Field-angle dependence of thermal transport in Kitaev-$\Gamma$ model

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Abstract. We investigate the magnetic field effect on the Kitaev model with the $\Gamma$-type interaction, which plays an essential role in understanding the magnetic properties of real materials. We examine the mean-field phase diagram and thermal Hall conductivity using the linear spin-wave theory. We find that the $\Gamma$ interaction substantially changes the field-angle dependence of the thermal Hall conductivity and suppresses its magnitude. The suppression is caused by the enhancement of the low-energy magnon gap while increasing the $\Gamma$ interaction.

1. Introduction

The quantum spin model proposed by A. Kitaev has attracted considerable attention in strongly correlated electron systems [1, 2]. This is called the Kitaev model and realizes a canonical quantum spin liquid (QSL) as a ground state due to strong quantum fluctuations and correlations. The Kitaev model is believed to dominate magnetism in compounds including 4$d$ or 5$d$ transition metal ions with strong spin-orbit coupling [3]. Among them, $A_2$IrO$_3$ ($A =$ Li, Na) and $\alpha$-RuCl$_3$ whose magnetism are governed by $j_{\text{eff}} = 1/2$ pseudospins, have been intensively studied as candidate materials of the Kitaev QSL [4]. However, other interactions, such as the Heisenberg and off-diagonal $\Gamma$ terms, are present in real materials. These contributions lead to the appearance of a magnetic order [5]. While the additional interactions destabilize the Kitaev QSL state, they cause a wide variety of magnetically ordered states [6, 7]. In particular, a zigzag-type magnetic order, which appears in $A_2$IrO$_3$ ($A =$ Li, Na) and $\alpha$-RuCl$_3$ at low temperatures, is stabilized by the competition between the Kitaev and Heisenberg/$\Gamma$ interactions.

Recent experiments clarified that the Kitaev candidate material $\alpha$-RuCl$_3$ exhibits the half-quantization of the thermal Hall conductivity in the region where the zigzag-type magnetic order disappears by applying the magnetic field [8], and the thermal Hall conductivity is strongly depends on the magnetic-field direction [9]. These observations are considered to be convincing evidence for a Majorana chiral edge mode. Stimulated by these results and related experiments, magnetic field effects on the Kitaev-related systems have been examined theoretically [10]. In addition to the Majorana picture consistent with the result in the Kitaev model [11], theoretical calculations based on the magnon picture have been made in the extended Kitaev models with the Heisenberg and $\Gamma$ interactions [6, 7]. Although the thermal Hall effect has been examined in the Kitaev-Heisenberg-$\Gamma$ model [2, 12, 13] for specific magnetic-field directions, the field-angle dependence of the thermal Hall effect ascribed to the magnons remains unclear in the Kitaev-$\Gamma$ model.

In this study, we investigate the thermal transport in the Kitaev-$\Gamma$ model on a honeycomb lattice under magnetic fields. By applying mean-field approximation and linear spin-wave theory, we examine the
thermal Hall conductivity by changing the direction systematically. We find that the direction of the magnetization deviates from that of the magnetic field by introducing the $\Gamma$ interaction and a peculiar magnetic order appears around the perpendicular direction to the honeycomb plane. Moreover, the $\Gamma$ interaction suppresses the thermal Hall conductivity by enhancing the low-energy magnon gap. We also clarify that the field direction vanishing the thermal Hall conductivity depends on the magnitude of the $\Gamma$ interaction, which is in contrast to the effect of the Heisenberg interaction.

2. Model and Method
We consider the Kitaev-$\Gamma$ model with $S = 1/2$ on the honeycomb lattice, which is given by

$$\mathcal{H} = \sum_{\gamma=x,y,z} \sum_{i,j} \left[ K S_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha) \right] - h \cdot \sum_i S_i,$$

(1)

where $K$ and $\Gamma$ is the Kitaev and off-diagonal interaction, respectively, and $h$ is the magnetic field. $(ij)_{\gamma}$ stands for the nearest neighbor site on the $\gamma$ bond ($\gamma = x, y, z$) presented in Fig. (1a). The indexes $\alpha$ and $\beta$ are such that $(\alpha, \beta, \gamma)$ is a cyclic permutation of $(x, y, z)$. In this study, we focus on the ferromagnetic Kitaev coupling, namely, $K = -1$, and the magnetic field is fixed to be $h = 0.05$.

