Gapless spin liquids in frustrated Heisenberg models

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New Horizon of Strongly Correlated Physics, June 2014

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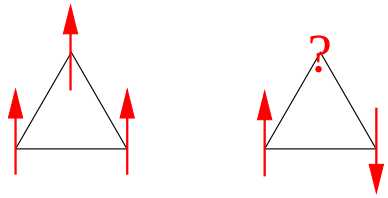
A. Parola (Como), D. Poilblanc (CNRS, Toulouse), and S. Sorella (SISSA)

Ultimate frustration?

Looking for a magnetically disordered ground state



- Many theoretical suggestions since P.W. Anderson (1973)

  Anderson, Mater. Res. Bull. **8**, 153 (1973)

  Fazekas and Anderson, Phil. Mag. **30**, 423 (1974)

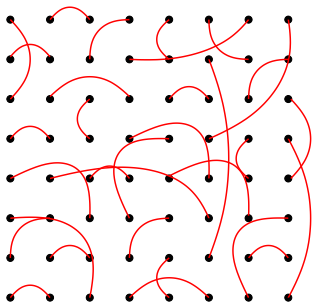
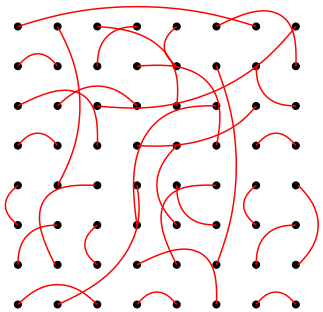
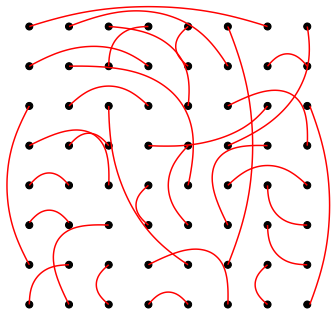
"Resonating valence-bond" (quantum spin liquid) states

Idea: the best state for two spin-1/2 spins is a valence bond (a spin singlet):

$$|VB\rangle_{\mathbf{R},\mathbf{R}'} = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_{\mathbf{R}}|\downarrow\rangle_{\mathbf{R}'} - |\downarrow\rangle_{\mathbf{R}}|\uparrow\rangle_{\mathbf{R}'}\right)$$

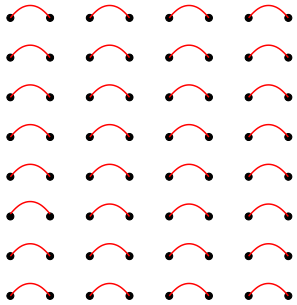
Every spin of the lattice is coupled to a partner

Then, take a superposition of different valence bond configurations

$\Psi =$  $+$  $+$  $+ \ldots$

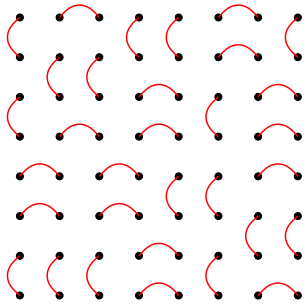
Valence-bond states: liquids and solids

Valence-bond solid



breaks translational/rotational symmetries

Short-range RVB



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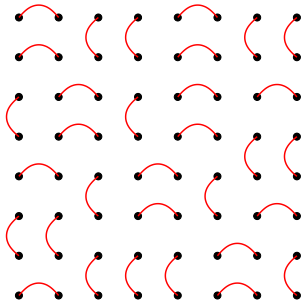

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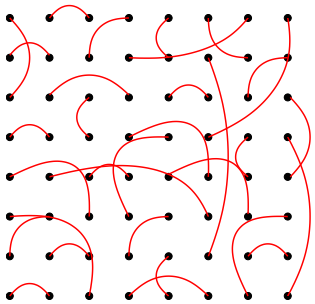
Long-range RVB



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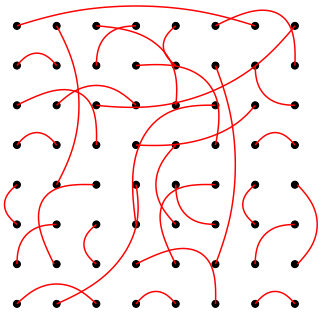
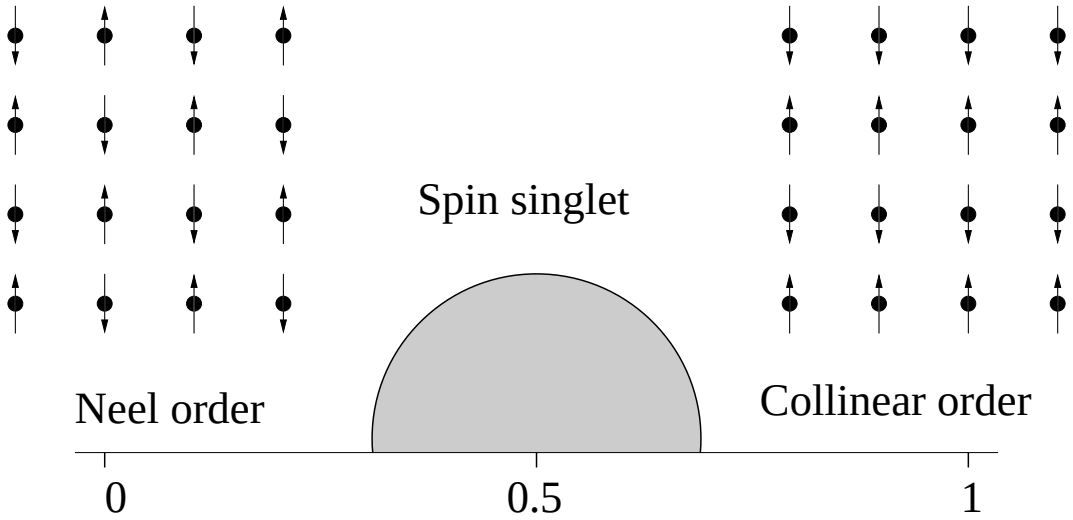


+ ...

The Heisenberg model on the frustrated square lattice

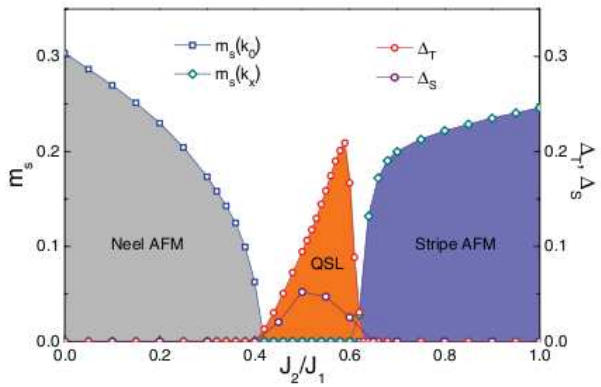
$$\mathcal{H} = J_1 \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{\langle\langle ij \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$



- 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 $VOMoO_4$ ($J_2 < 0.5 J_1$)

Recent DMRG calculations

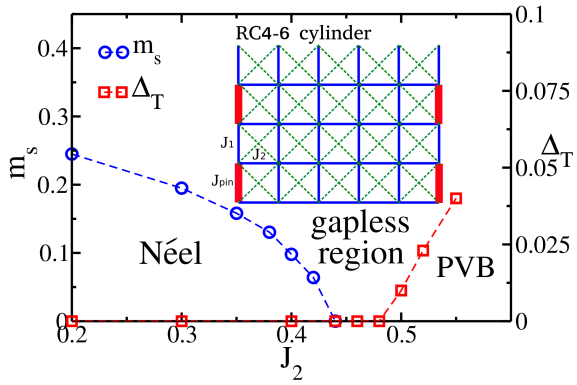


Jiang, Yao, and Balents, PRB **86**, 024424 (2012)

- It has been criticized by Sandvik (possible dimer order)

Sandvik, PRB **85**, 134407 (2012)

- More recent calculations with both spin-liquid and dimer phases



Gong, Zhu, Sheng, Motrunich, Fisher, arXiv:1311.5962

Describing magnetically disordered phases

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

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

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

- At the mean-field level:

