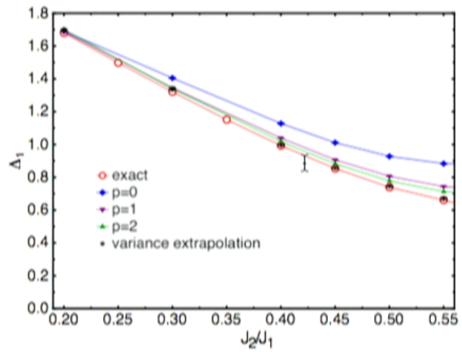


Spin excitations

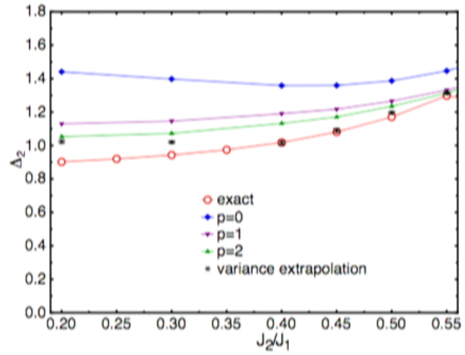
- The S=2 gap vanishes in the Néel phase
- The S=1 gap at $k = (\pi, 0)$ is instead finite in the Néel phase

The Lanczos extrapolation is performed on each state separately

Calculations on the 6×6 cluster vs exact results

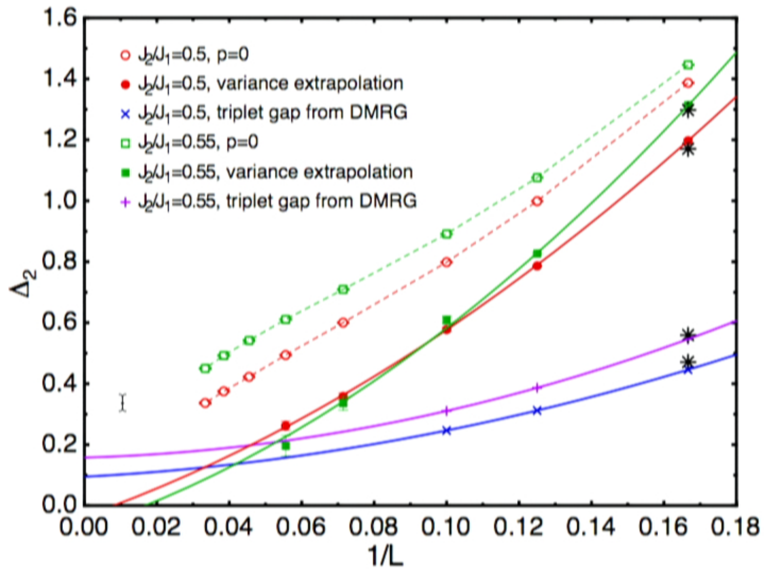


S=1 gap



S=2 gap

The S=2 spin excitation for large sizes



- $J_2/J_1 = 0.5 \longrightarrow \Delta_2 = -0.04(5)$
- $J_2/J_1 = 0.55 \longrightarrow \Delta_2 = -0.07(7)$

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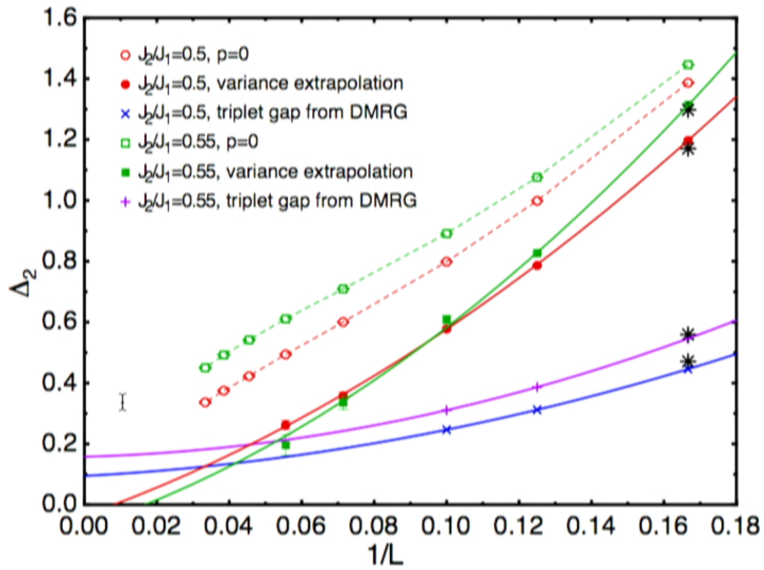

