Energy Dynamics in the Heisenberg-Kitaev Chain

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We investigate the Heisenberg-Kitaev chain in order to uncover the interplay between two qualitatively different integrable points in the physics of heat transport in one-dimensional spin liquids. Based on linear response theory and analytical as well as numerical approaches, we explore several directions in parameter space including exchange-coupling ratios, anisotropies, and external magnetic fields. We show the emergence of purely ballistic energy transport at all integrable points, manifest in pronounced Drude weights and low-frequency suppression of regular-conductivity contributions. Moreover, off integrability, we find extended quantum chaotic regions with vanishing Drude weights and well-defined DC conductivities. In the vicinity of the Kitaev point, we observe clear signatures of the topological gap in the response function.

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Introduction. Fractionalized excitations with unconventional statistics in condensed matter could be at the center of future information technologies [1]. Yet, confinement to one spatial dimension (1D) and strong electron correlations have long been the only route to fractionalizing electrons into spinons and holons [2 6]. Starting, however, with the quantum Hall effect, topological matter and topological order [7] have surfaced as far more general schemes, unifying concepts of emergent gauge fields with fractional charges in Hall states [8], magnetic monopoles in frustrated magnets [9], and Majorana fermions in topological (super)conductors [10–12]. A milestone in this context has been Kitaev’s exact solution of a quantum spin model on the honeycomb lattice with strong exchange anisotropy [13]. This model harbors a spin liquid in two dimensions, with either gapped or gapless emergent Majorana-fermion excitations, Z2 gauge fluxes, and a field-induced phase with non-Abelian quasi-particle excitations [13 14]. Early on, Mott-insulating layered iridates A2IrO3, which display strong spin-orbit coupling, have been suggested as promising material candidates for Kitaev’s model. However, additional SU(2) invariant Heisenberg exchange interactions beyond the bare Kitaev model have also been realized as an inevitable ingredient in any realistic context [15 17].

Remarkably, the notion of Majorana particles withstands the truncation of Kitaev’s model via n-leg ladders down to 1D chains [18 19], where remnants of gauge-field physics can remain active through an extensive number of conservation laws [20]. On the one hand, the dynamics of bare Kitaev chains has met an upsurge of interest in the context of transport through 1D topological superconductors [21 22], where Majorana edge modes may have been observed [23]. On the other hand, transport through pure Heisenberg chains has come under intensive scrutiny ever since the observation of colossal spinon heat-conduction in 1D cuprates [24 26] and the discovery of diverging transport coefficients in S = 1/2 Heisenberg chains [27 30].

Integrability of Heisenberg chains has surfaced the key to anomalous spinon transport. Notably, the spin heat-current is a conserved quantity of the XXZ chain, which results in a finite Drude weight (DW) for heat transport [29 30] and explains the large heat conduction observed experimentally [24 26]. However, the spectrum of the spin-current response, including the question of a finite DW for spin transport, remains an issue only partially solved even after more than two decades [24 28 30 39].

Due to its singular nature, transport in the XXZ chain is highly susceptible to integrability-breaking interactions, e.g., further-neighbor exchange [30 40 41], lattice degrees of freedom [42 44], and disorder [45]. In this context Kitaev’s anisotropic exchange is rather remarkable since it allows to tune between two completely different integrable points, namely, the Heisenberg and the Kitaev chain. Yet, the interplay between these two types of exchange interactions regarding transport properties of spin chains has never been studied. Therefore, the aim of this Letter is to advance the field of both, topological matter and low-dimensional quantum magnetism by studying energy transport in the Heisenberg-Kitaev chain. As our main finding, we uncover ballistic transport with reduced low-frequency spectral weight at all integrable points, embed in a range of extended quantum chaotic regions with well-defined DC conductivities.