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

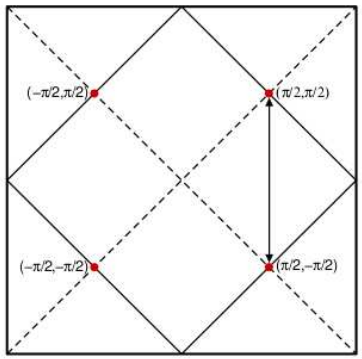
$$\langle c_{i,\alpha}^\dagger c_{i,\alpha} \rangle = 1 \qquad \langle c_{i,\alpha} c_{i,\beta} \rangle \epsilon_{\alpha\beta} = 0$$

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

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

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

Symmetry of the mean-field ansatz

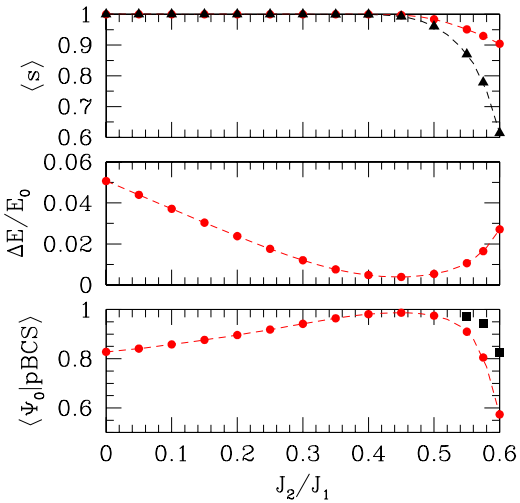


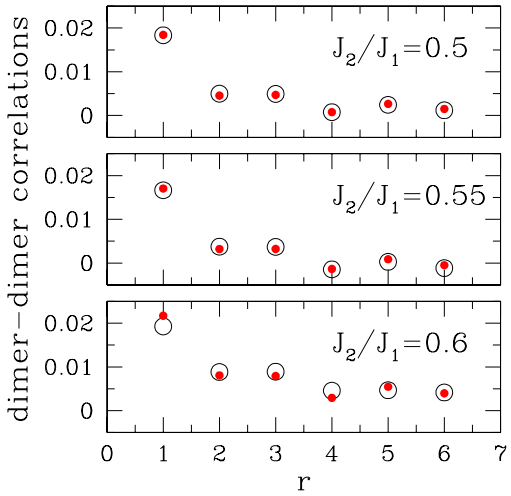
In 2001, we guessed:

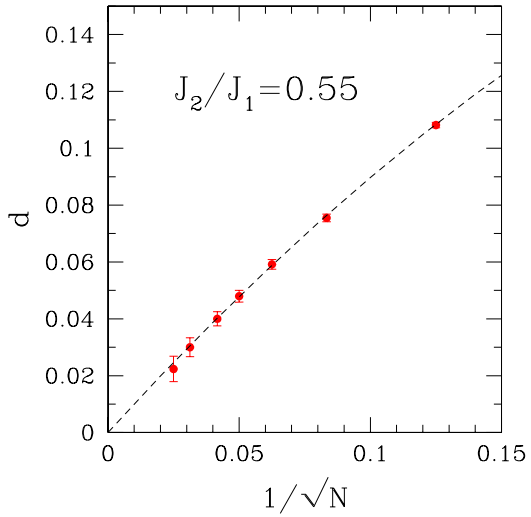
$\chi_k = 2t(\cos k_x + \cos k_y)$

$\eta_k = \Delta_{x^2-y^2}(\cos k_x - \cos k_y) + \Delta_{xy}(\sin 2k_x \sin 2k_y)$

After Wen, called Z2Azz13







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

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

Towards the exact ground state

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

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

- 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)

The variance extrapolation

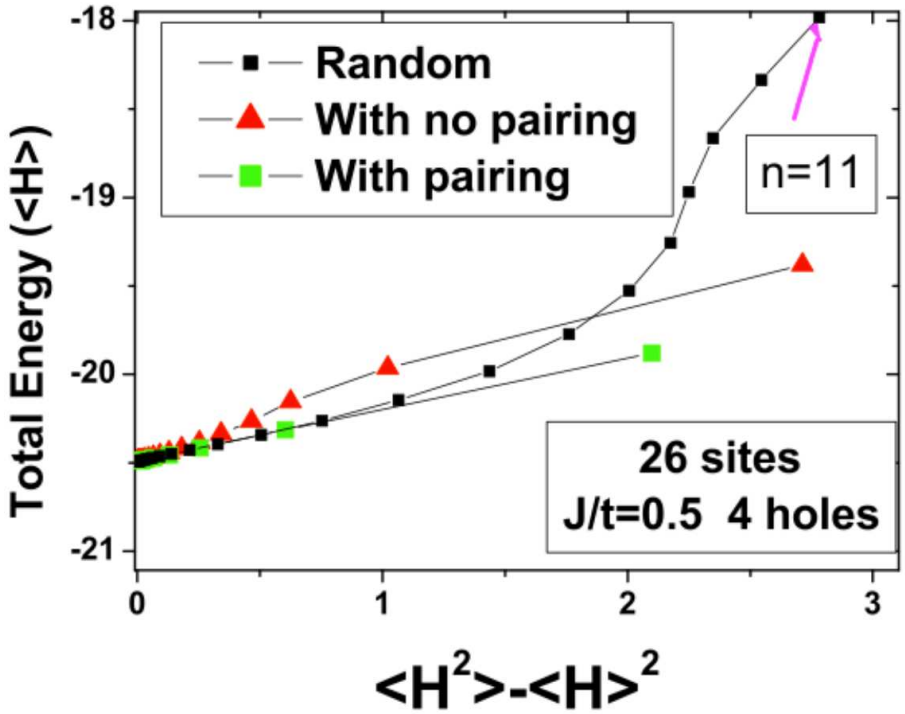
- A zero-variance extrapolation can be done

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



Going to the excitation spectrum

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

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

After a Bogoliubov transformation:

$$\mathcal{H}_{\mathrm{MF}} = \sum_{k} (E_k \psi^{\dagger}_k \psi_k - E_k \phi^{\dagger}_k \phi_k)$$

The ground state is:

$$|\Phi^0_{\mathrm{MF}}\rangle = \prod_k \phi^{\dagger}_k |0\rangle$$

Excited states are obtained by:

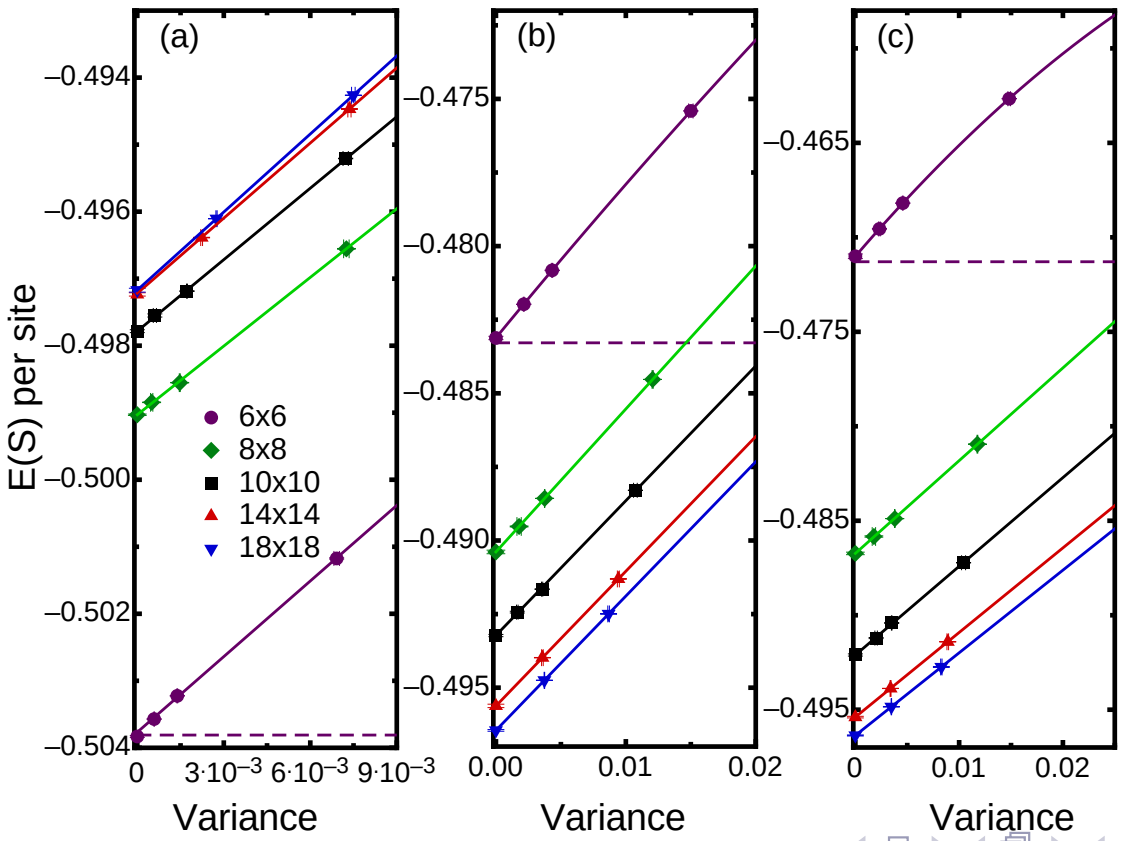
$$\phi_{q_1} \dots \phi_{q_n} \psi^{\dagger}_{p_1} \dots \psi^{\dagger}_{p_m} |\Phi^0_{\mathrm{MF}}\rangle$$

