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.\textsuperscript{[Yan, et.al., Science, 332, 1173 (2011)]}. In particular, the most promising gapped $\mathbb{Z}_2$ SL (the $\mathbb{Z}_2[0,0,0,\pi,\pi]$ state) conjectured to describe the ground state\textsuperscript{(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.

### Abstract:

In particular, the most promising gapped $\mathbb{Z}_2$ spin liquid is always 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. In particular, the most promising gapped $\mathbb{Z}_2$ SL (the $\mathbb{Z}_2[0,0,0,\pi,\pi]$ 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 antiferromagnet model on the kagome:
  \[ H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + J' \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_i \cdot \mathbf{S}_j \]

**Fermionic variational wave functions:**
- $\Psi = \int d^2 \Lambda \, \langle \Lambda | \hat{\phi} \rangle \Psi_0$, $\hat{\phi} = \sum_{\langle i,j \rangle} \chi_i \hat{c}_{i,\alpha} \chi_j \hat{c}_{j,\beta} + h.c.$, with $\chi_i = \chi_j$ and $\Delta_{ij} = \Delta_{ji}$.
- $| \Psi_{\Lambda} \rangle = B \Psi_0 | \psi_{\Lambda} \rangle$

**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. $\{ \chi'_i \} - \{ \chi_i \} = \epsilon \to 0$ is very small.
- This small $\epsilon$ 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 $U(1)$ gauge breaking is not realized up to 3rd NN and 6 of these have vanishing NN bond.

**Gauge breaking parameters:**
- 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 $\mathbb{Z}_2[0,0,0,\pi,\pi]$ SL.

### Extended $U(1)$ Dirac spin liquid and valence bond crystal patterns

**Summary of results:**
- The most promising gapped SL conjectured to describe the ground state discovered in the DMRG study, the $\mathbb{Z}_2[0,0,0,\pi,\pi]$ 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.
- At least 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.