Kitaev model and energy current. We begin with the bare Kitaev chain, for which we obtain analytic results. In one dimension, and with periodic boundary conditions, its Hamiltonian reads [10 18]

$$H = \sum_{l=1}^{L/2} h_l, \quad h_l = J_1 S_{2l-1}^x S_{2l}^x + J_2 S_{2l-1}^y S_{2l+1}^y,$$

where L is an even number of sites, $S^x_r, S^y_r$ are the x, y components of spin-1/2 operators at site r, and $J_1, J_2 \in \mathbb{R}$ are exchange coupling constants. The unit cell contains two bonds. We note that Kitaev’s chain allows for $L/2$
mutually commuting $Z_2$ invariants $S_{x}^{z} S_{x+1}^{z}$ and $S_{z}^{x} S_{x+1}^{x}$.

The energy current follows from the continuity equation $[27]$

$$ J = \sum_{i=1}^{L/2} -i[J_{i}, J_{i+1}] = J_{1} J_{2} \sum_{i=1}^{L/2} S_{2i}^{x} S_{2i+1}^{x} S_{2i+2}^{x}. \quad (2) $$

This operator acts on three adjacent sites and contains also the $z$ component of spin-1/2 operators.

Both, the Hamiltonian and the energy current can be brought into a spinless-fermion representation using the Jordan-Wigner transformation. At that point, the Hamiltonian can also be rewritten as a model of Majorana fermions $[18]$, where Eq. $2$ refers to its associated energy flow. Fourier and Bogoliubov transformation diagonalizes the spinless-fermion Hamiltonian into $H = \sum_{k} (H_{k}^{x} c_{k}^{\dagger} c_{k} + H_{k}^{z} d_{k}^{\dagger} d_{k})$, with a one-particle dispersion $H_{k}^{x, z} = \pm \sqrt{J_{1}^{2} + J_{2}^{2} + 2 J_{1} J_{2} \cos 2 k}$ consisting of two branches for $c_{k}^{\dagger}$ and $d_{k}^{\dagger}$ fermions $[18, 40]$. We note that the momentum $k = 2 \pi j / L$, $j = 1, 2, \ldots, L/4$ is confined to $k \leq \pi / 2$ and that two ‘zero modes’ $H_{k}^{3, 4} = 0$ exist.

The heat current in Eq. $2$ can also be written in terms of $c_{k}^{\dagger}$ and $d_{k}^{\dagger}$, but will be non-diagonal in this representation. E.g., for $J_{1} = J_{2}$, the Hamiltonian is $H = J_{1} \sum_{k} \cos k (c_{k}^{\dagger} c_{k} - d_{k}^{\dagger} d_{k})$, however, the energy current reads

$$ J = \frac{J_{1}^{2}}{4} \sum_{k=0}^{\pi/2} \sin 2 k (c_{k}^{\dagger} c_{k} + d_{k}^{\dagger} d_{k} + c_{k}^{\dagger} d_{k} + d_{k}^{\dagger} c_{k}). \quad (3) $$

Obviously, and in contrast to the Heisenberg chain, $[H, J] \neq 0$. Moreover, we find that the Hamiltonian’s zero modes do not contribute to the energy current.

In general the current operator comprises four eigenvalues $J_{k}^{4} = J_{1} J_{2} \sin(2k)/2$ with its own three zero modes $J_{k}^{3, 4} = 0$. Interestingly, $H_{k}^{4} J_{2}^{2} \partial J_{k}^{1}/\partial k = -J_{k}^{2}$.

**Energy-current autocorrelation.** In the following we investigate the energy-current autocorrelation $C(\omega) = 1/(2 \pi) \int_{-\infty}^{\infty} d \omega \exp(-i \omega t) \langle J(\omega) J(0) \rangle_{\text{eq}}$, in frequency space $\omega$, where $\langle \ldots \rangle_{\text{eq}}$ labels equilibrium averages at inverse temperatures $\beta = 1/T$ and time arguments refer to the Heisenberg picture. The quadratic nature of the theory allows for analytic results.

