論文の内容の要旨

Functional Renormalization Group Study on Kitaev Quantum Spin Liquid

(Kitaev 量子スピン液体の汎関数繰り込み群による研究)

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In this doctoral dissertation, we address two topics related to the realization of the Kitaev quantum spin liquid in condensed matter physics. The first one is the study on the feasibility of it in ultracold molecular systems trapped in the optical lattice rather than in solids. The other is the study on the realization of the Kitaev quantum spin liquid in the high-spin materials. As a method to tackle these studies, we use the functional renormalization group (FRG) method, especially pseudo-fermion functional renormalization group (PFFRG) method. This is a numerical method for studying frustrated quantum spin systems, and it still has been intensively extended recently. Chapter 2 and 3 are devoted to introduce general fermionic FRG and PFFRG, respectively, in detail.

In Chapter 4, we discuss the feasibility of the Kitaev quantum spin liquid in ultracold polar molecular systems trapped in the optical lattice, based on the realization of Kitaev-type interactions proposed in 2013 [S. R. Manmana *et al.*, Phys. Rev. B **87**, 081106 (2013), A. V. Gorshkov, K. R. Hazzard, and A. M. Rey, Mol. Phys. **111**, 1908 (2013)]. Referring to the above proposals, we define dipolar Kitaev model on the honeycomb lattice as

$$\begin{aligned}\mathcal{H} = -\frac{1}{2}\sum_{i,j}^{i\neq j}\frac{1}{3r_{ij}^3}\Bigg\{ & J_x[1-2\cos\left(2\Phi_{ij}-\frac{4\pi}{3}\right)]S_i^x S_j^x \\ & + J_y[1-2\cos\left(2\Phi_{ij}-\frac{2\pi}{3}\right)]S_i^y S_j^y \\ & + J_z[1-2\cos\left(2\Phi_{ij}\right)]S_i^z S_j^z\Bigg\}. \end{aligned} \tag{1}$$

Here, $\boldsymbol{r}_{ij}$ is the vector connecting from site i to site j. In addition, $r_{ij} = |\boldsymbol{r}_{ij}|$ and $\Phi_{ij} = \mathrm{Arg}(r_{ij,x} + \mathrm{i} r_{ij,y})$. These definitions are shown in Fig. 1. In the dipolar Kitaev model, the interactions between the nearest-neighboring sites are consistent with the Kitaev model, but those between sites farther than the nearest-neighbor are more complicated. We apply PFFRG to this model to investigate the ground state at each parameter. The results show that FM order and zigzag AFM order are realized in the FM and AFM dipolar Kitaev model, respectively, for all anisotropy parameters. As a example, we show the momentum dependence of the (z-component) static spin susceptibility (χ^{zz}) of the isotropic ($J_x = J_y = J_z$) ferromagnetic (FM) and antiferromagnetic (AFM) dipolar Kitaev model at each ordering scale $\Lambda = \Lambda_{\mathrm{c}}$ in Fig. 2 (a) and (b), respectively. Furthermore, in order to investigate the connection between the (nearest-neighbor) Kitaev model and the dipolar Kitaev model, we introduce an artificial range of interactions L_{int} and calculate the susceptibility when approaching the dipolar Kitaev model with long-range interactions from the Kitaev model with only nearest-neighbor interactions. From this calculation, it is clarified that the spin liquid state realized in the Kitaev model is quickly collapses, as the range of interactions L_{int} is extended. These behaviors of the susceptibility are shown in Fig. 2 (c). We only display the susceptibility in $\Lambda \geq \Lambda_{\mathrm{c}}$ for the model with $L_{\mathrm{int}} \geq 6$ for visibility. From these results, it can be concluded that the dipolar Kitaev model does not host the quantum spin liquid due to its long-range nature. This is in contrast to the dipolar Heisenberg model, which obtains frustration stronger than the nearest-neighbor Heisenberg model due to its long-range nature, and hosts quantum spin liquids.

After the proposals of Kitaev-type interaction in ultracold polar molecular systems by microwave irradiation in 2013, the calculation based on these proposals has not been performed, and whether Kitaev quantum spin liquid state is actually realized has remained an open question. We address this issue with PFFRG and elucidated the above results for the first time.

