Thermal transport in one-dimensional spin gap systems

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We study thermal transport in one dimensional spin systems both in the presence and absence of impurities. In the absence of disorder, all these spin systems display a temperature dependent Drude peak in the thermal conductivity. In gapless systems, the low temperature Drude weight is proportional to temperature and to the central charge which characterizes the conformal field theory that describes the system at low energies. On the other hand, the low temperature Drude weight of spin gap systems shows an activated behavior modulated by a power law. For temperatures higher than the spin gap, one recovers the linear $T$ behavior akin to gapless systems. For temperatures larger than the exchange coupling, the Drude weight decays as $T^{-2}$. We argue that this behavior is a generic feature of quasi one dimensional spin gap systems with a relativistic-like low energy dispersion. We also consider the effect of a magnetic field on the Drude weight with emphasis on the commensurate-incommensurate transition induced by it. We then study the effect of nonmagnetic impurities on the thermal conductivity of the dimerized XY chain and the spin-$\frac{1}{2}$ two leg ladder. Impurities destroy the Drude peak and the thermal conductivity exhibits a purely activated behavior at low temperature, with an activation gap renormalized by disorder. The relevance of these results for experiments is briefly discussed.

I. INTRODUCTION

The past many years have seen a resurgence of interest, both theoretical and experimental in quasi-one dimensional spin gap systems. Well known examples of systems with a gap are spin chains with dimerization, frustration and anisotropy. Another interesting example is the two leg spin $S = \frac{1}{2}$ ladder which was proposed as a toy model for the pseudogap phase in high temperature superconductors. Renewed interest in these systems was triggered by the availability of anisotropic materials in which the magnetic properties of the insulating phase could be ascribed to one or quasi-one dimensional spin systems. The dynamical properties of these quasi-1d spin phases have been extensively studied using standard techniques like neutron scattering and NMR measurements. More recently, heat transport is being used as a complementary probe to study low dimensional spin systems. Measurements of thermal conductivity have been carried out in systems such as the spin chain materials SrCu$_2$O$_2$ and Sr$_2$CuO$_2$Cl$_2$, the spin Peierls system CuGeO$_3$, and the spin ladder materials (Sr,Ca,La)$_4$Cu$_2$O$_8$. The huge anisotropy seen in the thermal conductivity in the directions parallel and perpendicular to the chains or the ladders, indicates that magnetic excitations of these quasi-1D systems do play an important role in heat transport. This is further confirmed by measurements in the presence of a magnetic field.

Various attempts have been made to extract from these measurements, the purely magnetic contribution to the thermal conductivity. This is often done by subtracting a phonon background calculated within a Debye model. However, in order to account for the entire magnetic contribution, one needs to understand the interactions of the spin excitations of the low dimensional spin systems with themselves and, with defects and phonons. This is a non-trivial problem since the spin excitations are usually rather complicated. Consequently, experimental results have been fitted using various phenomenological kinetic theory expressions for non-interacting spinons or magnons. This effort to obtain the purely magnetic contribution to the thermal conductivity has stimulated theoretical studies of thermal transport in spin chain and spin ladder systems. In the absence of extrinsic scattering such as phonons or defects, some studies showed that the frequency dependent thermal conductivity $\kappa(\omega,T) = \pi\tilde{k}(T)\delta(\omega)$, where $\tilde{k}(T)$ is the thermal Drude weight. However, the Drude weight extracted from finite size zig-zag ladders seems to be at odds with the idea of an infinite thermal conductivity in spin systems without disorder.

In this paper, we use analytical methods to revisit the problem of the thermal conductivity for various quasi 1d spin systems with special emphasis on the two leg spin-$\frac{1}{2}$ ladder. In the absence of impurities, we present results...
which should be valid for spin gap systems possessing low energy triplet excitations and gapless systems irrespective of the details of the nature of the interaction. A schematic representation of the thermal Drude weight for a spin gap system is shown in Fig. 1. We also study the effect of one/many impurities on the thermal conductivity of the spin ladder and show that in the presence of impurities, the thermal conductivity is not simply given by the Drude weight times a temperature independent scattering time.

The paper is organized as follows: in Sec. II, we discuss the temperature dependence of the Drude weight for different spin systems ranging from gapless integrable spin chains to spin gap systems like the spin ladder and the spin−1 chain. In Sec. III, we discuss the effect of impurities on the thermal conduction. In particular, we use the Landauer approach to evaluate the effect of a single non-magnetic impurity on the thermal conductivity of the ladder and the XY-chain. We then study the effect of a finite concentration of impurities on the ladder. Finally, we present a comparison of our results to experiments and other theoretical work on the subject.

II. TRANSLATIONALLY INvariant SYSTEMS

In this section, we briefly outline the general definitions of the thermal current and the thermal conductivity calculated within linear response theory. We then use this formalism to calculate the dc thermal conductivity of various spin systems with and without a gap to low energy excitations. The examples considered are: gapless integrable spin chains described by a conformal fixed point, the spin−1/2 ladder, the dimerized XY chain and lastly the case of massive bosons. We also consider the effect of a magnetic field on the thermal Drude weight.