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

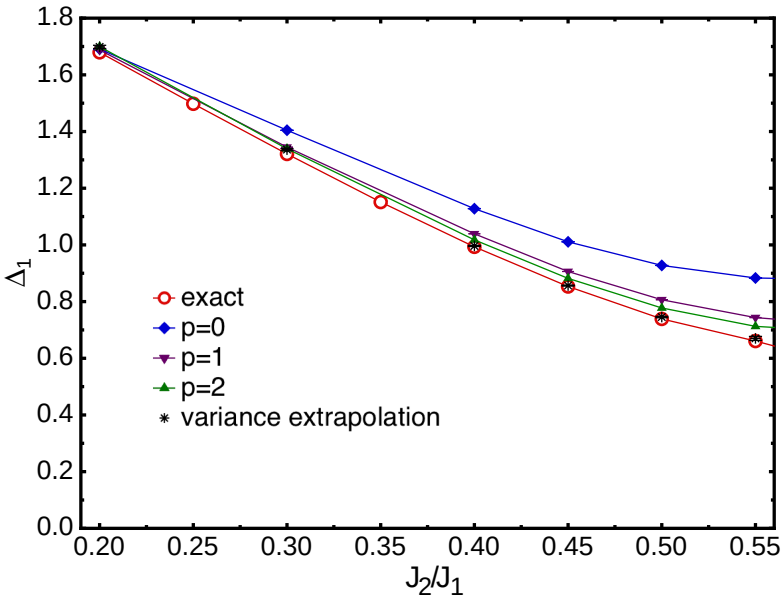


Spin excitations

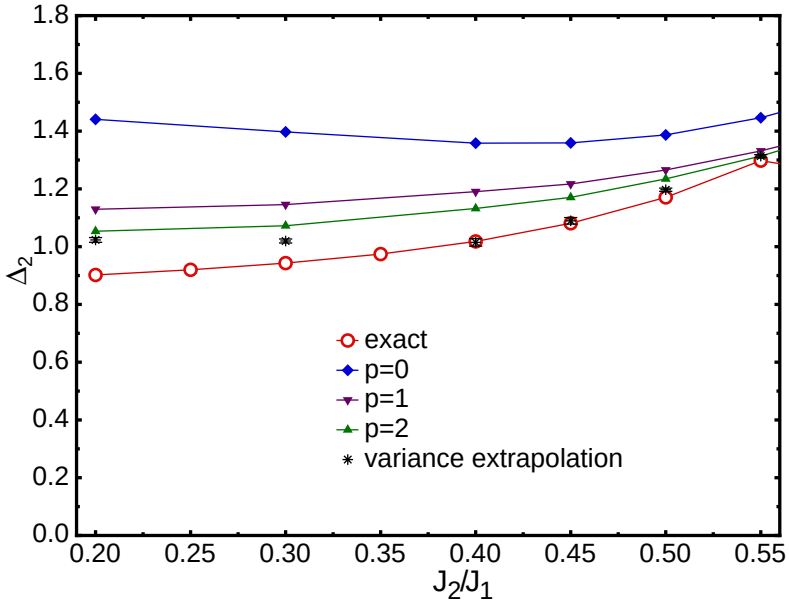
- The S=2 gap vanishes in the Néel phase
- The S=1 gap at $k = (\pi, 0)$ is instead finite in the Néel phase

