Thermal Hall conductivity near field-suppressed magnetic order in a Kitaev-Heisenberg model

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We investigate thermal Hall conductivity $\kappa_{xy}$ of a $J$-$K$ Kitaev-Heisenberg model with a Zeeman field in the $(111)$ direction in the light of the recent debate surrounding the possible re-emergence of Ising topological order (ITO) and half-quantized $\kappa_{xy}/T$ upon field-suppression of long-range magnetic order in Kitaev materials. We use the purification-based finite temperature Tensor Network approach making no prior assumptions about the nature of the excitations: Majorana, visons or spin waves. For purely Kitaev interactions and fields $h/K \gtrsim 0.02$ sufficient to degrade ITO, the peak $\kappa_{xy}/T$ monotonously decreases from half-quantization associated with lower fields - a behavior reminiscent of vison fluctuation corrections. In our $J$-$K$ model (with ferro-$K$ and antiferro-$J$), in the vicinity of field-suppressed magnetic order, we found $\kappa_{xy}/T$ to be significant, with peak magnitudes exceeding half-quantization followed by a monotonous decrease with increasing $h$. We thus conclude that half-quantized thermal Hall effect, if found in our model in the vicinity of field suppressed magnetic order, is a fine-tuning effect and is not associated with a Majorana Hall state with ITO.

Thermal Hall conductivity has become a very important transport diagnostic for emergent phenomena in insulating magnetic systems such as the underdoped cuprates [1], frustrated magnets such as pyrochlores [2], kagome systems [3], and more recently a Kitaev material $\alpha$-RuCl$_3$ [4–7]. Specifically in the Kitaev material, one set of studies [4–6] has reported the half-quantized thermal Hall effect at finite magnetic fields comparable to the magnetic ordering scale, suggesting a re-emergent Majorana Hall insulator state originally predicted [8] for the honeycomb Kitaev model at very small magnetic fields and low temperatures, which is a deconfined phase with robust Ising topological order (ITO). This view has been challenged [7, 9] in recent experiments where half-quantization has been ruled out. Nevertheless $\kappa_{xy}/T$ is found to be large, sometimes even exceeding the half-quantized value at temperatures and fields comparable to the magnetic ordering scale, implying half-quantized peaks/plateaus of $\kappa_{xy}/T$, if observed near field suppressed magnetic order, are a consequence of fine tuning and do not represent re-emergence of a deconfined ITO phase. The authors of Refs. [7, 9] offered an alternate explanation based on a spin wave picture. Theoretical studies have relied on various interacting quasiparticle pictures, with spin wave approximations [10–14] most commonly used. Since spin wave approximations in frustrated spin-1/2 magnets are best justified at high fields or in the presence of long-range magnetic order, the possibility of half-quantization at low temperatures near field-suppressed magnetic order (not seen in spin wave treatments) cannot be completely ruled out. Other theoretical approaches begin from the fractionalized quasiparticles, and suppression of half-quantized $\kappa_{xy}/T$ by external magnetic field or finite temperatures is understood from the perspective of vison (gauge field) fluctuations that couple to the Kitaev spinons [15], or from thermal excitation of bulk Majorana fermions [16]. Although the fractionalization analyses are based around expansion from the ITO phase, even here it is not clear whether ITO can re-emerge through field-suppression of long-range magnetic order. These challenges motivated us to take a different route of numerically estimating $\kappa_{xy}$ without making any quasiparticle approximation - whether fractionalized or spin waves - which forms the basis of existing theoretical approaches. We obtain the thermal Hall current and conductivity numerically using purification-based Tensor Network techniques[17]. To our knowledge, this is the first use of the Tensor Network technique for thermal Hall calculation of an interacting many-body system.

