Phase diagram and thermal Hall conductivity of spin-liquid Kekulé-Kitaev model

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In this work we study the phase diagram of Kekulé-Kitaev model. The model is defined on a honeycomb lattice with bond dependent anisotropic exchange interactions making it exactly solvable in terms of Majorana representation of spins in close analogy to the Kitaev model. However, the energy spectrum of Majorana fermions has a multi-band structure characterized by Chern numbers 0, ±1, and ±2. We obtained the phase diagram of the model in the plane of exchange couplings and in the presence of a magnetic field and found chiral topological and trivial spin-liquid ground states. If the absence of magnetic field most part of the phase diagram is a trivial gapped phase continuously connected to an Abelian phase, while in the presence of the magnetic field a topological phase arises. Furthermore, motivated by recent thermal measurements on the spin-liquid candidate α-RuCl₃, we calculated the thermal Hall conductivity at different regimes of parameters and temperatures and found the latter is quantized over a wide range of temperatures.

I. INTRODUCTION

In recent years, there has been a surge of interests in strongly correlated Mott insulators with exotic and nontrivial ground states featuring novel states of matter. Of particular interest is the insulating quantum magnets where the strong quantum fluctuations prevent the formation of any long-range magnetic ordering even at zero temperature, the so-called spin-liquids. Despite being a long-sought problem since the original idea proposed by Anderson, the experimental realization of spin liquids in materials has remained elusive until the experimental verification of the absence of magnetic ordering in the quasi-two-dimensional organic materials. The organic compounds κ-(ET)₂Cu₂(CN)₃ and EtMe₃Sb[Pd(dmit)]₂ have triangular-lattice structure and are Mott insulators at ambient pressure with no signature of magnetic ordering, nor anomalies in the specific heat and/or thermal conductivity up to lowest measured mili-Kelvin temperatures. Beside the organic compounds, in the mineral herbertsmithite ZnCu₃(SO₄)₂(OH)₆Cl₂ with underlying kagome lattice no indication of magnetic ordering was observed at very low temperatures yielding yet another spin-liquid ground state. The electronic structure of these materials at half-filling is mainly dominated by spin-1/2 ions located at the vertices of the underlying lattices. In the Mott phase the underlying low-energy physics can be simply described by the Heisenberg Hamiltonian $H = J_H \sum_{<i,j>} S_i \cdot S_j$, where $S_i$ is the spin operator at site $i$ and $J_H$ denotes the Heisenberg antiferromagnetic exchange coupling between nearest-neighbor sites. The boson or fermion representation of spins gives rise to a plethora of spin-liquid ground states, gapless or gapped spectrum, and fractionalized excitations, which can partially explain the experimental measurements.

The next generation of two-dimensional magnetic Mott insulators with ground states proximate to a spin-liquid phase arises in materials with 4$d$/5$d$ elements, e.g., the materials containing Ru, Rh, Os, and Ir elements, where the strong spin-orbit coupling manifests large degree of frustration and anisotropic magnetic interactions. In magnetic iridate compounds (Li, Na)$_2$IrO₃, the Ir$^{4+}$ ions are located on the vertices of honeycomb lattices stacked along the crystallographic c-axis. The low-energy effective Hamiltonian contains the magnetic exchange coupling between the $J_z = 1/2$ local moments of Ir$^{4+}$ ions, and is described by the Kitaev’s model augmented by an isotropic Heisenberg interaction:

$$H = J_H \sum_{<i,j>} S_i \cdot S_j + J_K \sum_{<i,j>, \gamma} S_i^\gamma S_j^\gamma,$$

where the second term with $\gamma = x, y, z$ is anisotropic and bond-dependent, a.k.a., the Kitaev’s interactions. Though the model shows a phase transition from a magnetically ordered phase to the Kitaev spin-liquid phase by deceasing $J_H$, the inelastic neutron scattering clearly shows an ordered phase at temperatures below $T_N \sim 15K$. This observation confirms that in these materials the Heisenberg interaction between magnetic moments is rather strong spoiling the spin-liquid phase. Nevertheless, to understand the underlying zigzag ordered phase, a large degree of anisotropy should be included in the Hamiltonian.

