Projected wave function for frustrated spin models

Federico Becca

Y. Iqbal and D. Poilblanc

CNRS and Laboratoire de Physique Theorique, Université de Toulouse

Y. Iqbal, FB, and D. Poilblanc, Phys. Rev. B 83, 100404(R) (2011)

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

Y. Iqbal, FB, and D. Poilblanc, New J. Phys., in press (2012)

Y. Iqbal, FB, S. Sorella, and D. Poilblanc, arXiv:1209.1858 (yesterday)

KITP, September 2012

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
Poilblanc	12- or 36-site VBC		QDM
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

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:

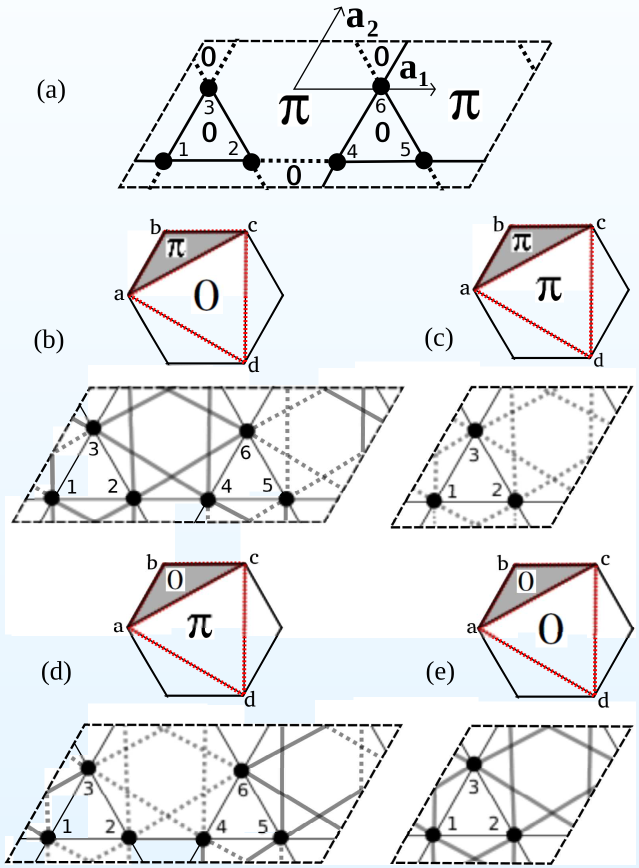
$$\mathcal{H}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu \delta_{ij}) c^\dagger_{i,\alpha} c_{j,\alpha} + \sum_{i,j} \{ (\Delta_{ij} + \zeta \delta_{ij}) c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + \mathrm{h.c.} \}$$

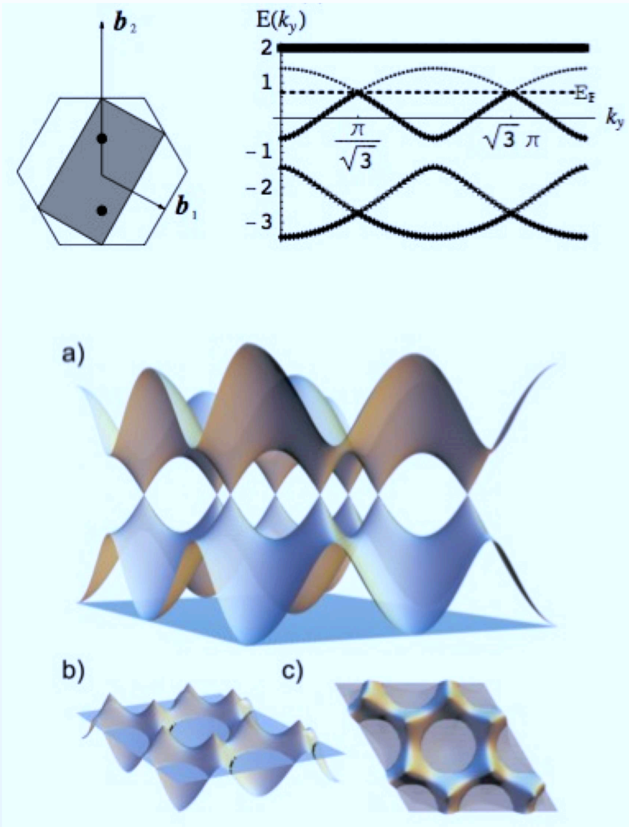
$$\langle c^\dagger_{i,\alpha} c_{i,\alpha} \rangle = 1 \qquad \langle c_{i,\alpha} c_{i,\beta} \rangle \epsilon_{\alpha\beta} = 0$$

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





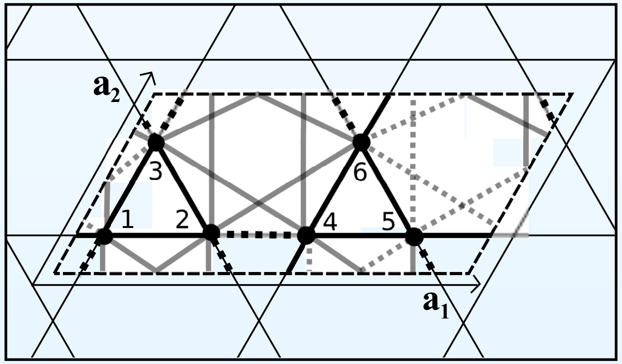
The U(1) gapless (Dirac) spin liquid is a good variational ansatz

