Competing phases of the $S = \frac{1}{2}$ Kagomé quantum Heisenberg antiferromagnet: A variational Monte Carlo approach

A gapless U(1) or a gapped $\mathbb{Z}_2$ spin liquid?

Yasir Iqbal [1], Federico Becca [2], and Didier Poilblanc [1]

[1]Laboratoire de Physique Théorique (IRSAMC), CNRS and Université Paul Sabatier, Toulouse, France

[2]Democritos National Simulation Center, Istituto Officina dei Materiali del CNR and Scuola Internazionale Superiore di Studi Avanzati (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

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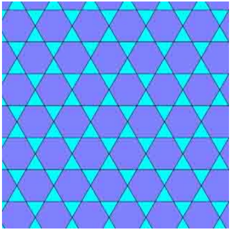
The Heisenberg Hamiltonian:

$$\hat{\mathcal{H}} = J(|\mathbf{r}|) \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j \quad (1)$$



What makes the nearest neighbour antiferromagnetic Heisenberg model on the kagomé lattice so special?

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A particular example of such a *magnetically disordered* ground state is a 'spin liquid'.

What makes the search for the ground state of $S = 1/2$ kagome QHAF so challenging and elusive?

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It is this energetic proximity of many competing states shown above and their sensitivity to small perturbations, that makes this search so challenging and elusive.

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Defying conventional wisdom

Since, ordinarily according to band theory we should have a conductor.

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- They are examples of quantum ordered states and are distinguished by their projective symmetry groups.

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$$\hat{\mathcal{H}}_{\mathrm{MF}} = \sum_{i,j,\alpha} (\chi_{ij} + \mu \delta_{ij}) c^{\dagger}_{i,\alpha} c_{j,\alpha} + \sum_{i,j} \{ (\Delta_{ij} + \zeta \delta_{ij}) c^{\dagger}_{i,\uparrow} c^{\dagger}_{j,\downarrow} + h.c. \}, \tag{3}$$

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Project this non-correlated fermionic state onto the physical Hilbert space of one-fermion per site:

$$|\Psi_{\mathrm{VMC}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle = \mathcal{P}_G |\Psi_{\mathrm{MF}}(\chi_{ij}, \Delta_{ij}, \mu, \zeta)\rangle, \tag{4}$$

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where $\mathcal{P}_G = \prod_i (1 - n_{i,\uparrow} n_{i,\downarrow})$ is the full Gutzwiller projector enforcing the one-fermion per site constraint.
$\Rightarrow$ The χ_{ij}, Δ_{ij}, μ, ζ are the *ansatz* of a given state, and serve as the variational parameters.

Numerical method

We use Stochastic reconfiguration iteration method to optimize the wave function. (S. Sorella, Phys. Rev. B 71, 241103(R) (2005).)
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- In the SR method, we use square distance between two normalized wave functions as opposed to cartesian distance used in standard steepest descent method.
- SR method captures cases when:
  (a) Small change of the variational parameters corresponds to a large change of the wave function.
  (b) Conversely, a large change of the variational parameters can imply only a small change of the wave function.

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- This method is indispensable when the energy landscape is very flat, i.e. when the energy nearly converges but the parameters do not.

$$\Downarrow$$

In this case, optimization of parameters is possible because forces are calculated by correlated sampling and not by energy differences.
Note: The $U(1) \to \mathbb{Z}_2$ transition on the kagomé falls in this category, as we will see later

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- $SU(2) \times SU(2)$ SLs: The low energy gauge group is larger as compared to high energy gauge group.
  Types: gapless, linear.