A. Definition of thermal current and thermal conductivity

We consider a system defined by a Hamiltonian density $\mathcal{H}(x)$ so that the total Hamiltonian is $H = \int dx \mathcal{H}(x)$. Conservation of energy leads to the continuity equation

$$\partial_t \mathcal{H}(x, t) + \partial_x j_e(x, t) = 0,$$

where $j_e$ is the energy(thermal) current of the system. In the absence of charged excitations, the energy and thermal current are equivalent. Eq. (1) permits a definition of the thermal current in terms of the Hamiltonian density. Within linear response theory the energy current response function at temperature $T > 0$ reads:

$$\chi(\omega, T) = \int dx \int_0^\infty dt e^{i\omega t} \langle [j_e(x, t), j_e(0, 0)] \rangle,$$

where $\langle \rangle$ indicates both quantum and thermal averaging. It is often easier to use the imaginary time formalism to calculate $\chi(i\omega_n)$ where $\omega_n$ are the Matsubara frequencies and then analytically continue to real frequencies $i\omega_n \rightarrow \omega + i0$ to obtain $\chi(\omega, T)$. The frequency dependent thermal conductivity is then given by:

$$\kappa(\omega, T) = \frac{1}{i\omega T} [\chi(0, T) - \chi(\omega, T)],$$

In general, in the absence of phonons or impurities, the total thermal current $J_e(t) = \int dx j_e(x, t)$ is conserved. This conservation permits an alternative but equivalent formulation of the thermal conductivity

$$\kappa(\omega, T) = \frac{1}{2L^2} \int_0^\infty dt \langle \{J_e(t), J_e(0)\} \rangle e^{i\omega t},$$

where $L$ is the system size. Since $J_e$ is conserved, the total current is time independent and

$$\kappa(\omega, T) = \frac{\pi}{LT^2} (J_e^2) \delta(\omega) = \tilde{\kappa}(T) \delta(\omega).$$

This implies an infinite dc thermal conductivity, with a temperature dependent Drude weight $\tilde{\kappa}(T)$ which vanishes at zero temperature. This thermal Drude weight has been studied numerically for some spin gap systems in Refs. [22,23]. In the following sections, we present an analytical discussion of the behavior of the Drude weight in various gapless and gapped quasi-one dimensional spin systems.

B. Gapless Integrable Spin Chains

In this section, we present results for the thermal Drude weight of integrable spin chains which are characterized by a vanishing singlet-triplet gap. One example of such a system is the integrable spin−1/2 Heisenberg model, which is known to have a Drude weight that vanishes linearly as temperature goes to zero $\tilde{\kappa} = \pi^2 v T/3\hbar$, where $v$ is the velocity of spin excitations. Other interesting systems, are the various integrable generalizations of the spin−1/2 Heisenberg spin chain, like the spin−S chain model and $SU(N)$ spin chain models. This description allows one to easily obtain the low temperature thermal conductivity of these chains. The long wavelength behavior of these integrable systems are described by a conformal invariant fixed point. This
description allows one to easily obtain the low temperature thermal Drude weight of these chains. The effective Hamiltonian of these systems has the generic form

$$H = \int dx [\mathcal{H}_R(x) + \mathcal{H}_L(x)]$$ (6)

where $\mathcal{H}_R$ and $\mathcal{H}_L$ describe right and left moving chiral modes. In addition, chirality imposes the constraints $\mathcal{H}_R(x, t) = \mathcal{H}_R(x - vt)$ and $\mathcal{H}_L(x, t) = \mathcal{H}_L(x + vt)$. This leads to the following relation

$$\partial_t (\mathcal{H}_R(x, t) + \mathcal{H}_L(x, t)) = -v \partial_x (\mathcal{H}_R(x, t) - \mathcal{H}_L(x, t))$$ (7)

which results in a thermal current density:

$$J_c = v \int dx [\mathcal{H}_R(x) : - : \mathcal{H}_L(x) :]$$ (8)

As before, since $[H, J_c] = 0$, the Drude weight is given by

$$\hat{k}(T) = \frac{\pi}{LT^2} \langle J_c^2 \rangle$$ (9)

Moreover, since there is no interaction between the right and the left moving modes, $\langle J_c^2 \rangle = v^2 \langle H^2 \rangle$. One thus immediately obtains the result $\hat{k}_{WZ}(T) = \pi C_v(T) v^2$, where $C_v$ is the specific heat of these modes. For conformally invariant modes with a central charge $c$, the specific heat is given by $C_v(T) = \frac{2\pi T}{3\hbar} c$, leading to a thermal Drude weight:

$$\hat{k}(T) = \frac{\pi^2 T v}{3 T^2}$$ (10)

For the integrable spin-1 chain at the Takhtajan-Babujian point, this weight can also be recovered from explicit calculations using the Majaron formalism to be discussed in the forthcoming sections. For a theory described by a free massless boson like the spin-$\frac{1}{2}$ Heisenberg chain, which has a central charge $c = 1$, this weight is $\pi^2 T v/3$, which can also be checked by direct calculations of the thermal susceptibility. For systems with a Luttinger liquid like description $\mathcal{H}/\mathcal{L}$ with a Luttinger exponent $K$, the present derivation illustrates clearly that the weight $\hat{k}$ is independent of the Luttinger exponent or equivalently, the compactification radius of the free bosonic Luttinger field. Considering the case of XXZ chains, this result implies that the thermal Drude weight is independent of the anisotropy $J_z/J_{xy}$ which is in agreement with Bethe Ansatz calculations on the XXZ spin chain in the Luttinger liquid regime.

