Thermal transport in a two-dimensional $\mathbb{Z}_2$ spin liquid

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We study the dynamical thermal conductivity of the two-dimensional Kitaev spin-model on the honeycomb lattice. We find a strongly temperature dependent low-frequency spectral intensity as a direct consequence of fractionalization of spins into mobile Majorana matter and a static $\mathbb{Z}_2$ gauge field. The latter acts as an emergent thermally activated disorder, leading to the appearance of a pseudogap which partially closes in the thermodynamic limit, indicating a dissipative heat conductor. Our analysis is based on complementary calculations of the current correlation function, comprising exact diagonalization by means of a complete summation over all gauge sectors, as well as a phenomenological mean-field treatment of thermal gauge fluctuations, valid at intermediate and high temperatures. The results will also be contrasted against the conductivity discarding gauge fluctuations.

I. INTRODUCTION

Thermal transport is an important tool to study elementary magnetic excitations in local moment materials. This has been demonstrated in a large variety of systems displaying excitations, which range from conventional spin waves to exotic fractional quasiparticles, including magnons \([1–8]\), triplons \([9, 10]\), spinons \([11–16]\), and emergent magnetic monopoles \([17, 20]\). Most recently, the first thermal transport measurements have appeared in systems with strong spin-orbit coupling (SOC), which are potentially proximate to 2D spin-liquid states \([21,22]\).

Quantum magnets with SOC have attracted considerable interest, because they allow for directionally dependent highly anisotropic super-exchange, which can lead to strongly frustrated quantum magnets \([23–27]\). Among them is Kitaev’s model on the honeycomb lattice \([28]\). It constitutes the rare case of a 2D spin system with an exactly known spin-liquid ground state and fractionalization of spins in terms of bulk Majorana fermions and $\mathbb{Z}_2$ gauge fields \([25,28,32]\). Part of its quantum phases are perturbatively equivalent to the toric code \([33]\), providing a direct link to paradigmatic models of topological order \([34,35]\).

In finite magnetic fields the $\mathbb{Z}_2$ vortices acquire non-abelian anyonic statistics and the Majorana Dirac spectrum opens a gap displaying a chiral edge mode \([25]\).

There is an ongoing quest for Kitaev materials with 2D honeycomb variants $\text{Na}_2\text{IrO}_3$ \([39]\), $\alpha$-$\text{Li}_2\text{IrO}_3$ \([37]\), $\alpha$-$\text{RuCl}_3$ \([38]\), and 3D polymorphs $\beta$-$\gamma$-$\text{Li}_2\text{IrO}_3$ \([39,40]\), as well as triangular lattice versions $\text{Ba}_3\text{IrT}_2\text{O}_9$ under scrutiny \([41]\). Presently, all compounds show significant non-Kitaev exchange. The role of coupling to extrinsic degrees of freedom, such as phonons, is an open issue \([29]\). In pursuit of signatures of fractionalization, an enormous amount of research has been performed on the spin dynamics in Kitaev models and materials, including the dynamic structure factor \([42,44]\), Raman scattering \([45,46]\), and nuclear magnetic resonance \([47]\). Thermal conductivity measurements on $\alpha$-$\text{RuCl}_3$ \([21,23]\) have yet been confined to the longitudinal component $\kappa_{xx}$ and reveal \([24]\) that the heat transport seems intimately related to spin-phonon coupling. Observations of putative chiral edge modes, using off-diagonal $\kappa_{xy}$ at finite magnetic fields are still lacking.

Theoretically, fractionalization has long been a topic for magnetic transport in 1D quantum magnets, due to the existence of spinons in Heisenberg chains and dimerized or frustrated variants thereof \([48,49]\). One key question is the dissipation of currents, which has been investigated extensively at zero frequency (dc) and momentum in connection with the linear response Drude weight (DW) \([50,51]\), which is the non-dissipating dc part of the current autocorrelation function and, if existent, indicates a ballistic channel of the fractional quasiparticles.

First theoretical studies of heat transport in Kitaev models have been carried out on chains \([57]\) and ladders \([58]\) with very different conclusions. In the former, gauge fields are absent and the chain is found to be a perfect, ballistic heat conductor with a finite thermal DW. The ladder is the simplest quasi-1D descendant of the honeycomb lattice model featuring both, matter fermions and $\mathbb{Z}_2$ gauge fields. It is found to display no ballistic channel and a zero frequency insulating pseudogap. This is a direct consequence of fractionalization, with the static gauge fields acting as an emergent, thermally induced disorder, which scatters the current carrying mobile Majorana matter. Since dimensionality of the Majorana matter could have a significant impact on the scattering from the gauge field, the prime motivation of the present work is to extend the ideas of Ref. \([58]\) to 2D. As our central results, we find that similar to Ref. \([58]\), ballistic channels are suppressed and finite low-frequency spectral weight is generated in the dynamical conductivity by scattering from the gauge field. However, in sharp contrast to the ladder, the pseudogap does not fully survive the thermodynamic limit in 2D, leading to a dissipative heat conductor, rather than an insulator.
The paper is organized as follows. In Section II we provide details of the Kitaev model as needed for this work. In Section III we summarize magnetic heat transport theory in the linear response regime. In Section IV we present and compare our results, derived from three complementary methods, i.e. exact diagonalization (ED), Sec. IV A; average gauge configuration (AGC) calculations, Sec. IV B; and zero vortex sector (ZVS) analytic evaluations, Sec. IV C. Lastly, Sec. V contains our conclusions.

