Tensor Netowkr Study on $S = 1$ Bilinear-Biquadratic Kitaev model

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The $S = 1/2$ honeycomb lattice Kitaev model has been extensively studied as a model for investigating the properties of two-dimensional spin liquids [1, 2]. Similarly, Kitaev models with higher S are also believed to have spin liquid ground states. However, unlike the $S = 1/2$ case, Kitaev models with higher S are not exactly solvable, making numerical analysis crucial. In spin systems with higher S, in addition to conventional magnetic order, the nematic order, which is absent in $S = 1/2$ spin systems, can also be stabilized. Recently, the competition between Kitaev and other interactions have been analyzed using semiclassical approximations [3]. However, due to the limitations of these approximations, Kitaev spin liquid could not be precisely treated, and the phase structure near the spin liquid has not been sufficiently analyzed.

To elucidate the competition between the $S = 1$ Kitaev spin liquid and nematic order, we analyzed bilinear-biquadratic (BBQ) Kitaev model [3] this year. The Hamiltonian of the BBQ-Kitaev model is given as

$$\hat{H}_{\mathrm{BBQ-K}} = \sum_{\gamma=x,y,z} \sum_{\langle i,j\rangle_\gamma} \hat{H}_{\langle i,j\rangle_\gamma}, \tag{1}$$

$$\hat{H}_{\langle i,j\rangle_\gamma} = J_1 \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + J_2 \left(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j\right)^2 + K \hat{S}_i^\gamma \hat{S}_j^\gamma. \tag{2}$$

Here, $\langle i,j\rangle_\gamma$ denotes the nearest neighbor pair on a γ bond. J_1, J_2, and K are the coupling coefficients for the Heisenberg, biquadratic, and Kitaev interactions, respectively. To analyze the phase structure of the BBQ-Kitaev model,

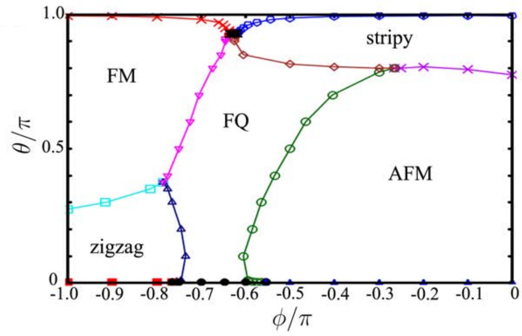

Figure 1: Phase diagram of the BBQ-K model in the region of $0.0 \leq \theta/\pi \leq 1.0$ and $-1.0 \leq \phi/\pi \leq 0.0$. FQ stands for the ferro-quadrupolar phase, and in the vicinity of $\phi/\pi = 0$ and 1, we observed an extended spin liquid phase. (Adapted from Ref. [5])

we employed the infinite projected entangled pair state (iPEPS) method, which can directly calculate the ground state of an infinitely large system. To optimize the tensors in iPEPS, we used imaginary time evolution combined with the truncation of the bond dimension by the simple update. The calculation of the physical quantities was performed by the corner transfer matrix renormalization group method. The entire calculation was done using TeNeS [4], which supports MPI and OpenMP hybrid parallelization.

In Fig. 1, we show the phase diagram of the BBQ-Kitaev model for $J_2 < 0$ [5]. We represented the interaction coefficients with two parameters θ and ϕ as $(J_1, J_2, K) \equiv (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$. We found that the BBQ-Kitaev model has a rich phase structure, including both ferro and anti-ferro Kitaev spin liquids, the quadrupolar order, and several magnetic orders. Interestingly, there is a direct phase transition between the ferroquadrupolar (FQ) ordered and the Kitaev spin liquid phases. Note that both phases are characterized by the absence of magnetic order. In this sense, we can consider that such direct transition is induced by quantum fluctuations, and there is no classical counterpart.

In addition to this point, in the case of ferro Kitaev spin liquid, we observed an extension of the spin liquid phase around $\phi = \arctan(2) \simeq -0.648\pi$, where the BBQ interaction is reduced into the pure quadrupolar interaction, without Heisenberg interaction. This result indicates that the ferro Kitaev spin liquid is robust against the quadrupolar interaction. This would be useful not only for the search for Kitaev spin liquids in real compounds but also for understanding the nature of general spin liquids.

References

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