We apply the mean-field approximation to the Kitaev-$\Gamma$ model given in Eq. (1) and determine the stable magnetic-order pattern at zero temperature. Under the spin configuration, we calculate the magnon dispersions and thermal Hall conductivity using the linear spin-wave theory. In this theory, the Hamiltonian is approximately written as a bilinear form of the bosonic operators describing the magnon excitations as follows:

$$\mathcal{H}_{sw} = \frac{1}{2} \sum_k \mathcal{A}_k^\dagger M_k \mathcal{A}_k,$$

(2)

where

$$\mathcal{A}_k^\dagger = \left( a_{1,k}^\dagger \cdots a_{M/2,k}^\dagger a_{1,-k} \cdots a_{M,-k} \right).$$

(3)

Here, $a_{l,k}$ is the annihilation operator of a boson with momentum $k$ on sublattice $l$ with $M$ being the number of sublattices. In Eq. (2), $M_k$ is a $2M \times 2M$ Hermitian matrix, which is obtained by the Holstein-Primakoff transformation [13]. By diagonalizing $M_k$ using the Bogoliubov transformation with the transform matrix $\mathcal{F}_k$, we evaluate the magnon energy $\epsilon_{n,k}$ for the $n$th branch. We also calculate the thermal Hall conductivity $k^{ab}$, which is defined by $\langle J^a_{Q/T} \rangle = \epsilon^{ab}(-\nabla_b T)$, where $\langle J^a_{Q/T} \rangle$ is the expectation value of the thermal current along the $a$ axis in the presence of the thermal gradient $\nabla_b T$ along the $b$ axis [see Fig. (1a)]. This quantity is evaluated using the linear spin-wave theory, which is written as [15]

$$k^{ab} = -\frac{T}{V} \sum_{n=1}^M c_2(f_{BE}(\epsilon_{n,k})) \Omega_{n,k},$$

(4)

where $V$ is the volume, $c_2(x) = \int_0^1 dt [\ln(1 + t) - \ln t]^2$, and $\Omega_{n,k}$ is the Berry curvature given as

$$\Omega_{n,k} = i \left[ \sigma_3 \frac{\partial \mathcal{F}_k^\dagger}{\partial k_a} \sigma_3 \frac{\partial \mathcal{F}_k}{\partial k_b} \right]_{1n} + \text{H.c.},$$

(5)

with $(\sigma_3)_n = +1$ for $n \leq M$ and $(\sigma_3)_n = -1$ for $n > M$. 

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This property is clearly seen in Fig. b enhanced, but there are several nodal points where it remains zero for the temperature evolution. In the ferromagnetic Kitaev model under the magnetic field. With increasing temperature, "with the magnon branch a fields applied along the T several temperatures, and (c) its spherical plot at T = 0.05. (d) Spin-wave dispersions under the magnetic fields applied along the a direction at T = 0.05. The line color indicates the value of \( \Omega_{n,k} \) associated with the magnon branch \( \varepsilon_{n,k} \).

\[ \begin{align*} \text{Figure 1. (a) Schematic picture of the honeycomb lattice on which the Kitaev-\( \Gamma \) model is defined.} \\
\text{The lattice axes, } a, b, \text{ and } c, \text{ and the spin axes, } S^x, S^y, \text{ and } S^z, \text{ are also presented. (b) Thermal Hall conductivity } \kappa_{ab}/T \text{ as a function of the field direction in the Kitaev model with } \Gamma = 0 \text{ for } h = 0.05 \text{ at several temperatures, and (c) its spherical plot at } T = 0.05. \text{ (d) Spin-wave dispersions under the magnetic fields applied along the } a \text{ direction at } T = 0.05. \text{ The line color indicates the value of } \Omega_{n,k} \text{ associated with the magnon branch } \varepsilon_{n,k}. \end{align*} \]

3. Result and Discussion

3.1. Magnetic field effect on pure Kitaev model
First, we focus on the case without the \( \Gamma \) interaction. In this case, a spin-polarized state appears regardless of the field direction. Figure \( \text{II(b)} \) shows the field-angle dependence of \( \kappa_{ab}/T \) at several temperatures in the ferromagnetic Kitaev model under the magnetic field. With increasing temperature, \( \kappa_{ab}/T \) is enhanced, but there are several nodal points where it remains zero for the temperature evolution. In particular, for the magnetic field parallel to the \( b \) axis, \( \kappa_{ab} \) vanishes because of the symmetry \[ \{13\}. \]

The other nodal points are located on the planes spanned by two of three spin axes \( S^x, S^y, \) and \( S^z \). This property is clearly seen in Fig. \( \text{II(c)} \), and it is maintained even in the presence of the Heisenberg interaction but is not for the \( \Gamma \) one \[ \{13\}. \]

The sign of \( \kappa_{ab} \) depends on the direction of the applied magnetic field. The thermal Hall conductivity is positive for \( h \parallel a \) while it is negative for \( h \parallel c \) [Figs. \( \text{II(b)} \) and \( \text{II(c)} \)]. The nonzero thermal Hall conductivity comes from the finite Berry curvature \( \Omega_{n,k} \). Figure \( \text{II(d)} \) shows the Berry curvature for the magnon excitations in the magnetic field applied to the \( a \) direction. In this case, the low-energy magnon branch possesses the negative Berry curvature around the \( K \) and \( M \) points, which leads to the positive thermal Hall conductivity.