II. KITAEV MODEL

In this section we briefly summarize several points, clarifying the use of Kitaev’s model [28] in this work. The Hamiltonian reads

\[ H = \sum_{\langle l,m \rangle, \alpha(l,m)} J_\alpha \sigma^\alpha_l \sigma^\alpha_m, \]  

where \( \langle l,m \rangle \) refers to the sites on the nearest neighbor bonds of the honeycomb lattice. For simplicity, in this work, we will envisage the honeycomb lattice to be deformed into the so-called brickwall lattice (BWL) [29,30], shown in Fig. 1. \( J_\alpha \) and \( \sigma^\alpha \) are the exchange coupling constants and Pauli matrices respectively for coordinates \( \alpha = x, y, z \). The relation \( \alpha(\langle l,m \rangle) \) can be

\[ J_\alpha \text{referred to the left by } 45° \text{, with unit vectors } e_x, e_y \text{ (light blue shaded region). The exchange interactions for the ESL are } J_x \text{ and } J_y \text{ along the } e_x \text{ and } e_y \text{ directions respectively. The flux operator } \Phi_j \text{ of the } j\text{-th plaquette is the product of the } 6 \text{ spin operators around the plaquette, as shown in the dark yellowish highlighted region. The eigenvalue of the flux operator on that plaquette is equal to the product of the two corresponding } \eta \text{ fields belonging to the same plaquette, i.e., } \Phi_j = \prod_{l=1}^6 \sigma_{jl}^{\alpha(l)} = \eta_{j,1} \eta_{j,2}. \]

read off from the red, green, and blue bond coloring in Fig. 1. It is known that this model can be mapped onto free spinless (‘matter’) fermions in the presence of static \( Z_2 \) gauge fluxes. The allowed values \( \pm 1 \) of the latter are related to the eigenvalues of the conserved operator \( \Phi = \prod_{l=1}^6 \sigma_{jl}^{\alpha(l)} \) around each plaquette, Fig. 1, where \( \alpha(l) = x, y, z \), refers to that component of the exchange link which is not part of the loop passing site \( l \) [28]. For the remainder of this work we set \( h, k_B, \) and the lattice constant \( a \) to unity, and choose \( J_z \) as the unit of energy.

Several routes have been established to map the spins in Eq. (1) to fermions, e.g. using overcomplete sets of Majorana fermions [28], Jordan-Wigner transformation [29,30], or bond algebras [31]. The resulting final Hamiltonian reads [30]

\[ H = \sum_r h(r), \tag{2} \]

with \( h(r) \) the single particle local energy

\[ h(r) = J_x(d_r^+ + d_r)(d_{r+e_x}^+ - d_{r+e_y}) + J_y(d_r^+ + d_r) \times(d_{r+e_y}^+ - d_{r+e_x}) + J_z \eta_r(2d_r^+d_r - 1). \tag{3} \]

\( d_r^+ \) and \( \eta_r = \pm 1 \) refer to the spinless matter fermions and the gauge fields, which can be visualized to be located on the sites of a dual lattice of the \( z \)-bonds of the BWL, forming an effective square lattice (ESL), Fig. 1. In the fermionic representation \( \Phi_r = \eta_r \eta_{r+e_x} \) for the brickwall lattice, and \( \Phi_r = \eta_r \eta_{r+e_y} \) for the ESL. From the preceding, it is rather apparent that the ESL model lacks \( C_4 \) symmetry and the two diagonal directions \( e_x \pm e_y \) are distinct.

While the focus of our work is on bulk transport properties, we state three remarks of caution regarding boundary conditions. First, the mapping from Eq. (1) is exact only if periodic boundary conditions (PBCs) are used along the \( e_x \) direction of the BWL [29,30]. Requiring PBCs also along the \( x, y \)-chains (\( e_1 \) direction of the BWL), requires consideration of surface terms [30,32], as known from any Jordan-Wigner type of mapping. It has been shown recently, that for bulk thermal transport on Kitaev ladders such surface terms have no relevant effect [58], and therefore we discard them. Second, to describe bulk properties based on the ESL, it is natural to apply PBCs along the \( e_x, e_y \) directions of the lattice. This implies nonstandard \( O(1/L) \) finite size corrections for a system of \( N = L \times L \) sites. We do not expect these to be of any qualitative relevance. Third, and finally, the spectrum of the Kitaev model is highly degenerate. The relevance of this for the current correlation function is briefly commented on in App. A.
III. THERMAL TRANSPORT

The primary goal of this work is to evaluate the dynamical equilibrium \textit{bulk} thermal conductivity of the Kitaev model. In this section, and for completeness, we recollect the basic ingredients for this.