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)

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



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

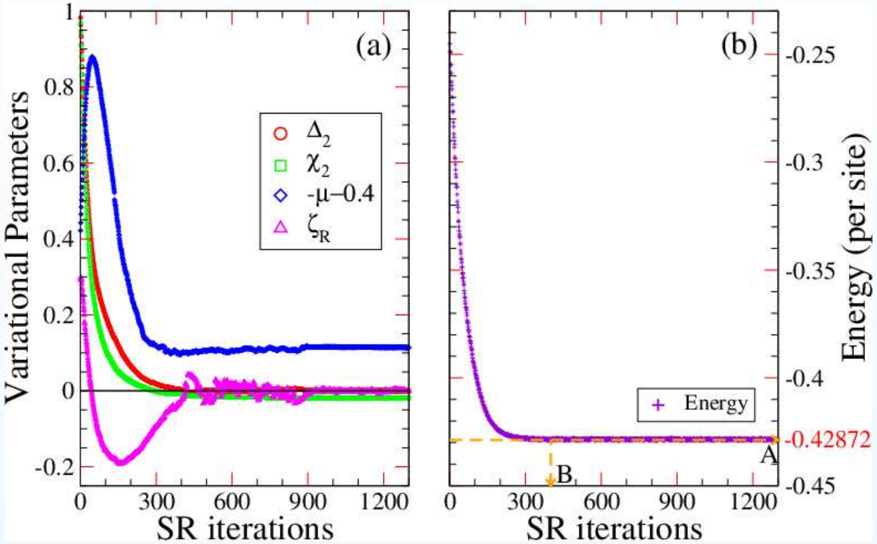
Only ONE gapped SL connected with the U(1) Dirac SL:

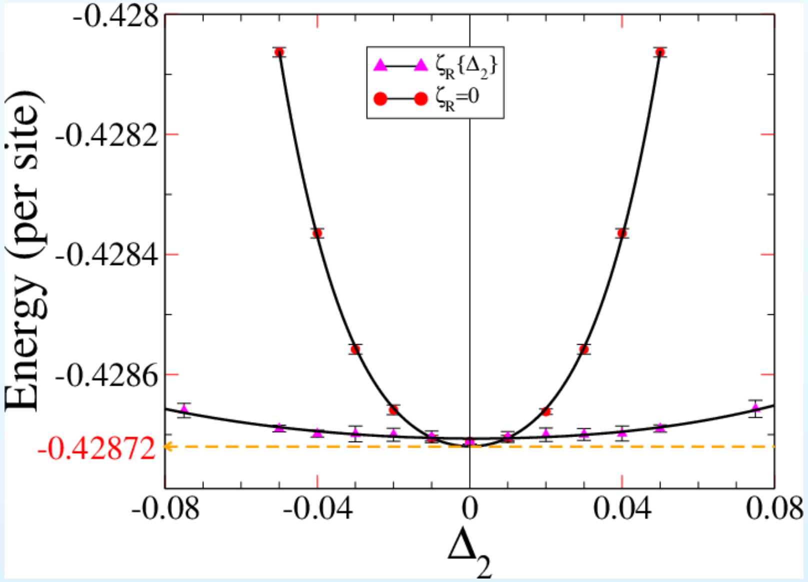
The $Z_2[0,\pi]\beta$ spin liquid

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

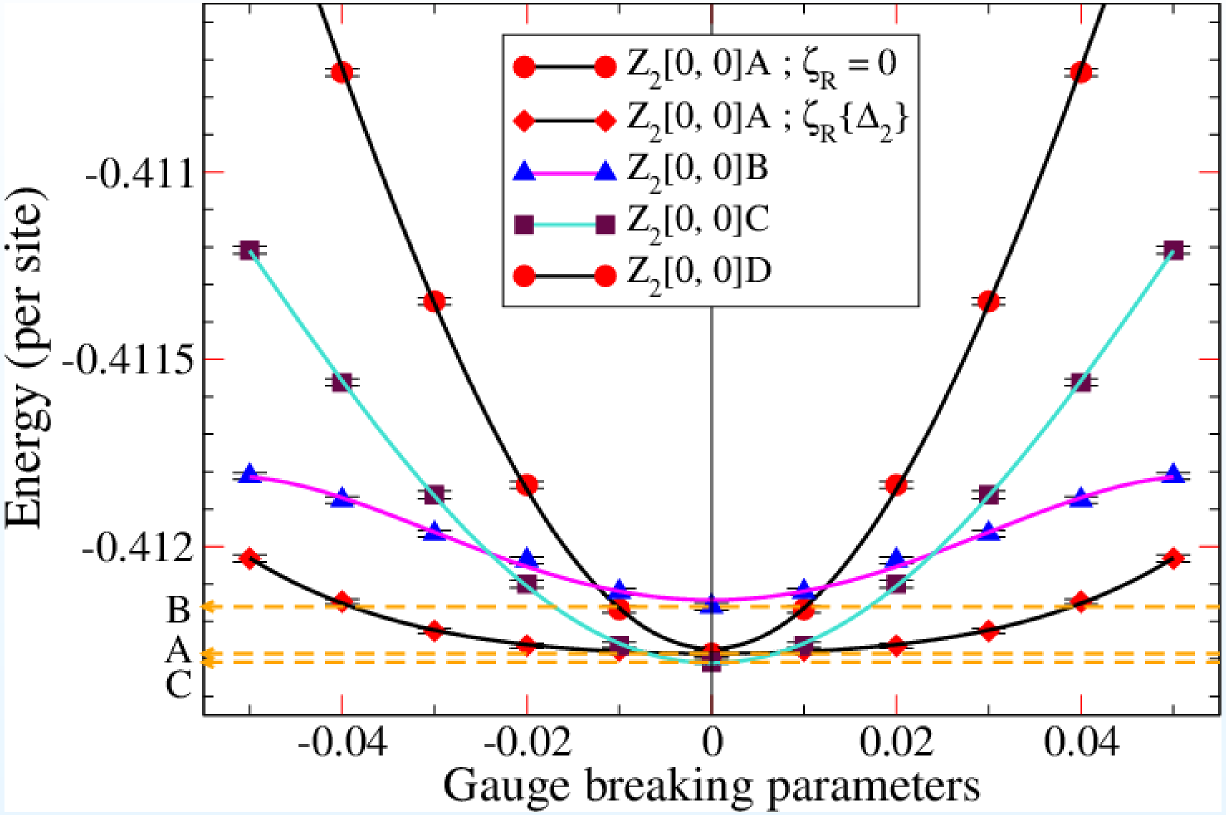
$Z_2[0,0]A$, $Z_2[0,0]B$, $Z_2[0,0]C$, $Z_2[0,0]D$

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





...and also the Uniform U(1) spin liquid is stable



The gapless U(1) Dirac SL is very stable

- Against dimerization
- For breaking the gauge structure down to Z_2

Even the Uniform U(1) SL is stable against Z_2 SLs

Possibility of a VBC ground state?

Recent studies with quantum dimer models established an exceptionally large quasi-degeneracy of GS manyfold

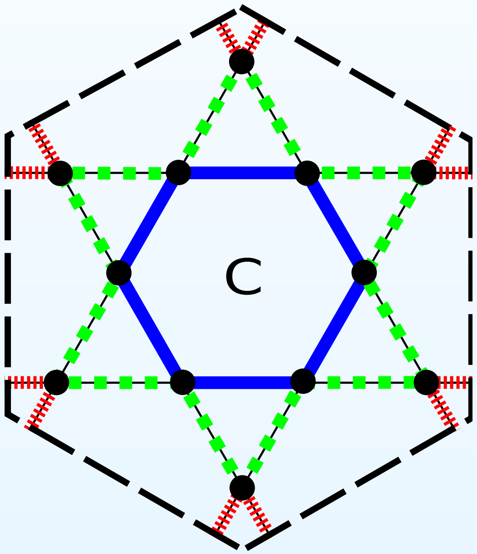
Poilblanc and Misguich, PRB 84, 214401 (2011)

We want to study VBC perturbation to the U(1) Dirac (gapless) SL

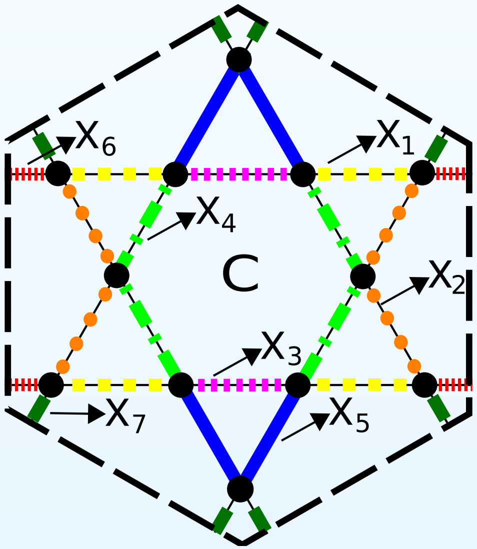
How many VBC are there?

Can they destabilize it by opening a gap?