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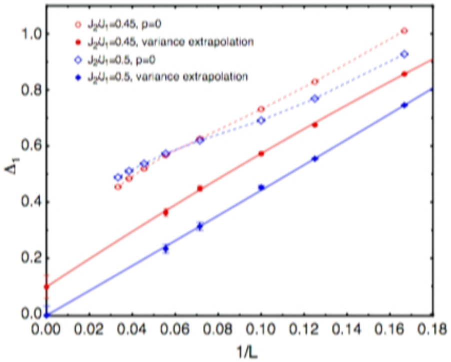
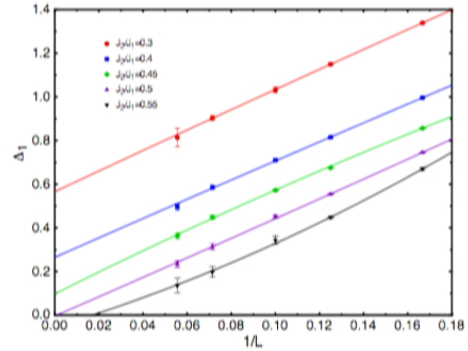
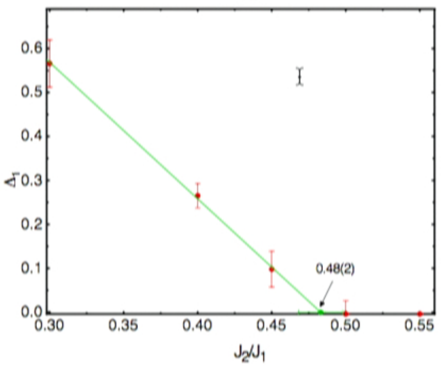




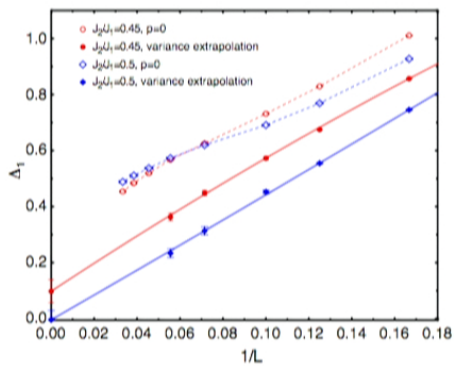


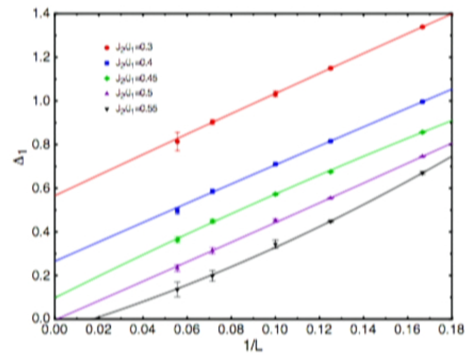
The spin gap is FINITE for $J_2/J_1 < 0.48$

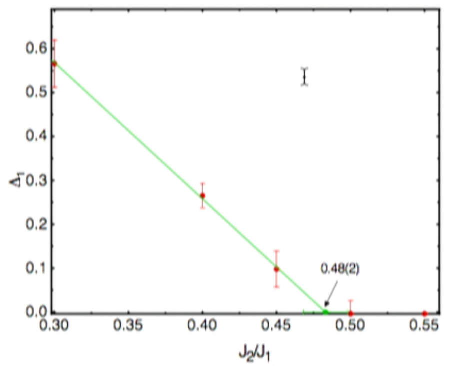
Instead, it vanishes for $J_2/J_1 > 0.48$

NON-trivial aspect of the SL phase!

The S=1 spin excitation for large sizes







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Conclusions (first part)

- Very good energies
  With few (TWO-THREE) variational parameters: Educated guess
  To be compared with about 16000 parameters in DMRG: Brute-force calculation
- Direct calculation of the spin gap for S=2 and S=1 excitations
  In both cases, we find evidence for a GAPLESS spin liquid

Our calculations are done on $L \times L$ clusters with PBC in both directions

DMRG calculations are done on $2L \times L$ cylinders with OBC along x and PBC along y (but the gap is computed only in the central part of the cluster)

Our approach may capture both gapless and gapped states

DMRG algorithm favors low-entangled (gapped) states

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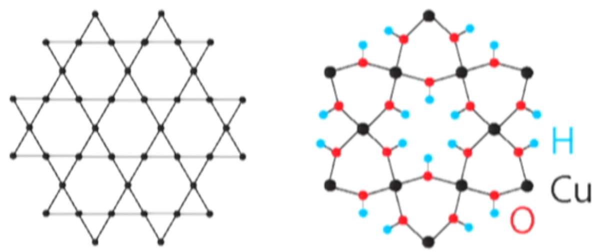
The Heisenberg model on the Kagome lattice

$$\mathcal{H} = J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \dots$$



- No magnetic order down to 50mK (despite $T_{CW} \simeq 200$K)
- Spin susceptibility rises with $T \to 0$ but then saturates below 0.5K
- Specific heat $C_v \propto T$ below 0.5K
- No sign of spin gap in dynamical Neutron scattering measurements