To start, linear response theory with respect to a real space dependent local equilibrium temperature \(T + \delta T(r)\) has to be performed, based on a canonical density matrix \(\rho = \exp[-\int d^3 r \left(\beta + \beta \delta T(r)\right) h(r)]\), where \(\beta = 1/T\), and \(h(r)\) is a local energy density which has to fulfill \(H = \int d^3 r h(r)\), where \(H\) is the Hamiltonian. In this framework, the linearized expectation value of the \(\mu\) component of the energy current \(J_{\mu}\) in \(d\) dimensions is obtained from the dynamical thermal conductivity tensor \(\kappa_{\mu\nu}(q, \omega)\) at wave vector \(q\) and frequency \(\omega\) through

\[
\langle J_{\mu}(q, \omega) \rangle = \sum_{\nu=1}^{d} \kappa_{\mu\nu}(q, \omega) \partial_\nu T(q, \omega). \tag{4}
\]

The equilibrium thermal expectation value \(\langle A \rangle\) reads \(\langle A \rangle = \text{Tr} A e^{-\beta H}/Z\), with \(Z = \text{Tr} e^{-\beta H}\) the partition function. The spectrum \(\kappa_{\mu\nu}(\omega)\), namely the real part of the thermal conductivity, follows from the Fourier transform of the current correlation function, \(C_{\mu\nu}(\omega)\),

\[
\kappa'_{\mu\nu}(\omega) = \frac{\beta}{2\omega} \left(1 - e^{-\beta \omega}\right) C_{\mu\nu}(\omega), \tag{5}
\]

\[C_{\mu\nu}(\omega) = \int dt e^{i\omega t} C_{\mu\nu}(t), \quad C_{\mu\nu}(t) = \frac{1}{N} \langle \dot{J}_{\mu}(t)J_{\nu} \rangle. \tag{6}\]

It is customary to decompose \(C_{\mu\nu}(\omega)\) as \[C_{\mu\nu}(\omega) = 4\pi D_{\mu\nu} T^2 \delta(\omega) + C_{\mu\nu}^{eg}(\omega), \tag{7}\]

where the \textit{regular} part refers to \(C_{\mu\nu}^{eg}(\omega) = C_{\mu\nu}(\omega \neq 0)\) and the \textit{Drude} weight (DW) \(D_{\mu\nu}\) is a measure for the ballistic contribution to the heat flow

\[
D_{\mu\nu} = \frac{\beta^2}{2Z^2} \sum_{E_l = E_m} e^{-\beta E_l} \langle \{J_{\mu}(m)\{m|l\}\rangle. \tag{8}\]

Because of Eq. (5), \(\kappa'_{\mu\nu}(\omega) = 2\pi D_{\mu\nu}\delta(\omega) + \kappa_{\mu\nu}^{eg}(\omega)\). Whenever \(D_{\mu\nu} \neq 0\), the system is a perfect heat conductor in channel \(\mu\nu\). Otherwise it is a dissipative conductor with a limiting dc heat conductivity of \(\kappa_{\mu\nu}^{dc} = \kappa'_{\mu\nu}(\omega \to 0)\). If both, \(D_{\mu\nu} = 0\) and \(\kappa_{\mu\nu}^{dc} = 0\), the system is an insulator in channel \(\mu\nu\).

To determine the energy current \(\mathcal{J}\) we turn to a real space version of the continuity equation \(\partial_t h(r) + \nabla \cdot \mathcal{J}(r) = 0\), which is more amenable to describe the spinless fermions of Hamiltonian \[H = H_d\] and \[H = H_{\mu\nu}\], which comprise a real space dependent potential by virtue of \(\eta_r\). To this end we use the polarization operator \[P = \sum_r r h(r)\],

\[
\mathcal{J} = i[H, P], \quad \text{with} \quad P = \sum_r r h(r), \tag{9}\]

which yields the same current operator as the continuity equation in the limit of \(q \to 0\) for a homogeneous system. For the Kitaev model on the ESL and using our \textit{definition} of the energy density, given in Eq. (3), we arrive at the energy current

\[
\mathcal{J}_{\mu} = 2i\mu \sum_r \left[ J_z \eta_r b_r b_{-\mu} + \tau_{\mu} J_y \eta_y b_r + e_{\mu} \right], \tag{10}\]

where \(b_r = (d_r^+ + d_r^-)\), \(\mu = y(x)\) and \(\tau_{\mu} = +(-)\) for \(\mu = x(y)\). From the expression above, one can readily see that also the energy current operator is diagonal in the gauge fields.

We caution that the only requirement for \(h(r)\) is that \(H = \int d^3 r h(r)\). This may be a reason for differing \textit{quantitative} results for the Drude weight and the regular conductivity spectrum, obtained in recent studies of various frustrated and spin ladder models \[54-61\]. However, it is generally believed that universal \textit{qualitative} statements, concerning the existence or absence of finite Drude weights and dc conductivities are insensitive to the freedom of choice for the energy density.

IV. EVALUATION OF HEAT CURRENT CORRELATION FUNCTIONS

Even though Kitaev’s model comprises free fermions, the distribution of the \(\eta_r\) in real space, renders analytical evaluation of thermal traces infeasible. Numerically, quantum Monte-Carlo (QMC) methods have been used for a variety of observables \[63-65\]. Regarding thermal transport, to the best of our knowledge, exact diagonalization (ED) \[58\], summing over all gauge configurations, supplemented also by approximate methods, has been used first to evaluate \(C_{\mu\nu}(t)\) for the Kitaev Hamiltonian on a ladder \[58\]. Here we will extend this work to \(d=2\) dimensions analyzing the \textit{longitudinal} heat transport properties, i.e. \(C_{\mu\nu}, \kappa'_{\mu\nu}\), and \(D_{\mu\nu}\), at finite temperatures, using unbiased exact diagonalization, as well as an approximate ensemble of average gauge configurations. In addition, we perform an illustrative evaluation of \(C_{\mu\nu}(\omega)\), and \(D_{\mu\nu}(T)\) based on only the uniform gauge. In following, we focus on the isotropic gapless point \(J_x = J_y = J_z\) unless mentioned otherwise.

