

SPIN LIQUIDS IN QUANTUM  
ANTIFERROMAGNETIC MODELS ON TWO  
DIMENSIONAL FRUSTRATED LATTICES

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24th September 2012

# OUTLINE

- ✱ **Spin Liquids:** *The colorful world beyond Landau's theories.*
- ✱ **“Hot” playgrounds:** *The “infamous” kagome spin-1/2 Heisenberg antiferromagnet and its experimental realizations.*
- ✱ **Maths for spin liquids:** *Slave particle constructions.*
- ✱ **Numerical methods:** *Monte Carlo methods.*
- ✱ **Competing phases:** *Spin liquids vs Crystals.*
- ✱ **The winner:** *The “algebraic”  $U(1)$  Dirac spin liquid.*
- ✱ **Conclusions and perspectives.**

# WHAT ARE SPIN LIQUIDS & WHERE TO FIND THEM?

Phases of matter which even at  $T=0$  do not spontaneously break *any* symmetries. **Anderson' 73**

\* “Different” spin liquids *cannot* be distinguished only on the basis of physical symmetries such as lattice space group and time-reversal, and they lack order parameters in the conventional sense of Landau. **Wen' 2002**

\* They possess deeper *internal* “patterns” which are related to symmetries of complex ground state wave functions, which enables one to distinguish them.

Expected to exist in systems with *strong* quantum fluctuations

\* Systems with low dimensionality ( $d = 2$ ), non-bipartite lattices with low coordination number, low spin value ( $S = 1/2$ ), frustrating antiferromagnetic interactions of Heisenberg type.



Melted ground state:  $\langle \hat{\mathbf{S}}_i \rangle = 0$

# S=1/2 HEISENBERG ANTIFERROMAGNET ON THE KAGOME LATTICE

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



A quantum paramagnetic ground state has been shown to exist from several numerical studies using exact diagonalization, series expansion, *etc.*

Zeng' 90

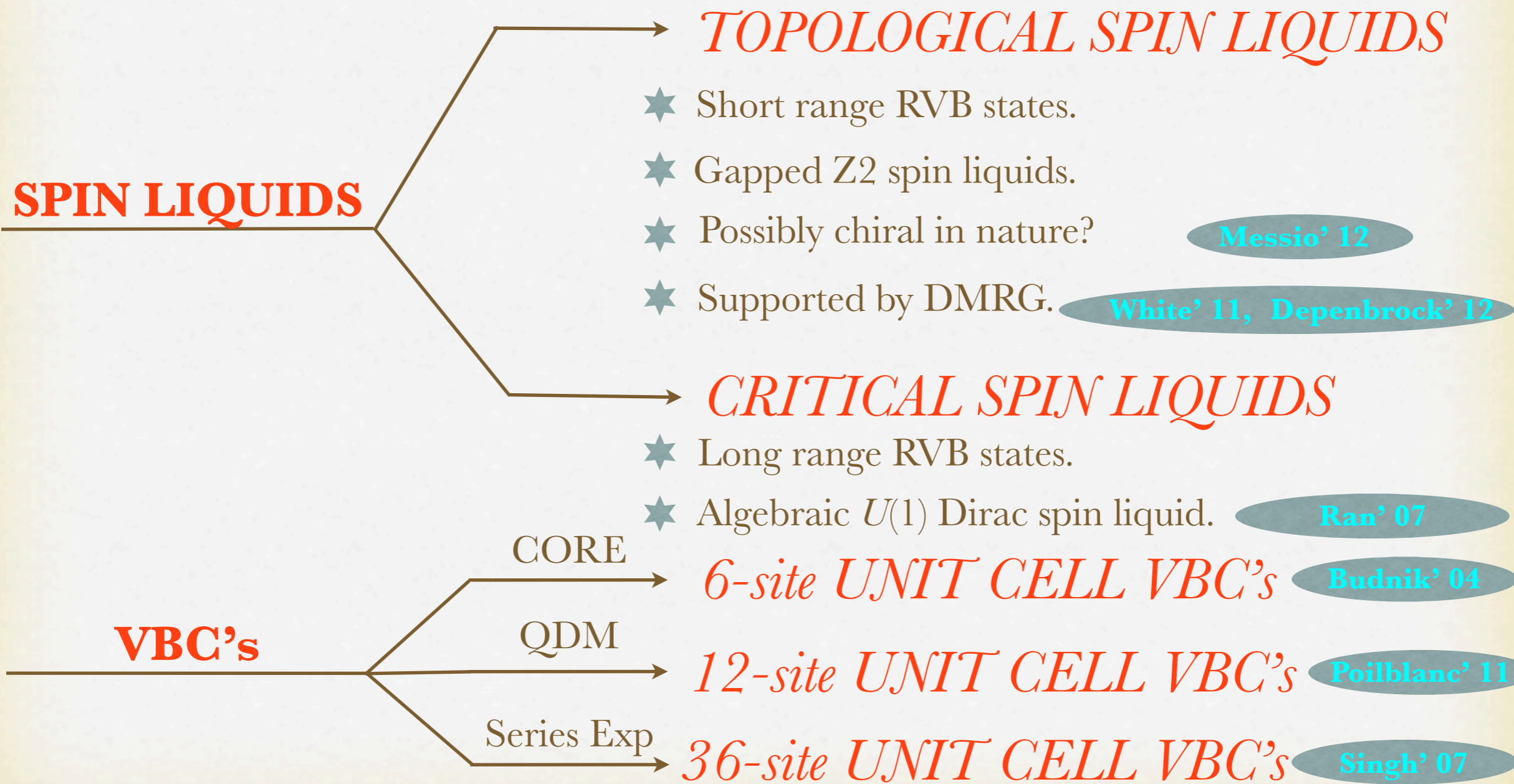
Singh' 92

\* The ground state manifold is highly *quasi-degenerate* with a myriad of competing ground states lying within a very narrow band of energy.  
*Quantum critical point?*

Sindzingre' 09 , Poilblanc' 11

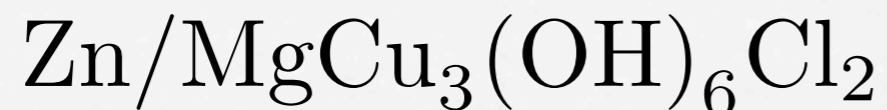
\* Different approximate numerical methods have vouched for different ground states, and the claims from one method have not been backed by another.

# COMPETING PHASES



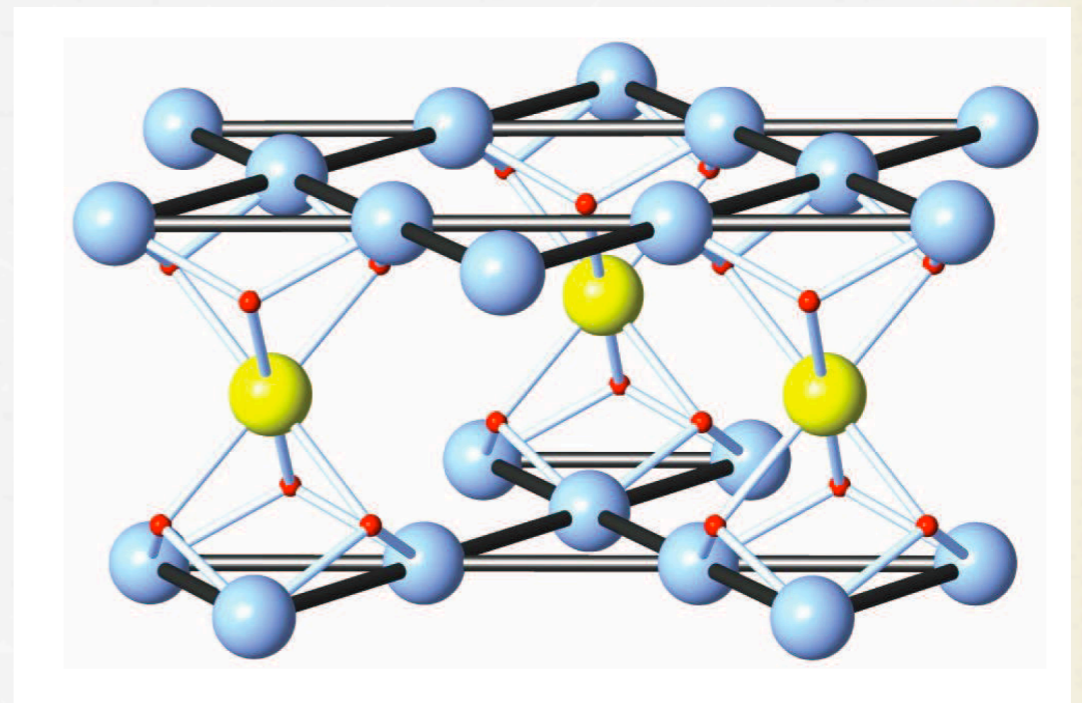
# EXPERIMENTS

The  $S=1/2$  QHAF is well replicated in “Herbertsmithite”.