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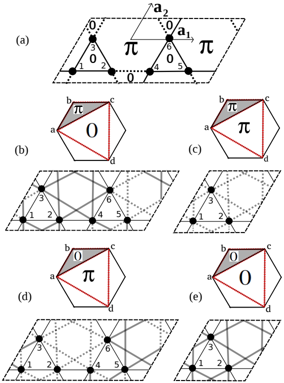
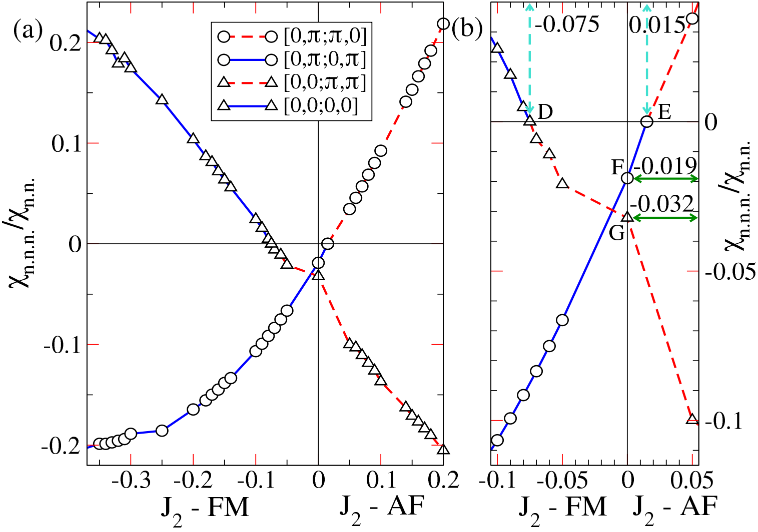
Y. Iqbal, F. Becca and D. Poilblanc PRB 83, 100404(R) (2011).

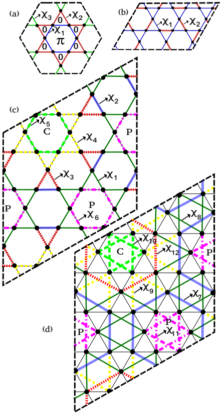


Extending the U(1) DSL to 2nd NN

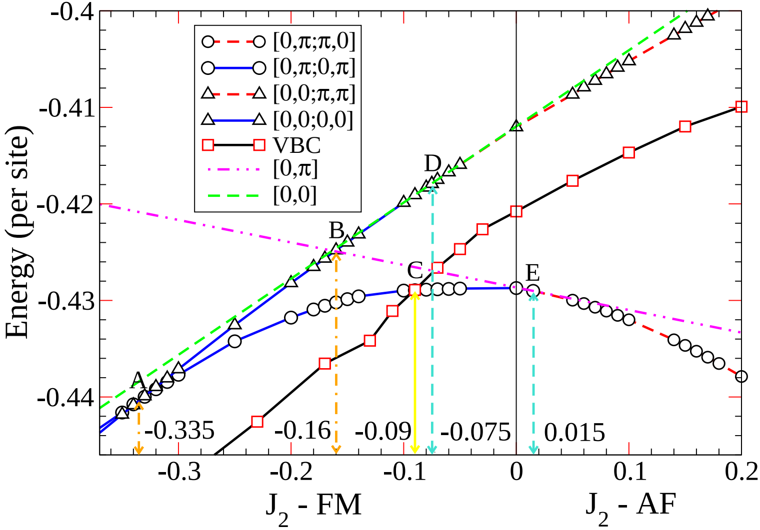


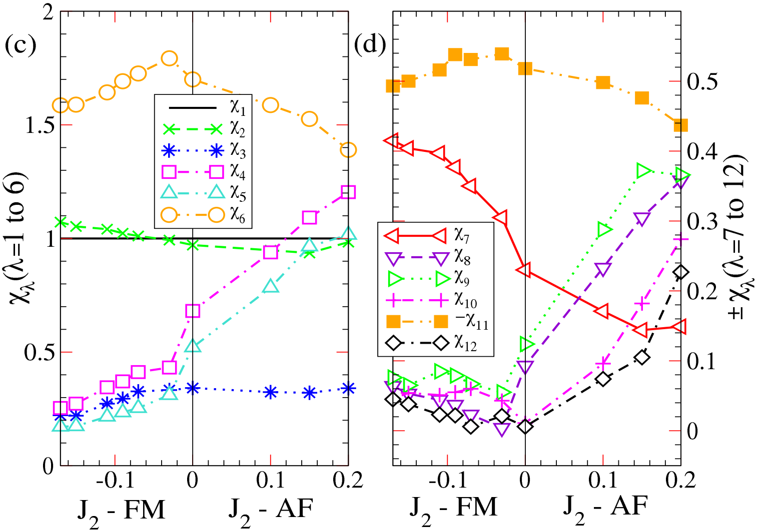
VBC patterns - possible instabilities of U(1) DSL