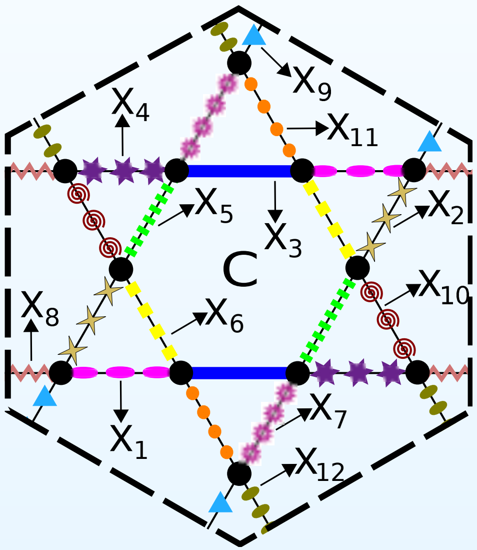
Competing 12-site unit cell VBCs



SVBC, Hastings 2000

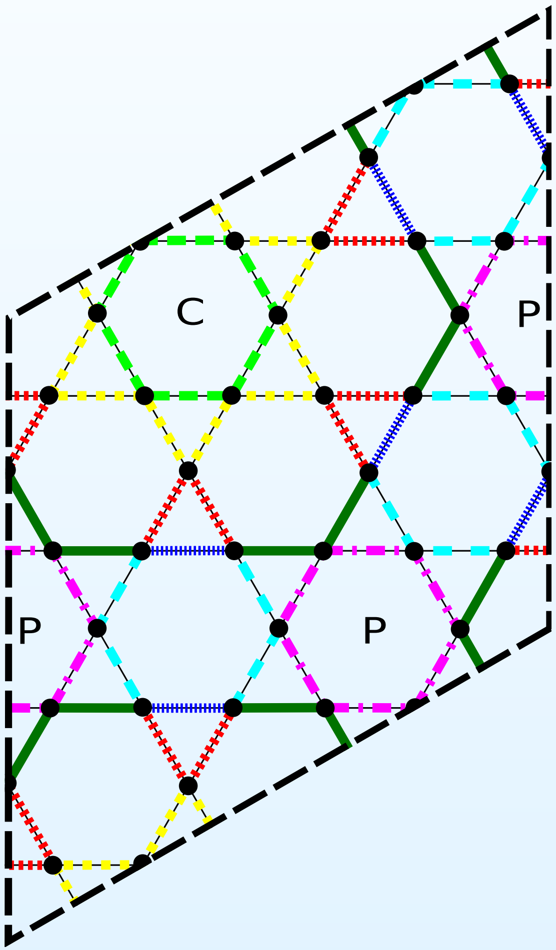


DVBC, White 2011

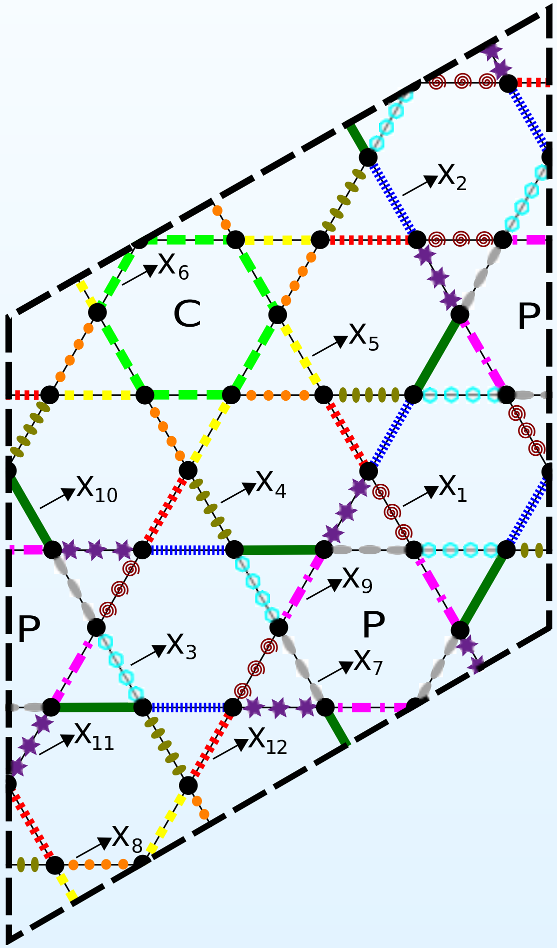


VBC_3 Poilblanc 2011

Competing 36-site unit cell VBCs