We consider for concreteness a ferromagnetic (FM) Kitaev model with a competing antiferromagnetic (AFM) Heisenberg interaction ($J$-$K$ model), subjected to a Zeeman field along the $c = (1, 1, 1)$ direction,

$$H = -K \sum_{\langle ij \rangle; \gamma \in \text{links}} S_i^\gamma S_j^\gamma + J \sum_{\langle ij \rangle} S_i \cdot S_j + h \sum_{i, \gamma} S_i^\gamma.$$  

(1)

Here $\gamma = x,y,z$ denote the bond dependent spin axes on the honeycomb lattice. Thermal Hall conductivity of this model has recently been studied using spin wave approximations [12]. In the Kitaev limit ($J/K = 0$), there is a fairly large window of magnetic fields (e.g. $h_{[c]} \gtrsim 0.02 K$) [18, 19] where ITO is significantly degraded (see also S.M. [33] for a similar signature in the topological entanglement entropy $\gamma(h)$) but interacting spin wave analysis [13] shows that magnons are good quasiparticles for $h/K \gtrsim 1$ although not at significantly lower fields due to interaction broadening. Fields in the range $0.02 \lesssim h/K \lesssim 1$ thus constitute an interpolating region between the ITO and spin wave regimes not easily lend-
ing to quasiparticle-based analyses, and we focus on this window. Likewise for the spin density wave (SDW) ordered states of the $J$-$K$ model, we are interested in the range of magnetic fields starting from field-suppressed SDW to deeper in the spin-polarized phase, where the nature of excitations may be changing.

Our main findings are as follows. In the Kitaev limit, near the lower end of our field range $h/K \approx 0.02$, $\kappa_{xy}/T$ peaks at small finite temperatures, with peak heights smaller but comparable to the half-quantized value $\pi/12$ associated with the ITO phase (see Fig. 2). With increasing $h$ as well as temperature $T$, $\kappa_{xy}/T$ declines sharply and monotonously, reminiscent of vison fluctuation effects discussed recently [15]. Thermal excitation of the bulk majoranas also suppresses half-quantization within the ITO phase [16]; however we are outside this regime. Our result qualitatively differs with the spin wave calculations in Ref. [13] where a non-monotonous temperature dependence with a peak-dip feature together with a nonzero high temperature value was reported. In the magnetically ordered phase, we studied $\kappa_{xy}/T$ at intermediate fields corresponding to suppression of magnetic order in order to test the possibility of field-revived quantized thermal Hall effect. We found $\kappa_{xy}/T$ to large and with an opposite sign relative to the Kitaev limit, with peak values that can even exceed half-quantization, consistent with experimental reports [9]. Further increasing the magnetic field decreases the extrema, which monotonously approach zero at high fields like in the Kitaev limit. We posit that half-quantized thermal Hall effect appears in the ITO phase and possibly its immediate vicinity. Therefore in the field-suppressed SDW regime, we do not accord physical significance to any isomagnetic of $\kappa_{xy}/T$ showing extremum near half-quantization since the isomagnetics commonly peak at much larger values for nearby fields.

**Strategy:** Thermal currents can be readily expressed in terms of local microscopic degrees of freedom (spin operators in our case) and do not require any knowledge of quasiparticles, which was the approach followed in Kitaev’s original work [8]. Kitaev’s prescription for calculation of edge thermal currents is however difficult to implement numerically in a general nonintegrable situation because of the large temperature differences used to mimic the bulk and vacuum regions. An alternate way of using the Kubo linear response approach is also numerically challenging because it involves small differences of two large contributions represented by the energy-current correlators and the bound energy magnetization contributions [20]. Our strategy is similar to Kitaev’s except that the system is immersed in a uniform temperature bath. Although there is no net transport Hall current, it is because of cancellation of equal and opposite contributions of the two edges. Then, for gapped systems that are sufficiently long, the thermal Hall current associated with one edge is simply obtained by summing over the Hall currents from the relevant edge to the center. This method assumes the thermal Hall currents are essentially due to edge modes and the Hall current deep inside the bulk is insignificant; hence the decay of thermal Hall currents away from the bulk needs to be checked every time. This also ensures that the left and right edge currents do not overlap.