(a) Hastings, PRB. 63, 014413 (2000). (b) Marston and Zeng, J. Appl. Phys. 69, 5962 (1991) (c) Nikolic and Senthil, PRB. 68, 214415 (2003), Singh and Huse, Phys. Rev. B. 76, 180407(R) (2007). (c) and (d) Y. I, F. B and D. P, PRB 83, 100404(R).



Energetics of SL and VBC phases




(c)
$\chi_\lambda(\lambda=1$ to $6)$
χ_1
χ_2
χ_3
χ_4
χ_5
χ_6
J$_2$ - FM
J$_2$ - AF
(d)
χ_7
χ_8
χ_9
χ_{10}
$-\chi_{11}$
χ_{12}
$\pm\chi_\lambda(\lambda=7$ to $12)$

Comparison of energies of proposed competing Ground states of $S = 1/2$ kagome QHAF

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Start exploring the plethora of gapped $\mathbb{Z}_2$ spin liquids.

Y.-M. Lu, Y. Ran, and P. A. Lee, PRB. 83, 224413 (2011).

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- Positive feature shared by these 12 $\mathbb{Z}_2$ SLs:
  All of them are continuously connected to some $U(1)$ gapless SL.

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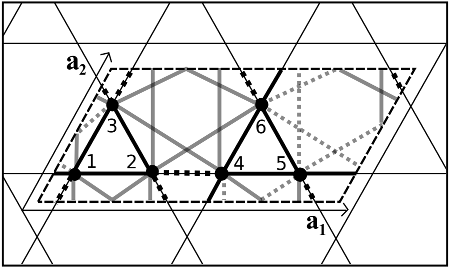
- The $\mathbb{Z}_2[0, \pi]\beta$ state can be obtained from the $U(1)$ DSL by continuously tuning on a gauge breaking parameter.

$$\mathcal{H}_{\mathrm{MF}}\{\mathbb{Z}_2[0,\pi]\beta\} = \chi_1 \sum_{\langle ij\rangle,\alpha} \mathrm{s}_{ij} c^\dagger_{i,\alpha} c_{j,\alpha} + \sum_{\langle\langle ij\rangle\rangle} \nu_{ij}\{\chi_2 \sum_{\alpha} c^\dagger_{i,\alpha} c_{j,\alpha} + \Delta_2 (c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} + h.c.)\} + \sum_i \{\mu \sum_\alpha c^\dagger_{i,\alpha} c_{i,\alpha} + \zeta_{\mathrm{R}} (c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow} + h.c.)\}, \quad (5)$$



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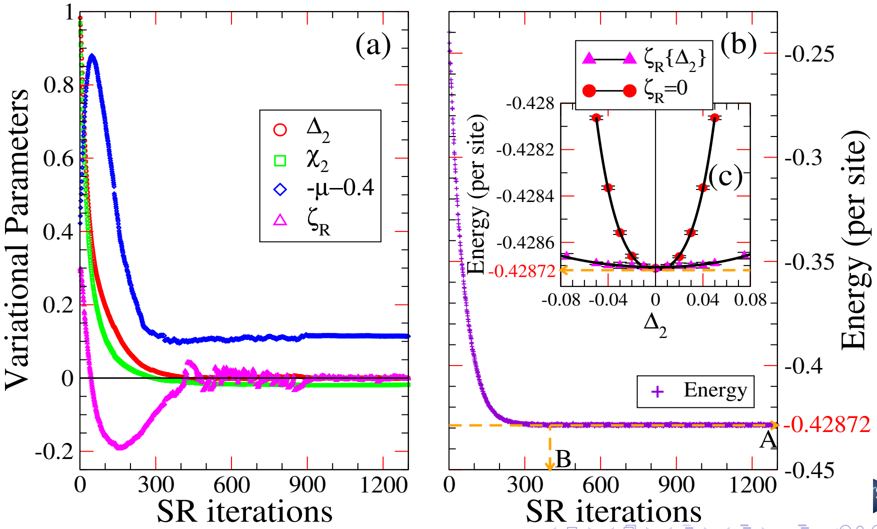
- Hence, a finite Δ_2 breaks the U(1) gauge structure down to $\mathbb{Z}_2$, and opens up an energy gap via the Anderson-Higgs mechanism.