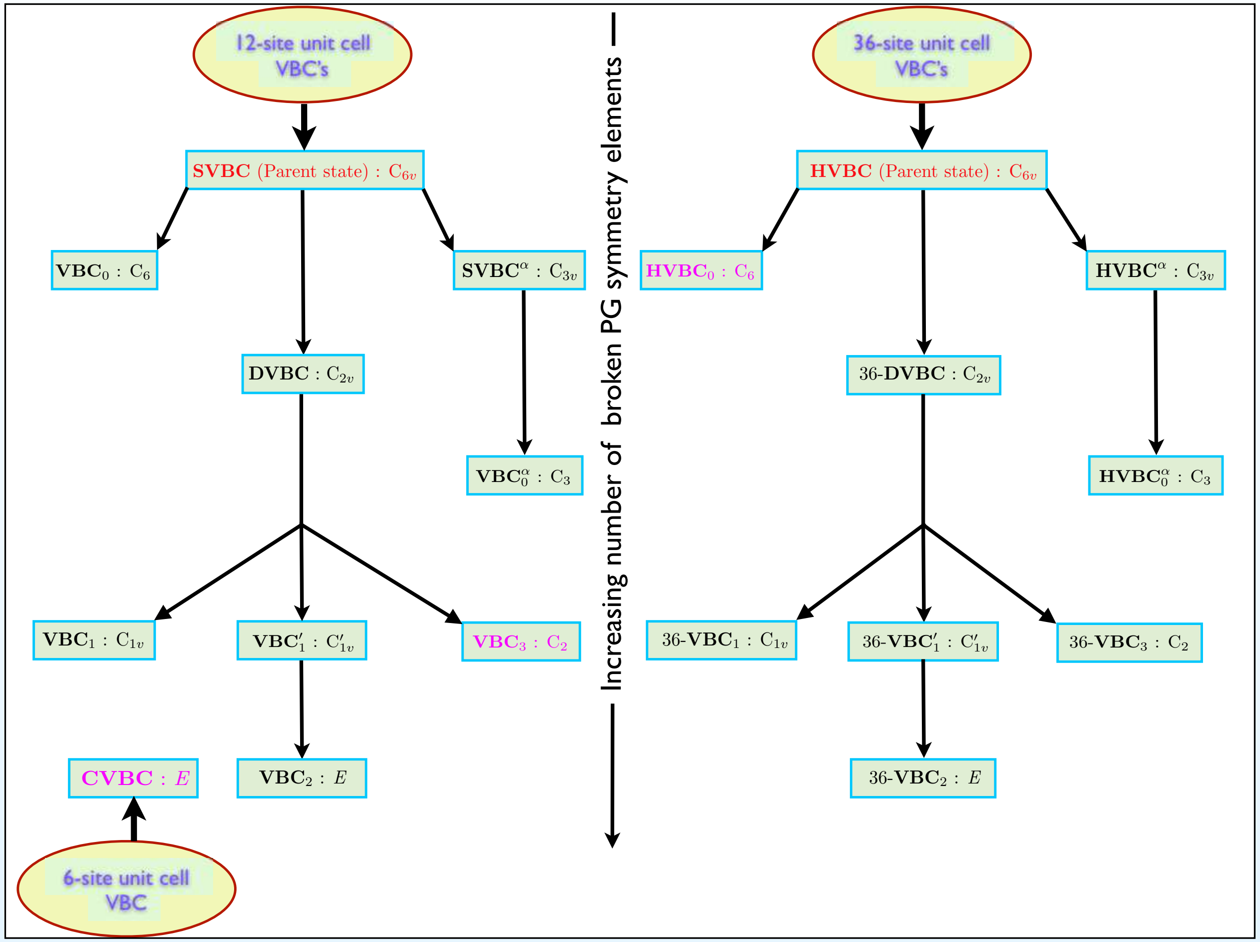


HVBC



HVBC$_0$

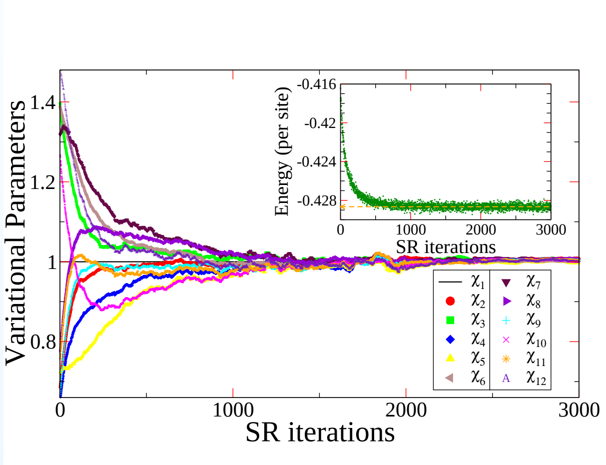
VBC patterns: Symmetry classification



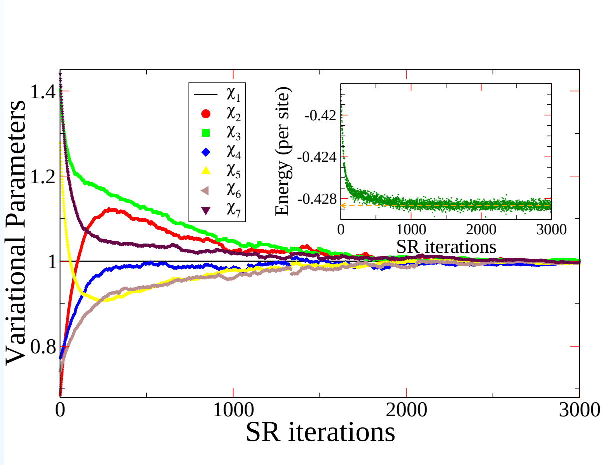
Iqbal, Becca, Poilblanc, arXiv:1203.3421 (to appear in NJP)