Mendels *et al.*, PRL 98, 077204 (2007)

Helton *et al.*, PRL 98, 107204 (2007)

Bert *et al.*, PRB 76, 132411 (2007)

Some of the previous results

Nearest-neighbor Heisenberg model on the Kagome lattice

Author	GS proposed	Energy/site	Method used
P.A. Lee	$U(1)$ gapless SL	$-0.42866(1)J$	Fermionic VMC
Singh	36-site HVBC	$-0.433(1)J$	Series expansion
Vidal	36-site HVBC	$-0.43221\ J$	MERA
Poilblanc	12- or 36-site VBC		QDM
Lhuillier	Chiral gapped SL		SBMF
White	Z_2 gapped SL	$-0.4379(3)J$	DMRG
Schollwoeck	Z_2 gapped SL	$-0.4386(5)J$	DMRG
Xie *et al.*	gapped SL	$-0.4364(1)J$	PESS

Ran, Hermele, Lee, and Wen, PRL **98**, 117205 (2007)

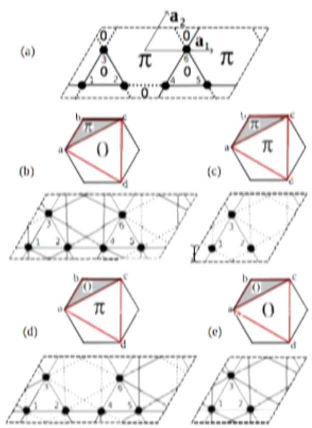
Yan, Huse, and White, Science **332**, 1173 (2011)

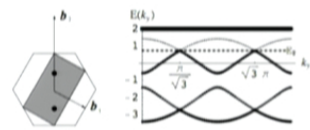
Results with projected wave functions

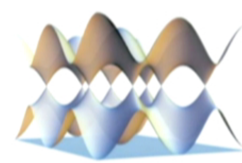
A variational ansatz with ONLY hopping but non-trivial fluxes has been proposed with

- π fluxes through hexagons and 0 fluxes through triangles
- Dirac points in the mean-field spinon spectrum

Ran, Hermele, Lee, and Wen, PRL **98**, 117205 (2007)







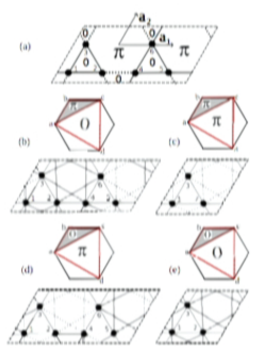
- 0 fluxes everywhere
- Fermi surface in the mean-field spinon spectrum

Can we have a Z_2 gapped spin liquid (as in DMRG)?

Projective symmetry-group analysis

Lu, Ran, and Lee, PRB **83**, 224413 (2011)

$$u_{ij} = \begin{pmatrix} \chi^*_{ij} & \Delta_{ij} \\ \Delta^*_{ij} & -\chi_{ij} \end{pmatrix}$$



No.	η_{12}	Λ_s	u_α	u_β	u_γ	$\tilde{u}_\gamma$	Label	Gapped?
1	+1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	$Z_2[0,0]A$	Yes
2	−1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	0	$Z_2[0,\pi]\beta$	**Yes**
3	+1	0	τ^2,τ^3	0	0	0	$Z_2[\pi,\pi]A$	No
4	−1	0	τ^2,τ^3	0	0	τ^2,τ^3	$Z_2[\pi,0]A$	No
5	+1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^3	$Z_2[0,0]B$	Yes
6	−1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^2	$Z_2[0,\pi]\alpha$	No
7	+1	0	0	τ^2,τ^3	0	0	–	–
8	−1	0	0	τ^2,τ^3	0	0	–	–
9	+1	0	0	0	τ^2,τ^3	0	–	–
10	−1	0	0	0	τ^2,τ^3	0	–	–
11	+1	0	0	τ^2	τ^2	0	–	–
12	−1	0	0	τ^2	τ^2	0	–	–
13	+1	τ^3	τ^3	τ^2,τ^3	τ^3	τ^3	$Z_2[0,0]D$	Yes
14	−1	τ^3	τ^3	τ^2,τ^3	τ^3	0	$Z_2[0,\pi]\gamma$	No
15	+1	τ^3	τ^3	τ^3	τ^2,τ^3	τ^3	$Z_2[0,0]C$	Yes
16	−1	τ^3	τ^3	τ^3	τ^2,τ^3	0	$Z_2[0,\pi]\delta$	No
17	+1	0	τ^2	τ^3	0	0	$Z_2[\pi,\pi]B$	No
18	−1	0	τ^2	τ^3	0	τ^3	$Z_2[\pi,0]B$	No
19	+1	0	τ^2	0	τ^2	0	$Z_2[\pi,\pi]C$	No
20	−1	0	τ^2	0	τ^2	τ^3	$Z_2[\pi,0]C$	No

