

Dear Editors of SciPost Physics,

Thank you for your recent correspondence and reports on our manuscript, “Spin-1/2 kagome Heisenberg antiferromagnet with strong breathing anisotropy”. We thank both referees for their positive reports and for recommending the publication of our paper in SciPost Physics after minor revisions.

We have responded to all comments of the two referees and we would like to resubmit our paper. We hope that with this, our manuscript is ready for publication in SciPost Physics.

Please find a list of changes and responses to all referee's comments below.

Sincerely Yours,
The Authors

List of changes:

- Fig 3 were modified in response to request of the referees and energies from other studies were added to the figure
- Fi 7-(a) was added to the paper and Fig. 7-(b) has now been improved
- Fig 8-(a) was updated with more accurate energies and Fig. 8-(b) was added to the in response to the referees
- Fig-9,10 were added to the paper
- Relevant discussions in response to the referee’s remarks were added to the manuscript in particular to Sec. 5

Anonymous Report 1 on 2020-1-31 Invited Report

Requested changes:

1. On page 6 and figure 5, the authors find that the scaling of the ground-state energy with respect to bond dimension follows a power law. Therefore, they claim a gapless state. I do not find this convincing. Is there any theoretical proof that a power law scaling with respect to bond dimension would necessarily imply a gapless state? And why does it indicate a U(1) (rather than Z₂) gapless spin liquid? The author shall provide more concrete discussion or clarify that it is an empirically numerical expectation.

Reply: It has previously been shown numerically that the ground state energy of critical (gapless) systems, both in one [Phys. Rev. B 86, 075117 (2012)] and two [PRL 118, 137202 (2017)] dimension, $\epsilon_0(\mathbf{D})$, converges algebraically with respect to bond dimension D. While this is not a formal theorem, it is usually taken as a good indicator of a plausible gapless state. Our energies obtained with both iPEPS and particularly with PESS show an algebraic convergence which is best extrapolated by a fitting function of the form $\epsilon_0(D) = \epsilon_0 + aD^{-\beta}$ shown in Fig.3. These results on top of the long-range spin-spin correlation of Fig.7 in the main text (which has been improved substantially in our new simulation) are therefore compatible with the fact that the underlying state is plausibly a gapless spin liquid. However, characterizing the U(1) or Z₂ nature of the state is a

numerically nontrivial task. The gapless spin liquid is expected to have long-ranged entanglement and correlation functions and the U(1) state has no well-characterized topological order. We calculated the reduced density matrix of the ground state obtained from our PESS simulation on bipartitions of a semi-infinite cylinder and calculated the entanglement entropy. We found no topological contribution to the entanglement entropy which is in agreement with that of a U(1) gapless spin liquid. Let us further note that the momentum-dependent excitation spectrum which was extracted from the DMRG transfer matrix of Ref [29,44], exhibits Dirac cones that match those of a π -flux free-fermion model (the parton mean-field ansatz of a U(1) Dirac spin liquid). Although we are not able to calculate the same information within the framework of our TN simulations, we provided evidences throughout the paper that our results are in agreement with these DMRG calculations of Ref. [44] and therefore we believe that the gapless state we capture at the isotropic point should be a U(1) spin liquid. This has now been clarified in the revised version of the manuscript.

A minor issue is, based on the plot it is hard to tell the scaling behaviour is a power law. Can the authors contrast it with other scalings such as eD/a and $\log D$?

Reply: We have extrapolated the convergence of the ground state energy at the isotropic point versus bond dimension D with different functions i.e., exponential decay: $\epsilon_0(D)=\epsilon_0+\exp(-D)$, logarithmic decay: $\epsilon_0(D)=\epsilon_0+\log(D)$ and finally the power-law decay: $\epsilon_0(D)=\epsilon_0+aD^{-\beta}$. The result has been shown below in Fig. R1. One can clearly see that the converges our PESS energies are best fitted with a power-law decay signaling a gapless underlying state. Let us also stress that the same fact holds for the iPEPS energies which has been shown to converge algebraically in the inset of the Fig .3 in the main text. This has also been clarified in the revised manuscript.