For simplicity, we discuss the case of $J_{1} = J_{2}$ first and focus on the high-temperature limit $\beta \to 0$. Here, $C(\omega)$ is a symmetric function of $\omega$ and can be written at $\omega \neq 0$ as $C(\omega) = 1/(L/2) \sum_{k} A_{k}^{2} \delta(\omega \pm \omega_{k})$ with the frequency $\omega_{k} = 2 |J_{1}| \cos k$ resulting from the energy difference of the off-diagonal transitions $c_{k}^{\dagger} d_{k}$ and $d_{k}^{\dagger} c_{k}$. The amplitude $A_{k} = J_{1}^{2} \sin(2k)^{2}/L$ is essentially the square of the corresponding matrix elements. In the thermodynamic limit $L \to \infty$, the $k$ sum can be converted into an integral over the density of states $|\partial k / \partial \omega_{k}|$, which can be carried out straightforwardly to yield the exact expression

$$ C(\omega \neq 0) = \frac{|J_{1}|^{3}}{32 \pi} \sqrt{1 - \left( \frac{\omega}{2 J_{1}} \right)^{2}} \left( \frac{\omega}{2 J_{1}} \right)^{2}. \quad (4) $$

Furthermore, since the integrated spectral weight $\int d \omega C(\omega \neq 0) = J_{1}^{2}/128$ is exactly half of the ‘sum rule’ $J_{1}^{2}/64$ $[40]$, we obtain $C(\omega) = C(\omega \neq 0) = J_{1}^{2} \delta(\omega)/128$, including a finite heat DW.

Figure $[1]$ (a) summarizes the frequency-dependence of $C(\omega)$. The finite DW at zero frequency is commonly expected for integrable models while counter examples exist (such as the vanishing spin DW in the gapped XXZ chain $[28, 34, 33, 36]$). The existence and form of the regular part is a non-trivial property of the Kitaev model. It is worth mentioning that the suppression of the regular part at low frequencies and in particular the $\omega^{2}$-behavior has been proposed for all gapless models with DWs $[39]$ even though a rigorous proof is lacking and arguments are based on numerical simulations of finite systems.

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**FIG. 1.** (color online) Energy-current autocorrelation $C(\omega)$ for the Kitaev model at $\beta \to 0$ and $(a) J_{1} = J_{2}$, $(b) J_{1} = 2 J_{2}$ for $L = \infty$. (c), (d) show (a), (b) for $L = 16$.

**FIG. 2.** (color online) Level-spacing distribution $P(s)$ for the Heisenberg-Kitaev model at $(a) J_{1, 2} = -2 J_{3}$, $(b) J_{1, 2} = -J_{3}$ for $L = 16$ in a single symmetry sector. Curves indicate both, the integrable Poissonian distribution and the nonintegrable Wigner distribution.
In the general case of \( J_1 \neq J_2 \), i.e., for a non-zero topological gap, \( C(\omega) \) can be obtained analogously. In Fig. 1(b) we show \( C(\omega) \) at \( J_1 = 2J_2 \). Clearly, the overall structure is similar to Fig. 1(a), but there is no spectral weight within a window of \( \delta \omega = J_1/2 \), which resembles the topological gap between the two branches of the one-particle dispersion. This gap vanishes at \( J_1 = J_2 \).

**Heisenberg-Kitaev model.** Now we add an XXZ type of Heisenberg exchange to Kitaev’s model

\[
H' = J_3 \sum_{r=1}^L S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z. \tag{5}
\]

This modification requires analytical approaches to be replaced by numerical methods. We will focus on the antiferromagnetic and isotropic case, \( J_3 > 0 \) and \( \Delta = 1 \), with a ferromagnetic choice of \( J_{1,2} < 0 \).

While Kitaev’s model is integrable and in 1D Heisenberg’s model is also in terms of the Bethe Ansatz, their sum \( H + H' \) will not be so in general. This is corroborated by the level-spacing distribution \( P(s) \), which is depicted in Fig. 2(b). It shows clear signatures of quantum chaos, especially if \( |J_{1,2}| \gg |J_3| \). Note that a proper evaluation of \( P(s) \) requires an ‘unfolding’ of the spectrum and a restriction to a single subspace of all ‘trivial’ symmetries, i.e., translation invariance, conservation of the even/odd particle number, as well as particle-hole symmetry.