Only ONE gapped SL connected with the U(1) Dirac SL:

FOUR gapped SL connected with the Uniform U(1) SL:

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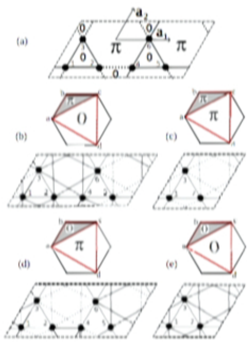

No.	η_{12}	Λ_s	u_α	u_β	u_γ	$\tilde{u}_\gamma$	Label	Gapped?
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3	+1	0	τ^2,τ^3	0	0	0	$Z_2[\pi,\pi]A$	No
4	−1	0	τ^2,τ^3	0	0	τ^2,τ^3	$Z_2[\pi,0]A$	No
5	+1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^3	$Z_2[0,0]B$	Yes
6	−1	τ^3	τ^2,τ^3	τ^3	τ^3	τ^2	$Z_2[0,\pi]\alpha$	No
7	+1	0	0	τ^2,τ^3	0	0	–	–
8	−1	0	0	τ^2,τ^3	0	0	–	–
9	+1	0	0	0	τ^2,τ^3	0	–	–
10	−1	0	0	0	τ^2,τ^3	0	–	–
11	+1	0	0	τ^2	τ^2	0	–	–
12	−1	0	0	τ^2	τ^2	0	–	–
13	+1	τ^3	τ^3	τ^2,τ^3	τ^3	τ^3	$Z_2[0,0]D$	Yes
14	−1	τ^3	τ^3	τ^2,τ^3	τ^3	0	$Z_2[0,\pi]\gamma$	No
15	+1	τ^3	τ^3	τ^3	τ^2,τ^3	τ^3	$Z_2[0,0]C$	Yes
16	−1	τ^3	τ^3	τ^3	τ^2,τ^3	0	$Z_2[0,\pi]\delta$	No
17	+1	0	τ^2	τ^3	0	0	$Z_2[\pi,\pi]B$	No
18	−1	0	τ^2	τ^3	0	τ^3	$Z_2[\pi,0]B$	No
19	+1	0	τ^2	0	τ^2	0	$Z_2[\pi,\pi]C$	No
20	−1	0	τ^2	0	τ^2	τ^3	$Z_2[\pi,0]C$	No

Only ONE gapped SL connected with the U(1) Dirac SL:

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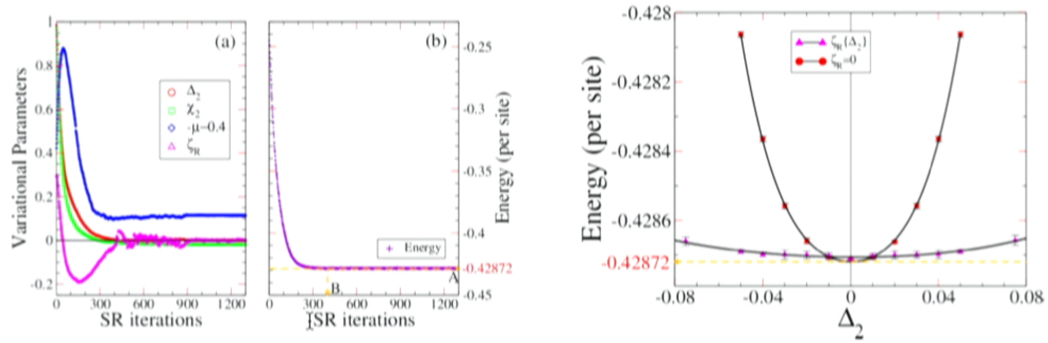
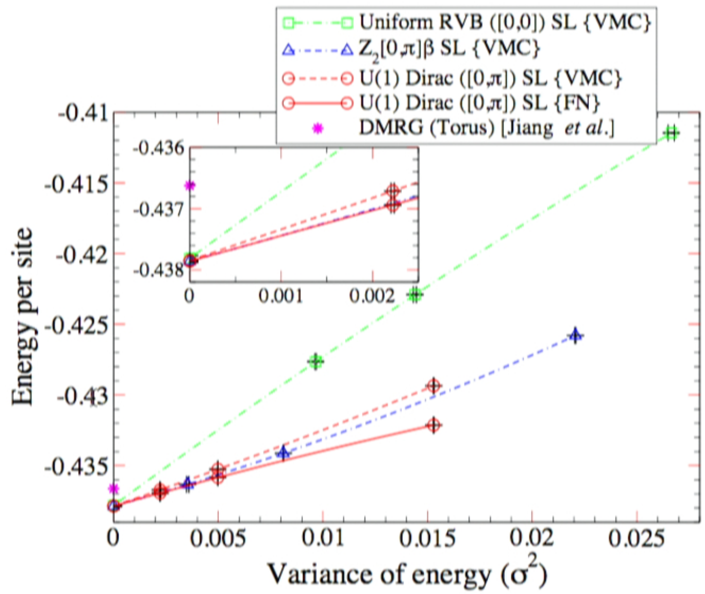
The Dirac U(1) SL is stable against opening a gap



