Improved variational wave functions for the Heisenberg model on the Kagome lattice

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Y. Iqbal, FB, and D. Poilblanc, Phys. Rev. B 84, 020407(R) (2011)

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The Heisenberg model on the Kagome lattice

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

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
Lhuillier	Chiral gapped SL		SBMF
White	Z_2 gapped SL	$-0.4379(3)J$	DMRG
Schollwock	Z_2 gapped SL	$-0.4386(5)J$	DMRG
Auerbach	"P6 chiral SL"		CORE

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

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

Schwinger fermion approach for projected wave functions

$$\vec{\mathbf{S}}_i = \frac{1}{2} c^{\dagger}_{i,\alpha} \vec{\tau}_{\alpha,\beta} c_{i,\beta}$$

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

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

At the mean-field level:

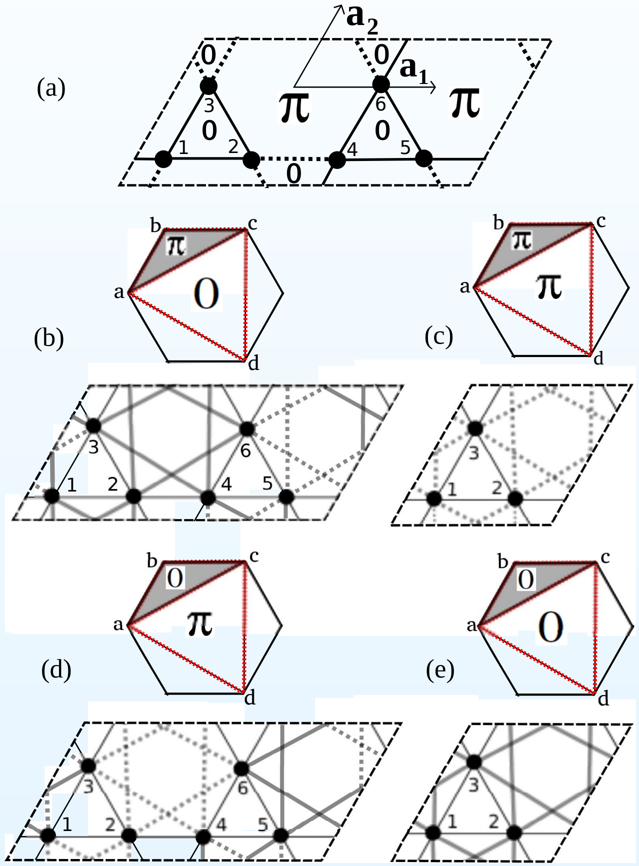
$$\mathcal{H}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu \delta_{ij}) c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{i,j} \{ (\Delta_{ij} + \zeta \delta_{ij}) c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + \mathrm{h.c.} \}$$

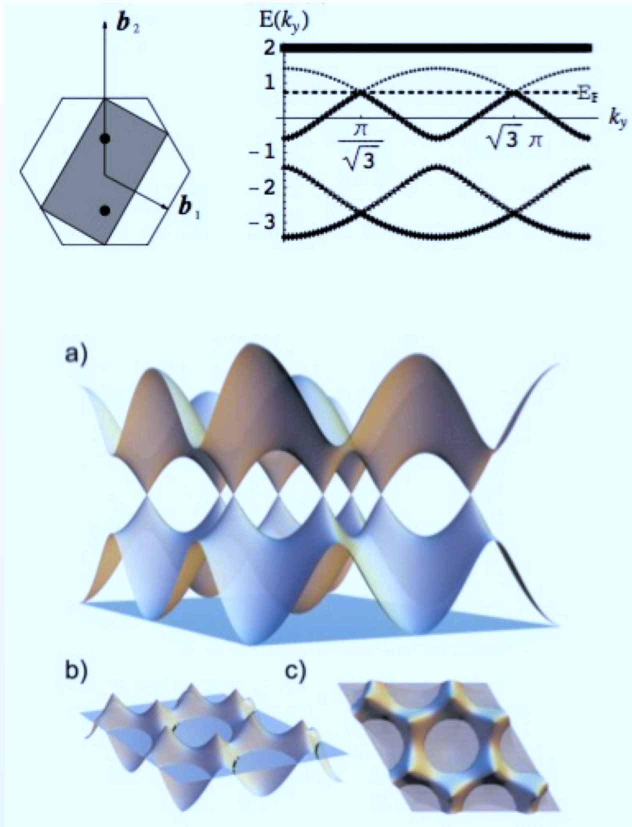
$$\langle c^{\dagger}_{i,\alpha} c_{i,\alpha} \rangle = 1 \qquad \langle c_{i,\alpha} c_{i,\beta} \rangle \epsilon_{\alpha\beta} = 0$$

