Competing phases of the kagome $S = 1/2$ quantum Heisenberg antiferromagnet.

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Abstract:

Within the class of *full* Gutzwiller projected fermionic wave functions, using quantum variational Monte Carlo simulations, we investigated the energetics of all possible $\mathbb{Z}_2$ spin liquids (SLs) on the kagome lattice which can potentially occur as ground states of the nearest-neighbor (NN) $S = 1/2$ QHAF. We conclusively show that all *gapped* and gapless $\mathbb{Z}_2$ SLs are higher in energy compared to the U(1) gapless SLs in whose neighborhoods they lie. These results contradict the recent proposal made using the density-matrix renormalization group method, that the ground state is a *fully* gapped $\mathbb{Z}_2$ SL. (Yan, *et.al.* Science, **332**, 1173 (2011)). In particular, the most promising gapped $\mathbb{Z}_2$ SL (the $\mathbb{Z}_2[0,\pi]\beta$ state) conjectured to describe the ground state (Lu, *et.al.* Phys. Rev. B **83**, 224413 (2011)) is always higher in energy compared to the U(1) Dirac SL for both the NN and NNN $S = 1/2$ QHAF. We also extended the U(1) Dirac SL and the uniform RVB SL to include 2nd NN hopping terms, and studied its *local* and *global* stability towards various valence bond crystal (VBC) patterns. In particular, we found that a non-trivial 36 site VBC is stabilized upon addition of a *small* ferromagnetic exchange coupling, whereas on the antiferromagnetic side we have a gapless U(1) Dirac state.

Model, wave function & numerics

Heisenberg Hamiltonian:

- We study the isotropic NN and NNN $S = 1/2$ quantum Heisenberg antiferromagnetic model on the kagome:

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

Fermionic variational wave functions:

- $\hat{\mathbf{S}}_i = \frac{1}{2} c^{\dagger}_{i,\alpha} \sigma^{\alpha,\beta} c_{i,\beta}$
- $\hat{\mathcal{H}}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu\delta_{ij}) c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{i,j} \{(\Delta_{ij} + \zeta\delta_{ij}) c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + h.c.\}$; with $\chi_{ij} = \chi^{*}_{ji}$ and $\Delta_{ij} = \Delta_{ji}$.
- $|\Psi_{\mathrm{VMC}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle = \mathcal{P}_G |\Psi_{\mathrm{MF}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle$

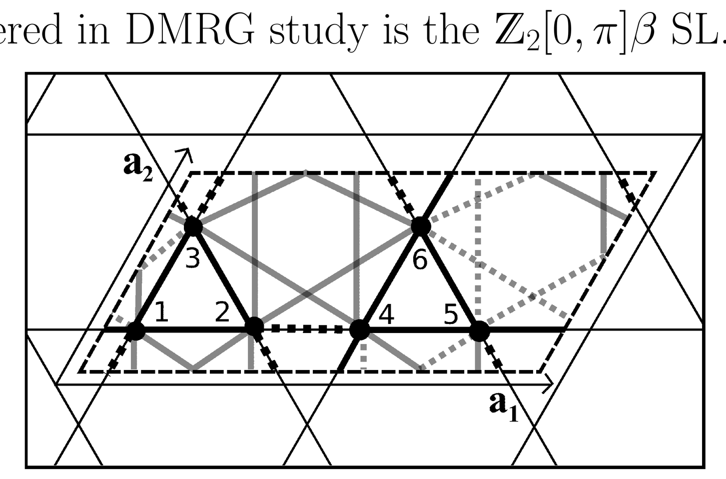
Stochastic reconfiguration optimization:

- Very accurate determination of the optimized parameters using correlated sampling & not by energy differences.
- Enhanced stability of iteration method for energy optimization. $\{\alpha'_i\} - \{\alpha_i\} = \epsilon \rightarrow$ is very small.
- This *small* ϵ is made possible by using the squared distance between two normalized wave functions.