The newly discovered ruthenate compound α-RuCl₃ (and very recently YbCl₃) inspired the realization of the spin-liquid phase, where it turns out the Heisenberg...
interaction is rather weak and therefore the ground state is possibly proximate to a spin-liquid phase. In the absence of the magnetic field and at low temperatures, i.e., $T < T_N \approx 7K$, the ground state of $\alpha$-RuCl$_3$ is characterized by a zigzag antiferromagnetic (AFM) order. The nuclear magnetic resonance and neutron scattering measurements indicate that the AFM order melts down in a tilted magnetic field applied to the sample when the in-plane component exceeds $\mu_0 H_0^\parallel = 7T$, and the spin-liquid phase appears$^{32}$. The measurements of the 2D thermal Hall conductance show a half-integer quantized plateau at temperatures below 6K and a possible signature of low-energy fractionalized excitations is demonstrated in microwave absorption measurements$^{33}$. Thermal transport through the chiral Majorana edge states and the role of bulk phonons discussed in Refs.$^{[34,35]}$ could account for the quantization observed experimentally.

While a complete understanding of the experimental results still remains to be a far-reaching problem, in most of the theoretical works done so far the focus has mainly been on the original Kitaev model with only two sites in a unite cell leading to a two-band model of Majorana fermions$^{22}$. In this work we instead consider an alternate of the Kitaev model with a multi-band spectrum, the so-called Kekulé-Kitaev model$^{13,14}$. The arrangements of anisotropic bond interactions on the underlying honeycomb lattice is shown in Fig. 1(a). We first obtain the phase diagram on the latter model. The size of the non-Abelian phase characterized by a finite Chern number does depend on the strength of the time-reversal symmetry-broken perturbation, while in the absence of the latter perturbation most of the phase diagram is characterized by an Abelian model defined on a dual Kagome lattice. Furthermore, we investigate how the multi-band spectrum affects the thermal Hall transport properties. In particular, we show that the thermal Hall conductivity assumes a large quantized value at low temperatures due to the nontrivial band topology of Majorana fermions in the non-Abelian phase. Also, in contrast to the two-band Kitaev model, where the thermal Hall conductivity contribution of the lower band is always positive$^{36}$ (or negative depending on the sign of the applied magnetic field), we found that in the multi-band Kekulé-Kitaev model the bands contribute with different signs in the thermal Hall conductivity resulting from the Berry curvature profile through the momentum space. The sign change of the thermal Hall conductivity of $\alpha$-RuCl$_3$ in a perpendicular magnetic field has been observed experimentally$^{37}$, an observation which may point toward the necessity of constructing a more realistic multi-band model to understand the physical properties of these materials.

The paper is organized as follows. We introduce the Kekulé-Kitaev model, lattice structure, and its general properties in Sec.II. The effects of time-reversal symmetry breaking and the phase diagram are discussed in Sec.III. We then present the results of thermal Hall conductivity in Sec.IV, and Sec. V concludes.

II. KEKULÉ-KITAEV MODEL AND FREE MAJORANA FERMION REPRESENTATION

The exactly solvable spin-1/2 Kekulé-Kitaev model$^{13,14}$ is comprised of two-body interactions between spins located at the vertices of a honeycomb lattice as shown in Fig. 1(a). The spin Hamiltonian of the model is given by

$$H_0 = - \sum_{<i,j>,\alpha} J_\alpha \sigma_\alpha^i \sigma_\alpha^j,$$  \hspace{1cm} (2)

where $\sigma_\alpha^i (\alpha = x, y, z)$ denote the Pauli matrices and $J_\alpha$ are exchange couplings. We take $J_\alpha > 0$ throughout. Note that the model is distinct from the famous Kitaev model$^{22}$, though both are defined on honeycomb lattice and are exactly solvable via Majorana fermionization as explained below. In contrast to the Kitaev model, the exchange interactions on the links around the plaquettes are not the same for all cells in the Kekulé-Kitaev model. We use three colors to keep track of the interactions emanating from each vertex. The red, green and blue links represent $\sigma^x \sigma^x$, $\sigma^y \sigma^y$ and $\sigma^z \sigma^z$ spin interactions, respectively. Now, it is easy to see that we can use the same colors to label the plaquettes. The color of a plaquette is determined by the color of the outgoing links. For instance, the red plaquette is the one with red outgoing links and the same holds for blue and green plaquettes; see Fig. 1(a).