- By optimizing the variational state, the breaking terms go to zero
- The best variational energy is obtained by the U(1) Dirac state

Calculations on the 48-site cluster

Our zero-variance extrapolation gives: $E/N \simeq -0.4378$



$E/N \simeq -0.4387$ by ED, A. Lauchli (seen at APS in Boston)
$E/N \simeq -0.4381$ by DMRG, S. White (private communication)

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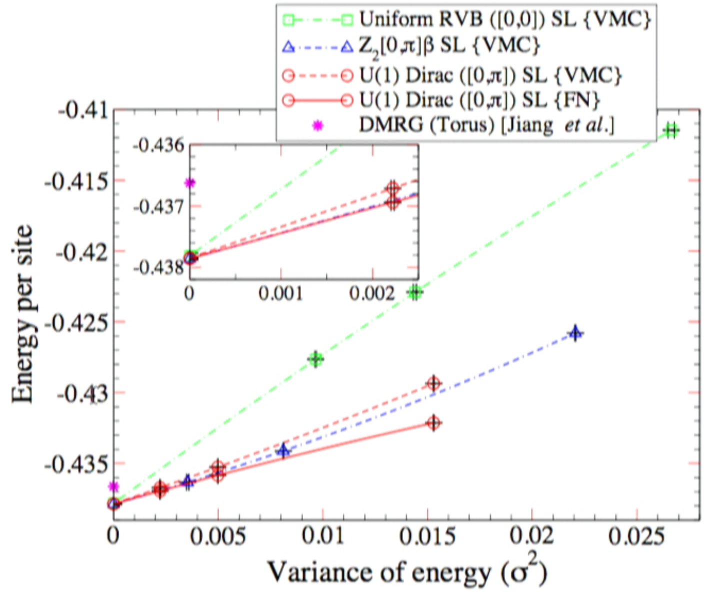

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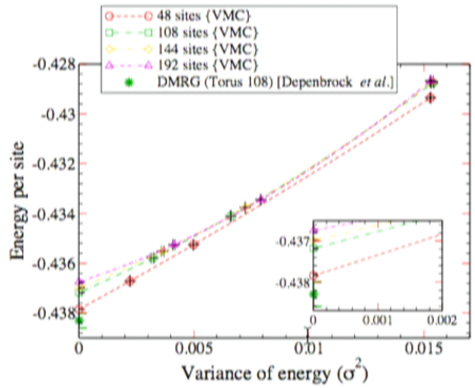
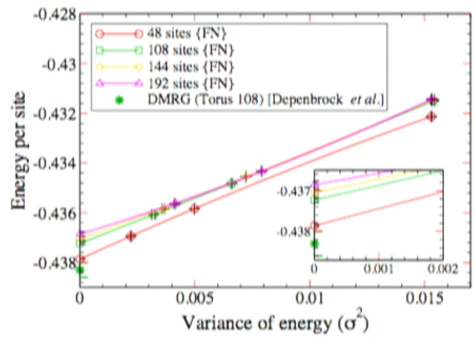
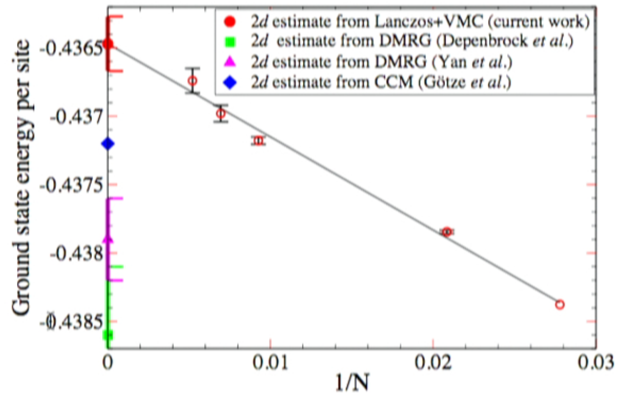
Calculations on larger clusters





