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Thermal Transport in a one-dimensional Z_2 Spin Liquid

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We study the dynamical thermal conductivity of the Kitaev spin model on a two-leg ladder. In contrast to the majority of conventional one-dimensional spin systems, we show the ladder to exhibit no ballistic channel and a zero-frequency pseudo-gap. This is a direct consequence of fractionalization of spins into mobile Majorana matter and a static Z_2 gauge field, which acts as an emergent thermally activated disorder. Our finding rests on complementary calculations of the current correlation function, comprising a phenomenological mean-field treatment of thermal gauge fluctuations, a complete summation over all gauge sectors, as well as exact diagonalization of the original spin model. The results will also be contrasted against the conductivity discarding gauge fluctuations.

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Thermal transport by magnetic degrees of freedom in insulating quantum magnets is a fascinating probe of spin dynamics. This includes conventional magnons in two-dimensional (2D) antiferromagnets (AFMs) with long range order (LRO) [1], but also more exotic elementary excitations, ranging from gapped triplons in quantum disordered 1D spin ladder compounds [2, 3], via fractional spinons in 1D Heisenberg AFM spin chains [4–6] and potentially also in 2D triangular AFMs [7], up to emergent monopoles in spin ice [8, 9]. Recently quantum magnets with strong spin-orbit coupling have experienced an upsurge of interest, since they may realize highly frustrated spin systems with *compass* exchange [10–12]. This includes Kitaev’s model [13], which represents a rare case of an exactly solvable, interacting quantum many-body system in 2D, where spin-1/2 moments on the honeycomb lattice fractionalize to form an infinite set of spin liquids with topological degeneracy, comprising Majorana fermions, coupled to a Z_2 gauge field [13–17]. In a broader context, Kitaev’s model is therefore related to topological insulators [18], superconductors [19], or fractional quantum Hall systems [20], as well as topological matter and order [21, 22]. Interestingly, the physics of Kitaev’s model can be generalized to 3D [23, 24] lattices as well as to 1D *ladder* versions of the Kitaev model, which allow for topological string order [14].

In this work we shed light on fractionalization as seen by magnetic heat transport in Kitaev ladders. First heat transport measurements in the proximate 2D Kitaev system α -RuCl₃ have surfaced only recently [25], with however phonons dominating. Transport in low-D quantum magnets has been investigated extensively at zero frequency (DC) and momentum regarding the Drude weight (DW) [26–41]. The DW is the nondissipating DC contribution to the current autocorrelation function and, if existent, signals a ballistic channel. While in general, the picture depends on the type of current [26], in integrable systems the *energy* conductivity is generically expected to be infinite, as for the Heisenberg chain [42–45], implying a finite thermal DW. Constructing nonintegrable

systems, e.g., by coupling Heisenberg chains to form spin ladders, routinely leads to normal dissipative heat conduction [34, 45–48], equivalent to a finite DC value, but a vanishing DW of the current autocorrelations. In contrast to this conventional behavior of translationally invariant quasi 1D spin systems, and as one of our prime results, we find that the Kitaev ladder has no ballistic channel and displays a zero-frequency pseudo gap indicative of a heat insulator.

This is a direct consequence of the matter-gauge-field interactions and can be viewed as a fingerprint of this Z_2 spin liquid in 1D. This behavior is also in sharp contrast to that of the Kitaev chain [49], which hosts no gauge field. To justify these claims, we consider results from complementary calculations, comprising analytical, phenomenological mean-field, and exact numerical evaluations of the dynamic energy current correlation function.

The Hamiltonian of the Kitaev ladder reads

$$H = \sum_{\langle m,n \rangle} J_{\alpha} \sigma_m^{\alpha} \sigma_n^{\alpha}, \quad (1)$$

with notations detailed in Fig. 1. It is known that this model can be mapped onto free Majorana fermions in the presence of static Z_2 gauge fluxes by various techniques [13, 14, 16]. Here we use the bond algebra method [12, 16], where each exchange link $\sigma_m^{\alpha} \sigma_n^{\alpha}$ in Fig. 1 is replaced by $i\eta_{mn} c_m c_n$, with Majorana fermions $c_{m(n)}$, with $c_m^2 = 1$ and $\{c_m, c_n\} = 2\delta_{mn}$, and a *static* Z_2 gauge field $\eta_{mn} = \pm 1$. As shown in refs. [12, 16], the complete Hilbert space of (1) is accounted for by constraining $\eta_{mn} \equiv 1$ along the $J_{x,y}$ -legs, i.e.