Corresponding to each colored plaquette, we define a plaquette operator which is product of Pauli spins located on vertices as follows:

$$W^B = - \prod_{i=1}^6 \sigma^z_i, \quad W^G = - \prod_{i=1}^6 \sigma^y_i, \quad W^R = - \prod_{i=1}^6 \sigma^x_i. \hspace{1cm} (3)$$

These plaquette operators define a set of integral of motions, since they commute with each other $[W^r, W^y] = 0$ and with the Hamiltonian $[H, W^r] = 0$, where $\gamma = R, G, B$ (for red, green and blue plaquette). Also, each plaquette operator square identity $(W^r)^2 = 1$. Therefore, the Hilbert space of the model is consist of sectors which are eigenspace of plaquette operators with eigenvalues $\omega = \pm 1$. Analogues to the Kitaev model, in each sector the dimension is still exponentially large calling for a Majorana representation of spin operators.

The Majorana fermions obey Clifford algebra, \{$c_i, c_j$\} = 2\delta_{ij} and $c_i^2 = 1$. Following Kitaev$^{22}$ we represent a spin operator by Majorana fermions $(b^r, b^y, b^z, c)$ as $\sigma^\alpha = ib^\alpha c$ with $i = \sqrt{-1}$. Hence, the Hamiltonian (2) becomes quadratic in terms of Majorana operators as

$$H_0 = \frac{i}{4} \sum_{<i,j>} 2J_{\alpha} u_{\alpha}^{i,j} c_i c_j,$$  \hspace{1cm} (4)

where $u_{\alpha}^{i,j} = ib^\alpha b_j^\alpha$ is the link operator associated with link $(i,j)$. The latter operators commute with each other.
Appendix A. (a) and Ψ Hamiltonian becomes phase is ascribed to the fact that both nodes appear at
trum becomes gapped. The fragile nature of the gapless
stronger than the others, or (ii) breaking the time rever-
the exchange coupling on one set of bonds, say red, to be
equal.
This has an important consequence on the stability of the
K high-symmetry lines of BZ in Fig. 2(a). This is in
composed of two superimposed Dirac cones at the center
J an energy scale. At equal coupling strength (i) making
K spectrum is also gapped by applying a magnetic field h/J0 = 0.2 and (d) the edge states arise due to
nontrivial band topology.

\[ u_{ij}^x, u_{ij}^y \] = 0 and with the Hamiltonian \[ u_{ij}^a, H \] = 0,
and they square to identity \( (u_{ij}^a)^2 = 1 \) with eigenvalues
\( u_{ij}^a = \pm 1 \). Thus there is \( \mathbb{Z}_2 \) gauge degrees of freedom on
each link. According to the Lieb theorem\(^{38}\) the ground
state of the model (4) is in zero-flux sector corresponding
to configuration with \( w^\gamma = 1 \) for all plaquettes. Note that
\( w^\gamma \) is defined as product of link operators around each
plaquette \( w^\gamma = \prod_{(i,j) \in \psi} u_{i,j} \). Since \( u_{ij}^x = -u_{ji}^x \), to avoid
obscurity we select a particular direction for each link.
We assume that \( u_{ij}^z = 1 \) when the site index i is even
and j is odd; see Fig. 1(a) for site numbering. In the
following we work in the zero flux sector with \( u_{ij}^z = 1 \).

By Fourier transformation to momentum space the Hamiltonian becomes
\[ H(k) = \frac{i}{2} \sum_k \Psi_k^T A(k) \Psi_{-k}, \]
where \( A(k) \) is an antisymmetric matrix given in Ap-
Appendix A, and \( \Psi_k^T = (c_{1k}, c_{2k}, c_{3k}, c_{4k}, c_{5k}, c_{6k}) \).