For calculations, we put our model on a cylinder along the $x$-direction with periodic boundary conditions along the $y$-direction, with a pair of open zigzag edges, see Fig. 1. The Hamiltonian is re-expressed as a sum of layer contributions, $H = \sum_i H_i$, connecting the two open edges. Links that cut the dual curve (dashed line in Fig. 1) separating adjacent layers, make equal contributions to the adjacent $H_i$. The energy current across the dual curve is obtained from the continuity equation,

$$\frac{dH_i}{dt} = -i[H_i, H] = \sum_j \hat{J}_{ij}, \quad \hat{J}_{ij} = -i[H_i, H_j]. \quad (2)$$

Here $\hat{J}_{ij}$ is the energy current from layer $j$ to $i$, (see S.M. [33] for expression of interlayer thermal currents) and we consider it as a sum of contributions $\hat{J}_{ij} (x)$ starting from one edge ($x = 0$) to the other ($x = L_x$). In situations where the thermal Hall currents are essentially due to the edge modes, the Hall current associated with one of the edges is given by $J_{ij}^H = \sum_{x \leq L_x/2} \langle \hat{J}_{ij} (x) \rangle$. The averaging includes both quantum and thermal. In the steady state, the labels $ij$ can also be dropped. Thermal Hall conductivity $\kappa_{xy}$ is obtained by taking the temperature derivative of $J^H$.

We use the standard purification-based finite temperature Tensor Network method [17] for performing the quantum and thermal averaging, where imaginary time evolution of the state is carried by applying the evolution operator as a matrix product operator (MPO) with W-II approximation, described in Ref. [21] – see S.M.
[33] for more details. Benchmarking of the finite temperature purification method was done (see S.M. [33]) against Exact Diagonalization (ED) calculation of one of the Kitaev plaquette fluxes at finite temperature and a small field of $h/K = 0.025$, and we found very good agreement between the two even at temperatures as low as $T/K = 0.01$. However the thermal Hall calculations at even smaller fields taking us well inside the ITO phase are substantially more expensive to implement numerically because of higher bond dimension and smaller Trotter size requirements. Note that the ITO phase is rather well-studied in the literature, and moreover the experimental interest is in magnetic fields that lie well outside the ITO - this further motivates us to focus in the field range upwards of those needed to suppress ITO.

Results: We consider first $\kappa_{xy}/T$ in the Kitaev limit $J/K = 0$, see Fig. 2. Introduction of a magnetic field hybridizes the dispersing majoranas with pairs of visons [22] whose excitation energy at zero field is $\Delta_{\text{pair}} \approx 0.065K$. The hybridization results in gapping of the bulk majoranas and appearance of chiral Majorana edge modes [8], vison fluctuations/hopping, and a suppression of topological order [17, 18] beyond $h \sim 0.02K$ with a concomitant gapping of the edge states [18]. Fractionalization may however survive to higher fields, as evidenced from quasiparticle stability analysis [23], and also experimentally from specific heat measurements [24]. At high fields $h/K \sim 1$, fractionalization is lost and local spin flips (magnons) constitute the elementary excitations.