$$H = i \sum_l [\eta_{l,1} c_{1l,1} c_{2l,1} + \eta_{l,2} c_{1l,2} c_{2l,2} + j_x (c_{1l,1} c_{2l,2} + c_{1l,2} c_{2l+1,1}) + j_y (c_{1l,2} c_{2l,1} + c_{1l+1,1} c_{2l,2})], \quad (2)$$

with $j_{x,y} = J_{x,y}/J_z$ and $J_z = 1$. Each *pair* of Majorana fermions $c_{1(2)l,j}$, can be replaced by *one* spinless fermion, $d_{l,j}^{(\dagger)}$, using $c_{1l,j} = d_{l,j}^{\dagger} + d_{l,j}$, $c_{2l,j} = i(d_{l,j}^{\dagger} - d_{l,j})$, mapping Eqn. (2) to a BCS Hamiltonian with a two-site basis. For

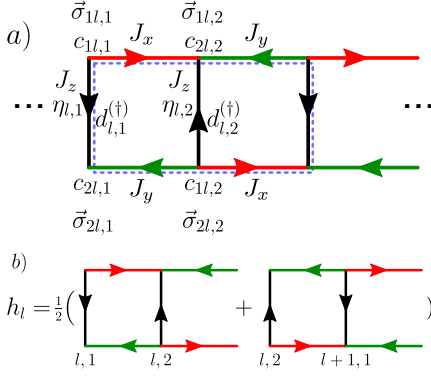


Figure 1: a) Kitaev ladder. Three equivalent representations: spins, Majorana fermions, and spinless fermions. $J_{x,y,z}$ exchange interaction. Index l refers to unit cell (PBC). $\vec{\sigma}_{il,j}$ Pauli matrix on leg(rung) $i(j)=1,2$. $c_{il,j}$ Majorana fermion of type(on rung) $i(j)=1,2$. $d_{il,j}^{(\dagger)}$ spinless fermion on rung j . Spins and Majorana fermions located at the vertices, spinless fermions at the center of the rungs. $\eta_{l,j} = \pm 1$ static Z_2 gauge fields. Arrows denote ordering of Majorana fermions on a bond [12]. Dashed blue loop of six sites refers to conserved flux operator Φ b) Local energy density used in this work.

periodic boundary conditions (PBC), each eigenstate of (2) is (at least) two-fold degenerate by changing sign of all $\eta_{l,j}$.

The main goal of this paper is to analyze the finite temperature energy current correlation function $C(t) = \langle J(t)J \rangle / N$ and its Fourier transform $C(\omega) = \int_{-\infty}^{\infty} dt C(t) \exp(i\omega t) = C_0 \delta(\omega) + C(\omega \neq 0)$, encoding the physics of the thermal conductivity [41]. Here, $\langle \dots \rangle$ is the canonical thermal trace at temperature $T = 1/\beta$ ($k_B = 1$). The energy current J follows from the energy polarization $P = \sum_l l h_l$ through $J = i[H, P]$ ($\hbar = 1$), where h_l is the energy density depicted in Fig. 1b). $D \equiv C_0/T^2$ is the Drude weight, which quantifies the non-dissipative current dynamics. Since the energy current is diagonal in the gauge fields, one may write

$$\langle J(t)J \rangle = \text{Tr}_{\eta} [Z_{d(\eta)} \langle J(t)J \rangle_{d(\eta)}] / Z. \quad (3)$$

The subscript $d(\eta)$ refers to tracing over matter fermions for a *fixed* gauge field state, and it can be done in different ways [53–55]. Here we consider three complementary types of calculations of the current correlation function. (i) To appreciate the impact of the thermal fluctuations of the gauge field on the transport, we first suppress the trace over $\eta_{l,i}$, and calculate $C(\omega)$ exactly in the ground state gauge, allowing however for finite temperatures. (ii) To treat large systems close to the thermodynamic limit, including gauge fluctuations, we approximate Tr_{η} by a partial trace characteristic of the *mean* gauge configurations. (iii) We perform exact summation over all gauge sectors on small systems and compare with ED of the original spin model.