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

$$|\Psi_{\mathrm{Proj}}(\chi_{ij}, \Delta_{ij}, \mu)\rangle = \mathcal{P}_G |\Psi_{\mathrm{MF}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle \qquad \mathcal{P}_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$$

Results with projected wave functions





The U(1) gapless (Dirac) spin liquid is a good variational ansatz:

Only hopping in the MF Hamiltonian: flux 0 (triangles) and π (hexagons)

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

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

Projective symmetry-group analysis Lu, Ran, and Lee, PRB **83**, 224413 (2011)

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

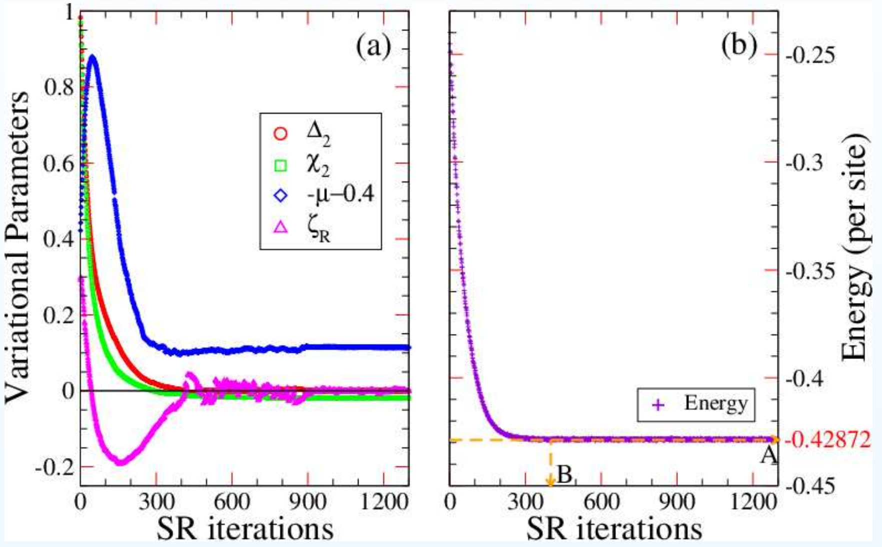
Only ONE gapped SL connected with the U(1) Dirac SL:

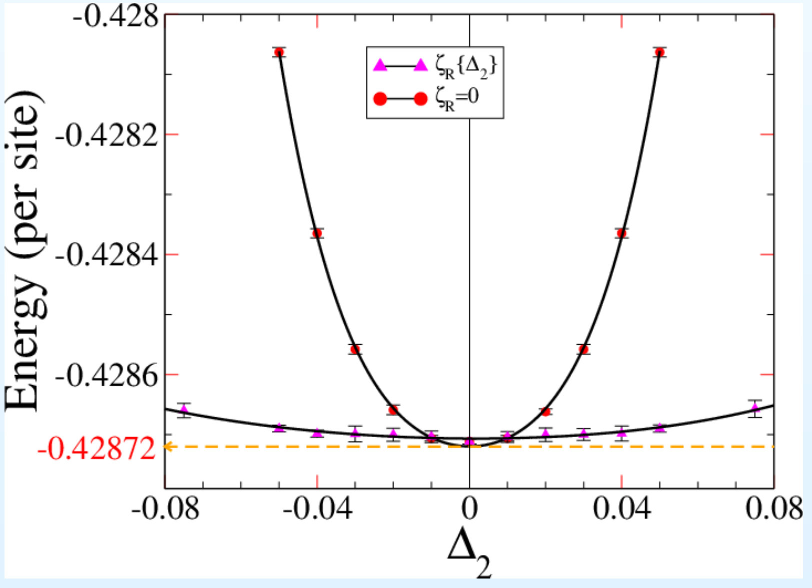
The $Z_2[0,\pi]\beta$ spin liquid

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

Z_2[0,0]A, Z_2[0,0]B, Z_2[0,0]C, Z_2[0,0]D

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





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)

The variance extrapolation

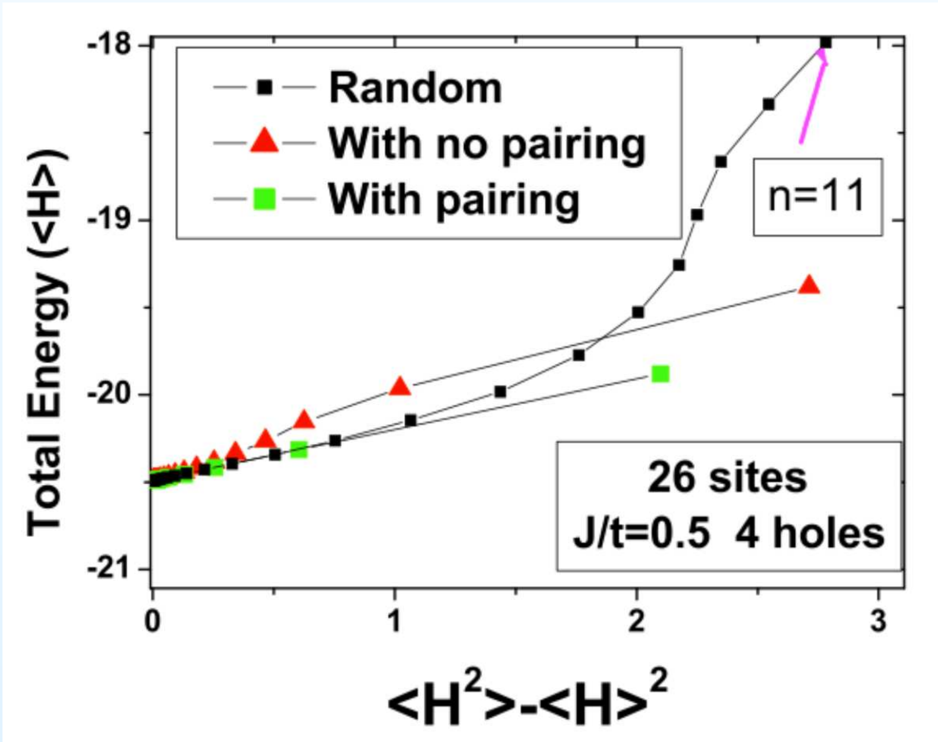
- A zero-variance extrapolation can be done
  Whenever $|\Psi\rangle$ is sufficiently close to the ground state:

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

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

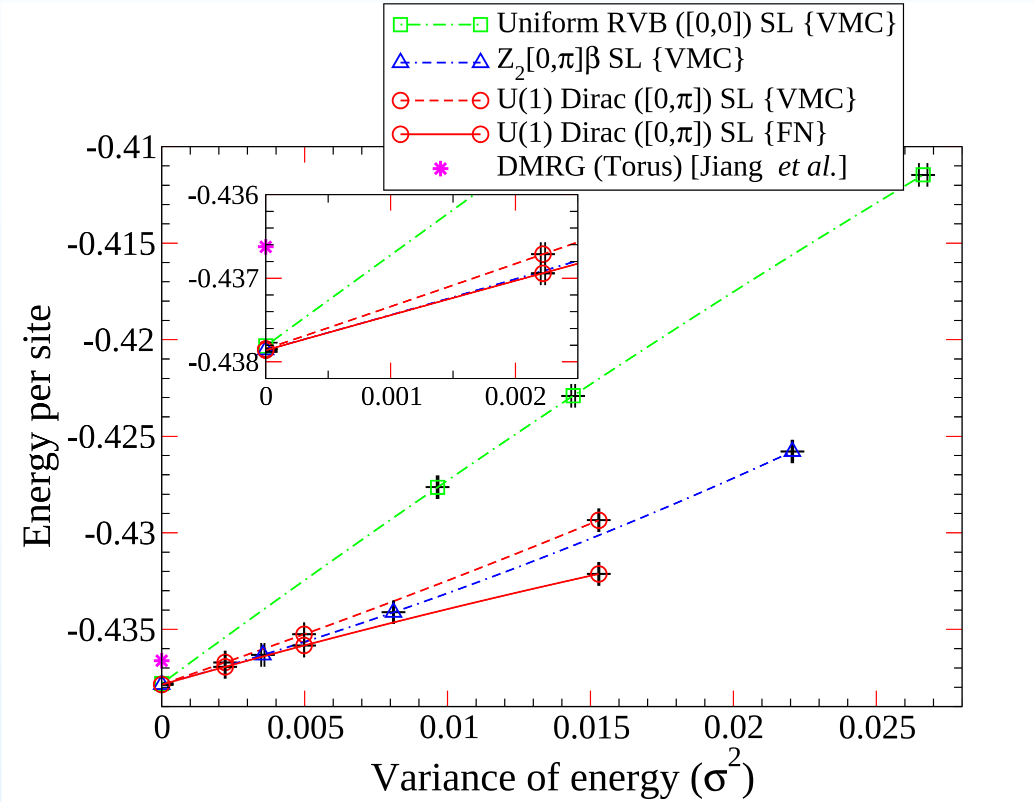
How does it work?