Figure 2 shows the temperature dependence of $\kappa_{xy}/T$ in the Kitaev limit for different values of $h$. Table I additionally shows the temperatures $T^*$ corresponding to the peak values of $\kappa_{xy}/T$, together with the calculated bulk gap $\Delta_{\text{bulk}}$ [25]. The $T^*$ all lie below $\Delta_{\text{bulk}}$, signifying the low temperature peaks are associated with gapped edge modes. This is also directly confirmed by our observation of rapidly decaying thermal Hall currents away from the edge and into the bulk (see SM [33]). For all fields except the lowest $h/K = 0.03$, we found $T^*$ is not very sensitive to the finite circumference of the edge - we confirmed this by increasing the edge size from $N_y = 6$ to $N_y = 8$ spins, and found no significant change in the position of $T^*$. An edge gap is known to appear upon transitioning out of the ITO phase [18]. For the lowest field shown in Fig. 2, $h/K = 0.03$, the peak value of $\kappa_{xy}/T$ reaches nearly 83% of the half-quantized value associated with the ITO phase, although topological order as measured by topological entanglement entropy $\gamma$ is significantly degraded, $\gamma(h)/\gamma(0) \approx 0.14$, (see S.M. [33]). We attribute the reduction here to vison fluctuations as analyzed in Ref. [15] since the peak is comparable to the half-quantized value at lower fields, and the alternate, interacting spin wave approximation becomes inaccurate at low fields $h/K \lesssim 1$ [13]. Further increase of $h$ monotonously decreases the peak values, while simultaneously pushing $T^*$ to higher temperatures. At high temperatures, the $\kappa_{xy}/T$ all tend to vanish and we see no signs of saturation predicted from an earlier spin wave [13]. We checked that $\kappa_{xy}/T$ has a similar behavior (although with an opposite sign) for fields along the crystallographic $a = (1, 1, 1)$ direction - a fact that is often the case experimentally. The sign of $\kappa_{xy}/T$ is dictated by that of the product $h_x h_y h_z$ as shown in Kitaev’s original work. We also verified that the effect vanishes along the $b = (1, -1, 0)$ direction - a consequence of the so-called $R^*$-symmetry [12, 15].

We now turn on the competing Heisenberg AFM interaction $J$. At $h = 0$, the Kitaev spin liquid phase is known to survive up to $J/K \approx 0.1$ [26, 27], beyond which a stripy SDW phase appears. The (111) Zeeman field competes with both topological and magnetic order [28], and at large values yields a trivial polarized phase. Recent field-theoretical phenomenology [29] as well as thermal Hall measurements of $\alpha$-RuCl$_3$ support the view that ITO re-emerges upon field-suppression of SDW order. However other experimental [7] and theoretical studies based on spin wave treatments [12, 13] disagree, and even the robustness of the reported half-quantization in this regime has been questioned. Before examining $\kappa_{xy}/T$, which depends on the excitations in the model, we first checked if the ground state shows re-emerged ITO by calculating $\gamma(h)$ for different values of $J/K$ (see S.M. [33]). For the magnetically ordered phase, $J/K > 0.1$, we found that there is indeed a small partial revival of $\gamma(h)$ from very small values to near $\gamma(h)$ associated with the the pure Kitaev model - this happens
for fields $h \sim J/3$. However the revival never takes $\gamma$ anywhere near the value $\ln(2)$ associated with ITO (see S.M.). In the discussion below we focus our attention in the vicinity of the fields where this partial revival of ITO takes place, since $\kappa_{xy}/T$ also peaks here.

Figure 3 shows isomagnetic curves of $\kappa_{xy}/T$ for different values of $J/K$ across the Kitaev spin liquid to stripy AFM transition. Consider the curve corresponding to $(J/K, h/K) = (0.1, 0.05)$. Apart from the sign reversal, $\kappa_{xy}/T$ shows a deep minimum that exceeds the half-quantized value, indicating we are well outside the ITO regime at such fields. This is also supported by the strong degradation of $\gamma(h)$ (see S.M. [33]) for the above parameters. We noticed that sign reversal of $\kappa_{xy}/T$ happens at $J/K = 0.02$, observed from the computation of the edge current in the ground state. Higher values of $J/K = 0.2, 0.3$ take us well within the stripy SDW phase at $h = 0$. We dial up the field to values where ITO is partially revived, and calculate $\kappa_{xy}/T$ in its vicinity. We find deep minima of comparable strength to the one seen for $(J/K, h/K) = (0.1, 0.05)$. Upon increasing the field, the minimum becomes shallower, very reminiscent of the intermediate field behavior of the Kitaev model where ITO has degraded. The temperature corresponding to the extremum, $T^*$, lies well within the bulk gap (see Table I) for these parameter values. In regimes with strong magnetic order and low fields ($h/J \ll 1$), we found that the Hall currents do not decay in the bulk for the length-scales we could study; consequently restricting us to the field-suppressed SDW regime and beyond. This is a limitation of our method that we have mentioned already - in cases where the bulk makes a significant contribution to the thermal Hall currents, our method of calculating the Hall current is invalidated. However it is encouraging for us that experimentally, the thermal Hall response at low fields in the SDW phase is not observed to be significant [4], and this is also the case in spin wave treatments [12] that are relevant for magnetically ordered states.