No sign of magnetic freezing has been observed down to 20 mK.

(i.e. four orders of magnitude smaller than  $J$ )



**Kermarrec' 11**

- \* Raman spectroscopic data, points towards a gapless (algebraic) spin liquid behaviour.

**Wulferding' 10**

- \* The SL phase survives DM interactions:  $\sim 0.01J$  &  $0.04-0.08J$  in- & out-of plane resp.

- \* There is  $\sim 5\%$  in-plane disorder  $\text{Zn}^{2+} \rightarrow \text{Cu}^{2+}$  and about  $\sim 15-20\%$  the other way.

**Mendels' 10**

# MATHS FOR SPIN LIQUIDS

$$\hat{\mathcal{H}}_{\text{MF}} = \sum_{ij} J_{ij} (\hat{\mathbf{S}}_i \cdot \langle \hat{\mathbf{S}}_j \rangle + \langle \hat{\mathbf{S}}_i \rangle \cdot \hat{\mathbf{S}}_j - \langle \hat{\mathbf{S}}_i \rangle \cdot \langle \hat{\mathbf{S}}_j \rangle) = 0 ? !!!$$

$$\Rightarrow \hat{\mathbf{S}}_i = \frac{1}{2} c_{i,\alpha}^\dagger \hat{\sigma}^{\alpha\beta} c_{i,\beta}$$

Spinons  $c_{i,\alpha}$ :  $S = 1/2$  charge neutral quasi-particles.  
Mathematical trick + fractionalization +  
 $SU(2)$  high energy gauge structure.

Baskaran' 87

Hubbard-Stratonovich transformation + Mean field approx.

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

$$\Rightarrow |\Psi_{\text{VMC}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle = \mathcal{P}_{\mathbf{G}} |\Psi_{\text{MF}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle$$

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

Enforcing one-fermion per site constraint, and hence including correlations into the system.

# NUMERICAL METHODS

The *energy*, its *variance* and the *correlation functions* in a state can be obtained using Monte Carlo methods.

- \* To find the optimal state  $|\Psi(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle$ : The variational parameters are optimized using stochastic reconfiguration optimization. **Sorella' 05, Yunoki' 06**
- \* The resulting state is studied using variational and fixed-node Monte Carlo. **ten Haaf' 95**

→ **Systematically improve the wave functions**

Apply a few Lanczos steps: 
$$|\Psi_{p\text{-LS}}\rangle = \left(1 + \sum_{k=1}^p \alpha_k \hat{\mathcal{H}}^k\right) |\Psi_{\text{VMC}}\rangle$$

**Sorella' 01**

For sufficiently accurate states:  $E \approx E_{\text{exact}} + \text{constant} \times \sigma^2$

Exact ground state energy & correlations are obtained using zero-variance extrapolation:



# U(1) DIRAC SPIN LIQUID

$$\hat{\mathcal{H}}_{\text{MF}} = \chi \sum_{\langle ij \rangle \pm 1} s_{ij} c_{j,\alpha}^\dagger c_{i,\alpha} + \text{h.c.}$$

Ran' 07

$$e^{i\phi} = \prod_{\text{plaquette}} s_{ij}$$

Hermele' 08

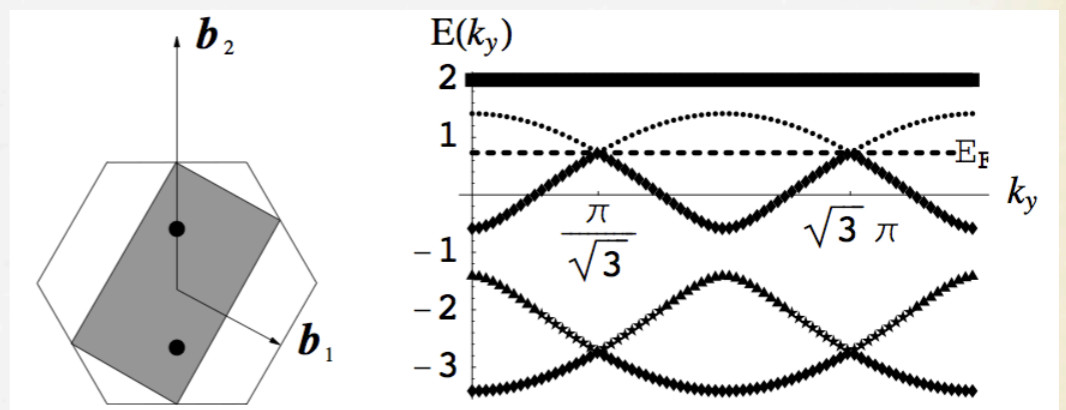
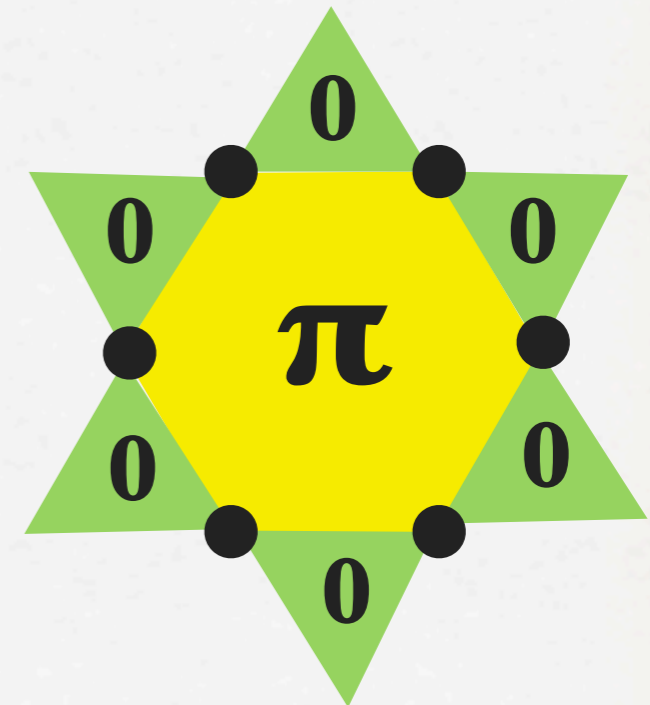
$$\langle S_i S_j \rangle \propto \frac{1}{r^4} \quad (\text{Algebraic spin liquid})$$

Gives the lowest variational energy *till date*, for a fermionic wave function, e.g. on a 48-site cluster

$E/J = -0.4293510(4)$  per site, from VMC

$E/J = -0.4387$  per site, ED

Lauchli' 12



# Z<sub>2</sub> SPIN LIQUIDS

DMRG calculations claim for a *fully* gapped, *fully* symmetric, Z<sub>2</sub> topological spin liquid GS, with  $E/J = -0.4386(5)$

Depenbrock' 12, White' 11

Using PSG classification we get “20” fermionic Z<sub>2</sub> spin liquids.