$\mathbb{Z}_2$ spin liquids on the kagome lattice

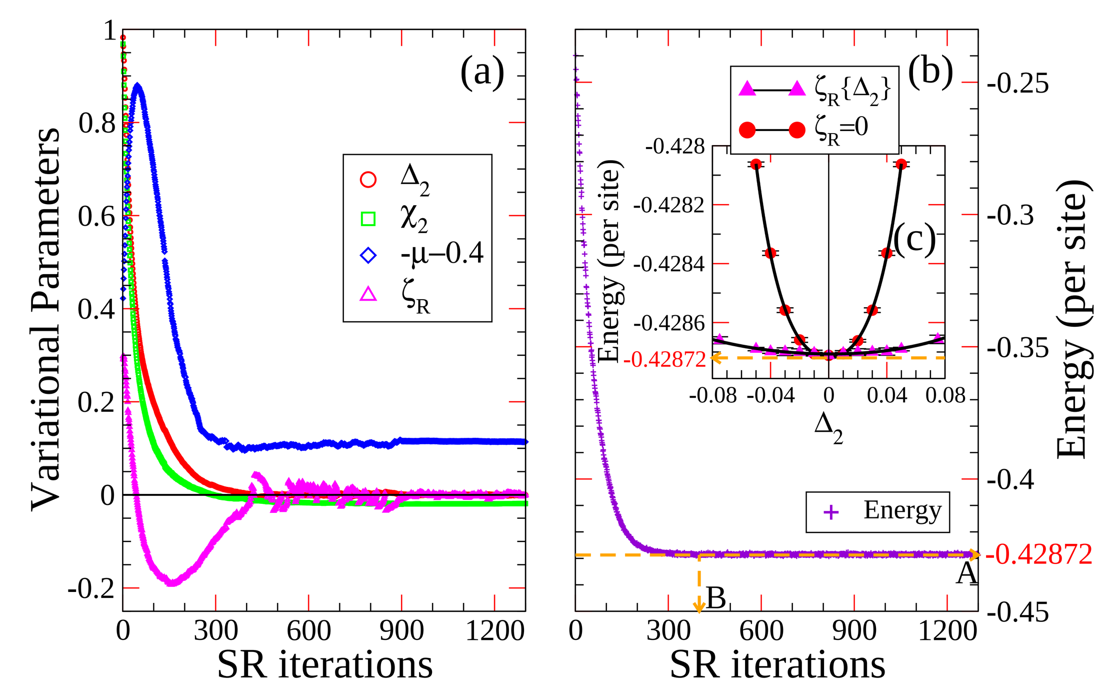
Classification:

- There are 20 fully symmetric $\mathbb{Z}_2$ mean-field spin liquids.
- Out of these, in 8 SLs the U(1)$\rightarrow \mathbb{Z}_2$ gauge breaking is not realized upto 3rd NN and 6 of these have vanishing NN bond $\Rightarrow$ Unlikely GSs of NN $S = 1/2$ QHAF.
- Remaining 12 SLs are continuously connected to some U(1) gapless SL.
- Out of these *only* 5 are gapped. 1 connected to the U(1) Dirac SL and 4 connected to the uniform RVB SL.
- Hence, the most promising candidate to act as the GS discovered in DMRG study is the $\mathbb{Z}_2[0,\pi]\beta$ SL.



$\mathbb{Z}_2[0,\pi]\beta$ state: SR optimization results

Y. Iqbal, *et.al.* arXiv: 1105.0341, PRB (in press)



- On optimization, $(\Delta_2, \zeta_{\mathrm{R}}) \rightarrow 0$. Thus, returning back to the 2nd NN U(1) Dirac SL, the $[0,\pi;\pi,0]$ state.
- Close to the U(1) Dirac SL, the energy landscape along the manifold connecting to the $\mathbb{Z}_2[0,\pi]\beta$ SL is *very* flat.
- The remaining 3 gapless $\mathbb{Z}_2$ SLs in the neighbourhood of the U(1) Dirac SL are also energetically higher.