A. Exact diagonalization (ED)

Since the energy current operator is diagonal in the gauge field, the correlation function \(C_{\mu\nu}(t)\) can be written as

\[
C_{\mu\nu}(t) = \frac{1}{ZN} Tr_{\eta} \left[ Z_{d(\eta)} \langle J_{\mu}(t)J_{\nu}\rangle_{d(\eta)} \right], \tag{11}\]

where \(N\) is the number of lattice sites, the subscript \(d(\eta)\) refers to tracing over matter fermions at a \textit{fixed} gauge
field state and the subsectors’ partition functions $Z_{d(\eta)}$ sum up to the total partition function $Z$. To numerically evaluate Eq. (11), we resort to ED. To this end, we define a $2N$ component operator $D^\dagger = (d_1^\dagger, ..., d_N^\dagger, a_1^\dagger, ..., a_N^\dagger)$ of the matter fermions. The indices $\{1, 2, ..., N\}$ label all sites $r$ of the ESL. In terms of $D^\dagger$ the Hamiltonian and the current are set up in real space as $H = D^\dagger h(\eta) D$, and $J_\mu = D^\dagger J_{\mu}(\eta) D$. Both $h(\eta)$ and $J_{\mu}(\eta)$ are $2N \times 2N$ matrices, which depend on the actual state of the gauge field $\eta = (\eta_1, \eta_2, ..., \eta_N)$. For each given $\eta$ we compute a Bogoliubov transformation $U$, which introduces canonical quasiparticle fermions $A^\dagger = (a_1^\dagger, ..., a_N^\dagger, a_1, ..., a_N)$ via $A = U^\dagger D$ and maps the Hamiltonian to $H = \frac{1}{2} A^\dagger E A$, where $E$ is diagonal and $\text{diag}(E) = (\varepsilon_1, ..., \varepsilon_N, -\varepsilon_1, ..., -\varepsilon_N)$, with $\varepsilon_j$ being the quasiparticle energies.

With these definitions, the current correlation function in a fixed gauge configuration reads

$$C^\eta_{\mu\mu}(\omega) = \frac{2\pi}{N} \sum_{klmn} L_{klm} \langle A_k^\dagger A_n \rangle \langle A_l A_m^\dagger \rangle \delta(\varepsilon_l - \varepsilon_k - \omega),$$

where $L = U^\dagger (\eta) U$ and $\langle A_{\mu}^{(1)} A_{\nu}^{(1)} \rangle$ is either zero, $f_j$, or $(1 - f_j)$, depending on the components of the spinor $A$ involved, and $f_j = 1/(e^{\varepsilon_j} + 1)$ is the Fermi-Dirac distribution. Since the partition functions $Z_{d(\eta)}$ are byproducts of the ED for each gauge subsector, tracing the latter and Eq. (9), as in Eq. (11) completes the evaluation of $C_{\mu\mu}(\omega)$.

In Fig. 2 we present the frequency dependence of the correlation function $C_{\mu\mu}(\omega)$ for three temperatures $T/J_z = 0.1, 2, 100$. We note that we focus only on the positive frequency spectrum, $\omega > 0$, because $C_{\mu\mu}(-\omega) = e^{-2\delta\omega} C_{\mu\mu}(\omega)$, as required by detailed balance. To reduce the computational effort for the evaluation of full traces over the $2^N$ possible gauge field configurations, we make use of translation symmetry. This allows us to reach systems up to $N = 36$ sites corresponding to an enormous Hilbert space dimension of the underlying spin model of $2^{72}$ states. The $\delta$ functions are binned in windows of $\delta\omega = 10^{-3}$, except for the lowest temperature, $T/J_z = 0.1$, at which a binning of $\delta\omega = 0.02$ has been chosen due to the larger finite size effects. The sharp peaks at finite frequencies are amplified by the very fine binning, and they are not expected to survive in the thermodynamic limit.

For all temperatures $T/J_z \gtrsim 1$ the spectrum is qualitatively different from that discarding gauge excitations, which will be analyzed in Section IV.C see Fig. 7. We understand this central result to be a clear indication of fractionalization, where the matter fermions scatter off gauge field degrees of freedom, with the latter acting as a thermally activated disorder. In fact, Eq. (12) allows for two types of spectral contributions, namely quasiparticle, i.e. $\varepsilon_\ell \varepsilon_k > 0$, or pairbreaking, i.e. $\varepsilon_\ell \varepsilon_k < 0$ transport. The high frequency spectral weight $(\omega/J_z \gtrsim 6)$ in Fig. 2 is solely generated by the pairbreaking terms, and it is only quantitatively affected by the gauge disorder. Contrarily, the quasiparticle contribution is related to the matter fermion density relaxation and therefore is strongly affected by scattering from the gauge fields. In the ground state gauge, the complete quasiparticle transport will accumulate into only a single $T$-dependent DW, see Sec. IV.C. In the presence of the gauge excitation however, most of the DW spreads over a finite low-$\omega$ range, which displays an increasing weight in Fig. 2 as $T$ increases. The latter is due to the temperature dependence of the matter fermion occupation number. We note that on any finite systems remnants of a DW will remain within the spectrum.