Y. Iqbal, F. Becca, and D. Poilblanc, PRB **00** 000400(R) (2011)



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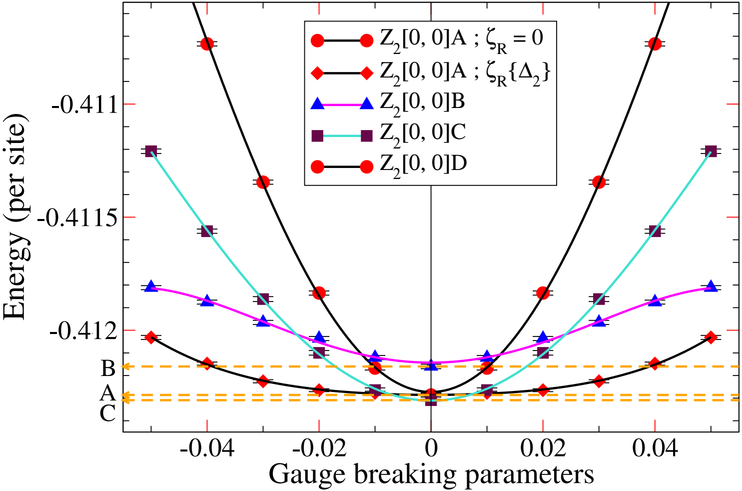
- All 4 SLs can be obtained from the $[0, 0]$ state by continuously tuning a gauge breaking parameter.

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

- *Ansätze* given only up to the neighbor at which the gauge symmetry is broken, in a form used by us in numerical simulations.
- The parameters highlighted in red are responsible for opening a gap by breaking the $U(1)$ gauge symmetry down to $\mathbb{Z}_2$.
- The $U_{3rd\rm n.n.}$ denotes bonds of length 2 connecting two sites and passing through a third site; instead, $\tilde{U}_{3rd\rm n.n.}$ denotes bonds of length 2 which dont pass through any site.

Energy Vs Gauge Breaking parameter plots



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- We recover the suitably extended, gapless 2nd NN U(1) Dirac SL.
- In particular, for $J'/J = 0.10$, this is the $[0,\pi;\pi,0]$ state with optimized $\chi_2 = 0.0924(2)$, and $E/J = -0.43200(2)$ per site; for $J'/J = -0.10$, this is the $[0,\pi;0,\pi]$ state with optimized $\chi_2 = -0.1066(2)$, and $E/J = -0.42898(2)$.

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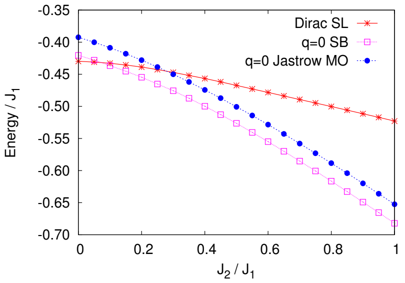
- Hence, *only* this $\mathbb{Z}_2$ SL can be made energetically competing.

T. Tay and O. I. Motrunich; Phys. Rev. B 84, 020404(R) (2011)



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- In particular, the most promising gapped SL conjectured to describe the ground state, the $\mathbb{Z}_2[0, \pi]\beta$ state, is always higher in energy than the U(1) Dirac SL.
- At least within the Schwinger fermion approach of the spin model, the U(1) Dirac SL has the best variational energy for the NN and NNN spin-1/2 QHAF on kagome lattice.

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- Explore the energetics of gapped $\mathbb{Z}_2$ SLs which break some symmetries such as time-reversal.
- 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.