To study the phase diagram we choose a plane in pa-
parameter space \((J_x + J_y + J_z = 3J_0)\). We set \( J_0 = 1 \) as
an energy scale. At equal coupling strength \((J_x = J_y =
J_z = 1)\) the spectrum is gapless and the dispersion is
composed of two superimposed Dirac cones at the center
of the Brillouin zone (BZ); see the bulk spectrum along
the high-symmetry lines of BZ in Fig. 2(a). This is in
contrast to the Kitaev model\(^{22}\), where the Dirac cones
appear at \( K \) and \( K' \) points. In the Kekulé-Kitaev model
the crossing of the Majorana bands occurs at the \( \Gamma \) point.
This has an important consequence on the stability of
the nodes. While in the former case the model remains gap-
less until the nodes meet at the center of BZ giving rise to
a finite region in the phase diagram known as B-phase,
the latter model is only gapless when all couplings are
equal.

In general there are two ways to open a gap in the spec-
trum and create a gapped spin-liquid phase: (i) making
the exchange coupling on one set of bonds, say red, to be
stronger than the others, or (ii) breaking the time rever-
symmetry. For the case (i), as shown in Fig. 2(b), by a
small deviation, from equal coupling strength the spec-
trum becomes gapped. The fragile nature of the gapless
phase is ascribed to the fact that both nodes appear at
the same point in BZ, making it susceptible to perturba-
tions, which can create the matrix elements between the
nodes. In the Kitaev model however a finite strength of
type (i) is required to move the nodes to the same point
and then annihilate them. The gapped phase around the
gapless point is connected to the gapped phase near the
corner of the phase diagrams without a phase transition,
and consequently, they should have the same low-energy
properties. Near the corners of the phase diagram one
of the exchange coupling becomes much larger than the
others, say \( J_z \gg J_x, J_y \). This limit is well suited for us-
using the degenerate perturbation theory to obtain a low-
energy description in terms of the original spin degrees
of freedom. The effective model becomes a \( \mathbb{Z}_2 \) lattice gauge
theory defined on the Kagome lattice\(^{14}\). The latter lat-
tice is obtained by shrinking the blue links, correspond-
ing to \( J_z \sigma^x \sigma^z \) coupling, of the honeycomb lattice to ef-
fective sites carrying a doublet of pseudospin-1/2 states.
Therefore the gapped phase in Fig. 2(b) is continuously
connected to a phase with Abelian anyon excitations.

III. BREAKING THE TIME-REVERSAL
SYMMETRY: CHIRAL SPIN LIQUID

Now we focus on the case (ii) mentioned in the pre-
ceeding section to open a gap in the spectrum. This
be achieved by applying an external magnetic field
\( H_B = \sum_i B \cdot \sigma_i \) to the system, i.e., \( H = H_0 + H_B \).
We assume that the magnetic field is small. Following
Kitaev\(^{22}\), the effect of the magnetic field can be studied
perturbatively giving rise to three-spin interaction terms
in the Hamiltonian \((2)\) as follows:
\[ H = \sum_{<i,j>,\alpha} J_{\alpha} \sigma_i^{\alpha} \sigma_j^{\alpha} - h \sum_{i,j,l} \sigma_i^{z} \sigma_j^{y} \sigma_l^{z}, \]
where \( h \simeq B^3/\Delta^2 \) and we treat it as an independent
parameter in the following. Here \( \Delta \) is the gap to the
excitations of the background fluxes\(^{22}\). Despite having
multi-spin interaction terms, the model remains to be
exactly solvable. Using the Majorana representation, the

FIG. 2: (a) Dispersion along high symmetry points for the equal coupling strength \((J_x = J_y = J_z)\) which is four fold degenerate
at the \( \Gamma \) point. (b) The dispersion away from the equal coupling point is gapped. Here we considered \( J_x = 1.0, J_y = 0.8 \) and
\( J_z = 1.2 \). (c) The bulk spectrum is also gapped by applying a magnetic field \( h/J_0 = 0.2 \) and (d) the edge states arise due to
nontrivial band topology.
above Hamiltonian is rewritten as

\[ H = \frac{i}{4} \sum_{<i,j>} 2\hat{J}^2_{i,j} u^*_{n_i} c_i c_j + i h \sum_{<i,j>} c_i c_j, \tag{7} \]