At very low temperatures, $T/J_z \lesssim 0.1$ the gauge excitations will start to freeze out and the correlation function will approach the form of $C_{\mu\mu}(\omega)$ within the ground state sector, Fig. 4. This regime suffers from large finite size effects and it is difficult to be tackled with our methods (see also the discussion in the context of Fig. 4).

The low-$\omega$ spectral hump in the correlation function displays a clearly visible, sharp dip as $\omega \to 0$, with $C(\omega \to 0) \approx 0$, as can be read off from Fig. 2(b). This is particularly obvious at elevated temperatures. The behavior of this low frequency pseudogap with system size is crucial in order to characterize the system as conducting or insulating in the thermodynamic limit, and requires a careful finite size analysis. Either the pseudogap will close as $L \to \infty$ and the system will have a conducting dc channel, or the pseudogap remains open. In the latter case the system will be characterized by the presence(absence) of a finite DW as an ideal conductor(insulator). These issues relate the system directly to questions of disorder in Dirac semi-metals [66, 67]. While our ED provides clear evidence for signatures of
fractionalization in the dynamical correlation function, a convincing answer to the behavior of the pseudogap with system size requires larger lattices, which we will tackle with the average gauge configuration approach, presented in Sec. [V.B]

Next, we focus on the temperature dependence of the ballistic contribution to the thermal conductivity, namely the DW, Eqs. (7), and (8). In Fig. 3 we present the temperature dependence of the DW for three different system sizes, acquired from the degeneracy plateau as usual [68]. The general form of the temperature dependence of the DW is that of a typical spin system exhibiting a maximum around $T \approx J_z$. With increasing system size, the magnitude of the DW is reduced. Note that this is different from the behavior of the DW obtained for other transport quantities in Ref. [65]. Although the system sizes at hand do not allow for a safe finite size extrapolation, our findings are suggestive of a vanishing DW in the thermodynamic limit. This picture is further corroborated by the AGC method, presented in Sec. [V.B] [69].

B. Average gauge configuration (AGC)

In this section, we introduce an approximate method to evaluate the current correlation function, capturing the main physics, and allowing to reach systems of $\sim 60 \times 60$ sites, i.e. $\sim O(100)$ larger than with ED, which is crucial to understand the low frequency regime of the correlation function. The main idea is to reduce the full trace $Tr_{\eta} \ldots$ to an average $\langle \ldots \rangle_{n(T)}$ over only dominant gauge configurations, set by a temperature dependent mean density $n(T)$ of elementary gauge excitations off the gauge ground state. I.e., we reduce the evaluation of $C_{\mu\mu}(t)$ to a disorder problem in a system of free fermions with an emergent temperature dependent defect density

$$C_{\mu\mu}(t) \approx \langle (J_{\mu}(t)J_{\mu})d(\eta) \rangle_{n(T)}.$$  

Several comments are in order for this approach. First, while the Hamiltonian (2-3) is formulated in terms of matter fermions and gauge fields $\eta$, the physical degrees of freedom are rather fermions and fluxes. In turn, depending on the temperature, fluctuations in $n(T)$ may be very large, rendering a mean field treatment in terms of the number of excited fluxes $\Phi(T)$ more appropriate. On the Kitaev ladder [58], this can be achieved by a direct mapping between $n(T)$ and $\Phi(T)$. On the honeycomb lattice this is not feasible. To make progress, we confine ourselves to temperatures above a scale $T_R$, which is elevated enough, such that a large number of fluxes is excited. Then, random gauge and flux ensembles will both behave similarly.

To approximate the scale $T_R$, we evaluate $n(T)$ and its fluctuations $\delta n(T)$, $\Phi(T)$ and its temperature derivative $\Phi'(T)$, as well as a thermodynamic observable, namely the specific heat $C_V$ exactly on a finite system of $N = 6 \times 6$ sites. We use

$$n(T) = \frac{1}{ZN}Tr_{\eta}Z_{d(\eta)}n_\eta,$$  

where $Z_{d(\eta)} = \sum_{\eta} e^{-\beta \Phi(\eta)}$ is the partition function of the averaged gauge configuration.

![Figure 3](image3.png)

Figure 3. Drude weight $D_{\mu\mu}(T)$ versus temperature for three different system sizes obtained via ED.

![Figure 4](image4.png)

Figure 4. (a) Temperature dependence of the mean density of gauge excitations $n(T)$, and the flux density $\Phi(T)$. A fit, $n(T) \sim 1/[\exp(\Delta/\Theta) + 1]$ is shown, with $\Delta = 0.06$, and $b = 3.5$. The infinite temperature limit of $n(T \rightarrow \infty) = n_{\infty} = 0.434$ is marked by a horizontal gray dashed line [69]. (b) Temperature dependence of the fluctuations of the mean density of gauge excitations $\delta n(T)$ and the derivative of the flux density $\Phi'(T)$ normalized to its minimum value at the cross over temperature $\Phi'(T_m) = -15.16$. Vertical dashed gray line: location of $T_m \approx 0.06J_z$. In addition, the specific heat is shown, obtained from ED and from the AGC methods, labeled accordingly. For the AGC, $n(T)$ as fitted to the ED result is used. All ED data from an $N = 6 \times 6$ sites system. The AGC data from an $N = 20 \times 20$ system, with $N_R = 20000$ realizations.
where \( n_q \) is the number of gauge fields flipped off the uniform ground state sectors, excluding degenerate ground state sectors. The flux density is defined by

\[
\Phi(T) = \frac{1}{ZN} \sum_{\{\eta_r\}} Z_{d(\eta)} \sum_r \Phi_r, \quad \Phi_r = \eta_r \eta_{r+s} \eta_{r+s}.
\]