$\mathbb{Z}_2$ spin liquids in the neighbourhood of the uniform RVB spin liquid

Y. Iqbal, *et.al.* arXiv: 1105.0341, PRB (in press)

Plots of Energy *vs* U(1)$\rightarrow \mathbb{Z}_2$ Gauge breaking parameters

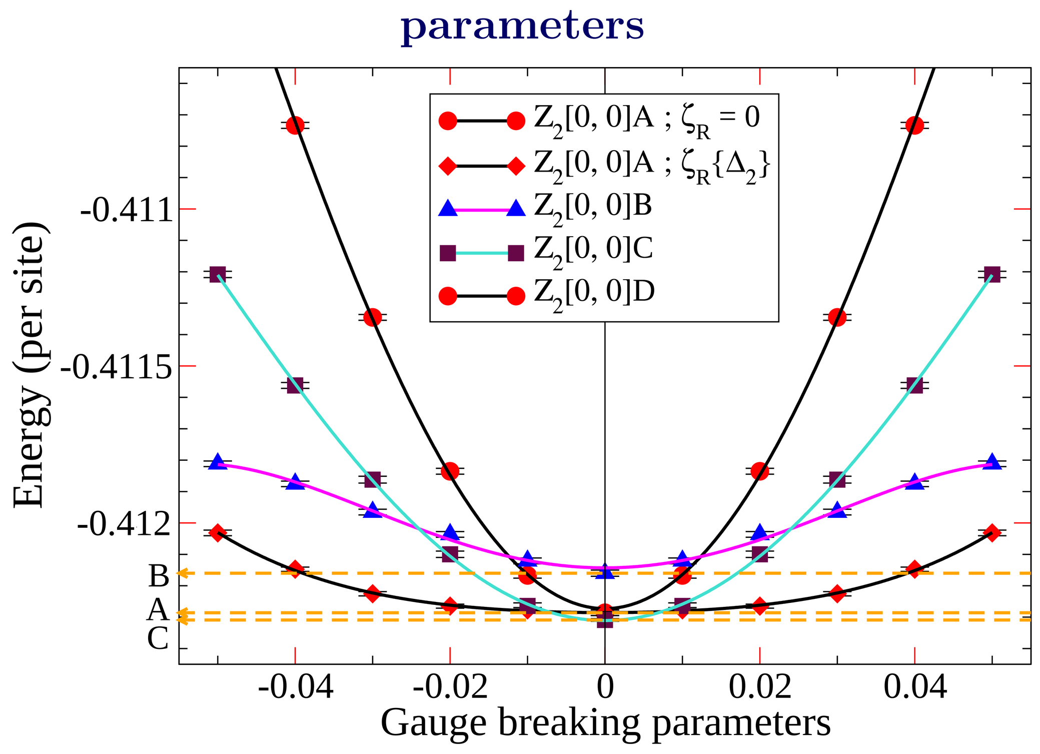


Table of Ansätze

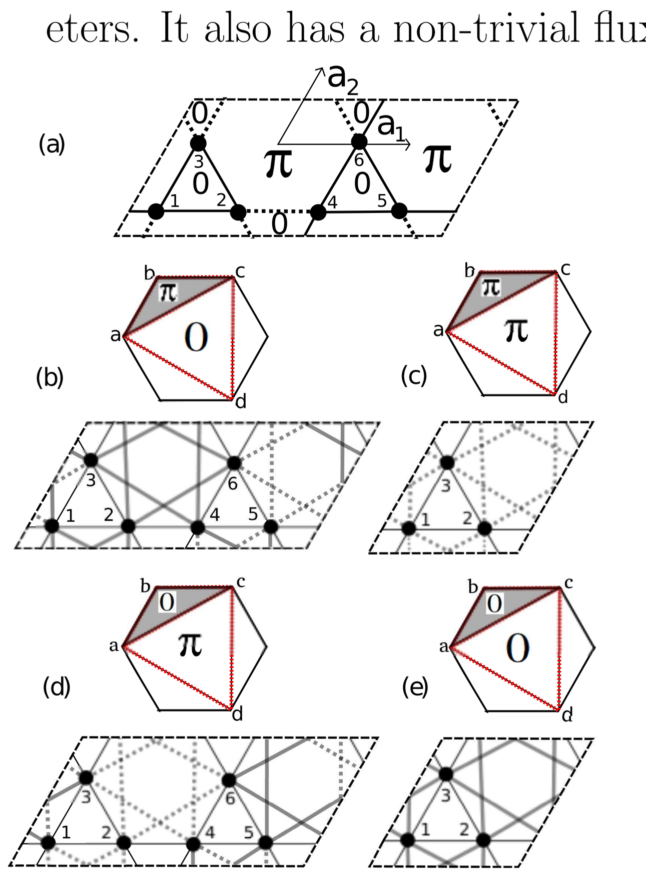
State	$\Lambda_{\mathrm{onsite}}$	$U_{\mathrm{n.n.}}$	$U_{2nd\mathrm{n.n.}}$	$U_{3rd\mathrm{n.n.}}$	$\tilde{U}_{3rd\mathrm{n.n.}}$
$\mathbb{Z}_2[0,\pi]\beta$	μ, ζ_{R}	χ_{R}	$\chi_{\mathrm{R}}, \Delta_{\mathrm{R}}$	0	0
$\mathbb{Z}_2[0,0]\mathrm{A}$	μ, ζ_{R}	χ_{R}	$\chi_{\mathrm{R}}, \Delta_{\mathrm{R}}$	0	0
$\mathbb{Z}_2[0,0]\mathrm{B}$	μ	$\chi_{\mathrm{R}}, \Delta_{\mathrm{I}}$	0	0	0
$\mathbb{Z}_2[0,0]\mathrm{C}$	μ	χ_{R}	χ_{R}	$\chi_{\mathrm{R}}, \Delta_{\mathrm{I}}$	χ_{R}
$\mathbb{Z}_2[0,0]\mathrm{D}$	μ	χ_{R}	$\chi_{\mathrm{R}}, \Delta_{\mathrm{I}}$	0	0