(i) *Ground state gauge:* In the thermodynamic limit, the ground state of Eqn. (2) is obtained from a choice of

$\eta_{l,j} \equiv \eta_j$, which is translationally invariant with respect to the unit cell [14, 50, 51]. For the parametrization of Eqn. (2) this is $\eta_1 = -\eta_2 = \pm 1$ [52]. After Fourier and Bogoliubov transformation to new spinless fermion quasiparticles $a_{k,i}^{(\dagger)}$ the Hamiltonian reads

$$H = \sum_{k,i} \epsilon_{k,i} (2a_{k,i}^{\dagger} a_{k,i} - 1) \quad (4)$$

with energies $2\epsilon_{k,1(2)} = 2[j_{\pm}^2 c^2 + (1 \pm j_{\pm} s)^2]^{-1/2}$, with $c = \cos(k/2)$, $s = \sin(k/2)$, $j_{\pm} = j_x \pm j_y$, and the Brillouin zone fixed to $k \in [0, 2\pi[$ [14]. For convenience we redefine the quasiparticles within the extended zone scheme $k \notin [0, 2\pi[$ to satisfy $\epsilon_{k,1(2)} = \epsilon_{-k,1(2)}$.

Using the energy density of Fig. 1b), expressed in terms of the *original* matter fermions $d_{lj}^{(\dagger)}$, deriving the current, and after transforming to Bogoliubov particles, one gets

$$J = \sum_{k,i} u_{k,i} (a_{k,i}^{\dagger} a_{k,i} + a_{-k,i} a_{-k,i}^{\dagger}) + j_{k,i} (a_{k,i}^{\dagger} a_{-k,i}^{\dagger} + a_{-k,i} a_{k,i}) \quad (5)$$

with $i = 1, 2$, $u_{k,i} = (j_{+}^2 - j_{-}^2) \sin(k)/2 + (-1)^i j_{-} \cos(k/2)$, and $j_{k,i} = (-1)^i |j_{+} \cos(k/2)|$. Using (4) and (5), solving for $C(t)$ is straightforward. For the Fourier transform $C(\omega)$ we obtain

$$C(\omega) = \frac{4\pi}{N} \sum_{k,i} \{ 2u_{k,i}^2 f_{k,i} (1 - f_{k,i}) \delta(\omega) + j_{k,i}^2 [f_{k,i}^2 \times \delta(\omega + 4\epsilon_{k,i}) + (1 - f_{k,i})^2 \delta(\omega - 4\epsilon_{k,i})] \}, \quad (6)$$

with f being the Fermi distribution, $f_{k,i} = 1/(e^{2\beta\epsilon_{k,i}} + 1)$. This result is of the form typical for a clean superconductor, comprising a zero frequency quasiparticle DW and two finite frequency pair breaking spectra, corresponding to the two quasiparticle energies of Eqn. (4).

In Fig. 2 the current correlation function is shown for two representative cases of $j_{x,y}$, referring to a gapless (gapped) matter sector at $j_{x,y} = 2, 1$ ($j_{x,y} = 2, 0.5$). Several comments are in order. First, the regular spectrum $C(\omega \neq 0)$ is depicted only for $\omega > 0$, since $C(-\omega) = e^{-\beta\omega} C(\omega)$, as required by detailed balance. Second, in the gapless case the regular spectrum for $\omega \ll 1$ shows a power law $C(\omega) \propto \omega^2$ due to $j_{\pi+q,i}^2 \propto q^2$, while displaying a van-Hove singular gap for $|j_{-}| \neq 1$. No qualitative difference arises in $C(\omega)$ between the topologically trivial and nontrivial phases, as to be expected for the current of a local energy density. At elevated energies two more van-Hove singularities arise, one at the onset of the the second quasiparticle excitations and one at the upper band edge. The insets Fig. 2b) and c) detail the DW versus temperature, relative to its integrated regular spectral weight $I(T) = \int_{-\infty}^{\infty} d\omega C(\omega)$, skipping the Drude peak, and relative to the high temperature value. Fig. 2b) shows that $D(T)$ is finite for any $T \neq 0$ and that