To summarize, we studied the temperature dependence of thermal Hall conductivity of the $J$-$K$ Kitaev-Heisenberg model for Zeeman fields in the (111) $\| c$ direction using a purification based finite temperature Tensor Network technique that goes down to $K/T \approx 100$. We make no prior assumption about the nature of the quasiparticles, whether fractionalized ones or spin waves. In the Kitaev limit, we focused on fields $h/K > 0.02$ where ITO has substantially degraded, extending the understanding of thermal Hall conductivity to the topologically trivial phase in the neighborhood of ITO. We found that $\kappa_{xy}/T$ features a low-temperature peak whose value approaches half-quantization at the lower end of our field range, and continuously declines with increasing $h$, approaching zero at larger fields. We associate the low-temperature peak with gapped edge modes expected in the absence of Ising topological order[30]. After peaking, $\kappa_{xy}/T$ monotonously decreases with increasing temperature reminiscent of vison fluctuation effects [15]. To understand the effect of Heisenberg perturbations we considered the cases $J/K = 0.1$ within the spin liquid phase (but close to the SDW phase boundary), and $J/K = 0.2, 0.3$ that lie well within the stripy SDW phase. Characteristically deep minima were seen in the isomagnetic curves of $\kappa_{xy}/T$ versus $T$, significantly exceeding half-quantization of the ITO phase, similar to the experimental observations in $\alpha$-RuCl$_3$. Although many of our observations are consistent with vison fluctuation effects, the large extrema in $\kappa_{xy}/T$ - exceeding half-quantization
- in the vicinity of field-suppressed magnetic order are not. At higher fields, any partially revived topological order seen after destruction of SDW order gets suppressed again, resulting in the polarized phase with small thermal Hall effects.

We did not find any intermediate field regime following field-suppression of SDW order where robust half-quantized $\kappa_{xy}/T$ associated with ITO exists. Although in the vicinity of the field-induced SDW suppression we do note a weak partial revival of topological order (as measured by the topological entanglement entropy $\gamma$), the revived $\gamma$ remain well below $\gamma = \ln 2$ associated with ITO. Since the magnitude of $\kappa_{xy}/T$ in the $J$-$K$ model may exceed the half-quantized value, it is possible to fine tune the field to bring it near half-quantization but that does not imply ITO. We believe that similar conclusions should also hold near field-suppressed SDW order even in the presence of other competing interactions like the anisotropic terms $\Gamma, \Gamma'$ - this is ultimately to be decided in future studies.

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I. PURIFICATION METHOD AND BENCHMARKING

For calculation of finite temperature quantities, we have used a purification based tensor network method [17]. The purification strategy involves expressing the mixed state as a pure state in an enlarged Hilbert space. We obtain the finite temperature ($T=1/\beta$) thermofield state (TFD) $|\psi_{\beta}\rangle$ by action of imaginary time evolution operator $\exp(-\frac{1}{2}H)$ on the infinite temperature state $|\psi_0\rangle$, which is constructed by Bell entangled pair of physical and ancilla spin 1/2 degree of freedom at each sites. Here, $H$ acts on the physical part of Hilbert space and we use the compact matrix product operator (MPO) representation for the finite temperature evolution operator with W-II approximation [21], provided in TenPy library [31]. Finite temperature expectation of a physical observable $\hat{O}$ is obtained from $\langle \hat{O}_{\beta} \rangle = \langle \psi_{\beta} | \hat{O} | \psi_{\beta} \rangle$. The purification method works best at higher temperatures. Figure 4 shows the benchmarking of the method against Exact Diagonalization (ED) calculation of one of the Kitaev plaquette fluxes $\langle W_{\beta} \rangle$ at finite temperatures and a small field of $h/K = 0.025$ for $N = 18$ site system. We find very good agreement between the two even at temperatures as low as $T/K = 0.01$. At higher temperatures, the discrepancy between purification and ED results is actually on account of the latter being inadequate (insufficient number of excited states taken into consideration).