It is seen that the three-spin term translates to second-neighbor hopping for Majorana fermions, and the Hamiltonian retains its bilinear form in fermion operators. In momentum space a Bloch Hamiltonian similar to (5) is obtained where the antisymmetric matrix is replaced with \( A(k) + B(k) \), and the expression for \( B(k) \) is given in Appendix A.

The band structures for \( h = 0.2 \) is shown in Fig. 2(c). The spectrum becomes fully gapped throughout the BZ. We shall discuss that this gapped phase is distinct from the gapped phase in Fig. 2(b). The distinction can be made more explicit and quantitative by evaluating the first Chern number

\[ C_n = \frac{1}{2\pi} \int_{\text{BZ}} dk \Omega^x_n(k), \tag{8} \]

where \( \Omega^x_n(k) \) is the Berry curvature: \( \Omega^x_n(k) = i(\nabla_k u_n) \times (\nabla_k u_n) \) with \( u_n(k) \) as the periodic part of the Bloch wave function in the \( n \)-th band with energy dispersion \( \varepsilon_{nk} \), i.e., \( H(k)|u_n(k)\rangle = \varepsilon_{nk}|u_n(k)\rangle \). The integration is taken over the entire BZ.

Lets take \( J_x = J_y = J_z = J_0 \) and \( h/J_0 = 0.2 \) for the moment. The evaluation of the Chern number shows that the band structure shown in Fig. 2(c) is topologically nontrivial: the Chern numbers read as \( (0, -1, 2, -2, 1, 0) \) for the bands from lowest to highest energies. Hence the occupied Bloch bundle, the three occupied bands corresponding to half-filling, carries a total Chern number of \(+1\). This finding immediately implies that the model should carry gapless edge states along the one-dimensional boundary. We diagonalize the Hamiltonian (7) in a ribbon geometry, where the spectrum is shown in Fig. 2(d). It is clearly seen that the chiral edge modes cross the bulk band gap due to the topological bulk Bloch bands. The band structure is however trivial in regions far away from \( J_x = J_y = J_z = J_0 \) point in the parameter space and with small \( h \) as characterized by the Chern numbers as \( (0, 1, -1, -1, 0, 0) \) yielding occupied bands with total zero Chern number.

Having obtained a simple picture of the band structure for a few representative points in the parameter space, we now present the full phase diagram of the free Majorana model (7). We obtained two types of phase diagram. First we tune the \( J_z \) and \( h \) parameters across a wide range of values, and the obtained phase diagram is shown in Fig. 3(a). The region with total Chern number \( C = 1 \), as explained above, has the Chern number \((0, 1, -1, -1, 0, 0)\) for the Bloch bands. As we shall discuss in the next section it would have important consequences for the thermal Hall conductivity at low fields. The region with \( C = 0 \) is trivial with Chern number distribution for all band as \((0, 1, -1, -1, 0, 0)\). Second, we obtained a phase diagram in \( J_x + J_y + J_z = 3 \) plane at two values of magnetic field \( h = 0.4 \) and \( h = 0.2 \) as shown, respectively, in Fig. 3(b) and Fig. 3(c). For larger value of \( h \) the majority part of the phase diagram is occupied by the topologically nontrivial phase with \( C = 1 \). By decreasing the magnetic field this region shrinks to a smaller one around the isotropic point.

**IV. THERMAL HALL CONDUCTIVITY**

In the preceding section we obtained the phase diagram of the multi-band Majorana model (7) consisting of topological and trivial phases. In this section we want to see what are the implications of these phases and the phase transition between them on the outcomes of the experimental probes. A natural consequence of the former phase is the existence of gapless chiral states propagating along the edges of the system. Since the edge mode is chiral and topologically protected, a sort of quantization is expected to occur in appropriate measurements. Since the low-energy properties of the model are described by Majorana fermions, which are neutral particles, there...
is no charge response in the system. Yet, the thermal probes can measure the response of Majorana fermions as they can carry energy and consequently heat through a system subjected to a thermal gradient $\nabla_x T$, where $T$ is the temperature. A sketch of the measurement is shown in Fig. 1(b) in a close analogy with the set up used in recent experiments on $\alpha$-RuCl$_3^{32,37}$.

