Thermal Transport in a one-dimensional $\mathbb{Z}_2$ Spin Liquid

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(Dated: June 1, 2016)

We study the dynamical thermal conductivity of the Kitaev spin model on a two-leg ladder. In contrast to conventional integrable one-dimensional spin systems, we show that heat transport is completely dissipative. This is a direct consequence of fractionalization of spins into mobile Majorana fermions, coupled to a $\mathbb{Z}_2$ gauge field, which acts as an emergent thermally activated disorder. Our finding rests on three 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.

PACS numbers: 75.10.Jm, 75.10.Pq, , 75.10.Kt,

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 gaped triplons in quantum disordered 1D spin ladder compounds [2, 3], via fractional spinons in 1D Heisenberg AFM spin chains [4, 5] and potentially also in 2D triangular AFMs [6], up to emergent monopoles in spin ice [7, 8]. Recently quantum magnets with strong spin-orbit coupling have experienced an upsurge of interest, since they may realize highly frustrated spin systems with directionally dependent compass exchange [9, 10]. This includes Kitaev’s model [11], 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 $\mathbb{Z}_2$ gauge field [12, 13]. In a broader context, Kitaev’s model is therefore related to topological insulators [14], superconductors [15], or fractional quantum Hall systems [16], as well as topological matter and order [17, 18]. Interestingly, the physics of Kitaev’s model can be generalized to 3D [19, 20] lattices as well as to 1D ladder versions of the Kitaev model, which allow for topological string order [13].

In this work we shed light on fractionalization as seen by magnetic heat transport in Kitaev ladders. Theoretical studies of transport in quasi 1D quantum magnets have a long and fertile history. 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) [21–39]. The DW is the nondissipating DC part of the current autocorrelation function and, if existent, indicates a ballistic channel close to equilibrium. In generic non-integrable systems, it is unlikely, that DWs exist in the thermodynamic limit [32], while the picture is more involved in the integrable case and depends on the type of current [25]. In general however, the energy conductivity is expected [40] to be infinite, as for the Heisenberg chain [41, 42], which implies a finite thermal DW. This conventional wisdom has recently been confirmed also for Kitaev-Heisenberg chains [43], which exhibits several integrable points, at all of which the energy DW is finite. Breaking integrability, e.g., by coupling Heisenberg chains to form spin ladders routinely renders heat flow dissipative [44, 45, 46], suppressing the DW. Kitaev ladders, however, remain an integrable, translationally invariant 1D spin system suggesting infinite heat conductivity. Instead of this, and as a prime result of this work, we show that heat transport is completely dissipative. This is a direct consequence of the matter-gauge-field interactions and can be viewed as a fingerprint of this $\mathbb{Z}_2$ spin liquid in 1D. This behavior is also in sharp contrast to that of the Kitaev chain [44], which hosts no gauge field. To justify these claims, we calculate the dynamic energy current correlation function (i) analytically discarding gauge field excitations, (ii) contrast this against numerical evaluations on large systems allowing for gauge field excitations in a phenomenological mean-field approximation, as well as on smaller systems by (iii) complete summation over all gauge sectors, and (iv) exact diagonalization (ED) of the original spin model.

The Hamiltonian of the Kitaev ladder reads

$$H = \sum_{(m,n)} J_\alpha \sigma^\alpha_m \sigma^\alpha_n,$$

with notations detailed in Fig. 1. It is known that this model can be mapped onto free Majorana fermions in the presence of static $\mathbb{Z}_2$ gauge fluxes. The allowed values $\pm 1$ of the latter correspond to the eigenvalues of the conserved operator $\Phi = \prod_{l=1,6} \sigma^\phi_{\alpha(l)}$ around each six-site loop, indicated in Fig. 1 where $\alpha(l) = x, y, z$, refers to that component of the exchange link which is not part of loop passing site $l$ [12, 13]. This mapping can be achieved along different routes, e.g. using an overcomplete set of four Majorana fermions per site [13], the Jordan Wigner transformation [14], or bond algebras [12, 16]. Follow-
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 \[39\]. Here, $\langle \ldots \rangle$ is the canonical thermal trace at temperature $T = 1/\beta (k_B = 1)$. The energy current $J$ follows from the energy polarization $P = \sum_{I} h_I$ through $J = i[H,P]$ ($h = 1$), where $h_I$ is the energy density depicted in Fig. 1). $D \equiv C_0/T^2$ is the Drude weight \[35\], which quantifies the non-dissipative current dynamics. Since the energy current is diagonal in the gauge fields, one may write

$$\langle J(t)J \rangle = Tr_\eta[Z_d(\eta) \langle J(t)J \rangle_{d(\eta)}]/Z.$$  

The subscript $d(\eta)$ refers to tracing over matter fermions only at a fixed gauge field state. The trace over gauge field states $Tr_\eta$ can be treated in different ways \[54, 57\]. Here we consider two approaches: (i) we perform exact summation over all gauge sectors on small systems to compare with ED of the original spin model, and (ii) we approximate $Tr_\eta$ in a mean-field sense.