In Chapter 5, we discuss the feasibility of the Kitaev quantum spin liquid in high-spin candidate materials. Our two main interests related to the Kitaev quantum spin liquid with general spin length S are (i) the difference between Kitaev models with half-odd integer S and integer S, and (ii) the upper limit of S allowed for the realization of spin liquids in candidate materials. In the first part of the chapter, we calculate the susceptibility of the spin-S Kitaev model using PFFRG and its extension for general spin length S. As a result of our calculation, breakdown behaviors appear in the flows of the susceptibility for $S \geq 2$ cases, which seem to indicate phase transition to magnetic order. This result is shown in Fig. 3 (a). However, it is known that in the Kitaev model with general S, the spin correlations exist only between the nearest-neighboring sites strictly and the system does not undergo ordering. In fact, the spatial structure of the susceptibility we calculate is also finite only between the nearest-neighboring sites. Therefore, we can conclude that this breakdown-like behavior is an artifact of spin-S PFFRG. We can speculate that this artifact indicates that the quantum fluctuations are weak in Kitaev quantum spin liquid with $S \geq 2$, and the system is easily ordered by other magnetic interactions.

Moreover, we examine whether there is a difference between the case where S is half-odd integers and the case where S is integers. In Fig. 3 (b) we show the frequency dependence of the pseudo-fermion damping at the infrared limit $\Lambda = \Lambda_{\mathrm{IR}}$ for some S. As S increases, it only shows the converging behavior. Furthermore, we investigate the difference between the 2-particle vertices of half-odd integer spin systems and integer spin systems, and there is also no difference between them. Therefore, we conclude that the spin-S extension of the PFFRG does not reflect the differences in topology between the half-odd integer spin and integer spin Kitaev model.

In the second part of chapter 5, we calculate the phase diagram of the spin-S Kitaev-Heisenberg model

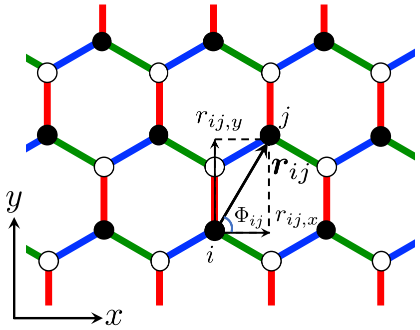

Figure1 Schematic figure showing the definition of $\boldsymbol{r}_{ij}$ and Φ_{ij} in the dipolar Kitaev model.

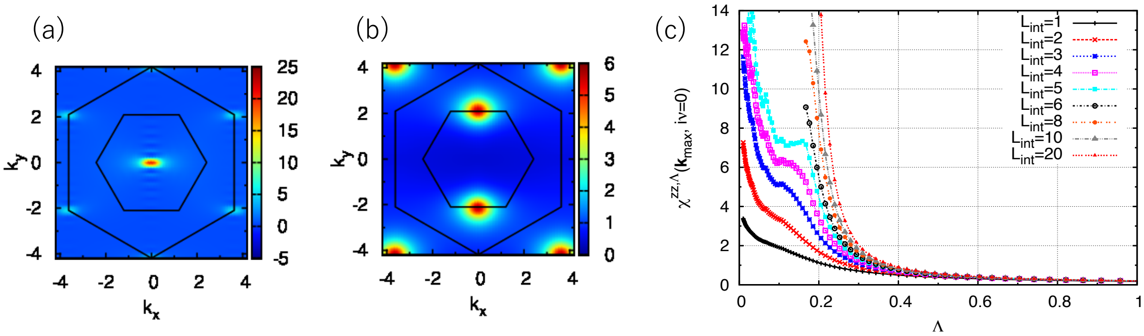

Figure2 The momentum dependence of the susceptibility (χ^{zz}) of the isotropic (a) FM and (b) AFM dipolar Kitaev model. (c) The susceptibility flows of the isotropic FM dipolar Kitaev model with the range of the interactions $L_{\rm int}$.

with $S = 1/2$-$5/2$ and $S = 50$. Its Hamiltonian is

$$\mathcal{H} = A \sum_{\mu} \sum_{\langle i,j \rangle_\mu} \left[2\sin(2\pi\xi) S_i^\mu S_j^\mu + \cos(2\pi\xi) \boldsymbol{S}_i \cdot \boldsymbol{S}_j \right]. \tag{2}$$

The obtained phase diagrams of the Kitaev-Heisenberg model for $S = 1/2$ and $S = 1$ are in general good agreement with the previous studies by other numerical methods. The phase diagram for $S = 50$ is also in good agreement with the previous study on the classical Kitaev-Heisenberg model by Monte Carlo simulation, except for some special points. These results are summarized in the S-ξ phase diagram and shown in Fig. 4. As a result of systematic calculations with different S, for $S \leq 3/2$, both the AFM and FM Kitaev spin liquid regions have a finite extent. For $S \geq 2$, no region showing Kitaev spin liquid state was found. Therefore, we believe that $S = 3/2$ gives an upper bound on the spins possessed by the candidate materials in which Kitaev quantum spin liquid is realized.