Quantum chaos prevails for all other ratios of \( J_{1,2,3} \) we have investigated, except for one additional integrable point at \( J_{1,2} = -2J_3 \), see Fig. 2(a). At this point, local rotation in spin space \( \mathbb{S}^2 \) maps the Heisenberg-Kitaev chain onto the Heisenberg chain only.

For the total Hamiltonian the energy current

\[
J = \sum_{l=1}^{L/2} \left[ (J_3 + J_1)(J_3 + J_2) \delta_{l1} S_{2l}^x S_{2l+1}^x - J_2^3 S_{2l}^y S_{2l+2}^y \right] S_{2l+1}^z + J_3 \Delta \left[ J_3 S_{2l+2}^y S_{2l+1}^y - (J_3 + J_1) S_{2l+1}^y S_{2l+2}^y \right] S_{2l+1}^z + J_3 \Delta \left[ J_3 S_{2l}^x S_{2l+1}^x - (J_3 + J_2) S_{2l}^x S_{2l+2}^x \right] S_{2l+2} \tag{6}
\]

turns into an operator with a rather involved structure, the numerical implementation of which is delicate. To check this, Fig. 2(c), (d) shows that our exact diagonalization perfectly reproduces the analytical result for \( C(\omega) \) of the Kitaev model. To this end, we have to compare numerically accessible chain lengths with finite-size analytic results, featuring only a few \( \delta \) functions, rather than Eq. 4. In the Kitaev limit the finite-size spectrum is particularly sparse because the \( L/2 \) \( Z_2 \) invariants imply a \( 2L/2 \) fold degeneracy.

Another important and non-trivial consistency check is \( C(\omega) \) for the Heisenberg model. In contrast to the conventional definition, the energy-current operator in Eq. 6 is not conserved, due to the two-site unit cell. While this emphasizes the well-known ambiguity of defining local energy densities, it has no consequence for the existence of a finite DW at zero frequency, as depicted in Fig. 3 (a). There, half of the total spectral weight is concentrated in the DW, similar to the Kitaev model. Moreover, the regular part shows a striking similarity to the one in Fig. 1(a). As a final check, \( C(\omega) \) at the Heisenberg-equivalent additional integrable point at \( J_{1,2} = -2J_3 \) turns out to be identical to that of the Heisenberg model, see Fig. 3 (a) and (b).

Next we investigate \( C(\omega) \) for the Heisenberg-Kitaev model within the nonintegrable region, and in particular for the case \( J_{1,2} = -J_3 \). In Fig. 4 we show \( C(\omega) \) at \( \beta \rightarrow 0 \) for finite chains of length \( L = 12, 14, \) and 16. Several comments are in order. First, at \( \omega \gg 0 \), \( C(\omega) \) is independent of \( L \) and a smooth function of \( \omega \), at least at a reasonable scale \( \delta \omega = 0.05 |J_3| \). Second, at \( \omega = 0 \), \( C(\omega) \) still depends on \( L \) due to the presence of a nonzero DW in finite chains; however, as shown in the inset of Fig. 4 this DW decreases exponentially with \( L \). Such finite-size scaling is commonly expected for nonintegrable quantum many-body systems.

Third, although the overall structure of \( C(\omega) \) is broad, a narrow ‘peak’ is clearly visible around zero frequency. Certainly, this peak may be interpreted as the broadening of the \( \delta \)
function, which is rather separated from the regular part at the three integrable points of the Heisenberg-Kitaev model, cf. Fig. 5 (a) and Fig. 5 (a), (b). The width of the ‘peak’ turns out to increase with \( \Delta \), although not shown explicitly here.

The situation is similar for \( J_1 \neq J_2 \). In particular, there is no low-frequency suppression of the regular part at intermediate \( J_3 \). Yet, at small \( J_3 \), we can clearly identify the topological gap even at high temperatures, see Fig. 5. The gap is only weakly dependent on \( J_3 \) up to \( J_3 = -0.14J_1 \), beyond which all signatures of the gap are hidden by high-temperature excitations \( \propto J_3^2 \), as expected from perturbation theory.