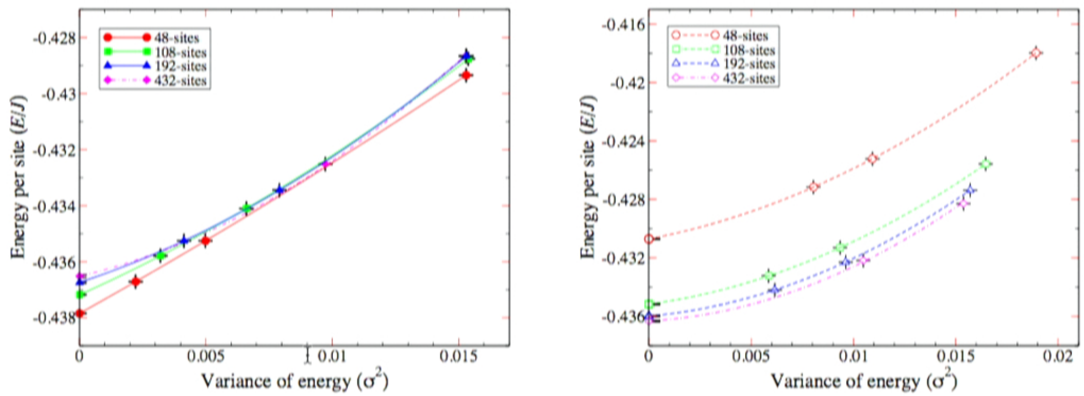
- NO substraction techniques to get the energy
- The state has ALL symmetries of the lattice
- The extrapolated values are essentially size consistent

The thermodynamic limit



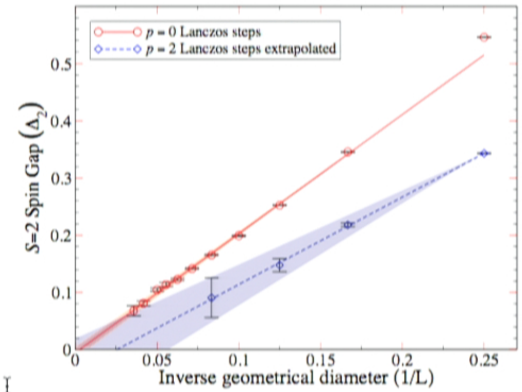
- OUR thermodynamic energy is: $E/J = -0.4365(2)$
- DMRG thermodynamic energy is: $E/J = -0.4386(5)$

The Lanczos step extrapolations



- We separately extrapolate both $S = 0$ and $S = 2$ energies
- Then the gap (zero-variance) gap is computed

The $S = 2$ gap of the kagome Heisenberg model



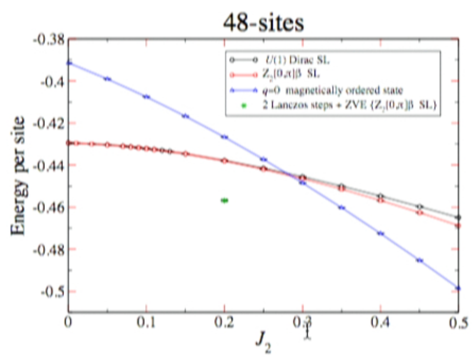
- The final result is $\Delta_2 = -0.04 \pm 0.06$
- The "upper" bound is given by $\Delta_2 \simeq 0.02$
- The $S = 1$ gap should be $\Delta_1 \lesssim 0.01$

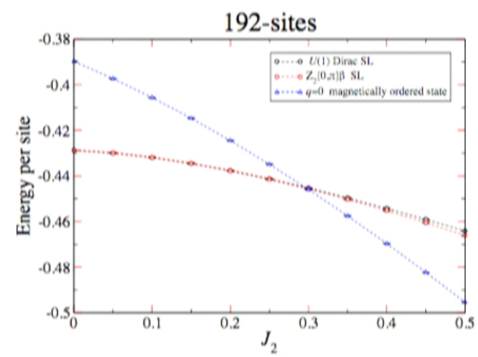
Much smaller than previous DMRG estimations

More similar to recent calculations by Nishimoto *et al.* $\Delta_1 = 0.05 \pm 0.02$

Nishimoto, Shibata, and Hotta, Nat. Commun. **4**, 2287 (2013)

Adding the next-nearest-neighbor super-exchange

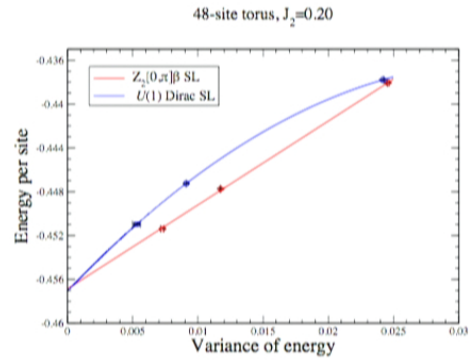




- The gapped Z_2 state overcomes the U(1) Dirac one for $J_2/J_1 > 0.1$
- The magnetic state with $q = 0$ (Jastrow) is stabilized for $J_2/J_1 > 0.3$

Adding the next-nearest-neighbor super-exchange

Applying Lanczos steps on 48 sites



- For finite J_2/J_1 the gapped Z_2 state has a "better" extrapolation with Lanczos steps
- Calculations on larger clusters are in progress...