Lu' 11

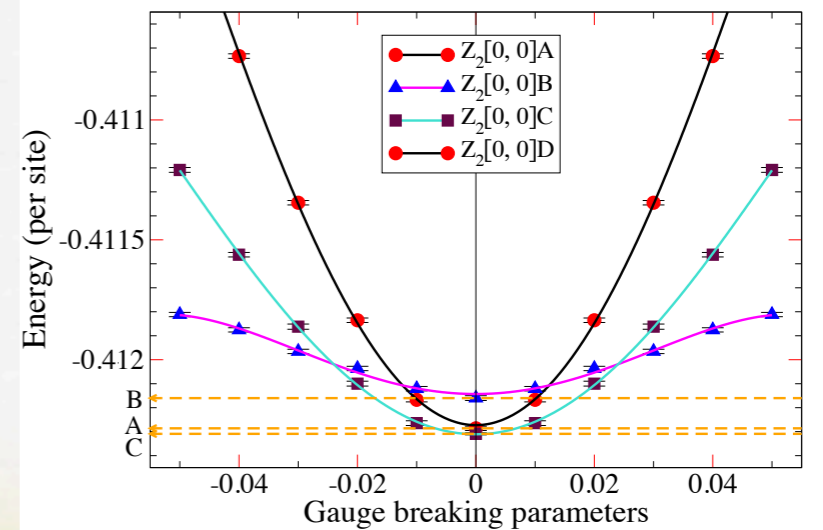
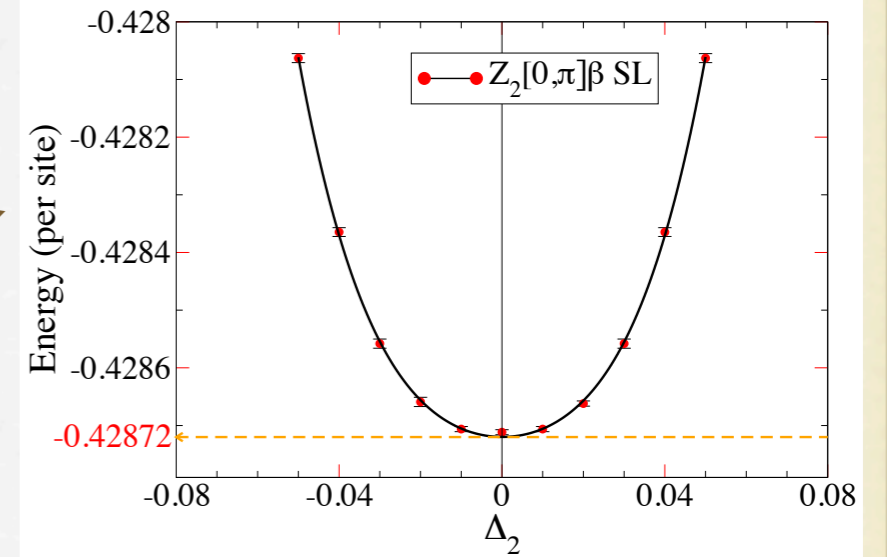
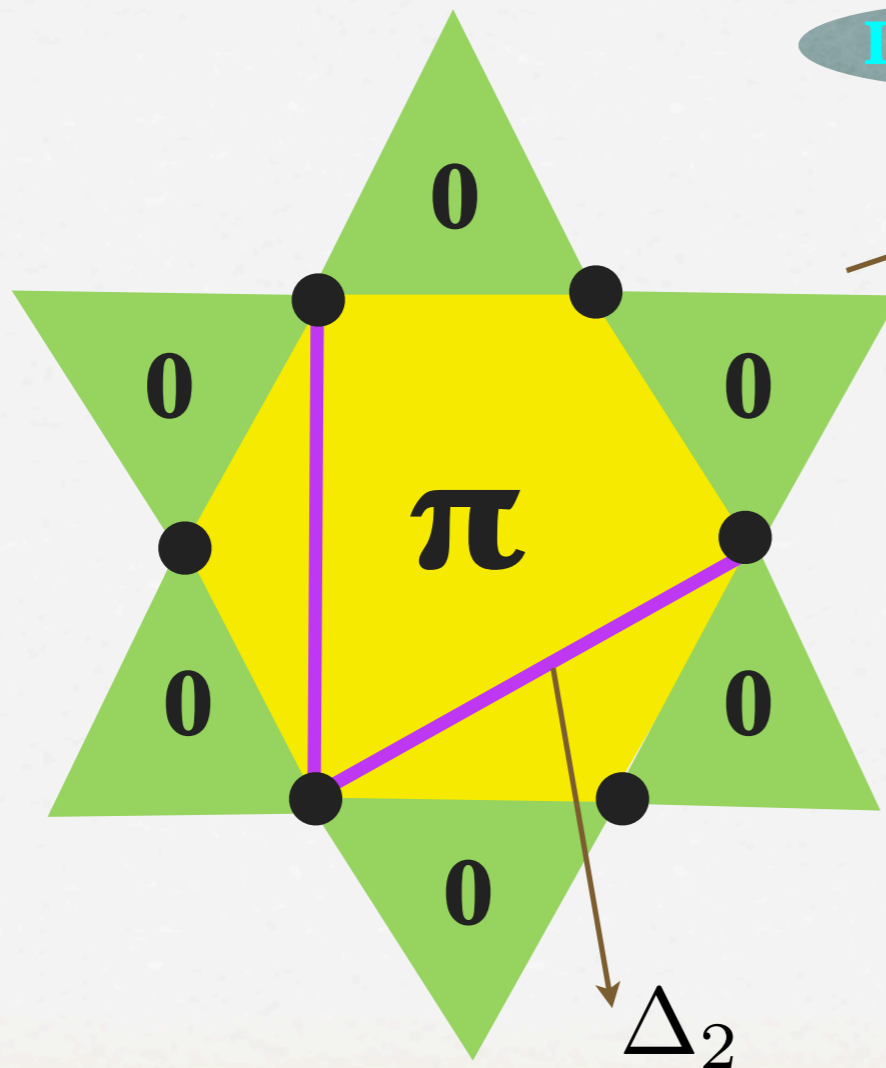
Only “5” of them are gapped.

Only “1” of them is continuously connected to the U(1) Dirac spin liquid, the  $\mathbb{Z}_2[0, \pi] \beta$  SL.

Rest “4” are continuously connected to the Uniform RVB spin liquid.

# Z<sub>2</sub> SPIN LIQUIDS

Energy *vs* Gauge breaking parameters



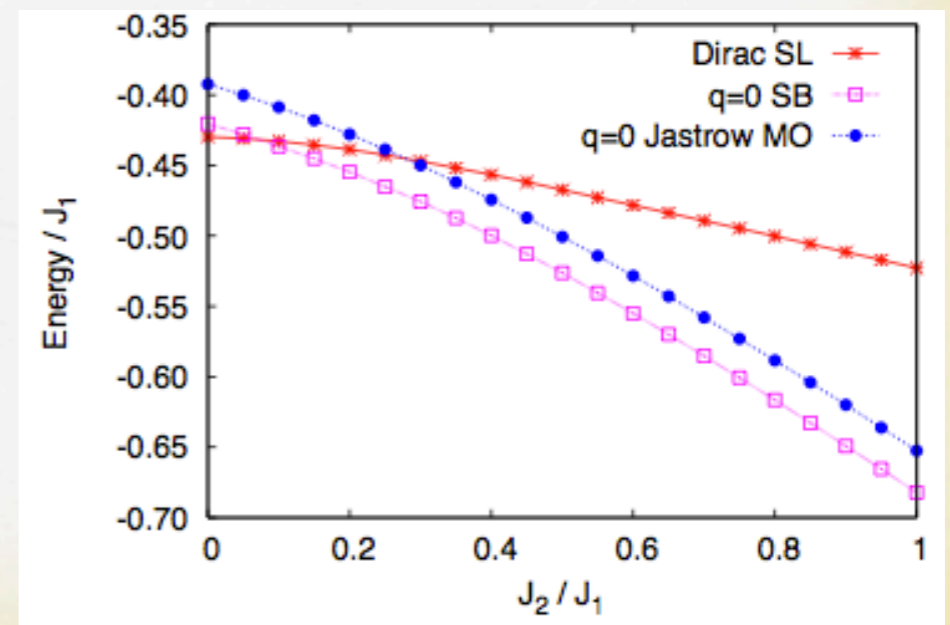
# PARTIAL CONCLUSION - I

- ✱ The U(1) Dirac and uniform RVB spin liquids are **stable** both *locally* and *globally* w.r.t. potential instabilities towards gapped and even gapless Z2 spin liquids.
- ✱ This stability remains preserved even in the presence of NNN exchange coupling of both antiferromagnetic and ferromagnetic type in the Hamiltonian.