3.2. Effect of \( \Gamma \) interaction
Next, we show the results in the presence of the nonzero \( \Gamma \) interaction. Figures \( \text{II(a)} \) and \( \text{II(b)} \) present the mean-field phase diagram on the plane of the field direction parametrized by \( (\theta, \phi) \) [see Fig. \( \text{II(a)} \)] at \( h = 0.05 \) for \( \Gamma = 0.1 \) and 0.2, respectively. As shown in these figures, the 6-site spin order presented in Fig. \( \text{II(g)} \) appears in the magnetic field applied around the \( c \) direction. On the other hand, when the magnetic field is away from the \( c \) axis, the magnetic order disappears, and the spin-polarized state is stabilized. In this polarized state, the total magnetic moment is not parallel to the field direction, unlike the case without the \( \Gamma \) interaction.

The field-angle dependence of \( \kappa_{xy}/T \) for \( \Gamma = 0.1 \) and 0.2 is shown on the sphere in Figs. \( \text{II(c)} \) and \( \text{II(d)} \), respectively. The feature seen in the pure Kitaev model is not observed in the presence of the \( \Gamma \)
interaction; the nodal lines are not on the planes spanned by the spin axes. We also find a large negative thermal Hall conductivity in the 6-site ordered phase and the suppression of $\kappa^\alpha/\mathcal{T}$ in the spin-polarized phase by the introduction of the $\Gamma$ interaction. To clarify the origin of this suppression effect, we examine the Berry curvature for $\mathbf{h} \parallel \mathbf{a}$. As shown in Figs. 2(e) and 2(f), the momentum dependence of $\Omega_{\mathbf{a},\mathbf{k}}$ is largely intact despite the increase of the $\Gamma$ interaction, but the excitation gap increases with increasing $\Gamma$. The enhancement of the gap leads to the suppression of the thermal Hall conductivity.

4. Conclusion
We have revealed the magnetic-field angle dependence of the spin configuration and thermal transport in the Kitaev-$\Gamma$ model using the mean-field approximation and the linear spin-wave theory. We have demonstrated that the $\Gamma$ interaction changes the nodal-line structure in the field-angle dependence of the thermal Hall conductivity. We also find that the 6-site magnetic order appears when the magnetic field is perpendicular to the honeycomb plane. We also find that the $\Gamma$ interaction suppresses the thermal Hall conductivity because of enhancing the low-energy magnon gap.

References
[1] Kitaev A 2006 Ann. Phys. 321 2–111 ISSN 0003-4916
[2] Motome Y and Nasu J 2020 J. Phys. Soc. Jpn. 89 012002
[3] Jackeli G and Khaliullin G 2009 Phys. Rev. Lett. 102(1) 017205
[4] Yamaji Y, Nomura Y, Kurita M, Arita R and Imada M 2014 Phys. Rev. Lett. 113(10) 107201
[5] Rau J G, Lee E K H and Kee H Y 2014 Phys. Rev. Lett. 112 077204
[6] Janssen L, Andrade E C and Vojta M 2016 Phys. Rev. Lett. 117 277202
[7] Chern I E, Kaneko R, Lee H Y and Kim Y B 2020 Phys. Rev. Research 2(1) 013014
[8] Kasahara Y, Ohnishi T, Mizukami Y, Tanaka O, Ma S, Sugii K, Kurita N, Tanaka H, Nasu J, Motome Y, Shibauchi T and Matsuda Y 2018 Nature 559 227–231
[9] Yokoi T, Ma S, Kasahara Y, Kasahara S, Shibauchi T, Kurita N, Tanaka H, Nasu J, Motome Y, Hickey C, Trebst S and Matsuda Y 2021 Science 373 568–572
[10] Gordon J S, Catuneanu A, Sorensen E S and Kee H Y 2019 Nat. Commun. 10 2470
[11] Nasu J, Yoshitake J and Motome Y 2017 Phys. Rev. Lett. 119(12) 127204
[12] Zhang E Z, Chern L E and Kim Y B 2021 Phys. Rev. B 103(17) 174402
[13] McClarty P A, Dong X Y, Gohlke M, Rau J G, Pollmann F, Moessner R and Penc K 2018 Phys. Rev. B 98(6) 060404
[14] Koyama S and Nasu J 2021 Phys. Rev. B 104(7) 075121
[15] Matsumoto R, Sindou R and Murakami S 2014 Phys. Rev. B 89 054420