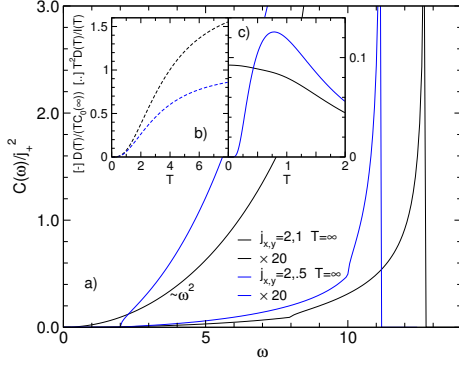


Figure 2: Black(blue) lines: infinite temperature dynamical current correlation function $C(\omega)$ versus frequency $\omega > 0$ using the ground state gauge for gapless(full) matter sector at $j_{x,y} = 2, 1(2, .5)$. Inset: DW $D(T)$ versus temperature T normalized to $I(T)/T^2 [TC_0(T = \infty)]$ dashed[solid].

$T^2 D(T)$ is comparable to $I(T)$ at sufficiently large temperatures. Fig. 2c) proves that $D(T \ll 1) \propto T$ as is true for 1D free fermions irrespective of their dispersion. In the gapped case $D(T)$ is exponentially activated. These results are in stark contrast with those when gauge fluctuations are taken into account, as it becomes apparent later on, Figs. 3 and 4.

(ii) *Average domain wall density approach:* Now we trace over gauge fluctuations in Eqn. (3) *approximately* by confining the full summation to a set of mean η -configurations [62]. Those characteristic configurations are chosen such that at any given temperature T they satisfy the *sole* constraint of containing a fixed number $n(T)$ of *domains* of η 's excited off the ground state. This approximation is justified as follows. First, at $T = 0$, forming a single domain in the ground state is gapped by Δ_L [13], with $\Delta_{L \rightarrow \infty}$ converging to some constant [57]. In other words, domain walls are deconfined. For simplicity we ignore the weak L dependence of Δ_L and we set $\Delta_L \approx \Delta$, with Δ evaluated by flipping a single $\eta_{i,i}$. Second, for multi-domain configurations, we attribute the same gap Δ to each additional domain. With these two steps the gauge field thermodynamics maps to lowest order to that of an $S = \pm 1$ nn-Ising chain with exchange constant $\mathcal{J} = \Delta/4$, i.e. a single domain increases the energy by $4\mathcal{J}$. The number of domain walls $n(T)$ can now easily be obtained from the average nn spin correlation function $\mathcal{C}(T) = \sum_{l=1}^{2N} \langle S_l S_{l+1} \rangle$. It is straightforward to see that $\mathcal{C}(T)$ satisfies the condition $\mathcal{C}(T) = 2N - 2n(T)$, which in turn yields $n(T) = 2N/(e^{\Delta/2T} + 1)$, rounded to multiples of two [58]. With this, Eqn. (3) reads

$$\langle J(t)J \rangle \approx \langle \langle J(t)J \rangle_{d(\eta)} \rangle_{n(T)}, \quad (7)$$

where $\langle \dots \rangle_{n(T)}$ now refers to random averaging over gauge domains with a number of walls set by $n(T)$. In turn, evaluating $\langle J(t)J \rangle$ reduces to a *disorder problem* with a temperature induced 'defect' density. We em-

phasize, that neither the neglect of fluctuations in $n(T)$, nor its specific dependence on T is qualitatively relevant for our main conclusions, as long as $n(T)$ interpolates between an exponential on-turn and a random state at $T = \infty$. Furthermore, our approach manifestly ensures that the ladder shows no LRO in the gauge field at any $T \neq 0$, since for $n(T) \neq 0$ domains of arbitrary size and location are included in the trace.