The Lanczos extrapolation is performed on each state separately

Calculations on the 6×6 cluster vs exact results

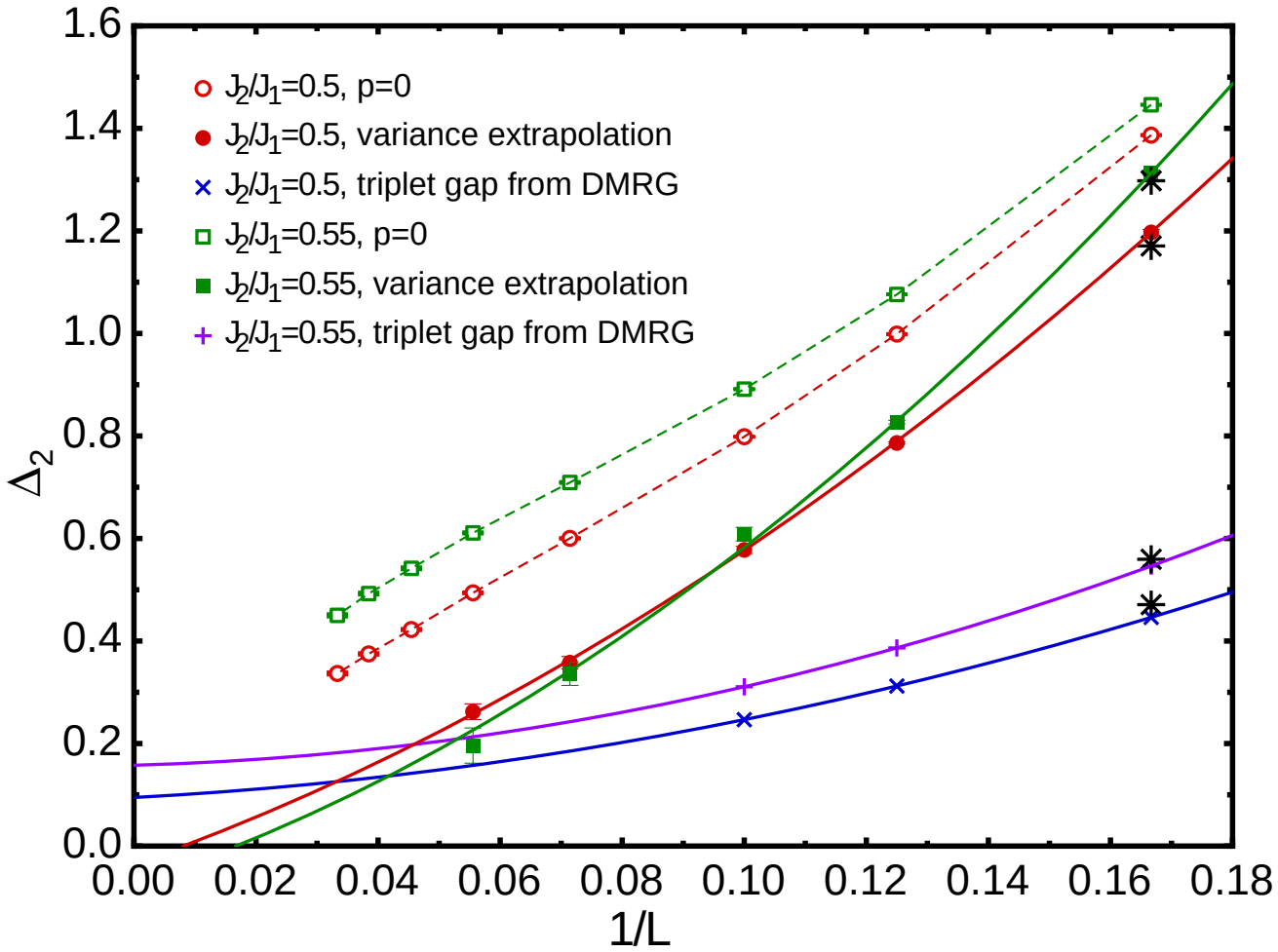


S=1 gap



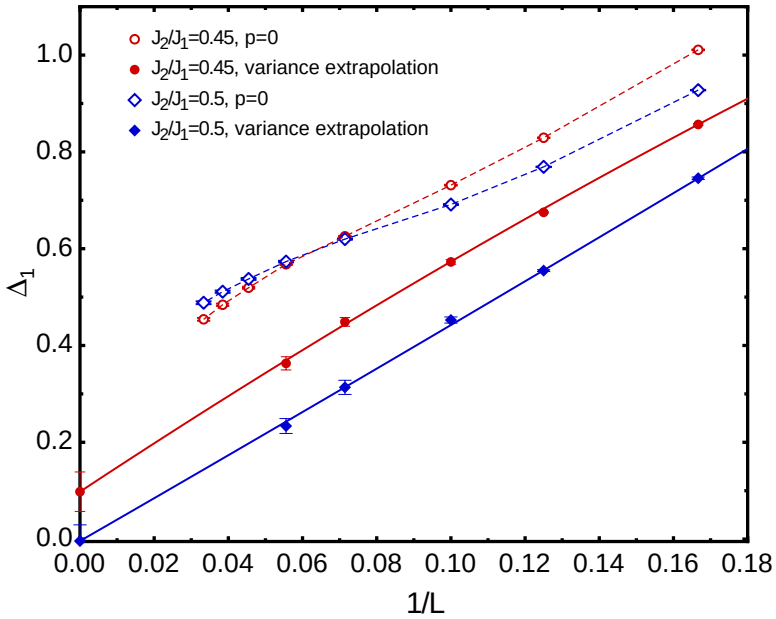
S=2 gap

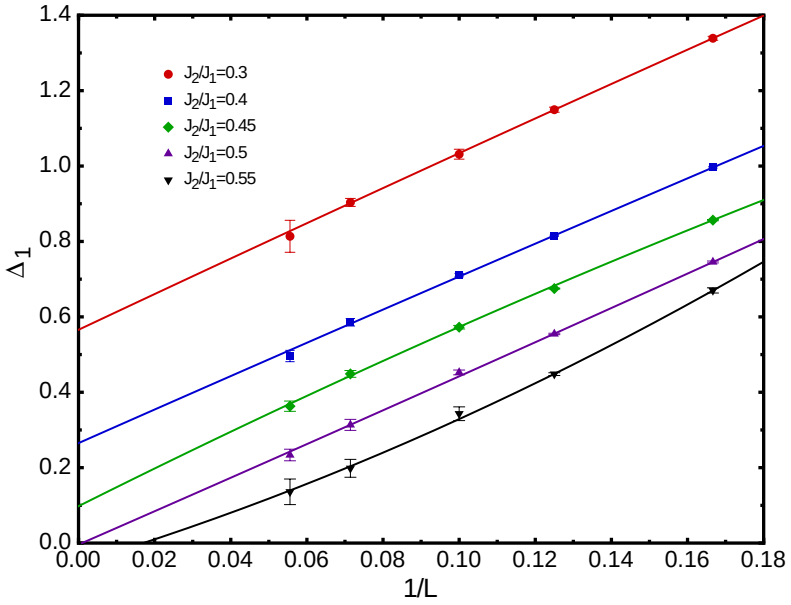
The S=2 spin excitation for large sizes

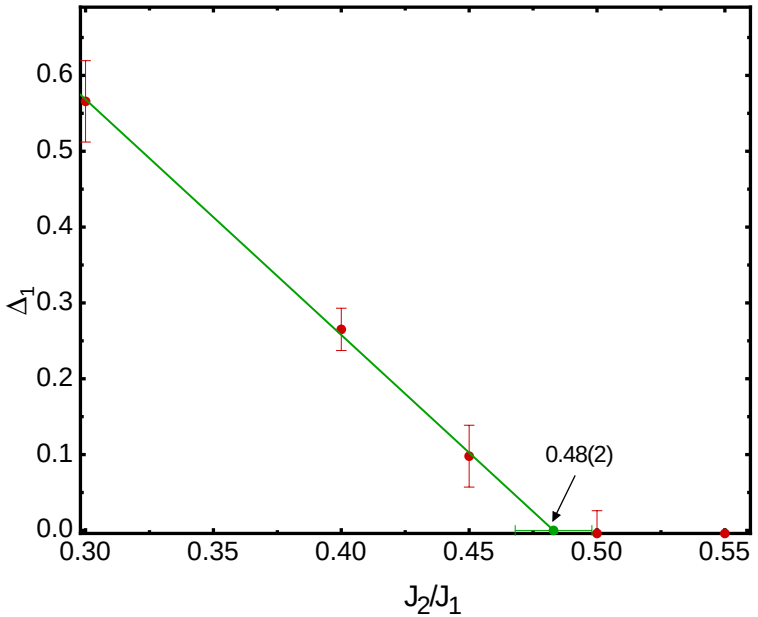


- $J_2/J_1 = 0.5 \longrightarrow \Delta_2 = -0.04(5)$
- $J_2/J_1 = 0.55 \longrightarrow \Delta_2 = -0.07(7)$

The S=1 spin excitation for large sizes







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!

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

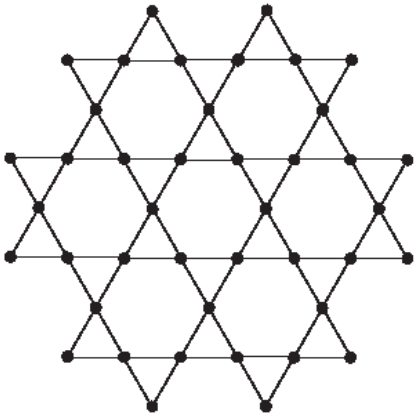
DMRG calculations are done on $2L \times L$ cylinders with OBC along x and PBC along y (but the gap is computed only in the central part of the cluster)

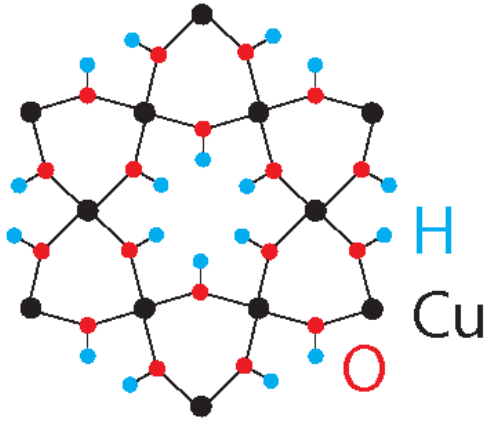
Our approach may capture both gapless and gapped states

DMRG algorithm favors low-entangled (gapped) states

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)

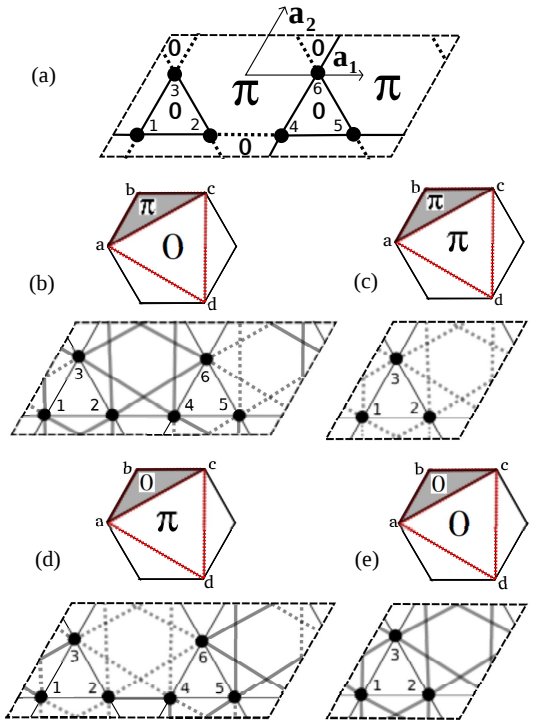
Yan, Huse, and White, Science **332**, 1173 (2011)