For the latter, we envisage tracing over $\eta$ by joining ground state gauge domains of either $\eta_1 = -\eta_2 = +1$ or $-1$ of arbitrary lengths $L$. At $T = 0$, forming a single domain in the ground state is gapped by $\Delta_L$, referring to the cost of creating two gauge fluxes at the domain walls \[39\]. The domain walls are deconfined, with $\Delta L \to \infty$ converging to some constant \[39\]. To simplify, we set $\Delta_L \approx \Delta$, with $\Delta$ evaluated by flipping a single $\eta_i$. Finally we approximate the preceding to remain true at $T \neq 0$, i.e. we discard thermal polarization effects on $\Delta$ from the matter fermions. This maps the gauge field thermodynamics to that of the $S = \pm 1$ nn-Ising chain with exchange constant $\Delta/4$. To perform the $Tr_\eta$ we then confine the summation to gauge field states, which only contain a temperature dependent mean, even number of domain walls $n(T)$. We fix $n(T)$ by using that the average nn spin correlation function $c_1 = \sum_{i=1}^{2N} \langle S_iS_{i+1} \rangle$, which is known for the 1D Ising model \[60\], satisfies $c_1 = 2N - 2n(T)$, yielding

$$n(T) = 2N/(e^{\Delta/2T} + 1),$$

routed to multiples of two. With this Eq. \[4\] reads

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

where $\langle \ldots \rangle_{n(T)}$ 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 emphasize, 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 $n(T)$ smoothly 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 $T \neq 0$, for since $n(T) \neq 0$ domains of arbitrary size and location are included in the trace.

To appreciate the impact of the thermal fluctuations of the gauge field on the transport, we first suppress the trace over $n_{l,i}$, and pick only the clean ground state gauge, allowing however for finite temperatures. Using the energy density of Fig. 1, expressed in terms of the original matter fermions $d_{l,i}^j$, deriving the current, and after transforming to Bogoliubov particles, one gets

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

$$+ j_{k,i} (a_{k,i}^\dagger a_{-k,i} + a_{-k,i} a_{k,i})$$

with $i = 1, 2$, $u_{k,i} = (j_2^2 - j_2^2) \sin(k)/2 + (-1)^i j_2 \cos(k)/2$, and $j_{k,i} = (-1)^i j_2 \cos(k)/2$. Using Equations 1 and 2, solving for $C(t)$ is straightforward. For the Fourier transform $C(\omega)$ we obtain

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

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 Drude peak and two finite frequency pair breaking spectra, corresponding to the two quasiparticle energies of Eqn. 3.

In Fig. 2 the current correlation function is shown for two representative cases of $j_{x,y}$, referring to a gapless (gaped) 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 $C(-\omega) = \bar{C}(\omega)$, as required by detailed balance. Second, in the gaped case the regular spectrum for $\omega \ll 1$ shows a power law $C(\omega) \propto \omega^2$ due to $j_x^2 q_i \propto q^2$, 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 second quasiparticle excitations and one at the upper band edge. The insets Fig. 2b) and c) detail the Drude weight versus temperature, relative to its integrated regular spectral weight $I(T) = \int_0^\infty d\omega C(\omega)$, skipping the Drude peak, and relative to the high temperature value. Fig. 2d) shows that $D(T)$ is finite for any $T \neq 0$ and that $T^2 D(T)$ is comparable to $I(T)$ at sufficiently large temperatures. Fig. 2e) proves that $D(T \ll 1) \propto T$ as is true for 1D free fermions irrespective of the actual dispersion. In the gaped case $D(T)$ is exponentially activated.
excitations. Similar physics, albeit weaker is visible also in Fig. 3b). Each inset in Fig. 3 details $C(|\omega| \ll 1)$, clearly evidencing a mobility gap with a vanishing DC correlation function $C(\omega \to 0) = 0$. We emphasize, that the energy scale of the mobility gap is unrelated to that of the $\omega^2$ power law of gapless case in Fig. 2. Rephrasing our results: heat localizes because the Kitaev ladder comprises 1D free matter fermions scattering off a disordered static gauge potential $[61]$. This also clarifies our results to be qualitatively insensitive to details of the form of $n(T)$ and the inclusion of fluctuations around Eq. 5. The fine structure in $C(\omega)$ comprises effects of finite size, finite domain realization number, but also scattering from “typical” clusters of excited gauge fields, as e.g. the clear case of impurity anti-bound states, visible in Fig. 3b) above the bare spectral cut-off. Nota bene, Eqn. 8) implies $C(\omega > 0, T = 0) = 4C(\omega > 0, T = \infty)$ and moreover, because of $n(T \to 0) = 0$, the spectrum from the numerical real space calculation should approach that of Fig. 2 up to a constant as $T \to 0$. This agrees with the evolution of Fig. 3a) to d).

To further substantiate our results, we also perform numerically exact evaluation of $C(\omega)$ in the full many body Hilbert space of the original spin model, to compare it with an evaluation in the full Hilbert space of the fermionic model. For the spin model, the canonical average of Eq. 4 is carried out on the Hamiltonian basis, obtained via ED, on systems up to 20 spins. For the purpose of this calculation, $\delta$-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 Eq. 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 the seemingly finite value of $C(\omega \to 0)$ is an artifact of the Lorentzian broadening of the $\delta$-functions combined with the steep 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 $C_0$ divided by the sum rule, i.e. $C_0 = N C_0/(J J')$, as a function of the inverse system size. This is in stark contrast to ED calculation for the DW of the Kitaev chain $[41]$, for which the DW is essentially independent of system size and finite.

In conclusion we have shown that, even though pure Kitaev ladders are translationally invariant and integrable spin systems, they are perfect heat insulators 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 Kitaev models with $d \geq 2$, thermal currents will scatter off thermally excited $Z_2$-links similarly, connecting this physics to transport in higher dimensional superconductors with a temperature dependent impurity concentration. Non-Kitaev exchange will lead to dispersion of gauge excitations, restoring translational invariance below some energy scale, where Majorana particle heat transport may dissipate by relaxing momentum into mobile gauge excitations.

Acknowledgments. We thank R. Steinigeweg, M. Vojta, S. Rachel, and J. van den Brink for fruitful discussions and comments. Work of W.B. has been supported
in part by the DFG through SFB 1143 and the NSF under Grant No. NSF PHY11-25915. W.B. also acknowledges kind hospitality of the PSM, Dresden.

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