Calculation of Eqn. (7) requires a numerical treatment. We define a $4N$ component operator $\mathbf{D}^\dagger = (d_{1,1}^\dagger, d_{1,2}^\dagger \dots d_{N,1}^\dagger, d_{N,2}^\dagger, d_{1,1}, d_{1,2} \dots d_{N,1}, d_{N,2})$ of the original matter fermions, in terms of which the Hamiltonian and the current are set up in real space as $H = \mathbf{D}^\dagger \mathbf{h}(\eta) \mathbf{D}$ and $J = \mathbf{D}^\dagger \mathbf{j}(\eta) \mathbf{D}$. Both, $\mathbf{h}(\eta)$ and $\mathbf{j}(\eta)$ are $4N \times 4N$ matrices, which depend on the actual state of the gauge field $\eta = \eta_{11}, \eta_{22} \dots \eta_{N1}, \eta_{N2}$. For each given η we compute a Bogoliubov transformation \mathbf{U} , which introduces canonical quasiparticle fermions $\mathbf{A}^\dagger = (a_{1,1}^\dagger, \dots a_{2N}^\dagger, a_1, \dots a_{2N})$ via $\mathbf{A} = \mathbf{U}^\dagger \mathbf{D}$ and maps the Hamiltonian to $H = \mathbf{A}^\dagger \mathbf{E} \mathbf{A}$, where \mathbf{E} is diagonal and $\text{diag}(\mathbf{E}) = (\varepsilon_1 \dots \varepsilon_{2N}, -\varepsilon_1 \dots -\varepsilon_{2N})$ are the quasiparticle energies. With these definitions the current correlation function reads

$$C(\omega) = \frac{2\pi}{N} \sum_{\kappa\lambda\mu\nu} L_{\kappa\lambda} L_{\mu\nu} (\langle A_\kappa^\dagger A_\nu \rangle \langle A_\lambda A_\mu^\dagger \rangle - \langle A_\kappa^\dagger A_\mu^\dagger \rangle \langle A_\lambda A_\nu \rangle) \delta(\omega - 2(\varepsilon_\kappa - \varepsilon_\lambda)), \quad (8)$$

where $\mathbf{L} = \mathbf{U}^\dagger \mathbf{j}(\eta) \mathbf{U}$ and $\langle A_\mu^\dagger A_\nu^\dagger \rangle$ is either zero, f_μ , or $(1 - f_\mu)$, depending on the components of the spinor \mathbf{A} involved.

Fig. 3 shows results for $C(\omega)$ from Eqn. (8), for $j_{x,y} = 2, 1$ on lattices with 1400 sites, by binning the δ -functions in windows of the order 10^{-2} . We perform an average over 1008 random gauge domain configurations, at various temperatures, so that $n(T)/N$ ranges from its maximum to the dilute limit. Both, the system size and T are chosen sufficiently large to simulate the thermodynamic limit and a finite domain wall *density*. The limit of only few domain walls is out of reach of our methods. Fig. 3 is in stark contrast to Fig. 2. First, no DW can be observed at any temperature. This will be corroborated by results from Fig. 4. At high temperatures, where the DW in the ground state gauge is a substantial fraction of the total integrated weight, Fig. 3a) displays significant low-frequency intensity. This can be interpreted by the lifting of degeneracies necessary for a DW [26, 34], due to scattering from the random gauge domains. I.e. the corresponding weight is 'shifted' into a finite frequency range of width $\sim O(j_{x,y})$. Similar physics, of weaker intensity is visible also in Fig. 3b), where the DW in the clean case would also be smaller. Each inset in Fig. 3 details $C(|\omega| \ll 1)$, clearly evidencing a zero-frequency pseudo-gap. Based on this data it is very tempting to conclude that the DC limit of the correlation function vanishes. We emphasize, that the energy scale of the

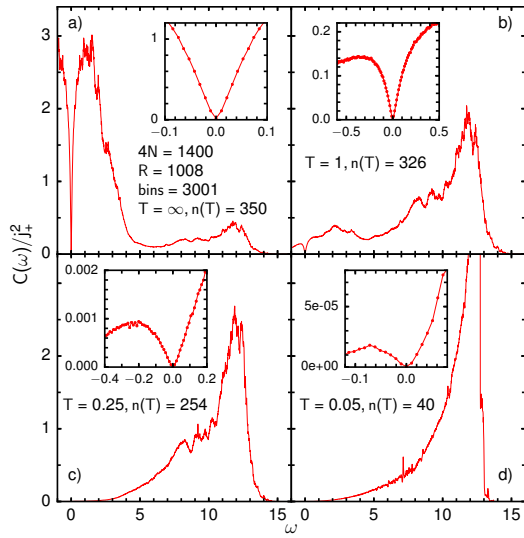


Figure 3: Current correlation function $C(\omega)$ versus frequency for $j_{x,y}=2, 1$ and various temperatures $T = \infty, \dots, 0.05$, from a) to d) corresponding to gauge domain wall numbers $n(T) = N, \dots, \ll N$. $\Delta(j_{x,y}=2, 1) \approx 0.279$. Inset: low- ω behavior.

mobility gap is unrelated to that of the ω^2 power law of gapless case in Fig. 2. The fine structure in $C(\omega)$ comprises effects of finite size and finite number of domain realizations, but also scattering from “typical” clusters of excited gauge fields, as eg. the impurity anti-bound states above the bare spectral cut-off in Fig. 3d). For consistency we note, that the overall shape and amplitude of the low- T section of Fig. 3 approaches $C(\omega)$ from Eqn. (6) at $T = 0$.