Of particular interest for our study of topological phases is to evaluate the thermal Hall conductivity $\kappa_{xy}$, which measures the transverse heat current $j_y^T = -\kappa_{xy} (\nabla_x T)$. The expression for $\kappa_{xy}$ is as follows:

$$\kappa_{xy} = \frac{-k_B^2}{A} \int d\epsilon f(\epsilon, T) \frac{\partial f(\epsilon, T)}{\partial \epsilon} \sum_{k,n} \Omega^x_n(k)$$

where $A$ is the area of the system, $k_B$ and $h$ are the Boltzmann and the reduced Planck constants, respectively. We set $k_B = h = 1$ in the following and restore when needed. Here $f$ is the Fermi-Dirac distribution function of the $n$-th band. The summation runs over the first BZ.

The results of $\kappa_{xy}/T$ for various cases are shown in Fig. 4. We begin by calculating the thermal Hall conductivity along a particular cut in the phase diagram Fig. 3(a). We set $J_z = 0.5$ and plot $\kappa_{xy}/T$ versus the magnetic field in Fig. 4(a) at different temperatures. Note that in these plots we restored $h$ and $k_B$. At low temperatures the value of $\kappa_{xy}/T$ in the trivial phase with $C = 0$ is nearly zero and a great enhancement is observed across the topological phase transition around $h/J_0 \approx 0.15$. The striking feature is that the value of $\kappa_{xy}/T$ saturates to a plateau quantized at $\pi/12$ as also expected from the number of chiral boundary mode. At high temperatures the increment around the phase transition is slightly smeared out, yet the quantization remains intact from the transition.

Next we study the variation of the thermal Hall conductivity with temperature in both phases. First we consider the case with $J_x = J_y = J_z = 1$, where the model is gapless in the absence of the magnetic field. As discussed in the preceding section a finite field opens a gap and the system immediately runs into a topological phase. In this phase the behavior of $\kappa_{xy}/T$ with temperature at different fields is shown in Fig. 4(b). A clear observation is that a robust quantized value of $\kappa_{xy}/T$ at $\pi/12$ occurs at a wide range of temperatures $T < 0.2$. At higher temperatures there is strong deviation from the quantized value. Indeed at the high temperatures the high energy band are thermally occupied by the Majorana fermions and consequently the contributions from all bands gives rise to a temperature dependent value. Note that at very high temperatures the $\kappa_{xy}$ in (9) is proportional to $\sum_{k,n} \Omega^x_n(k)$ over all bands which vanishes.

Fig. 4(c) shows the same plot of $\kappa_{xy}/T$ in the Abelian phase with $J_z = 1.3$. At small magnetic field where $C = 0$ the $\kappa_{xy}/T$ vanishes at low temperatures. A hump in $\kappa_{xy}/T$ is observed at temperatures around $T \approx 0.2$, which is likely due to the thermal occupation of bands with finite Chern number right above the gap. When the strength of the field is increased, a pronounced increment is observed in $\kappa_{xy}/T$ at low temperatures, which is again quantized to the value of $\pi/12$ akin to the nontrivial band topology with $C = 1$. Finally, we diagnose the contribution of different bands to thermal Hall conductivity. In all plots the saturation of $\kappa_{xy}/T$ at quantized values has a topological origin as discussed in main text.