Numerical results: optimization of the VBCs

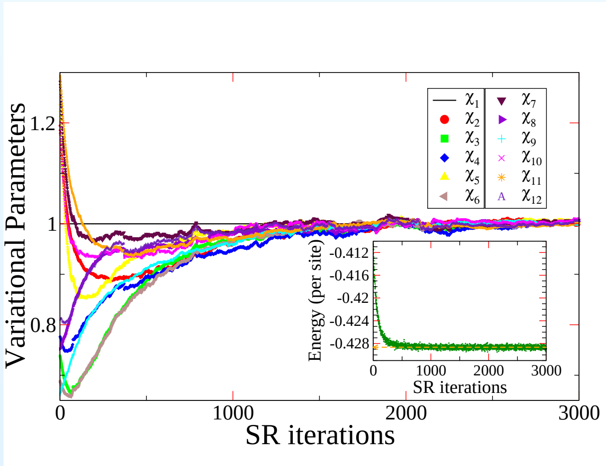
Results for the [0,π] U(1) SL



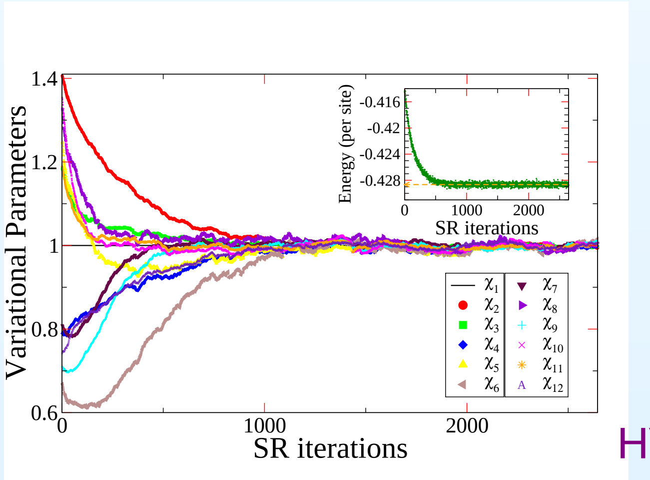
CVBC



DVBC



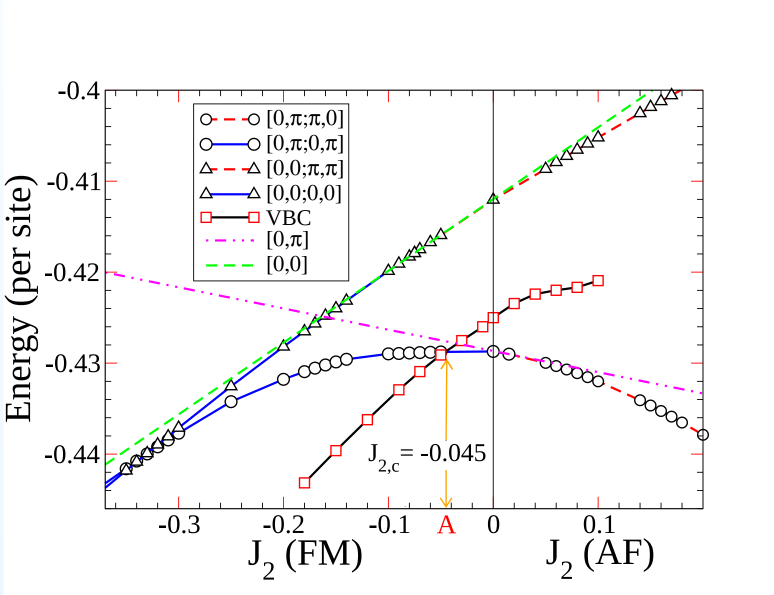
VBC_3

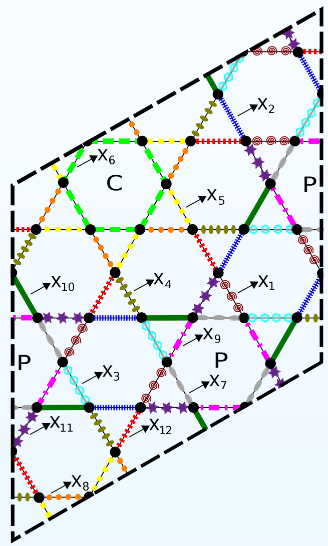


$HVBC_0$

Numerical results: optimization of the VBCs

Results for the [0,0] U(1) SL





HVBC$_0$

The U(1) Dirac SL is stable w.r.t. VBC order

The U(1) Uniform SL is unstable w.r.t. a 36-site VBC

A small ferromagnetic J_2 stabilizes a non-trivial dimerization

A small antiferromagnetic J_2 may lead to a gapped state

Tay and Motrunich, PRB **84**, 020404 (2011)

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 $p = 2$
- A zero-variance extrapolation can be done