Rephrasing these findings, heat transport in the Kitaev ladder is suppressed because it comprises 1D free matter fermions scattering off a disordered static gauge potential. The absence of a DW as well as the zero-frequency pseudo-gap may be related to established [59, 60], as well as to more recent [61] theories of disordered systems. Neither the specific form of the mean density $n(T)$ nor fluctuations around it affect this physics.

(iii) *Full Hilbert space exact results:* To further substantiate our arguments, we perform numerically exact evaluations of $C(\omega)$ in the full many body Hilbert space of the original spin model, using ED on systems up to 20 spins. These are compared to an exact all gauge sector summation in the fermionic description. For the purpose of this calculation, δ -functions are approximated by Lorentzians with a half width parameter of the order of 10^{-2} . Fig. 4 shows results for $\beta = 0$. First, the agreement of the two calculations is impressive. The differences are due to the neglect of boundary terms [17] in mapping Eqn. (1) to (2). Second, these results corroborate our findings from the disorder averaging scheme, with $C(\omega)$ being in good qualitative agreement with the high temperature results presented in Fig. 3a). Note that

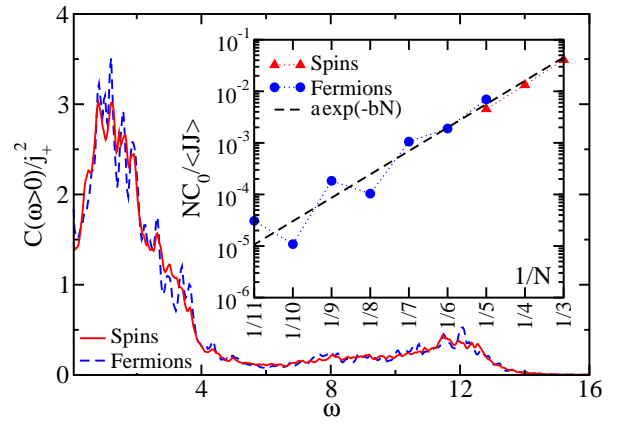


Figure 4: $C(\omega)$ from ED of the original spin Hamiltonian and from averaging over all sectors of the fermionic model obtained at $\beta = 0$ and for $N = 5$. Inset: Finite size scaling of the DW, evaluated in the spin and fermionic representations.

the seemingly finite value of $C(\omega \rightarrow 0)$ is an artifact of the Lorentzian broadening of the δ -functions combined with the step dip of $C(|\omega| \ll 1)$, observable in Fig. 3a). This cannot be captured on small systems. Inevitably for finite systems, we also find a finite DW, which however, scales to zero at least exponentially in the thermodynamic limit. This is shown in the inset of Fig. 4, where we present the normalized C_0 , on a semi-log scale, as a function of the inverse system size for both, spin and fermionic representations. Despite the odd-even effects [26, 37], as well as the boundary terms [17], we find that our data are nicely fitted by a single exponential function supporting our claim for a vanishing DW in the thermodynamic limit [62].

In conclusion we have shown that, though Kitaev ladders are translationally invariant systems, their heat transport has no ballistic channel and displays a zero-frequency pseudo gap, due to fractionalization of spins into mobile Majorana matter and static Z_2 gauge fields, which generate an emergent disorder at finite temperature. This is different from Kitaev chains in strictly $d = 1$, while similar phenomena should occur in $d \geq 2$. Many of the genuine properties of spin liquids are very susceptible to perturbations. Eg. non-Kitaev exchange can lead to dispersion of the gauge excitations or to a breakdown of the fractionalization which, to the best of our knowledge, we have probed by heat transport in the pure Kitaev case for the first time.

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