The accuracy of matrix product state (MPS) calculations requires enhancing the bond dimension $\chi$ and reducing the Trotter step size $\Delta \beta$ used in W-II approximation [21]. Figure 5 shows the $\kappa_{xy}/T$ (in the Kitaev limit as well as for the $J$-$K$ model) as a function of the Trotter step size. Calculations in the Kitaev limit typically require larger $\chi$ and smaller $\Delta \beta$ compared to the Heisenberg-perturbed cases that we studied. It is evident from Fig. 5 that fine-graining the Trotter steps from 0.04 to 0.02 does not affect the expectation values, while in the Kitaev limit we still see some sensitivity, especially at lower field values. We observed that for the bond dimensions that we work with ($\chi = 400$ and 600), Trotter errors are the main limitation on accuracy. For this reason, we limit our calculations in the Kitaev limit to fields greater than $h/K = 0.03$.

II. THERMAL HALL CURRENT DECAY IN THE BULK

In gapped phases, the low-temperature behavior of thermal Hall effect is governed by low-lying edge modes. Figure 6 shows the decay of the thermal Hall current along the $x$-direction (cylinder axis) for in the Kitaev limit for various values of the Zeeman field along the (111) direction. The current decays rapidly as we go deeper in the bulk allowing us to treat the left and right edge currents independently. Figure 6 shows the current decay in the $J$-$K$ Kitaev-Heisenberg model in the presence of a Zeeman field along the (111) direction. The ra-
Figure 5. Plot (a) shows the $\kappa_{xy}/T$ vs. $T/K$ with varying $(\Delta \beta)$ and $\chi$ in pure Kitaev limit for different magnetic field parameter range. $\kappa_{xy}/T$ is almost converged at high $\chi$ and lower $(\Delta \beta)$. Plot (b) shows $\kappa_{xy}/T$ vs. $T/K$ for J-K Kitaev-Heisenberg model with $J/K = 0.1$ for two magnetic field parameters $h/K = 0.05, 0.075$ and they found to be converged, implying accuracy of computation.

Figure 6. Plot (a) shows the decay of thermal Hall current along the the length of cylinder which is measured at the peak of $\kappa_{xy}/T$ in pure Kitaev limit with varying magnetic field strength. We show the current decay up to half of the chosen cylinder length ($L_x = 10$) and in other half current will be equal and opposite. It is evident from the plot that thermal current vanishes deep in the bulk. Plot (b) shows the current decay in field suppressed SDW phase. Here, we choose the cylinder length ($L_x = 20$) to make sure current decays well in bulk gap.

Figure 7. Ground state plaquette flux revival upon suppression of magnetic order. We considered the system size of $N_x = 10, N_y = 8$, where ground state is computed using finite DMRG method.
Figure 8. Field dependence of topological entanglement entropy $\gamma$. It is small in the magnetically ordered phase as well as at high fields but there is a small, partial revival at intermediate fields where magnetic field is comparable to magnetic ordering scale.

III. FLUX REVIVAL AND TOPOLOGICAL ENTANGLEMENT ENTROPY ($\gamma$) IN FIELD SUPPRESSED SDW PHASE

Motivated by seen experimental large thermal Hall in field revived SDW phase, we compute flux expectation value in ground state for J-K model with varying Zeeman field strength. We see that flux gets revived at Zeeman field strength $\sim J/3$ - see figure 7. We also compute topological entanglement entropy $\gamma$ using Kitaev and Preskill construction [32]. In this intermediate field regime, we see that the $\gamma(h)$ gets revived, albeit weakly, see Figure 8. We carried out this computation with system size of $N_x = 10, N_y = 8$ using finite DMRG method.

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