## A Schwinger boson perspective:

Tay' 11

A *gapped* bosonic Z2 spin liquid is stabilized upon addition of small NNN ( $\sim 0.08 J_1$ ) antiferromagnetic coupling.



# VBC ORDERING

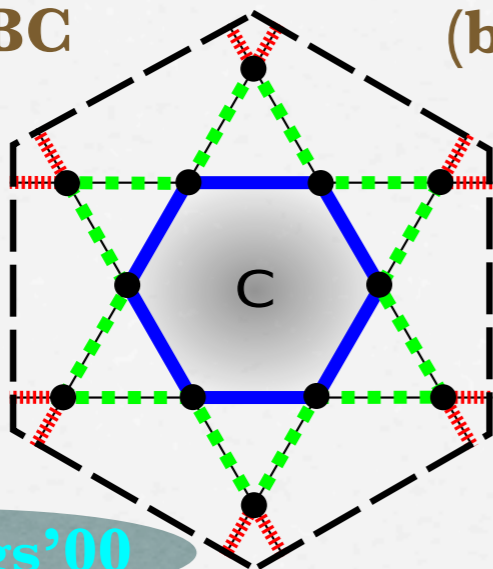
There is a stiff competition between many VBCs to occur as the ground state Poiblanç' 11



- ✱ What about Valence bond crystal perturbations to the  $U(1)$  gapless spin liquids?
- ✱ Can they destabilize them by opening a gap?
- ✱ If so, how many VBCs are there?, and what are they?