Example: the $t{-}J$ model



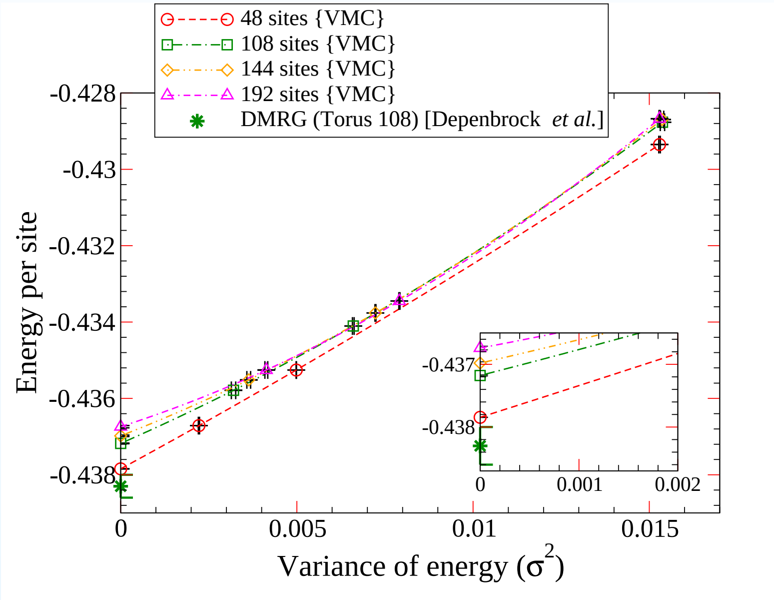
Calculations on the 48-site cluster

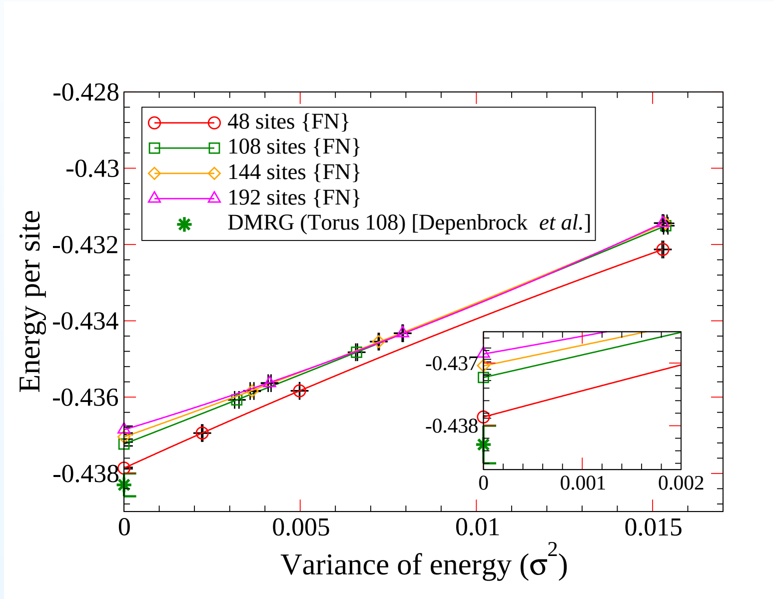
Our zero-variance extrapolation gives: $E/N \simeq -0.4378$