Conclusions

Results up to now:

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  With TWO variational parameters: Educated guess
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- Direct calculation of the $S = 2$ gap
  No evidence for a finite gap in thermodynamic limit

Pros

- Very flexible approach that may describe several different phases (gapped and gapless, not only low-entanglement states)
- Natural way of constructing and understanding low-energy excitations
- Applying few Lanczos steps allows for a sizable improvement

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- Still, it is a biased approach and more work must be done

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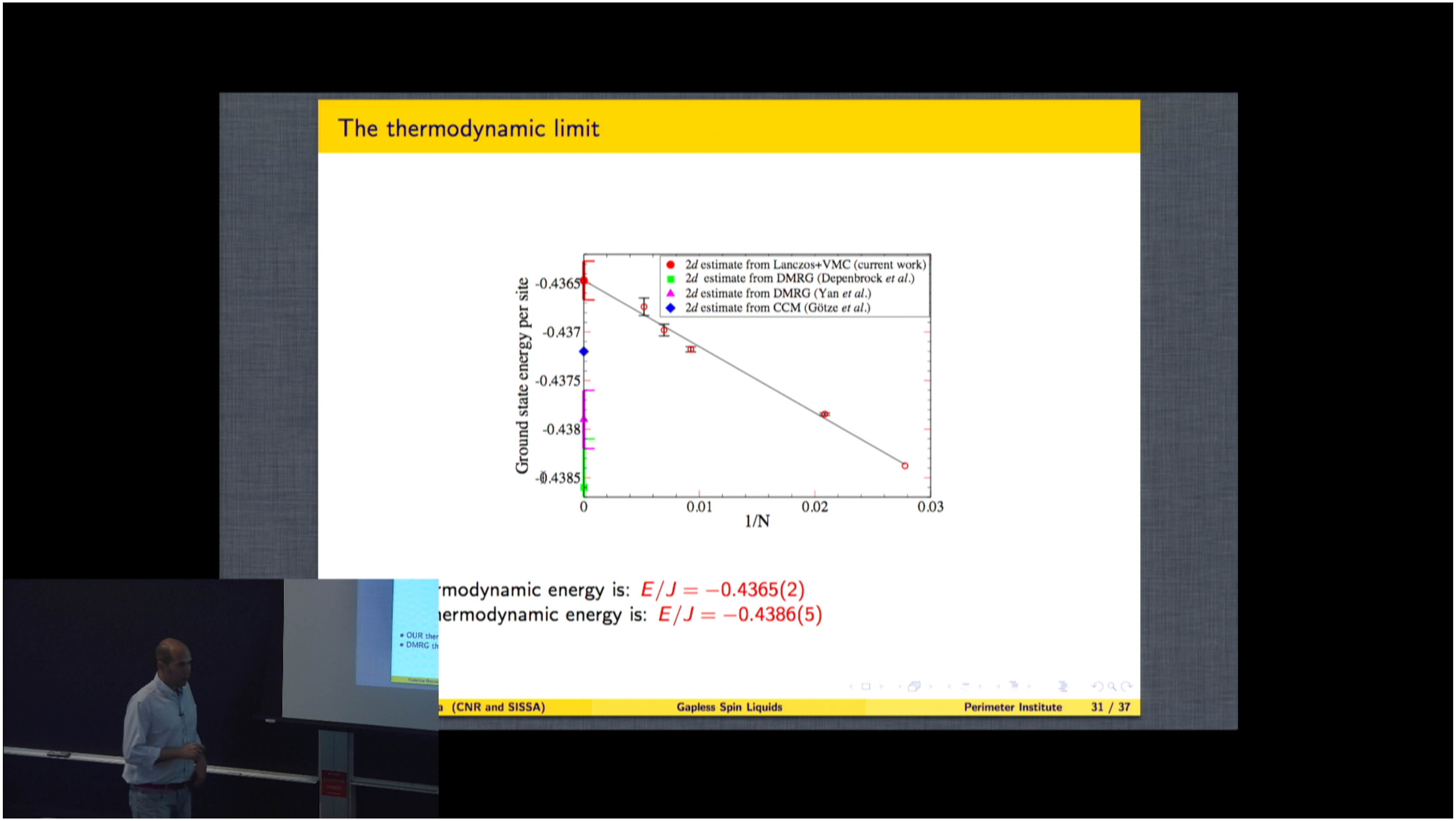