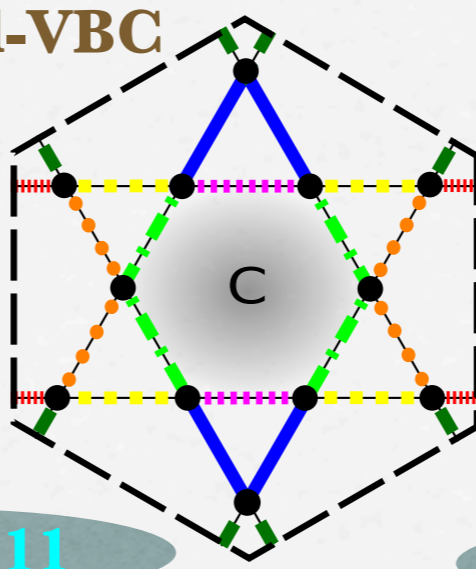
# 12 & 36 SITE VBC'S

(a) Star-VBC



Hastings'00

(b) Diamond-VBC



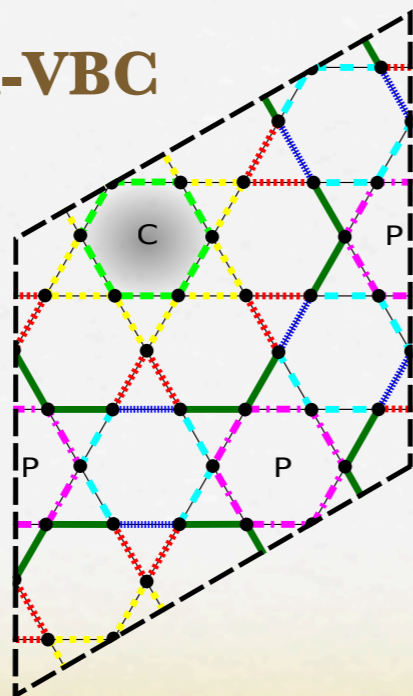
White'11

(c) VBC-3



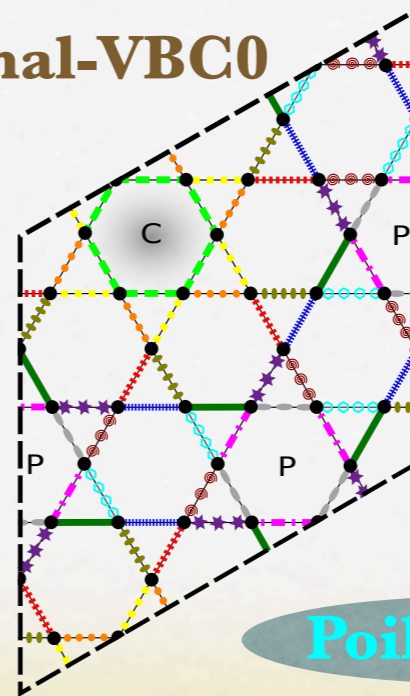
Poilblanc'11

(a) Hexagonal-VBC



Marston'91

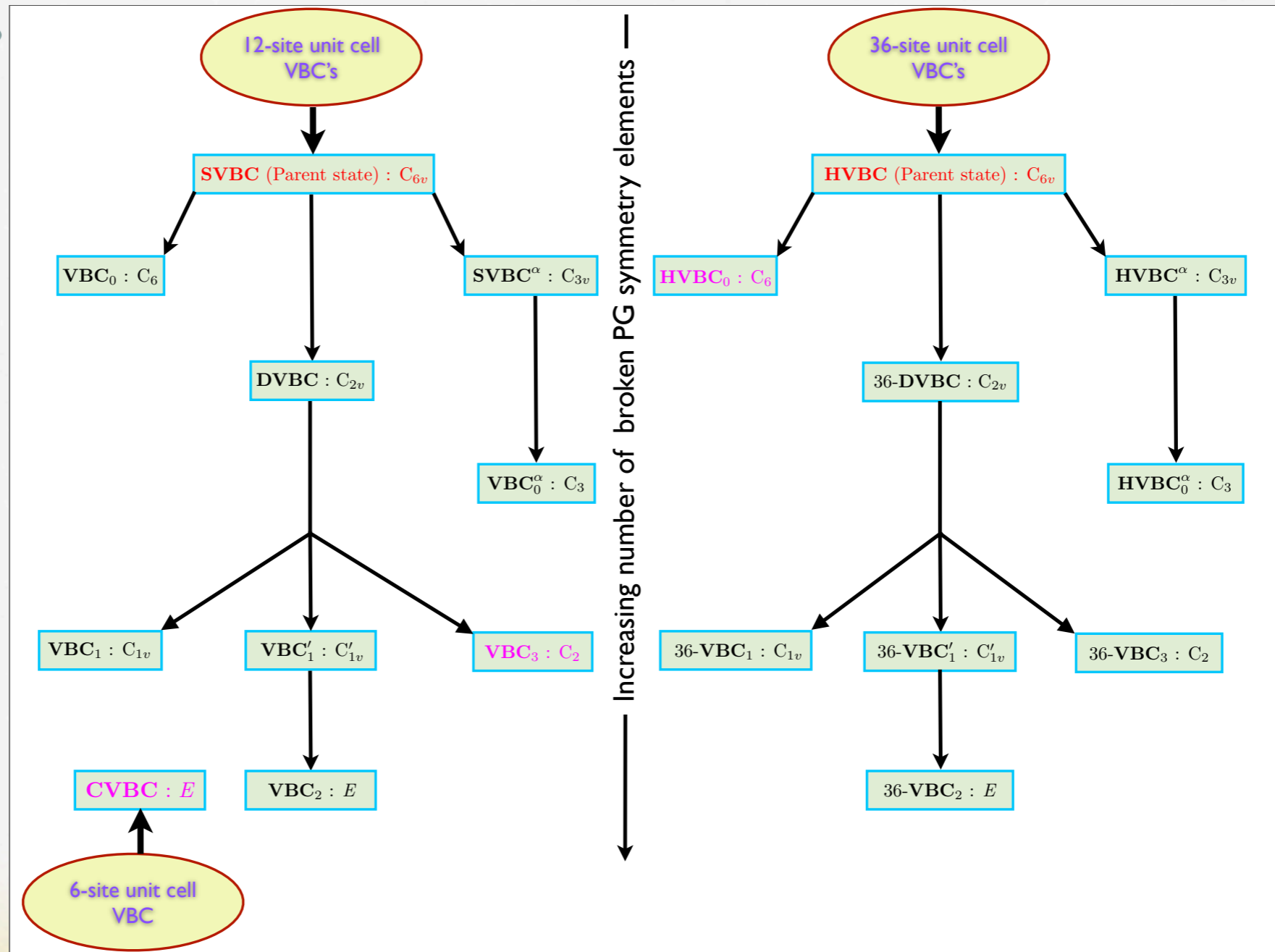
(b) Hexagonal-VBC0



Poilblanc'10