First, Fig. 4(a) shows that at very low temperatures, \( n(T) \) and \( \Phi(T) \) represent the gauge homogeneous ground state. Second, at temperatures \( T/J_z \sim 0.03 \), well below the single gauge flip gap \( \Delta_1/J_z \approx 0.263 \) [28], collective gauge excitations lead to a rapid increase of \( n(T) \), a downturn of \( \Phi(T) \), and a region of large fluctuations \( \delta n(T) > n(T) \). Third, and for \( T \geq 0.1J_z = T_R \), the system has essentially settled into a completely random gauge state with its proper infinite temperature limiting value of \( n_\infty \approx 0.434 \) for \( N = 6 \times 6 \) [69]. In this regime the system can be considered as free fermions scattering from a fully random binary potential.

In the crossover region \( n(T) \sim 1/[e(\Delta/T)^b + 1] \) with \( \Delta = 0.06 \), and \( b = 3.5 \) for the finite system [70]. This rather abrupt transition is likely due to gauge-gauge interactions and the large degree of degeneracy of the gauge fields for a given number of fluxes [71]. Considering the specific heat \( C_V \) in Fig. 4(b), there is a clear release of entropy of the fluxes or the gauges in the vicinity of \( T_m \approx 0.06J_z \) [65] [73]. In view of \( \delta n(T)/n(T) \) versus \( T \), as in Fig. 1(a,b), the AGC will work acceptably well for \( T \gtrsim T_R \). An indication of this is provided by evaluating the specific heat \( C_V \) within the AGC, using \( n(T) \) as from the ED, averaging over \( N_R = 20000 \) realizations, for a system with \( N = 20 \times 20 \). Obviously the agreement to the exact result is excellent down to \( T \approx T_R \), below which the AGC does not account for all of the entropy release. To conclude: we confine all subsequent AGC calculations to \( T_R \lesssim T < \infty \), using a fully random \( \eta \) ensemble, i.e. \( n(T) = 0.5 \).

In Fig. 5 we present the energy current correlation function obtained via the AGC method spanning three decades of temperature \( T/J_z = 0.1, 2.1, 100 \) and a binning of \( \delta \omega = 0.001 \). The left panels of the plot highlight the low frequency behavior of \( C_{\mu\mu}(\omega, T) \) while the right ones scan the complete positive frequency range. First, the qualitative and quantitative agreement between the ED and the AGC method for all temperatures shown is remarkable [68]. At high temperatures there is a low frequency hump, the weight of which reduces with temperature due to the occupation numbers of the matter fermions. At the same time, and since the sum rule does not change with temperature, more weight is accumulated at high frequencies, as in Fig. 2.

The left panels of Fig. 5 show, that apart from a smooth downturn at \( \omega/J_z \approx 1 \) there is a second, sharp dip structure within a very low energy range of \( \omega/J_z \ll 1 \). This narrow part of the pseudogap displays a strong system size dependence, in stark contrast to the rest of the frequency spectrum, for which larger system sizes merely render the spectra smoother. It is interesting to note that the system sizes which can be reached by ED do not display this low frequency structure, Fig. 5(e), rendering the use of the AGC method essential [68]. This low-\( \omega \) behavior with system size very much suggests the pseudogap to close in the thermodynamic limit. Therefore we extract a dc limit of the correlation function by fitting the data shortly before the dip. Because of the slight curvature within the data, we choose to fit a second order polynomial in the range [0.02 – 0.12], incorporating 100 frequency points, see also the inset of Fig. 5(d) and its discussion. The dc limit extrapolation for all three temperatures is marked by the gray arrows at the right panels of the plot. In addition, we note that we did not find any Drude weights for the systems analyzed [68]. In conclusion the system will be a normal dissipative conductor in the thermodynamic limit.

Next, in Fig. 6, we present the temperature dependence of the dc thermal conductivity, Eq. (5), for different system sizes. The overall behavior of \( \kappa_{dc}(T) \) versus \( T \) is typical for spin systems. It features a maximum at

\[
\kappa_{dc}(T) \approx \frac{1}{N^2} \sum_{\{\eta_r\}} Z_{d(\eta)} \sum_r \Phi_r, \quad \Phi_r = \eta_r \eta_{r+s} \eta_{r+s}.
\]
As compared to the previous sections, fixing the gauge to a ground state configuration, allows to obtain analytic expressions for the conductivity. While in principle this only represents the limit $T/\Delta \to 0$, it can nevertheless be used to check the approach to low temperatures of the ED and AGC results. Moreover it is instructive, to contrast a fictitious heat conductivity at $T/J_z = 0.1$, $N=40 \times 40$, and between $1$ and $2$ order polynomial to the low frequency regime of the correlation function. In the insets (b) and (c) this low frequency behavior of $C(\omega)$ for a system of $L=40$ at two temperatures $T/J_z = 0.1$, $N=40 \times 40$, and $T/J_z = 100$, $N=40 \times 40$, is shown, as well as, the corresponding linear and quadratic fit functions. The fitting range is restricted in the range $0.02 \leq \omega/J_z \leq 0.12$ for all the fits.