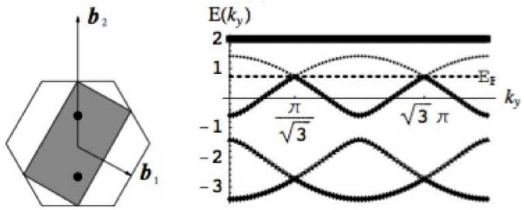
Results with projected wave functions

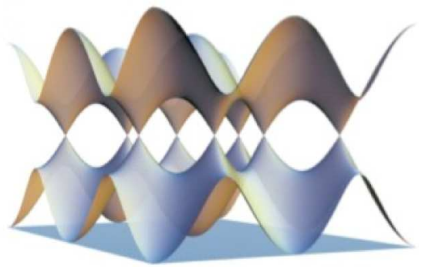
A variational ansatz with ONLY hopping but non-trivial fluxes has been proposed with

- 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)







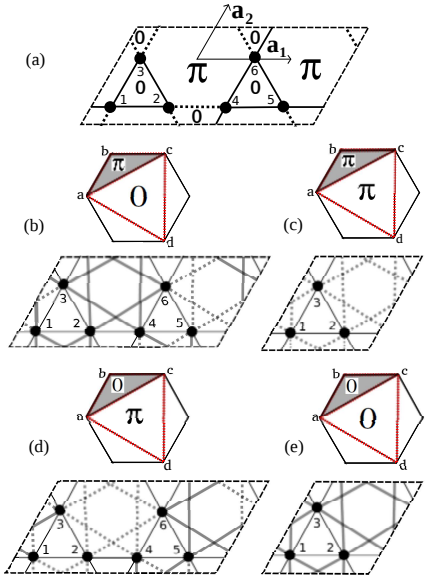
- 0 fluxes everywhere
- Fermi surface in the mean-field spinon spectrum

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

Projective symmetry-group analysis

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

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

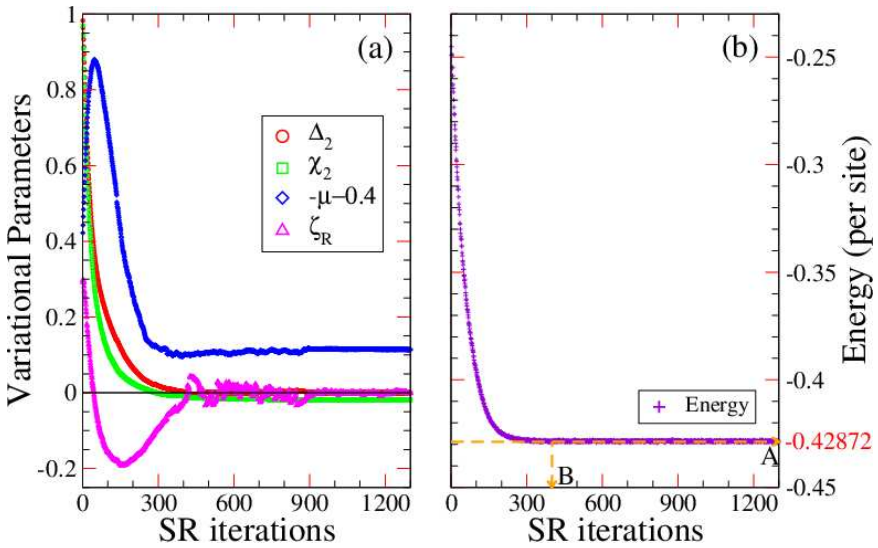


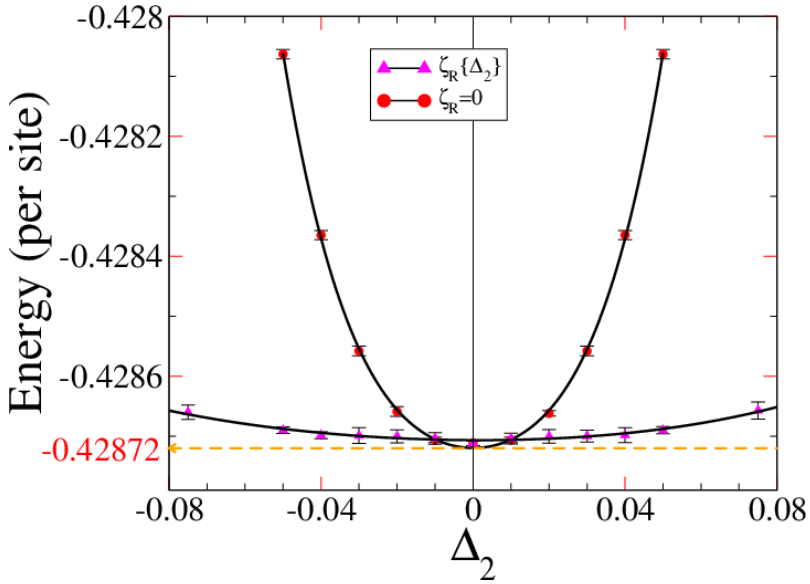
No.	η_{12}	Λ_s	u_α	u_β	u_γ	$\tilde{u}_\gamma$	Label	Gapped?
1	+1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	$Z_2[0,0]A$	Yes
2	−1	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	τ^2,τ^3	0	$\mathbb{Z}_2[0,\pi]\beta$	**Yes**
3	+1	0	τ^2,τ^3	0	0	0	$Z_2[\pi,\pi]A$	No
4	−1	0	τ^2,τ^3	0	0	τ^2,τ^3	$Z_2[\pi,0]A$	No
5	+1	τ^3	τ^2,τ^3	τ^3	τ^3	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:

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

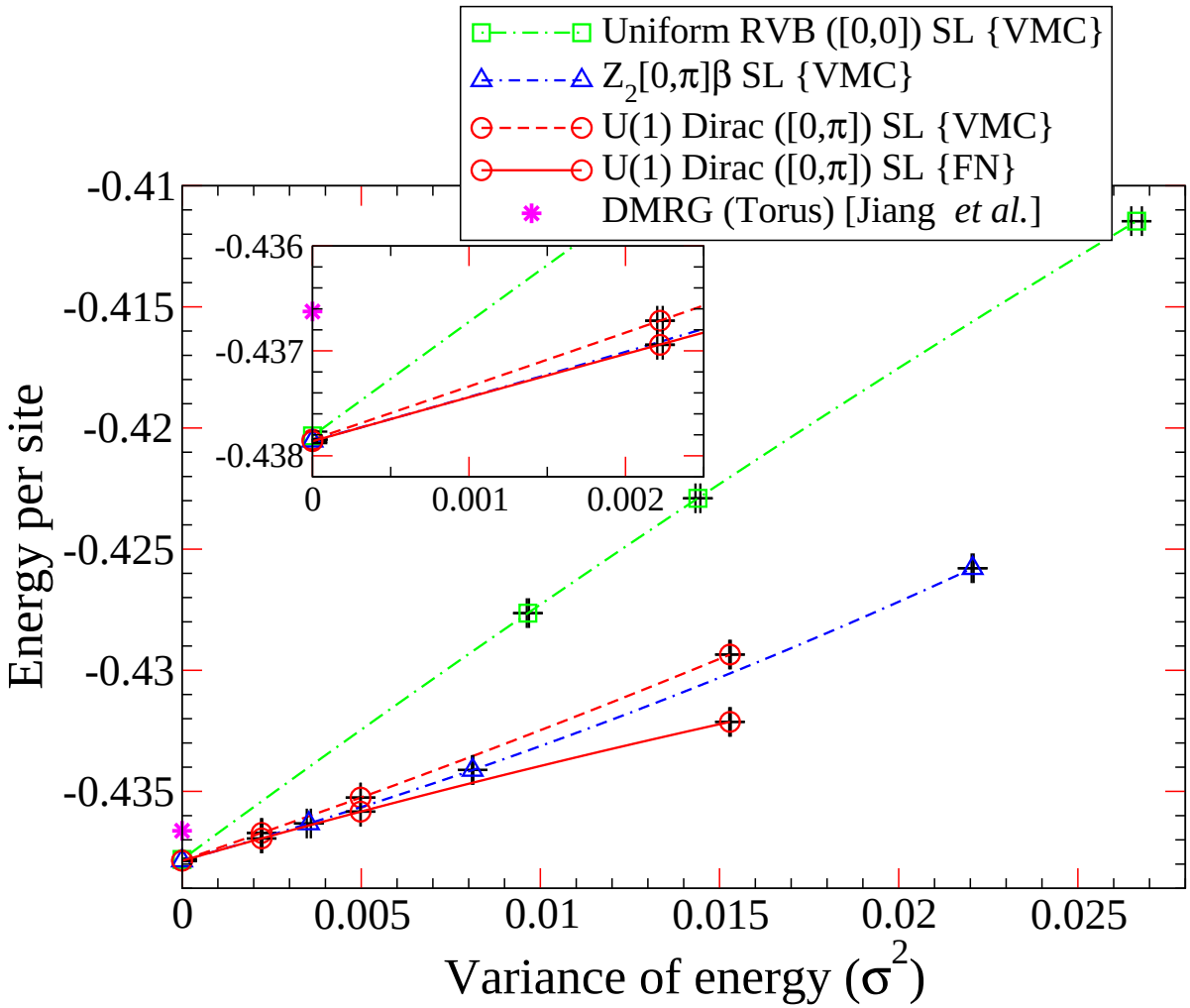




- By optimizing the variational state, the breaking terms go to zero
- The best variational energy is obtained by the U(1) Dirac state

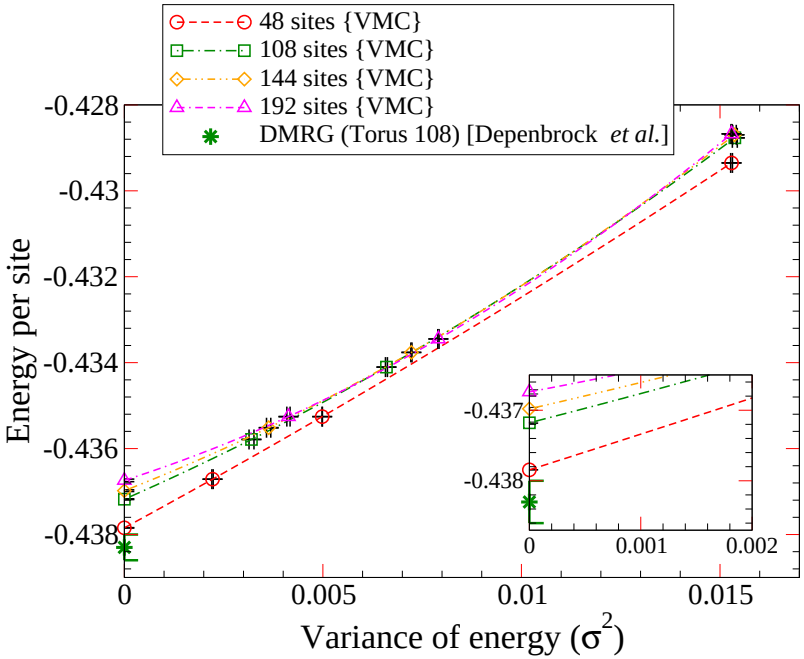
Calculations on the 48-site cluster

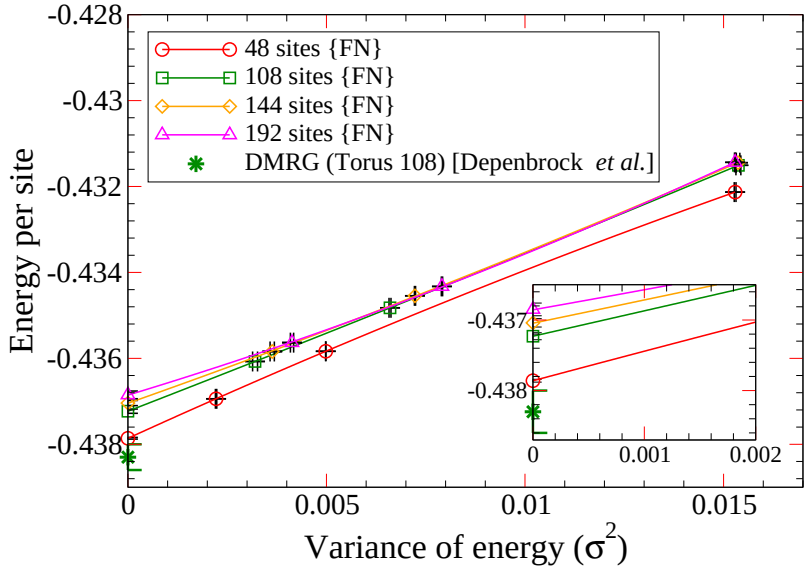
Our zero-variance extrapolation gives: $E/N \simeq -0.4378$