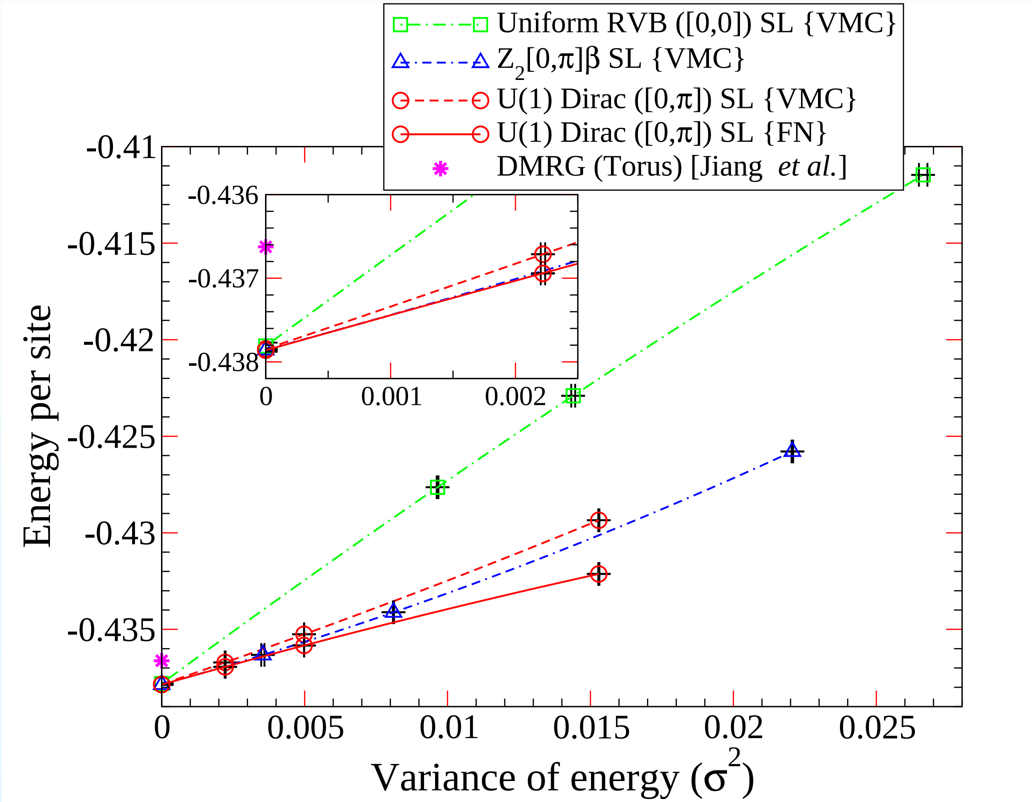
$$E \simeq E_0 + \text{const} \times \sigma^2$$

$E = \langle\mathcal{H}\rangle/N$

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

Calculations on the 48-site cluster

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

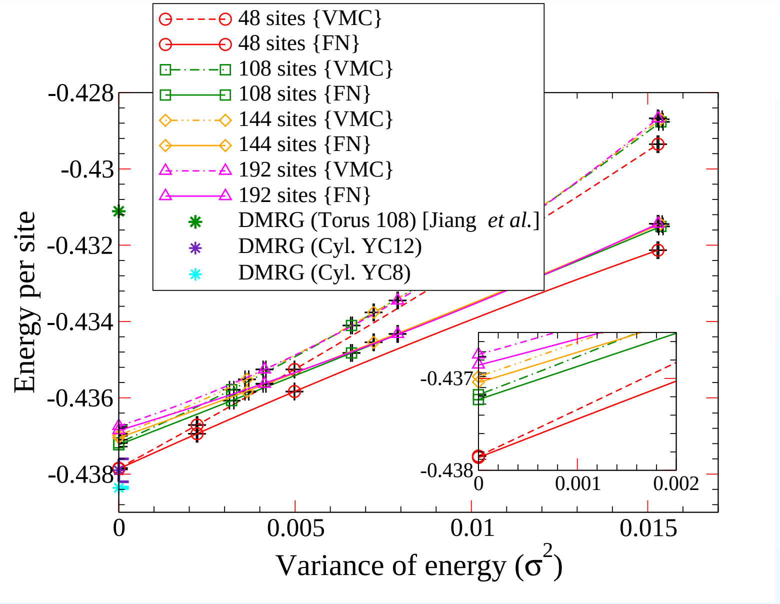


$E/N \simeq -0.4387???$ by ED (Lauchli) only seen in Boston

$E/N \simeq -0.4383(2)$ by DMRG

Depenbrock, McCulloch, and Schollwock, PRL **109**, 067201 (2012)