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

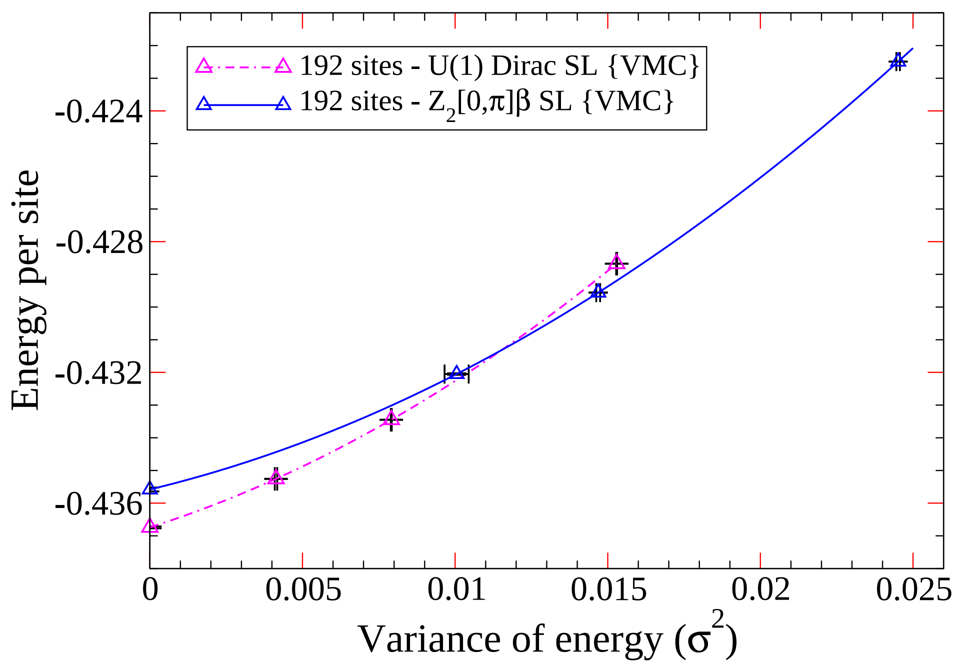
Calculations on larger clusters





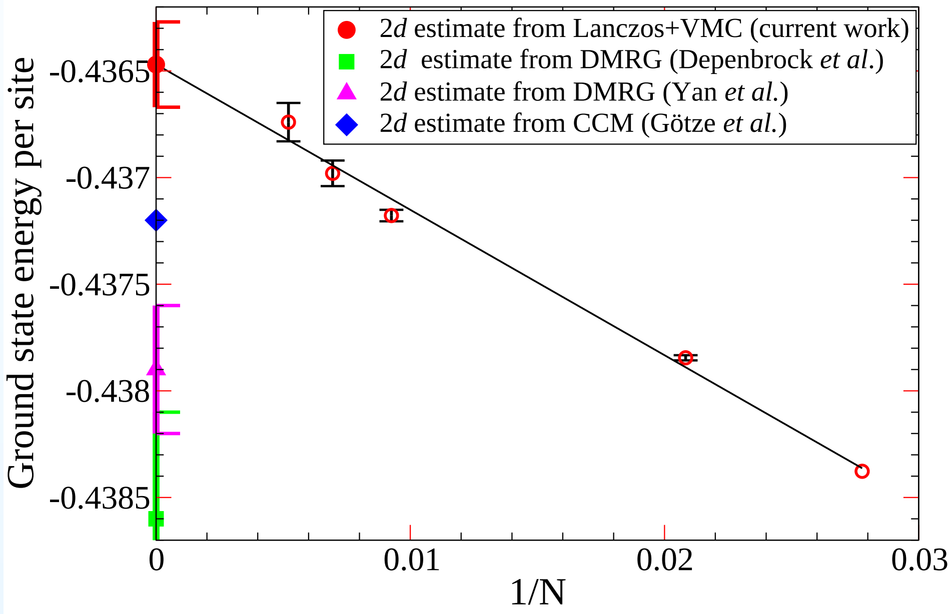
- NO substraction techniques to get the energy
- The state has ALL symmetries of the lattice
- The extrapolated values are essentially size consistent

U(1) versus Z_2 extrapolation



On large sizes, the extrapolation of the Z_2 state is higher than the one of the $U(1)$ state

The thermodynamic limit



- OUR thermodynamic energy is:

$$E/J = -0.4365(2)$$

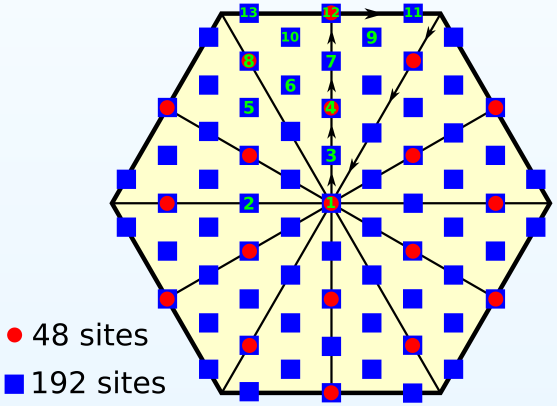
- DMRG thermodynamic energy is:

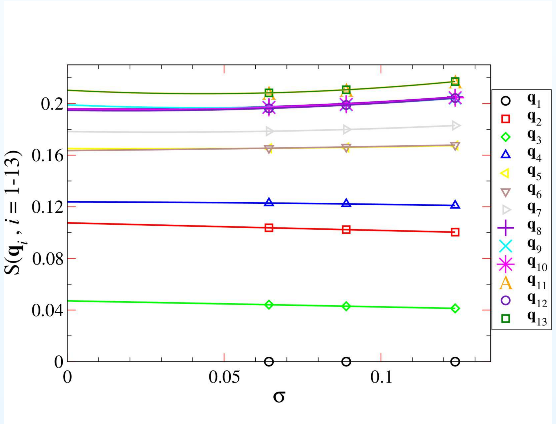
$$E/J = -0.4386(5)$$

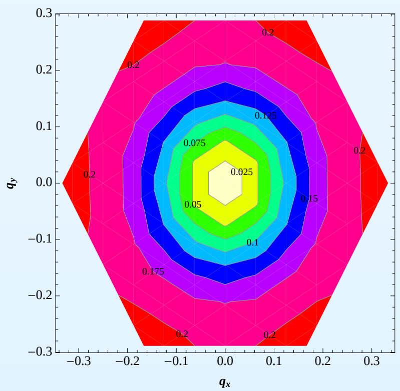
Equal in three errorbars

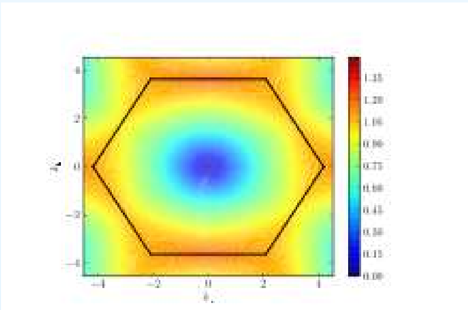
Static structure factor: momentum space

$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} \sum_{\mathbf{R}} e^{-\imath \mathbf{q}\cdot\mathbf{R}} S_{ij}(\mathbf{R})$$