FIG. 4: The variation of $\kappa_{xy}/T$ (a) across a topological phase transition at different low temperatures, (b) versus temperature at various magnetic fields at $J_x = J_y = J_z = 1$ and (c) away from the equal coupling exchanges, (d) the contributions of individual bands to thermal Hall conductivity. In all plots the saturation of $\kappa_{xy}/T$ at quantized values has a topological origin as discussed in main text.
V. SUMMARY AND CONCLUSIONS

In this work we have studied the Kekulé-Kitaev model\textsuperscript{13,14} whose spectrum is given by a multi-band model of Majorana fermions in terms of exchange couplings $J_x$, $J_y$, and a magnetic field $h$ as time-reversal breaking perturbation. Our main findings can be summarized as follows: we (i) found that at $J_x = J_y = J_z$ and $h = 0$ the spectrum is gapless and a gapped phase arises away from $J_x = J_y = J_z$ point continuously connected to an Abelian phase whose low-energy spectrum is given by abelian anyons on the Kagome lattice, (ii) numerically evaluated the field and temperature dependences of the thermal Hall conductivity and found that it shows a connected to an Abelian phase whose low-energy spectrum is given by abelian anyons on the Kagome lattice, (iii) systematically evaluated the field and temperature dependences of the thermal Hall conductivity and found that it shows distinct behaviors in topological and trivial phases, and (iv) observed a quantized plateau at low temperatures. The latter quantization is a resemblance of half-quantized plateau observed recently in thermal Hall measurements in compound $\alpha$-RuCl$_3$\textsuperscript{32}. Our results may suggest that the multi-band Kekulé-Kitaev model can also be considered as an alternative model and perhaps, when supplemented with other isotropic and anisotropic interactions, to describe other aspects of the experimental observations such as the sign change of thermal Hall conductivity, which we leave it for future study.

VI. ACKNOWLEDGEMENTS

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Appendix A: Antisymmetric skew matrices

In this appendix we present the full expression of skew antisymmetric matrices $A(\mathbf{k})$ and $B(\mathbf{k})$ appearing in the Bloch Hamiltonian on Majorana fermions. Let us assume that the primitive unite vectors of the honeycomb lattice are $\mathbf{a}_1 = (1, 0)$ and $\mathbf{a}_2 = (1/2, \sqrt{3}/2)$. The matrices are as follows:

\[
A(\mathbf{k}) = \begin{pmatrix}
0 & -J_z & 0 & -J_x e^{i\mathbf{k} \cdot \mathbf{a}_1} & 0 & -J_y \\
J_z & 0 & J_y & 0 & J_x e^{i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 \\
0 & -J_y & 0 & -J_z & 0 & -J_x e^{-i\mathbf{k} \cdot \mathbf{a}_2} \\
J_x e^{-i\mathbf{k} \cdot \mathbf{a}_1} & 0 & J_z & 0 & J_y & 0 \\
0 & -J_x e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & -J_y & 0 & -J_z \\
J_y & 0 & J_x e^{i\mathbf{k} \cdot \mathbf{a}_2} & 0 & J_z & 0
\end{pmatrix},
\]

\[
B(\mathbf{k}) = h \begin{pmatrix}
0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & -1 & 0 \\
0 & 1 & 0 & 0 & 0 & -1 \\
-1 & 0 & 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 1 & 0 & 0
\end{pmatrix}
+ \hbar \begin{pmatrix}
0 & 0 & e^{i\mathbf{k} \cdot \mathbf{a}_1} & 0 & e^{i\mathbf{k} \cdot \mathbf{a}_1} & 0 \\
0 & 0 & 0 & e^{-i\mathbf{k} \cdot \mathbf{a}_1} & 0 & 0 \\
e^{-i\mathbf{k} \cdot \mathbf{a}_1} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot \mathbf{a}_1} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]

\[
B(\mathbf{k}) = h \begin{pmatrix}
0 & 0 & e^{i\mathbf{k} \cdot \mathbf{a}_2} & 0 & e^{i\mathbf{k} \cdot \mathbf{a}_2} & 0 \\
0 & 0 & 0 & e^{-i\mathbf{k} \cdot \mathbf{a}_2} & 0 & 0 \\
e^{-i\mathbf{k} \cdot \mathbf{a}_2} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot \mathbf{a}_2} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
e^{-i\mathbf{k} \cdot (\mathbf{a}_1 - \mathbf{a}_2)} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}.
\]