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

Calculations on larger clusters

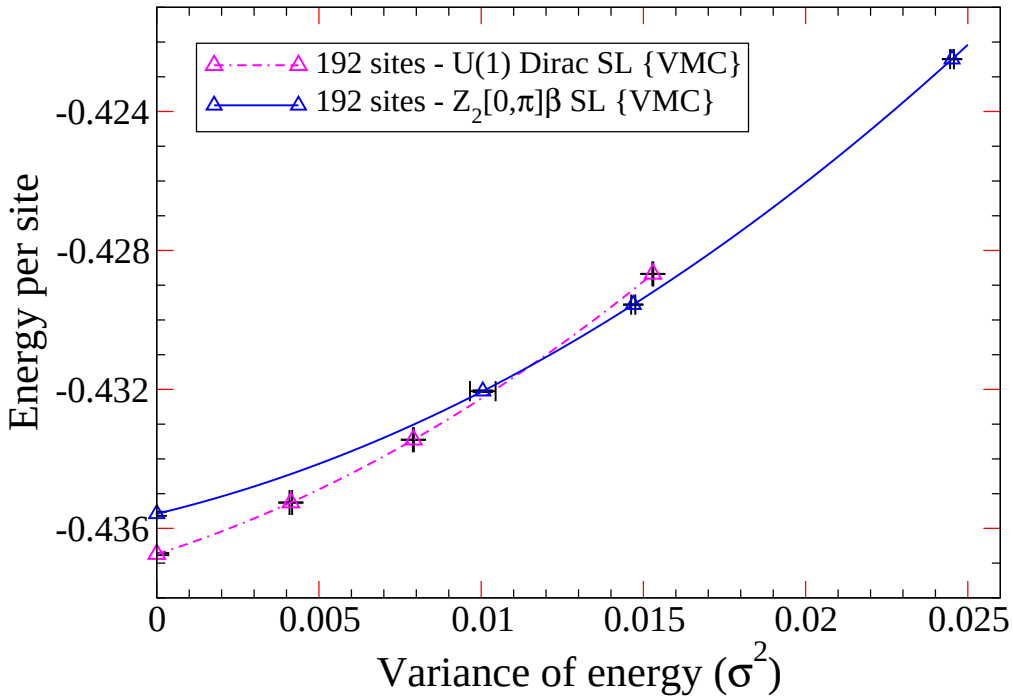




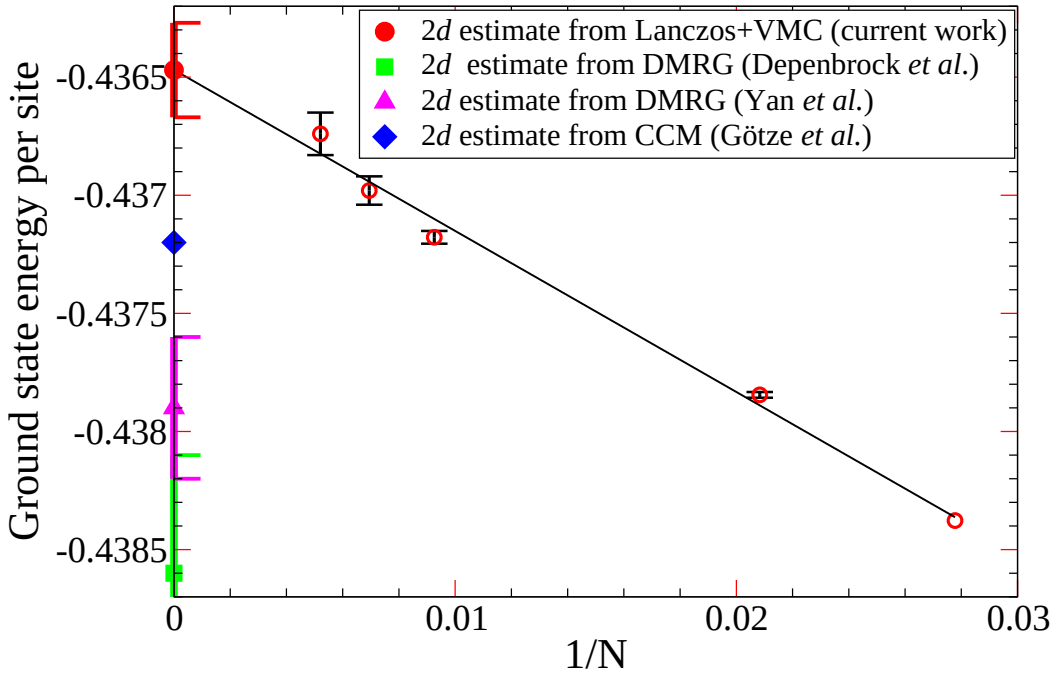
- NO substraction techniques to get the energy
- The state has ALL symmetries of the lattice
- The extrapolated values are essentially size consistent

Extrapolations for Dirac and Z_2 states

Starting from a Z_2 state the extrapolation is worse than for the Dirac state

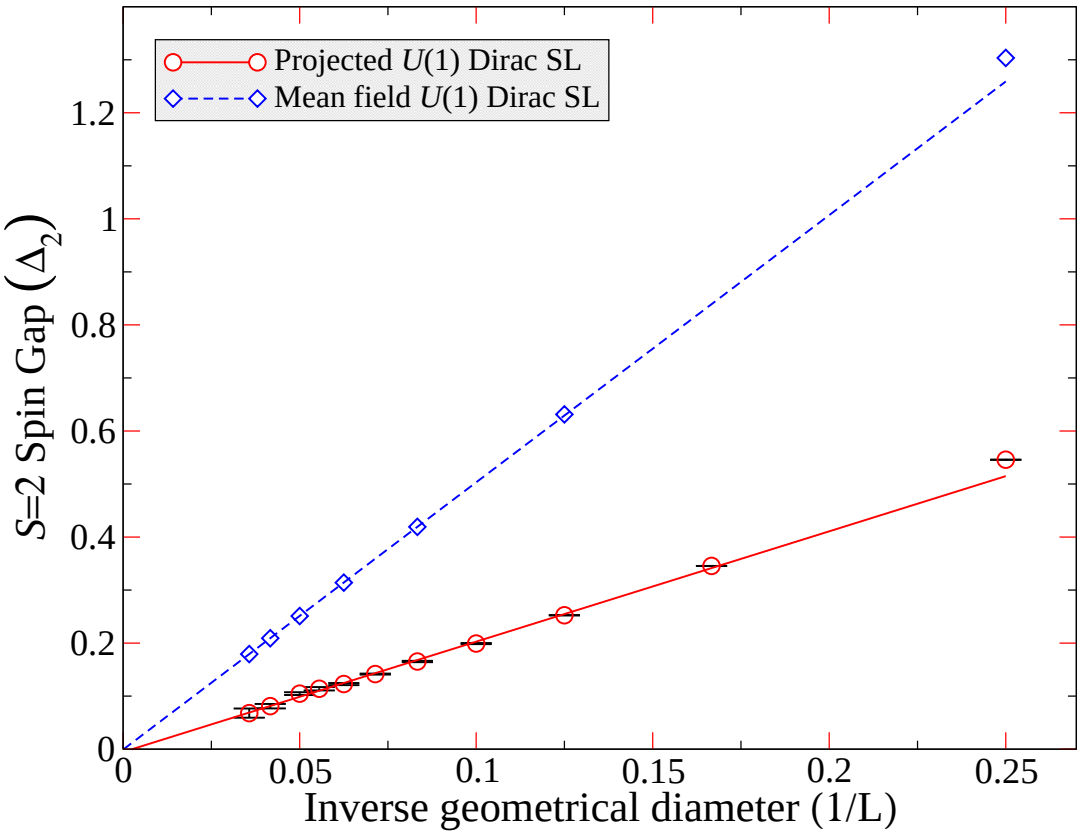


The thermodynamic limit



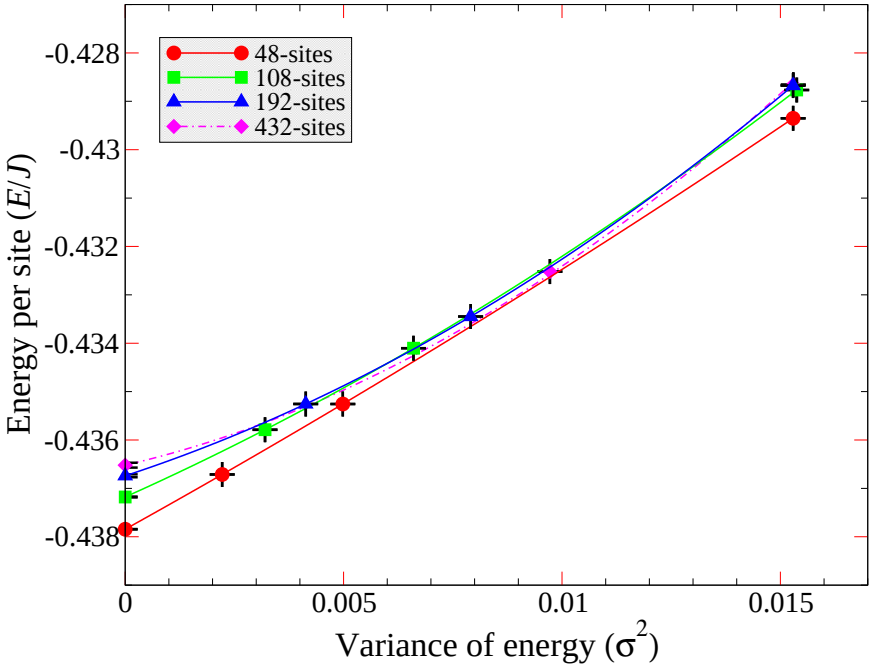
- OUR thermodynamic energy is: $E/J = -0.4365(2)$
- DMRG thermodynamic energy is: $E/J = -0.4386(5)$

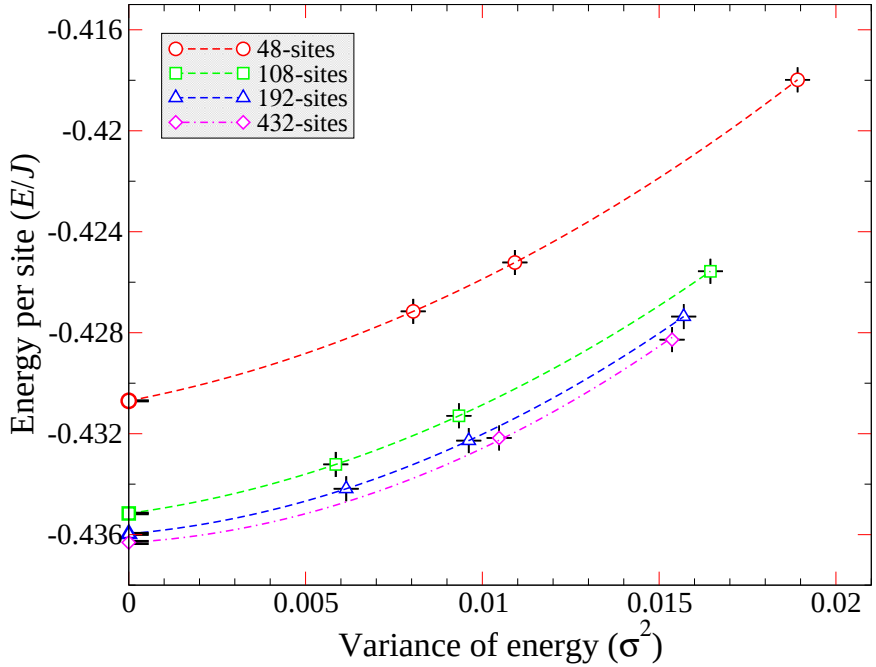
The variational $S = 2$ gap



- The Gutzwiller projected state is still gapless
- Remarkable stability of the $U(1)$ Dirac spin liquid

