Re: XW10449B

Comprehensive study of the global phase diagram of the J-K-Gamma model on a triangular lattice by Shi Wang, Zhongyuan Qi, Bin Xi, et al.

Dear Dr. Wang,

The above manuscript has been reviewed by two of our referees. Comments from the reports appear below for your consideration.

When you resubmit your manuscript, please include a summary of the changes made and a brief response to all recommendations and criticisms.

Yours sincerely,

Robert Konik

Associate Editor

Physical Review B

Email: [prb@aps.org](mailto:prb@aps.org)

https://journals.aps.org/prb/

Report of the First Referee -- XW10449B/Wang

The authors study the Heisenberg-Kitaev model with additional off-diagonal interactions which has been studied in the literature on a honeycomb lattice. Their study is on a triangular lattice which, based on symmetry arguments, they justify to have experimental relevance.

The purpose of the current study is to determine the system phase diagram. They accomplish that using exact diagonalization, Monte Carlo simulations (of the classical model), and analysis of the classical ground-state energy.

I think the study meets the PRB standards even from the academic point of view since the model is interesting and rich.

However, before the recommendation takes place, the authors should respond to the criticism and suggestion listed below.

1. Suggestion

Since the heat-bath method is explained, a few words about the over-relaxation MC method is also needed, just for the sake of self-containment and self-consistency.

1. Criticism

What is the effect of an asymmetric system for the ED calculations? Phases which break a real-space symmetry (such as stripes) may have different GS energy in asymmetric cluster when compared to symmetric one. Does it bias towards a stripe phase? Comments should be given in the main text.

1. Criticism

In Sec. 3A and in the caption of Fig. 2, use a more precise description. What is a quantum phase diagram? Is it the zero-T phase diagram or the finite-T phase diagram for the case of quantum spins?

What are the triangles in Fig. 4(i)?

1. Suggestion

In fig. 8, the ideal is that both vertical scales of the energy and of the second derivative are given. In the current version, it seems that the range of the former is small.

1. Criticism

Although the whole analysis is somewhat convincing, there is no consistent study on the second derivatives presented in Fig. 8. Could the authors state their findings of the peaks when compared to smaller systems? Is the finite-size effect consistent with a non-analyticity?

1. Suggestion

The arrows are hard to read in Figs. 10 and 12. Maybe, for clarity, the point sites (which are not necessary) may be dropped out.

1. Criticism

I find it important to precisely define the phases found here. What is the order parameter (nematic, stripe, etc)? The ordering vector?

1. Suggestion

I could not see the difference between the SSF of Figs. 4(a), (b), and (d), which are reported to be in different phases. It is only mentioned that these phases are different due to distinct peaks at the M points. I find this vague and confusing. Only much later in the text, different arguments are provided in order to clarify this point. Probably the authors should point out that further arguments will be provided. (Maybe with the clarifications of criticism 7 will help here.)

Report of the Second Referee -- XW10449B/Wang

The authors present a comprehensive study of the phase diagram of the J-K-Gamma model on the triangular lattice. They use exact diagonalization, classical Monte Carlo, etc. They are well-established methods and the authors seem to use them correctly. The study is apparently relevant to materials like Ba3IrTi2O9. Considering these facts, I would recommend the editor to accept this manuscript for publication in PRB.

An optional question is about the QSL phase. The claim that the observed QSL is a Z2 gapped spin liquid is rather weak. DSF is not a critical information for the determination. Can the authors do a parton mean-field theory calculation for this phase?