\[ H = \sum_k \mathbf{D}_k \mathbf{h}_k \mathbf{D}_k^\dagger, \quad J_\mu = \sum_k \mathbf{D}_k^\dagger \mathbf{L}_{k,\mu} \mathbf{D}_k, \]

where boldface $\mathbf{D}_k = (d^\dagger_k, d_k)$ are ‘spinors’, with $d_k^\dagger = \sum_k \exp(-ik \cdot r) d_k^\dagger$. We label the two entries by light symbols $\mathbf{D}_{k\alpha}$, with $\alpha = 1, 2$. Note that $\mathbf{D}_{k\alpha}$ are destruction(creation) operators depending on $\alpha = 1(2)$. Both, the Hamiltonian and current matrix elements, $h_k$ and $L_{k,x(y)}$ for the $x(y)$-directions are encoded in $2 \times 2$ matrices. From Eqs. (2), (3), and (10) we get

\[ h_k = \begin{bmatrix} e_k & i\Delta_k \\ i\Delta_k^* & -e_k \end{bmatrix}, \quad L_{k,\mu} = \mathbf{l}_{k,\mu} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{17} \]

where,

\[ e_k = 2[J_z - (J_x \cos(k_x) + J_y \cos(k_y))], \tag{18a} \]
\[ \Delta_k = 2(J_x \sin(k_x) + J_y \sin(k_y)), \tag{18b} \]
\[ l_{k,\mu} = 2[J_{\mu} J_z \sin(k_\mu) - J_x J_y \sin(k_\mu - k_\tau)], \tag{18c} \]

with $\bar{\mu} = y(x)$ for $\mu = x(y)$. After Bogoliubov transformation onto $h_k$’s quasiparticle (QP) basis $c^{\dagger}_k$, the Hamiltonian reads

\[ H = \sum_k \varepsilon_k(c_k^\dagger c_k - 1/2), \quad \varepsilon_k = \sqrt{e_k^2 + \Delta_k^2}. \tag{19} \]

Remarkably, the current operator is invariant under this Bogoliubov transformation. I.e. also in the QP basis $\mathcal{J}_\mu = \sum_k \mathcal{C}_k^\dagger \mathbf{L}_{k,\mu} \mathbf{C}_k$, with $\mathbf{L}_{k,\mu}$ identical to Eq. (17) and $\mathbf{C}_k = (c^{\dagger}_k, c^{\dagger}_{-k})$. Since $\mathbf{L}_{k,\mu}$ is not diagonal, the energy current has both, QP and pairbreaking contributions. It is satisfying to realize that $2l_{k,\mu} = \varepsilon_k \partial \varepsilon_k/\partial k_\mu$. Therefore, and because of Eqs. (16), and (17), the naive expectation that the energy current can be written as

\[ \mathcal{J}_\mu = \sum_k \varepsilon_k \frac{\partial \varepsilon_k}{\partial k_\mu} c_k^\dagger c_k + \text{pair breaking terms}, \tag{20} \]

is indeed satisfied by our definition of the local energy density Eq. (3).

Evaluating the current correlation function in the QP basis is straightforward. We get

\[ C_{\mu\mu}^n(\omega) = \frac{2n}{N} \left\{ \frac{1}{2} [2l_{k,\mu}]^2 [2f_k(1 - f_k) \delta(\omega) + f_k^2 \delta(\omega + 2\varepsilon_k) + (1 - f_k)^2 \delta(\omega - 2\varepsilon_k)] \right\}. \tag{21} \]

Where the superscript $0$ refers to the ground state gauge, the term $\sim \delta(\omega)$ represents the DW, and the remaining two addends are the pairbreaking contributions.

Figure 7(a) shows $C_{\mu\mu}^0(\omega)$ for two representative cases of $J_{x,y}/J_z = 1$ $(J_{x,y}/J_z = 0.25)$ referring to a gapless (gapped) matter sector. Several comment are in order. First, the regular spectrum at small $\omega$ reflects the gap structure of the low energy quasiparticle DOS combined with the energy current, leading to a power law $C_{\mu\mu}^0(\omega) \propto \omega^3$ in the gapless case, while displaying a linear onset above a finite gap. Second, within the spectrum a weak van-Hove singularity arises from the saddlepoint of

\[ \begin{array}{c}
\end{array} \]
Majorana matter and static gauge fields leaves a clear fingerprint on the spectrum of the current correlation function. In fact, thermally populated gauge excitations serve as an emergent disorder inducing an intrinsic energy scale for the relaxation of the matter fermion heat currents. This relaxation leads to a clearly observable low-$\omega$ accumulation of spectral weight in the current correlation function, increasing in intensity as the matter fermion density increases with temperature. We find this low-$\omega$ spectral weight to display a zero frequency pseudogap, which is strongly system size dependent. Based on finite size scaling, we have concluded that in the thermodynamic limit, part of the pseudogap closes, rendering the dc limit of the correlation function finite, albeit leaving a very sharp low-$\omega$ depletion within the spectrum behind. Therefore we have shown the 2D Kitaev model to be a normal dissipative heat conductor. This is in stark contrast to the Kitaev ladder, which is an insulator with a vanishing Drude weight and dc limit of the dynamical conductivity [58], as well as the one dimensional Kitaev chain, which is a ballistic conductor [57] and features a finite Drude weight (DW). We find, that for the 2D Kitaev model, the DW is finite only on small systems or when gauge excitations are completely neglected.