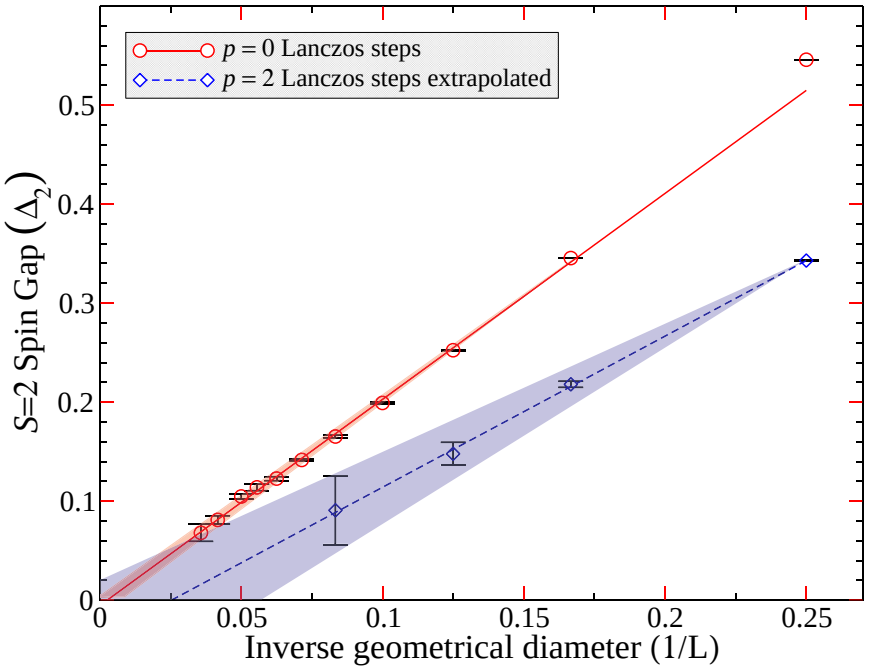
The Lanczos step extrapolations





- 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



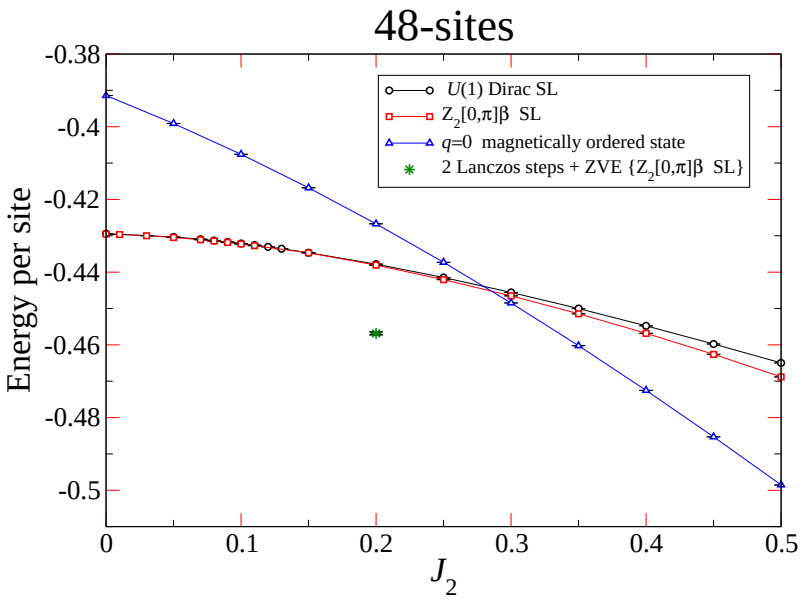
- The final result is $\Delta_2 = -0.04 \pm 0.06$
- The "upper" bound is given by $\Delta_2 \simeq 0.02$
- The $S = 1$ gap should be $\Delta_1 \lesssim 0.01$

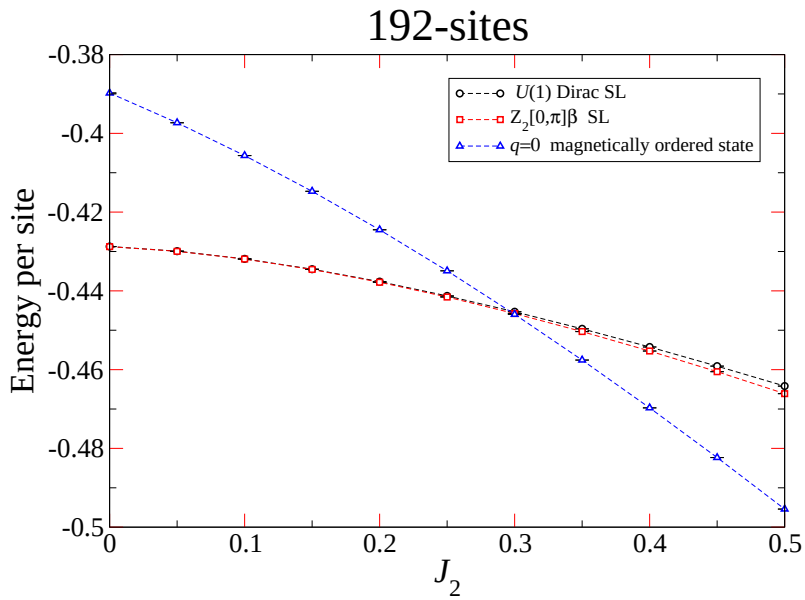
Much smaller than previous DMRG estimations

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

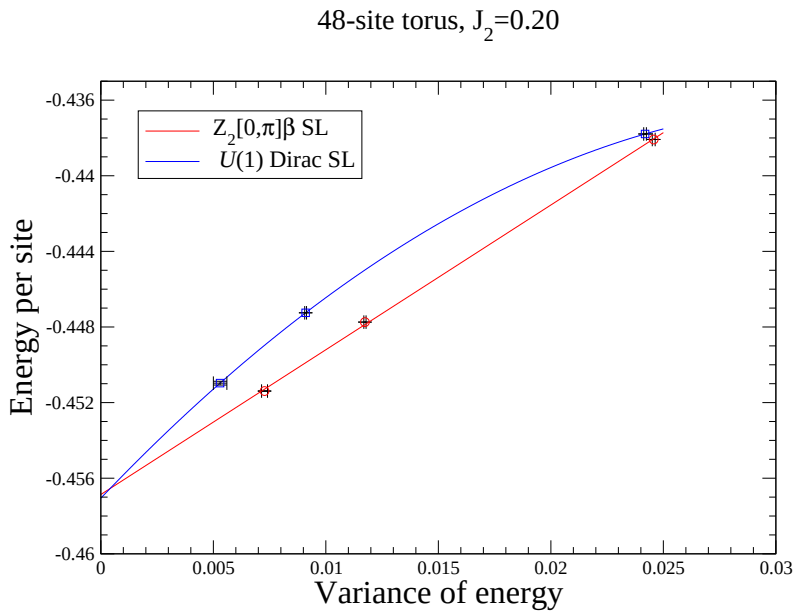




- The gapped Z_2 state overcomes the U(1) Dirac one for $J_2/J_1 > 0.1$
- The magnetic state with $q = 0$ (Jastrow) is stabilized for $J_2/J_1 > 0.3$

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:

- Very good energies
  With TWO variational parameters: Educated guess
  To be compared with about 16000 parameters in DMRG: Brute-force calculation
- 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

Cons

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

Different kinds of spin liquids

The folklore is that

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

We are trying to improve the quality of our liquids