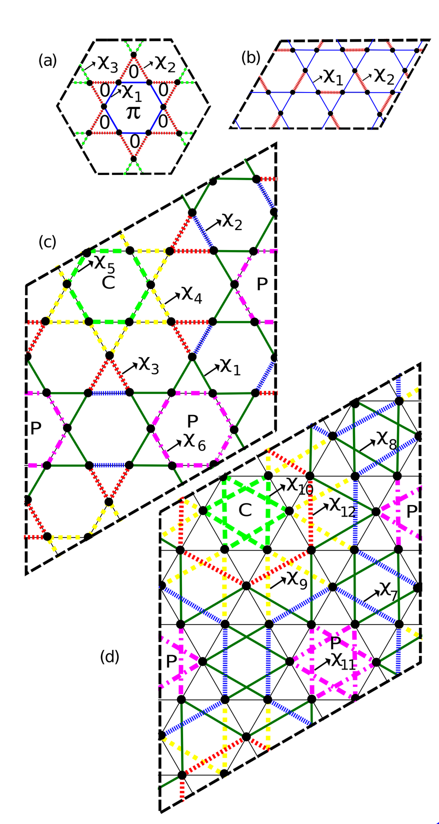
- For all 4 of these *gapped* $\mathbb{Z}_2$ SLs, the energy increases symmetrically and monotonically as the U(1)$\rightarrow \mathbb{Z}_2$ gauge breaking parameter (shown in red in the table) is tuned on from zero to a small finite value. The parameters in black are fixed to their optimized values.

Extended U(1) Dirac spin liquid and Valence bond crystal patterns

Y. Iqbal, *et.al.* PRB 83, 100404(R) (2011)

- The extended U(1) Dirac SL ((b) and (d)) and uniform RVB SL ((c) and (e)) lead to considerable improvement in energy for the $J - J'$ model.
- The NN Dirac SL (a) is *locally* and *globally* stable *w.r.t.* destabilizing into a 12 (a), 18 (b) or 36 (c) site unit cell VBC.
- Upon addition of a small ferromagnetic NNN J' exchange coupling, the extended uniform RVB SL dimerizes into a non-trivial 36 site unit cell VBC ((c) and (d)).
- This VBC is not a local instability of the $[0,0;0,0]$ SL, and possesses a large bond amplitude modulation in a variational space of 6 NN and 6 NNN variational parameters. It also has a non-trivial flux pattern.





Conclusions and future directions:

Summary of results:

- The most promising *gapped* SL conjectured to describe the ground state discovered in the DMRG study, the $\mathbb{Z}_s[0,\pi]\beta$ SL, is always higher in energy than the U(1) Dirac SL.
- In fact, all *gapped* $\mathbb{Z}_2$ SLs on the kagome are higher in energy compared to the U(1) SLs, of which they are continuous deformations.
- All gapless $\mathbb{Z}_2$ SLs on the kagome are also energetically higher compared to the U(1) gapless SLs.
- The U(1) Dirac SL is stable against various VBC and chiral SL perturbations.
- Atleast within the Schwinger-fermion approach of the spin model, the *gapless* U(1) Dirac SL has the best variational energy for the NN and NNN (AF) spin-1/2 QHAF on the kagome lattice.

Future directions:

- Consider further improvements of variational wave functions, based upon the application of a few Lanczos steps.
- Application of an approximated fixed-node projection technique.
- Explore the energetics of gapped $\mathbb{Z}_2$ SLs which break some symmetries.
- The possibility that the fully gapped SL found by the DMRG study possesses a different low energy gauge structure other than $\mathbb{Z}_2$ also remains open.