(a) XC16 system (196 sites)

Depenbrock et al.,

PRL **109**, 067201 (2012)

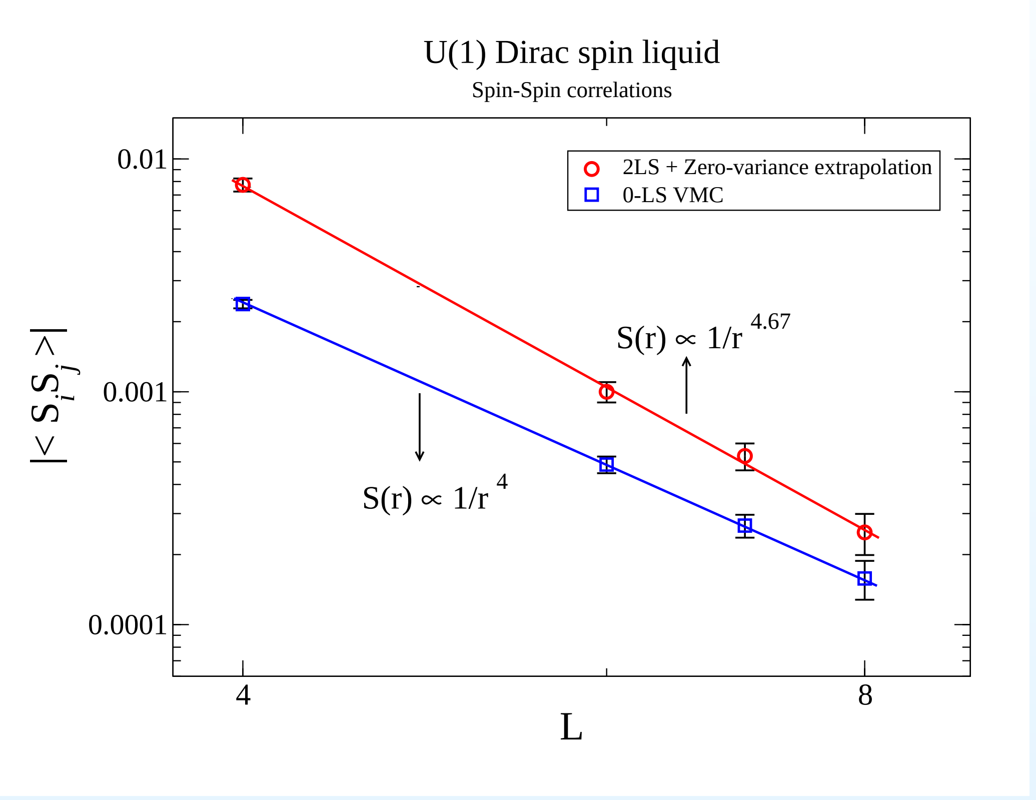
Small-q are important:

$S(q) \sim q^2 \rightarrow$ gap

$S(q) \sim q^2 \log q \rightarrow$ Dirac

Static structure factor: real space

Spin-spin correlation at the maximum distance



- The pure variational wave function gives $\langle S_0 S_R \rangle \sim \frac{1}{R^4}$
- The extrapolated data give $\langle S_0 S_R \rangle \sim \frac{1}{R^\alpha}$ with α slightly large than 4

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
- No evidence for changes in the spin-spin correlations

Subsequent works:

- Direct calculation of the spin gap
- Calculations for $J_2 > 0$

One key issue:

- Understand the large number of low-energy singlets
  Monopole excitations?
  Short-range singlets? ......