We now discuss the \( J_{1,2,3} \) dependence of the DW in detail. To this end, we introduce a parameter \( \alpha \in [0,1] \), rewriting the exchange coupling constants as \( J_3 = \alpha \) and \( J_{1,2} = \alpha - 1 \). In turn, the Kitaev model is realized for \( \alpha = 0 \) and the Heisenberg model for \( \alpha = 1 \). Figure (a) shows the high-temperature DW vs. \( \alpha \) for finite chains of length \( L = 10, 12, 14, \) and 16. Clearly, the DW takes on its minimum value at \( \alpha \sim 1/2 \). This minimum is merely a small fraction of the ‘sum rule’ for \( L = 16 \) and, in view of the inset of Fig. 5 it clearly approaches zero in the thermodynamic limit \( L \to \infty \). In the immediate vicinity of the integrable points at \( \alpha = 0, 1/3, \) or 1 such conclusions are less obvious. While the numerical data may be consistent with finite DWs \( D > 0 \) in the thermodynamic limit \( L \to \infty \), the system sizes are too small and would also be consistent with \( D = 0 \). Note that for \( J_1 \neq J_2 \) the peak at the point \( \alpha = 1/3 \) is shifted to other values of \( \alpha \) and, as a consequence of nonintegrability, vanishes for \( L \to \infty \), see Fig. 5 (b).

As an interesting side remark, for extreme anisotropy \( \Delta = 0 \), the parameter \( \alpha \) tunes from free Majorana to free XY fermions. In that case, as shown in Fig. 5 (a), (b), the DW is independent of \( \alpha \), corroborating a picture of free particles for all \( \alpha \).

**External Magnetic Field.** Finally, we also consider a \( z \) axis oriented external magnetic field \( B \) by including a Zeeman energy \( H'' = BS^z \). This leads to a magneto-thermal contribution \( J'' \) to the energy current

\[
J'' = \sum_{i=1}^{L/2} \frac{B}{2} \left[ J_3 S_{2i+1}^z S_{2i}^y - (J_3 + J_1) S_{2i+1}^y S_{2i+2}^x \right] + \frac{B}{2} \left[ J_3 S_{2i+1}^z S_{2i+2}^y - (J_3 + J_2) S_{2i+2}^y S_{2i+1}^x \right],
\]

which is a two-site operator and simplifies to the well-known spin current at \( J_{1,2} = 0 \) \cite{28, 30, 33, 36}.

We choose a ‘small’ \( B = 0.1 \) and repeat the calculation of the DW in Fig. 5 (a) for \( J_3 = \alpha \) and \( J_{1,2} = 1-\alpha \). The result of the calculation is depicted in Fig. 5 (c). Apparently, the DW at \( \alpha = 1/3 \) is extremely sensitive to \( B \) and seems to vanish in the thermodynamic limit \( L \to \infty \). In sharp contrast, the DW is much less sensitive for free particles at \( \Delta = 0 \) and remains finite for \( L \to \infty \).

**Conclusion.** In summary, we have studied energy dynamics in the Heisenberg-Kitaev chain which interpolates between two generic spin liquids in one dimension. Varying several parameters of the model including exchange coupling strength, ratio, and anisotropy as well as magnetic field, we showed that all integrable points (quantum chaotic regions) display finite DWs (vanishing DWs) and suppressed regular contributions at low frequencies (well-defined DC transport limits). We believe that our results are an essential first step towards understanding the transport in the Heisenberg-Kitaev model on 2D lattices, as well as transport experiments in novel local-moment materials with strong spin-orbit coupling.

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\[
\frac{\text{tr} \{ J^2 \}}{2L} = \frac{J_1^2}{128} + \frac{(J_3^2 \Delta^2 + B^2) [3J_3^2 + (J_3 + J_1)^2 + (J_3 + J_2)^2]}{128}.
\]