The phase diagram calculation of the Kitaev-Heisenberg model with a systematic change of spin S, as we perform here, has not been done before. This is the first study of the application of spin-S PFFRG to the Kitaev-Heisenberg systems. The results we obtain here provide a guideline for the recent intensive search for candidate materials of $S \geq 1/2$ Kitaev quantum spin liquid.

At last, in chapter 6, we summarize our studies and its findings with some further perspectives.

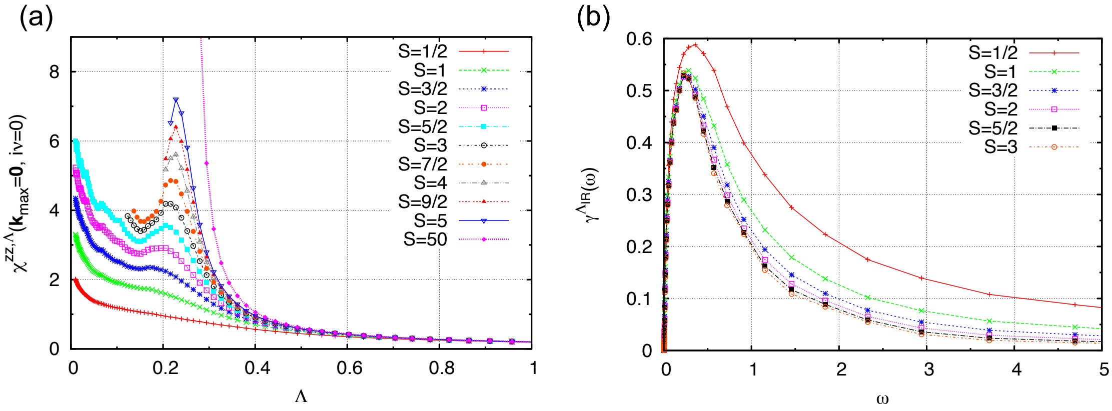

Figure3 (a) The susceptibility flow of the spin-S Kitaev model. (b) The Matsubara frequency dependence of the pseudo-fermion damping ($\simeq$self-energy) of the spin-S Kitaev model.

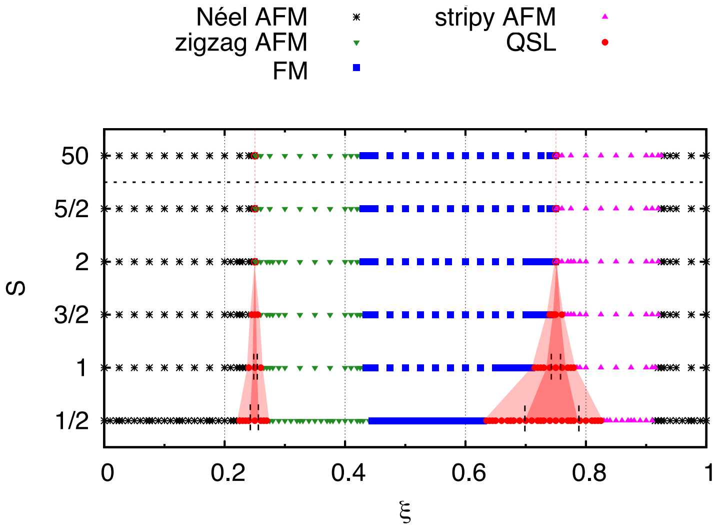

Figure4 S-ξ phase diagram of the spin-S Kitaev-Heisenberg model. The region where the spin liquid state was predicted by our calculations is shaded in light red. In the region enclosed by the dashed line, the spin liquid state was predicted by previous studies on the $S = 1/2$ and $S = 1$ Kitaev-Heisenberg model. The range in which the spin liquid state can be expected from previous studies and our study is colored in darker red.