# SYMMETRY CLASSIFICATION

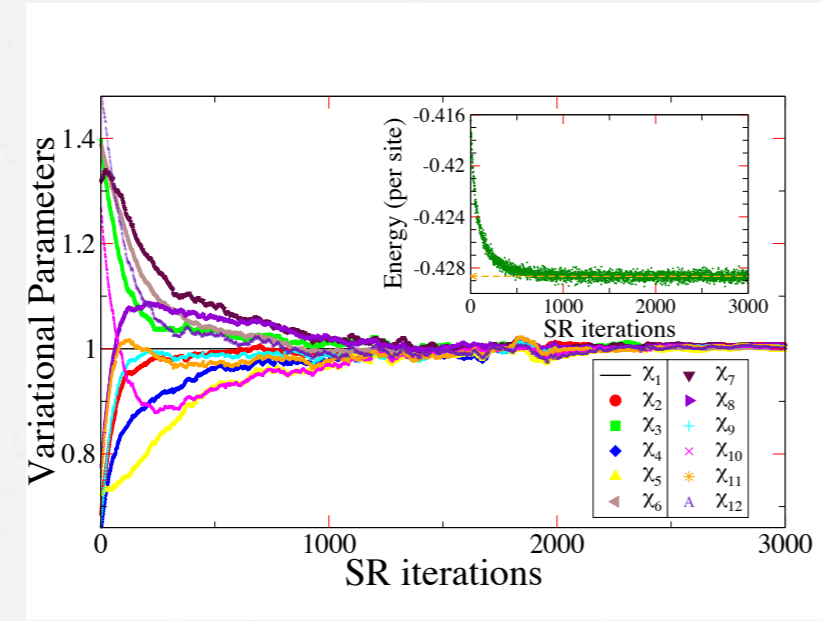
Iqbal' 12



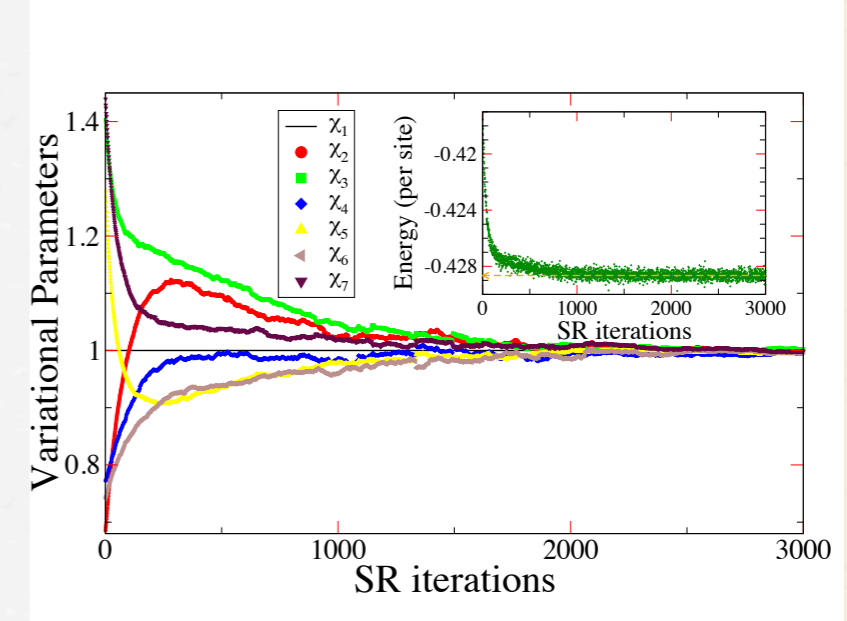
# OPTIMIZATION RESULTS

Iqbal' 12

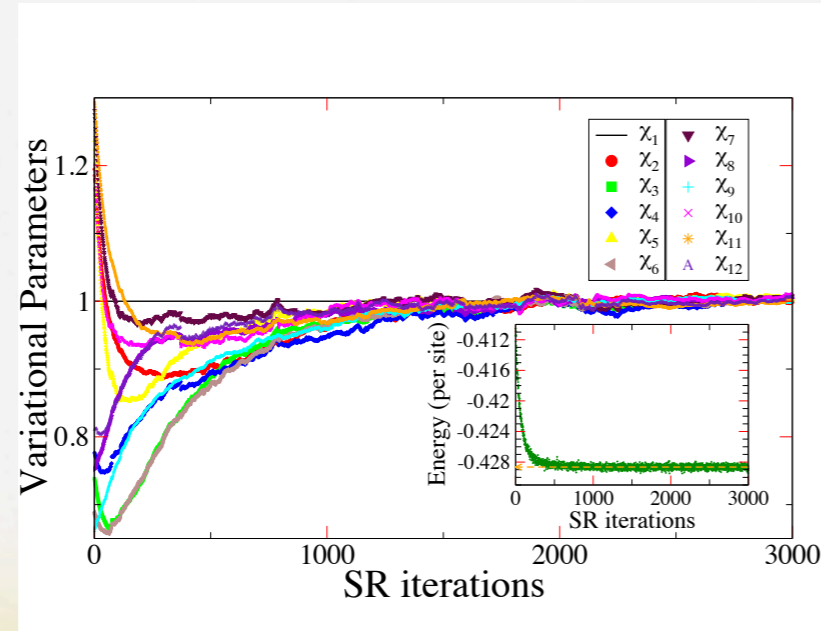
(a) C-VBC



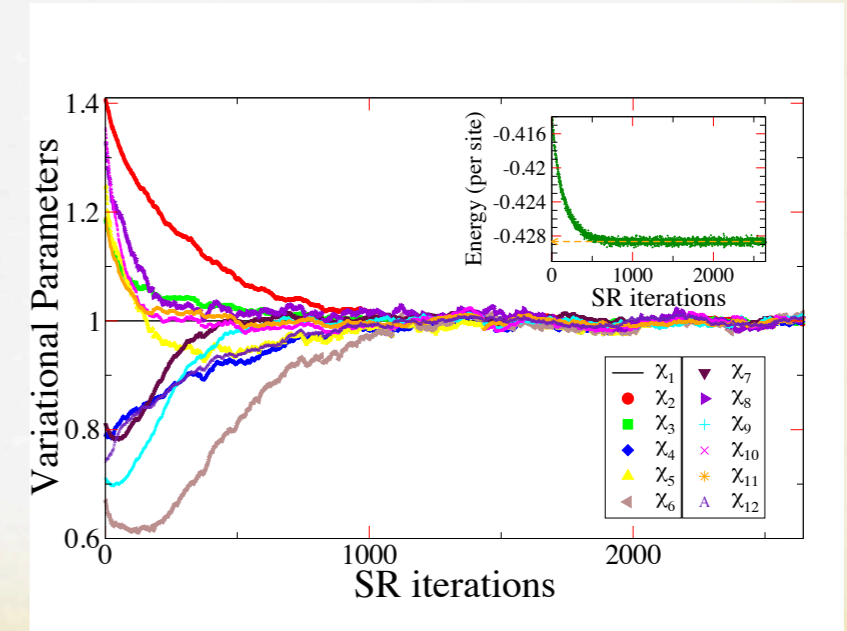
(b) D-VBC



(c) VBC-3



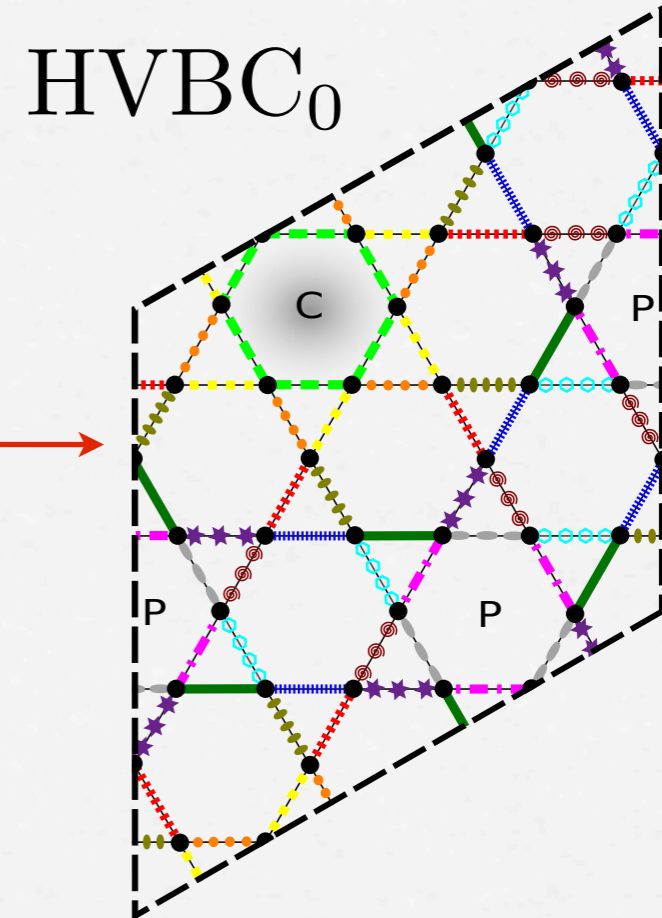
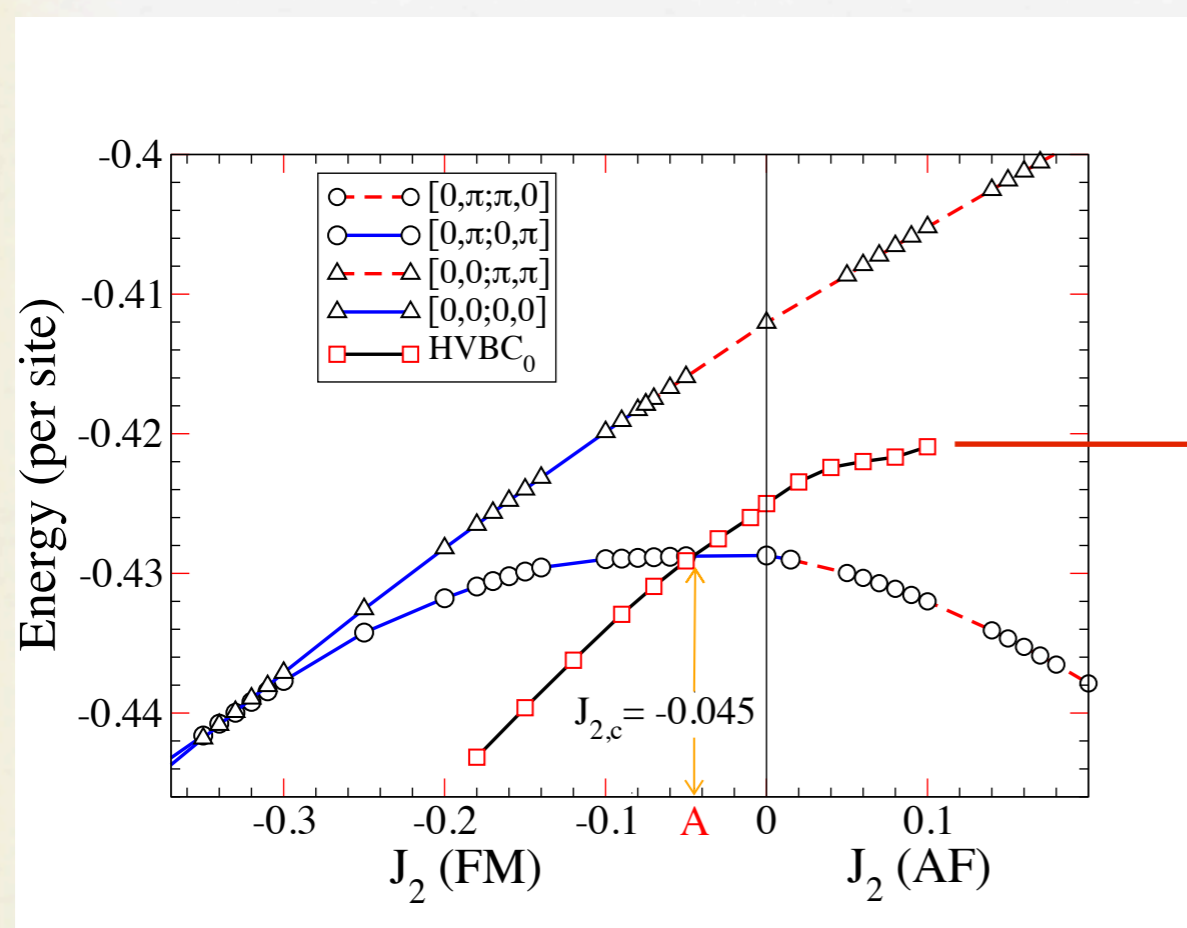
(d) H-VBC0