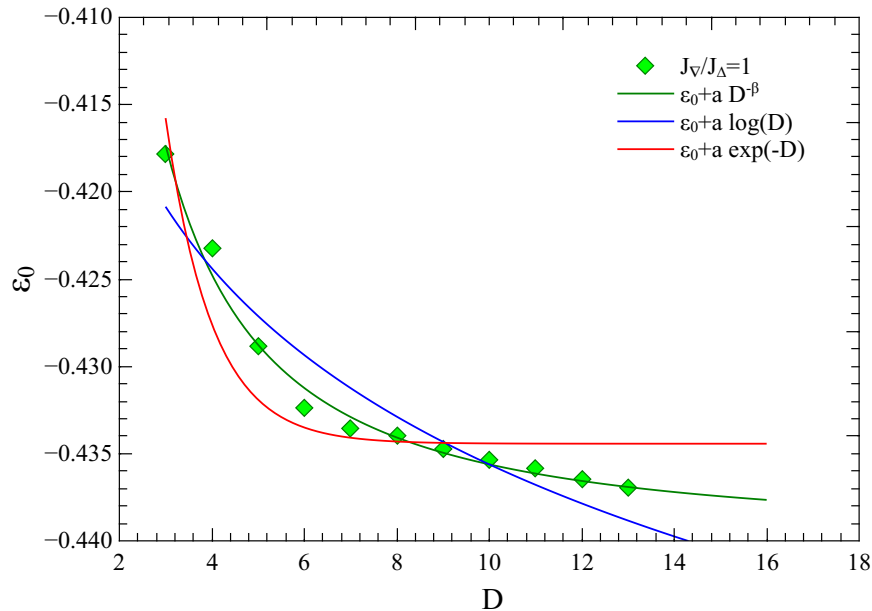


Fig. R1. Extrapolating the convergence of the PESS ground state energy as a function of bond dimension D with exponential, logarithmic and power-law decay functions. The best fitting is provided by the power-law decay function (green solid line).

2. In Figure 7, the correlation function at large distance r clearly falls off the power law

decaying. It is likely to be an artifact of finite bond dimension D . It would be good to plot the D -dependence of correlation function to show the trend that the power scaling becomes better as D increases.

Reply: It is already known that at the numerical level, any PEPS with finite bond dimension tends to be biased toward showing exponential decay of correlation which is typical of gapped states. However, one can still approximate gapless states with PEPS by increasing the bond dimension and allowing more entanglement on the virtual degrees of freedom. One can then observe that the long-range spin-spin correlation shows an algebraic decay at relatively small distances and then will decay with an exponential tail at larger distances. By increasing the bond dimension, the exponential tail will move to farther distances and the long-range correlation spreads to larger distances, giving rise to a better representation of the gapless state. (see Phys. Rev B 99, 205121 (2019), as well as Phys. Rev. B 78, 155117 (2008) for a similar example on 2d classical systems with tensor networks). In order to show that our TN results indeed obey the same trend, we have plotted the long-range spin-spin correlation, $C(r)$, for different bond dimension D at the isotropic point $J_{\nabla}/J_{\Delta}=1$ which is now shown in the new Fig. 7-(a) in the main text. The figure provides the log-log plot of the $C(r)$ for different D and the dashed line is the power-law fitting of $C(r)$ for $D=11$ at small distances. One can clearly see that by increasing the bond dimension the $C(r)$ approaches the dashed line, signaling a true power-law decay behavior in the thermodynamic limit.

3. The paper claims a first order phase transitions at $J_{\Delta}/J_{\nabla}=0.05$ based on the calculation with $D=13$. Is this statement sensitive to D ? More concretely, i) does the critical value shift as D is changing? ii) does the phase transition becomes more continuous as D increases? It is possible that the observation of a first order phase transition is an artifact of finite D .

Reply: In order to confirm both the location and the order of the phase transition more accurately, we performed a new set of large-scale TN simulations and carried out accurate entanglement scaling of the ground state energy, ε_0 , as well as the coefficients of the Taylor expansion of energy (Eq. (2) in the main text), c_1 and c_2 , for both large and small breathing anisotropy limits. The transition point was then captured from the level crossing of the energy series of the large and small breathing limits. The new Fig. 8-(b) demonstrates the scaling of the transition point with inverse bond dimension, $1/D$. One can clearly see that that transition point for $D>10$ has converged to 0.05 and does not show significant dependence to D at large bond dimensions.

In an attempt to draw conclusions about the infinite D limit, we have kept track of the evolution of the coefficients c_1 and c_2 with $1/D$. First of all, we have estimated the error bars on these coefficients. The new Fig. 9-(a-d) shows the fitting of PESS energies ($D=13$) using the c_1 and c_2 coefficients of Table 2. The error bars on the energies are very small, of the order 10^{-5} - 10^{-6} for different couplings, but they still lead to a non-negligible error threshold of the order 10^{-3} on the c_1 and c_2 coefficients. The resulting estimates for c_1 are plotted as a function of $1/D$ in Fig. 10, together with the DMRG results of Ref. [44] for the effective first-order model in the left panel, and with those of the RVB wave function of Ref. [58] in the right panel. This plot shows the difficulty in extrapolating our results as a function of $1/D$. The naive linear extrapolation suggested by the data if one forgets about the error bars can be excluded because it would lead to a value of c_1 much too small as compared to DMRG, and taking the error bars into account

leads to a very broad distribution. Besides, there is no theoretical prediction for the evolution of the results as a function of $1/D$ on which to rely to go beyond the naive linear extrapolation. The comparison with DMRG suggests that the coefficients c_1 must level off at larger D , but we are unfortunately unable to check this. Finally, we note that the coefficient c_1 of the p-RVB wave-function is not far but above the PESS values for both the nematic and $U(1)$ phases, in agreement with our finding that, at least for finite bond dimension D , this phase is not stabilized. These discussions were added to the text, and the conclusion has been modified accordingly.