The thermodynamic limit
2d estimate from Lanczos+VMC (current work)
2d estimate from DMRG (Depenbrock et al.)
2d estimate from DMRG (Yan et al.)
2d estimate from CCM (Götze et al.)
Ground state energy per site
-0.4365
-0.437
-0.4375
-0.438
-0.4385
0
0.01
0.02
0.03
1/N
rmodynamic energy is: $E/J = -0.4365(2)$
nermodynamic energy is: $E/J = -0.4386(5)$
a (CNR and SISSA)
Gapless Spin Liquids
Perimeter Institute
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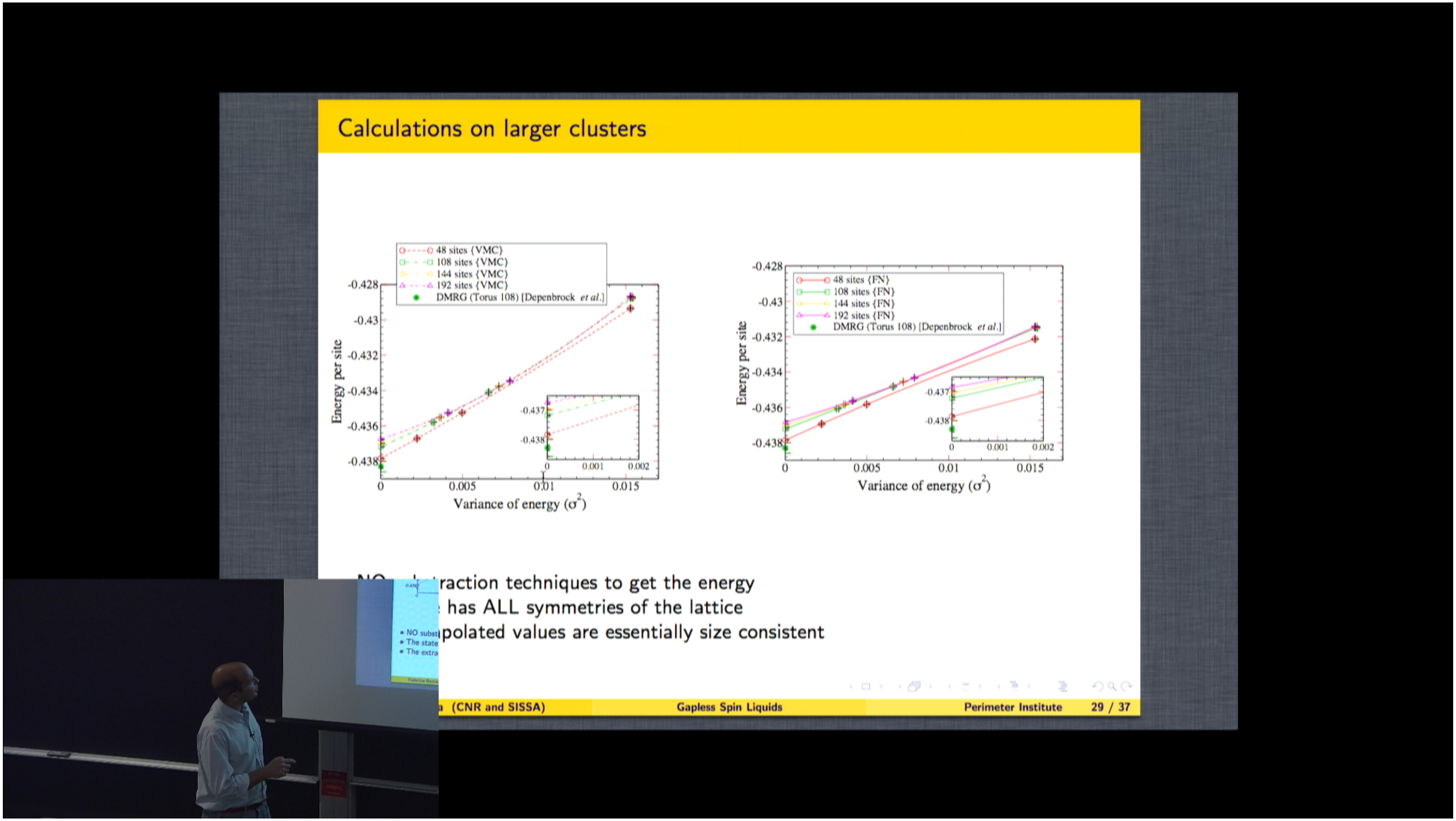
Calculations on larger clusters
48 sites {VMC}
108 sites {VMC}
144 sites {VMC}
192 sites {VMC}
DMRG (Torus 108) [Depenbrock et al.]
Energy per site
Variance of energy (σ²)
48 sites {FN}
108 sites {FN}
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