We caution that our finite size analysis cannot exclude extreme scenarios, in which at system sizes way beyond our reach, the pseudogap ceases to close and/or alters its variation with $\omega$, such as to remain with a zero dc conductivity.

While current materials, proximate to the Kitaev model display a heat transport, intricately intertwined with lattice degrees of freedom [21][23], it will be interesting to see if future systems might show Majorana matter heat transport as depicted in Fig. 6.

VI. ACKNOWLEDGMENTS

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Note added. – After completion of this work, we have become aware of related work by J. Nasu, J. Yoshitake, and Y. Motome. [arXiv:1703.10395]

Appendix A: Degeneracies

This appendix highlights the role of the degeneracies of the Kitaev model with respect to the observable considered, namely the heat current correlation function. First, we recapitulate that the spectrum of the Kitaev model is highly degenerate. This is due to the fact that a ‘chain-flip’, i.e. inverting the sign of $\eta_r$ located on all $z$-links at-
tached to any particular $xy$-chain is a unitary transformation \$2\$, leaving the fermionic spectrum invariant. We emphasize, that this degeneracy is a physical property and unrelated to spurious states which arise in some of the mappings \$2\$ from spins to fermions and $\mathbb{Z}_2$ fields for the Kitaev model. While only the case of open boundary conditions (OBCs) along the $xy$-chains is considered in Ref. \$2\$, the degeneracy remains in place using Eqs. \$2\$, and \$3\$ with PBCs on the torus and also for our square lattice geometry.

On any finite system of $N = L \times L$ sites, and restricting to even $L = 2k$ with $k \in \mathbb{N}$ hereafter, chain-flips will render each gauge configuration $2^{L-1}$ fold degenerate. On these finite systems, the ground state is either within the manifold of $\eta_r = 1 \forall r$ \$2\$, the homogeneous sector, or in a homogeneous sector, except for one ‘line-flip’, i.e. with $\eta_r = 1 \forall r$, except for a single ladder of $z$-links with $\eta_r = -1$. The energies $E_{\omega}(\eta)$ of these two types of configurations are the two lowest of the system. For a $4 \times 4$ system these two gauge sectors are shown in Fig. \$8\$ (a),(b). Fig. \$8\$ (c) shows the collapse of the ground state energies for these two lowest energy sectors versus $L$. As $L \to \infty$ this implies a $2^L$-fold degeneracy. Following the same logic, all energies of the model are at least $2^L$-fold degenerate in the thermodynamic limit.

The main point of this appendix is to exemplify, that not only the Hamiltonian, but also the physical observable $C_{\mu\mu}(\omega)$ is invariant under chain-flip operations. In Fig. \$8\$ (d,e) we show this for two sets of degenerate gauge configurations on a $4 \times 4$ system. Fig. \$8\$ (d) depicts $C_{\mu\mu}(\omega)$, using the first two gauge configurations from Fig. \$8\$ (a), while Fig. \$8\$ (c) employs the latter two gauges, with however gauge fields flipped on the two red sites. Obviously $C_{\mu\mu}(\omega)$ is identical within each of the two sets of gauges. Therefore, in the thermodynamic limit, the trace over $\eta$ in Eq. \$11\$ can in principle be restricted to one of the $2^L$ identical subtraces over gauge sectors, which are equivalent up to all chain-flip operations and a single line-flip.

**Appendix B: ED vs AGC for a small system**

In this appendix we make a direct comparison of the ED, Sec. \$V\$A and the AGC, Sec. \$V\$B methods for a small system of $N = 6 \times 6$ sites. In Fig. \$9\$ we plot the correlation function $C_{\mu\mu}(\omega)$, obtained via the ED and the AGC methods at three different temperatures $T/J_z = 0.1, 2, 100$ (from top to bottom). To anticipate finite size effects arising from the large mean level spacing of a system with a small linear dimension, we average over $N_B = 50000$ random configurations with $n(T) = 0.5$. At high temperatures and down to $T \approx J_z$, the agreement between the two methods is impressive. Not only is the overall behavior of $C_{\mu\mu}(\omega)$ quantitatively captured by the AGC method but also the fine structure yielded by singularities at the density of states. At the lowest temperature of $T = 0.1 J_z$, the AGC method clearly deviates from the exact high frequency structure of the correlation function, however the low frequency region $\omega < 4 J_z$ is still captured rather well.

Figure \$9\$ fortifies the physical conclusions extracted in the main text in the following two important aspects. First, it shows that the AGC method is capable of detecting the existence of a finite Drude weight (DW), although it fails to predict the correct weight of it. The latter does not come as a surprise since the evaluation of the DW involves only degenerate states and the AGC method is a random averaging approach. Therefore, the
absence of any trace of a DW for the larger systems displayed in Fig. 5 shows that the DW decays fast with system size, and the weight of the ballistic channel completely disappears in the thermodynamic limit. Second, Fig. 9 provides additional support for the notion of a closing of the low frequency dip with system size extracted from the AGC. Namely, according to Fig. 5 ED displays only a very shallow pseudogap. However Fig. 9 proves, that this is not at variance with the AGC, but solely due to the smaller system size of ED—which in turn we have overcome by using the AGC method.

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