# OPTIMIZATION RESULTS

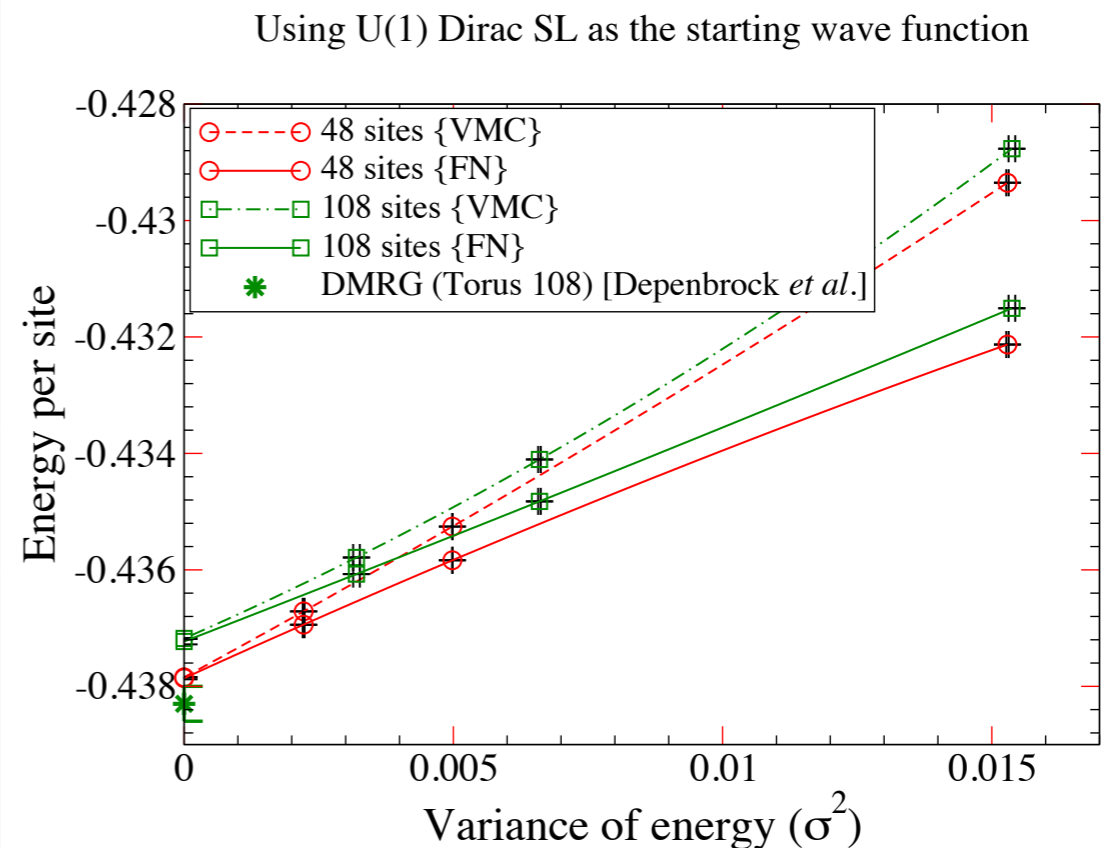
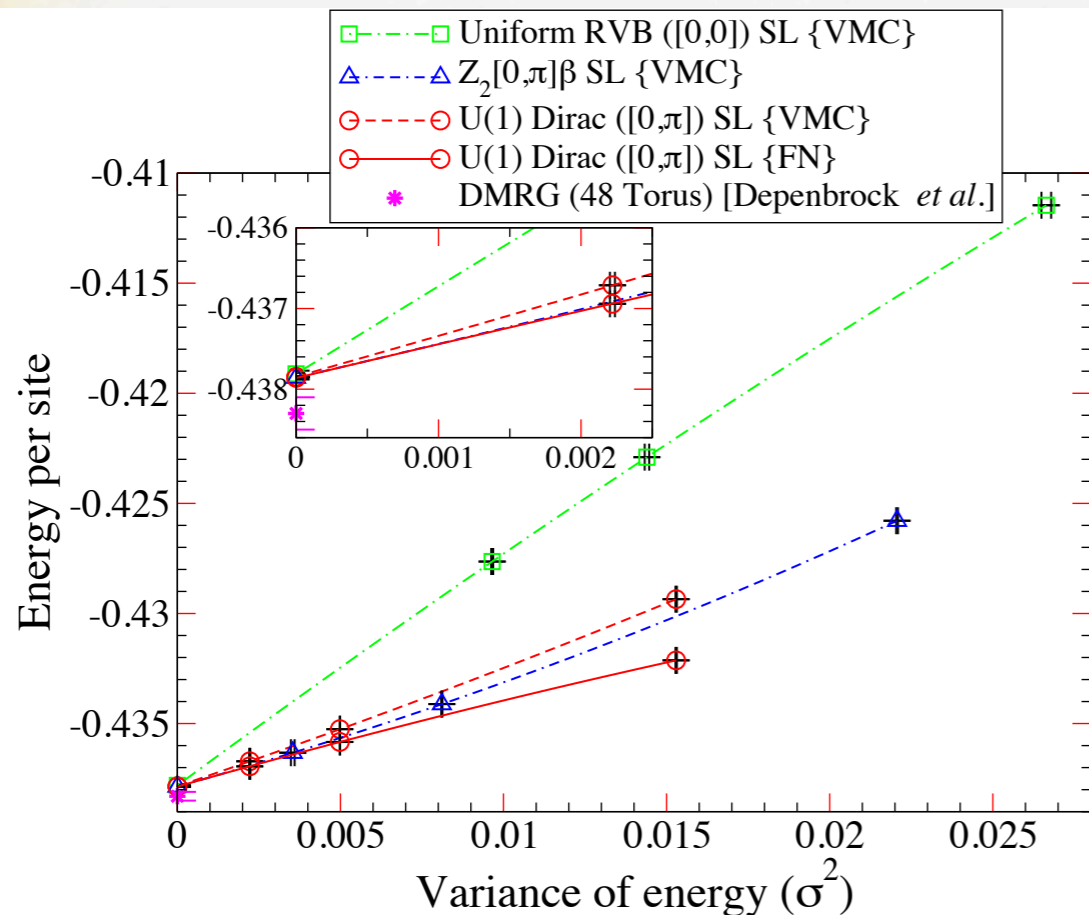
Iqbal' 12



- ✱ The  $U(1)$  Dirac spin liquid is stable towards all possible 6, 12, and 36 site unit cell VBCs.
- ✱ The Uniform RVB SL dimerizes into a 36 site VBC which is stabilized for small FM  $J_2$ .

# THE NATURE OF THE EXACT GROUND STATE

arXiv: 1209.1858

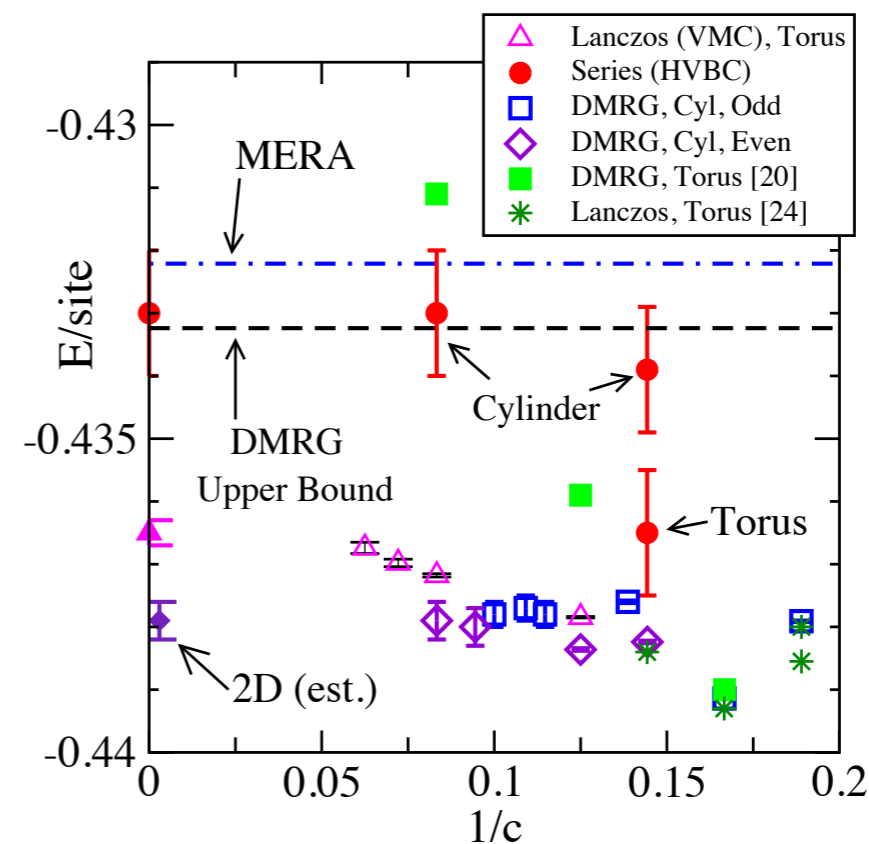
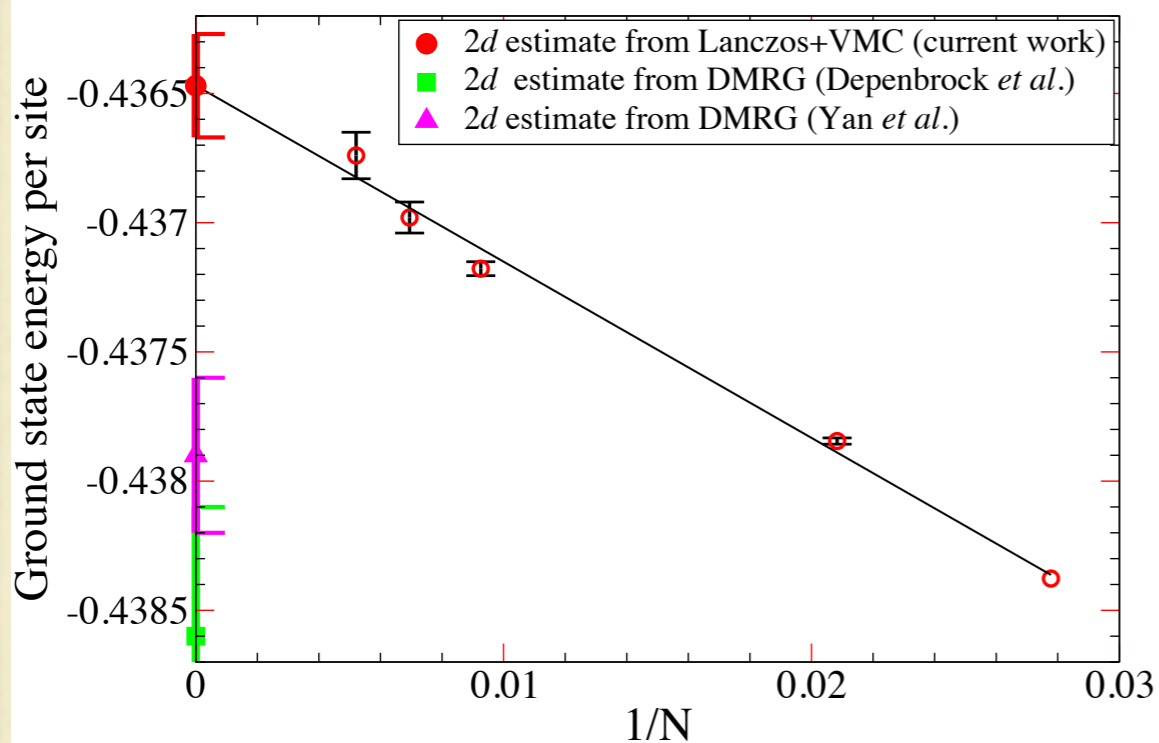