Calculations on larger clusters



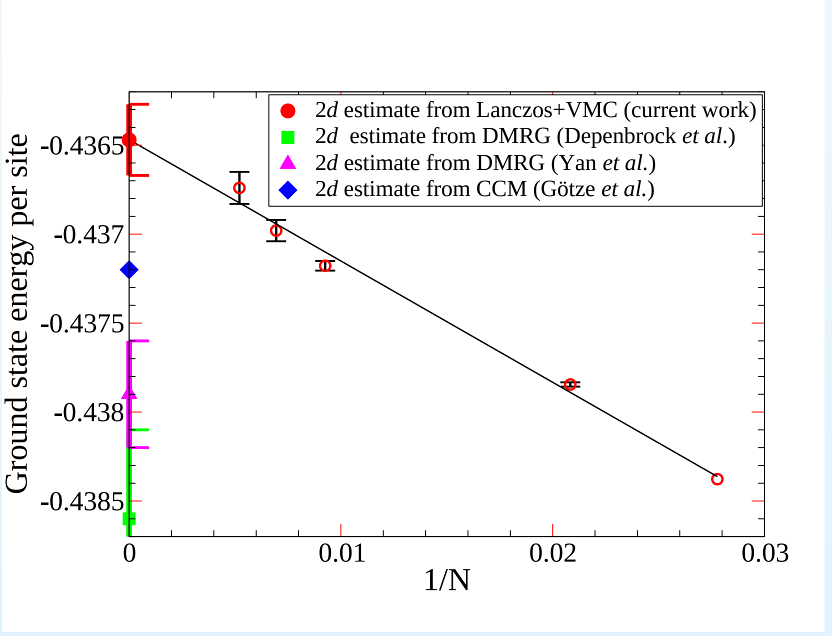
- NO substraction techniques to get the energy
- The state has ALL symmetries of the lattice
- OUR thermodynamic energy is:

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

- DMRG thermodynamic energy is:

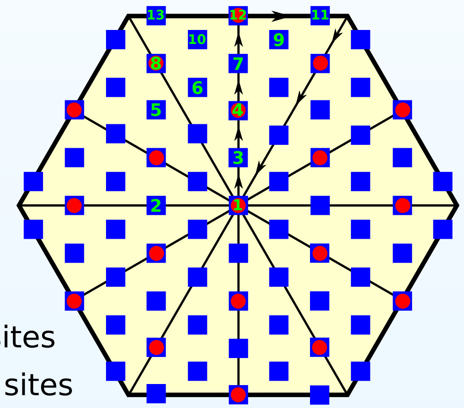
$$E/J = -0.4386(5)$$

Equal in three errorbars

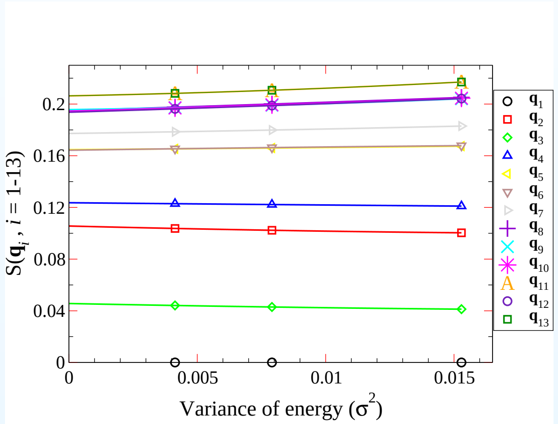


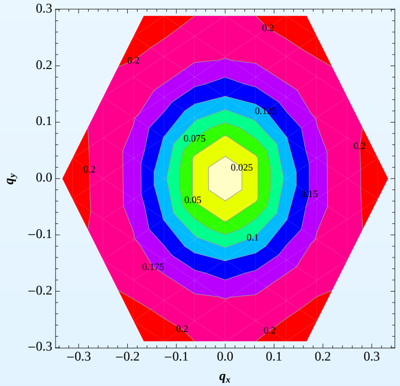
Static structure factor

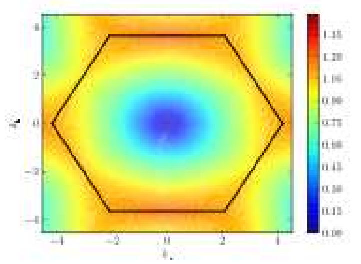
$$S(\mathbf{q}) = \frac{1}{N} \sum_{i,j} \sum_{\mathbf{R}} e^{-\imath \mathbf{q} \cdot \mathbf{R}} S_{ij}(\mathbf{R})$$



● 48 sites
■ 192 sites







(a) XC16 system (196 sites)

Depenbrock et al.,
PRL **109**, 067201 (2012)

Small-q are important:

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

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

?????

Conclusions

- Very good energies

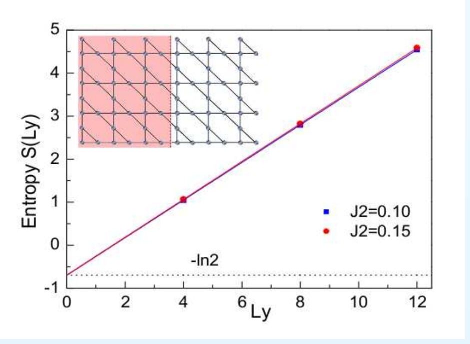
  With TWO variational parameters: Educated guess

  To be compared with about 16000 parameters in DMRG: Brute-force calculation

- No evidence for changes in the spin-spin correlations

Dimerization with a 36-site unit cell for $J_2 < 0$

gapped Z_2 spin liquid for $J_2 > 0$



Jiang, Wang, and Balents, arXiv:12054289

Is $J_2 = 0$ a critical point?

Is the U(1) state really stable (a phase in the Kagome)?