$$E/J \simeq -0.4378 \text{ (our work)}$$

$$E/J \simeq -0.4383 \text{ from DMRG (Depenbrock } et al., 2012)$$

$$E/J = -0.4387 \text{ from ED (Lauchli, 2012) } \textit{only seen in Boston?!}$$

# FINITE SIZE SCALING



$$E_{\infty}^{2D} / J = -0.4365(2)$$

$$E_{\infty}^{2D} / J = -0.4386(5) \text{ from DMRG (Depenbrock } et al., 2012)$$

★ The two estimates are the same within 3 error-bars.

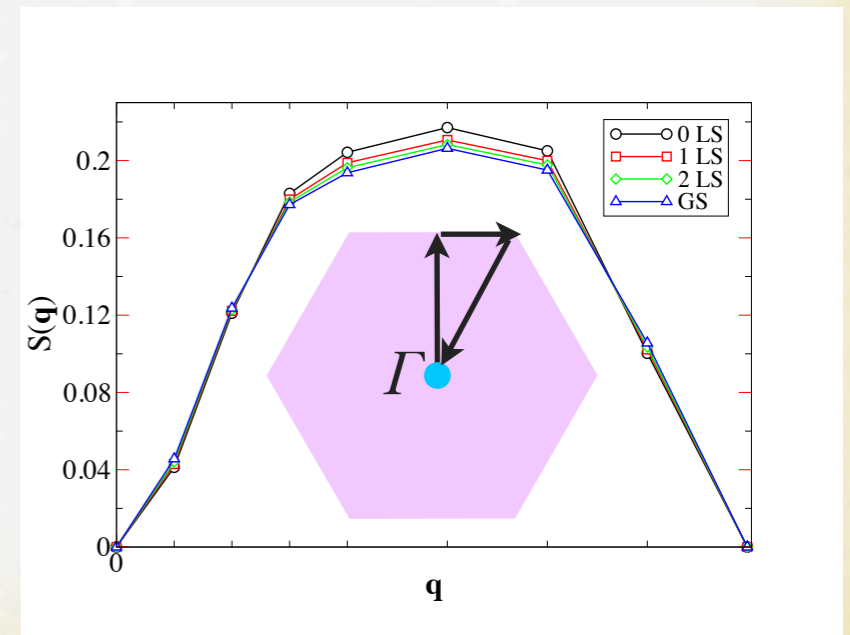
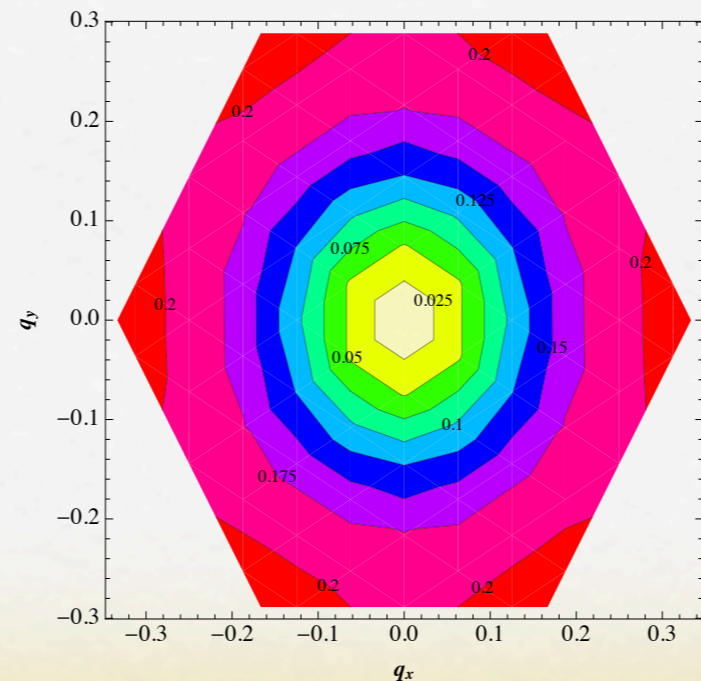
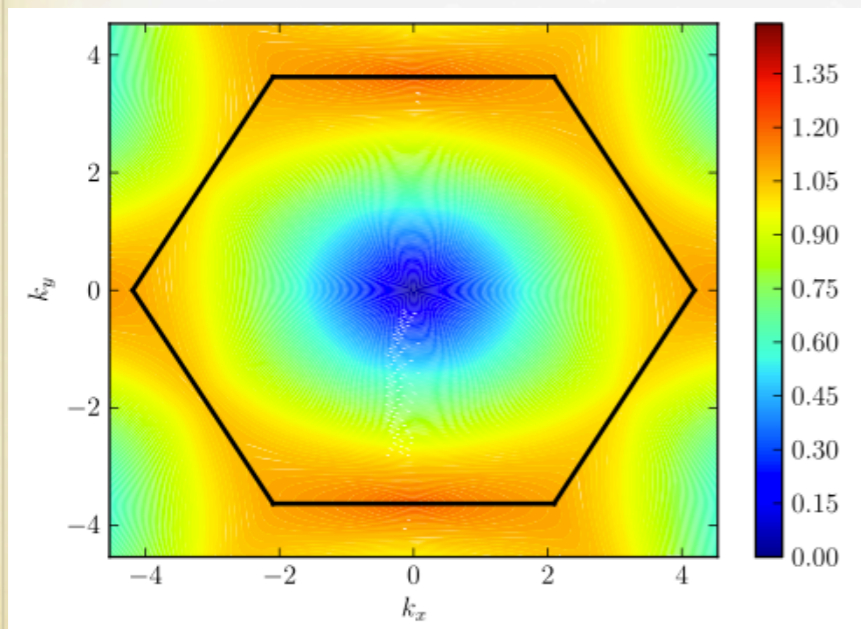
# STRUCTURE FACTORS

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

Results are obtained on the 192-site (8x8x3) cluster

DMRG (Depenbrock *et al.*, 2012)

VMC+Lanczos (Iqbal *et al.*, 2012)



# PARTIAL CONCLUSION - II

- ✿ Within the Schwinger fermion approach, the ground state is an algebraic  $U(1)$  Dirac spin liquid.
- ✿ Its energy is within 0.4% of DMRG estimates.
- ✿ Our energies, on all clusters, are the lowest estimates ever for a  $U(1)$  Dirac spin liquid, and in fact the lowest for any projected fermionic wave functions, till date.
- ✿ Our energies are obtained with a state that has all the symmetries of the lattice, while DMRG states are non-uniform (due to boundary effects) and one has to perform subtraction techniques.

# PERSPECTIVES

## Possible sources of discrepancy with DMRG results:

- ✿ The DMRG may have some issues with the finite-size extrapolation of the ground state energies, OR with the extrapolation of ground state energies with respect to the number of states/block going to infinity.
- ✿ It is probable that the true ground state contains a significant number of local two-*vison* quantum fluctuations, which are clearly missing in our wave functions, and are difficult to incorporate in a few LS's.
- ✿ A chiral  $Z_2$  topological spin liquid might also be stabilized.

*Thank You for  
your attention*

*The Kagome lattice is lovely, dark, and deep  
And there are miles to go before we sleep.*