C. Spin-$\frac{1}{2}$ ladder

Here and in the following sections, we focus exclusively on spin gap systems. We first apply the formalism of Sec. II to the clean two leg spin ladder. The Hamiltonian of the two leg spin ladder is

$$H = J_\parallel \sum_{p=1,2} \mathbf{S}_{i,p} \cdot \mathbf{S}_{i+1,p} + J_\perp \sum_i \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2},$$ (11)

where the $\mathbf{S}_{i,p}$ are spin-$\frac{1}{2}$ operators, and the exchange constants $J_{ij}/J_\perp > 0$. For weak interchain coupling $J_\perp \ll J_\parallel$, the spin ladder can be described by a continuum theory of spinless Majorana fermions. The continuum Hamiltonian reads:

$$H = \sum_{a=0}^{3} \int dx \mathcal{H}^a(x),$$ (12)

$$\mathcal{H}^a(x) = -\frac{i}{4} \left[ \xi_R^a \partial_x \xi_L^a(x) - (\partial_x \xi_R^a(x)) \xi_L^a(x) - \xi_R^a(x) \partial_x \xi_L^a(x) + (\partial_x \xi_R^a(x)) \xi_L^a(x) \right] + im^a \xi_R^a(x) \xi_L^a,$$ (13)

where the velocity of the Majorana fermions $v = \frac{\pi}{2} J_\parallel a$ (a is the lattice spacing). Physically, the Majorana modes $\xi_R^a_L$ $a = 1, 2, 3$ with masses $m_{1,2,3} = J_\perp/2\pi \equiv \Delta$ describe triplet excitations with a gap $\Delta$ and $\xi^0_R$ with mass $m_0 = 3J_\parallel/(2\pi) = -3\Delta$ describe singlet excitations. We remark that the bosonized version of the low energy Hamiltonian (12) describes more general spin ladder models than the one considered in (11). Using (14), the energy current for the ladder takes the form

$$j_e(x) = \sum_{a=0}^{3} j_e^a(x),$$ (14)

$$j_e^a(x) = -\frac{i}{4} \left[ m^a \xi_R^a \partial_x \xi_L^a -(\partial_x m^a \xi_R^a) \xi_L^a + m^a \partial_x \xi_R^a \xi_L^a - (\partial_x m^a \xi_R^a) \xi_L^a \right].$$

From (14) and (13), the total Drude weight for the spin ladder is found to be

$$\hat{k}(T) = \sum_a \hat{k}^a(T) = \hat{k}^0(T) + 3\hat{k}^3(T).$$ (15)

Since the Majorana fermions are essentially free, the correspondence between Majorana and Dirac fermions can be used to evaluate the Drude weight $\hat{k}^a(T)$

$$\hat{k}^a(T) = \frac{1}{8T^2} \int_{-\Lambda}^{\Lambda} \frac{dk}{\cosh^2 \left( \frac{\epsilon_a(k)}{2T} \right)},$$ (16)

where the energy dispersion $\epsilon_a(k) = \sqrt{(vk)^2 + m^2_a}$ and $\Lambda = \frac{2\pi}{a}$ is the lattice induced ultra-violet cutoff. The details of the calculation are presented in Appendix A. The thermal Drude weight of the spin ladder is now given by

$$\hat{k}(T) = \frac{3}{8T^2} \int_{-\Lambda}^{\Lambda} \frac{dk}{\cosh^2 \left( \frac{\epsilon_3(k)}{2T} \right)} + \frac{1}{8T^2} \int_{-\Lambda}^{\Lambda} \frac{dk}{\cosh^2 \left( \frac{\epsilon_0(k)}{2T} \right)}$$ (17)

At low enough temperatures $T \ll J_\perp/(2\pi)$, the triplet excitations are the dominant carriers of heat and

$$\hat{k}(T) = 3\sqrt{\frac{\pi \Delta^2}{2T}} ve^{-\Delta/T}$$ (18)
For temperatures $\Delta \ll T \ll J_{\parallel}$, the coupling between the two spin half chains becomes irrelevant and we recover $\tilde{\kappa} \propto T$ i.e., it is the sum of the Drude weights of two independent spin-\(\frac{1}{2}\) chains cf. Sec. 4.4. For temperatures $T \gg J_{\parallel}$, the temperature dependence in the integrand of Eq. (17) becomes negligible and since the $k$ integral is bounded on a lattice, the thermal Drude weight decays as $\tilde{\kappa} \propto T^{-2}$. The prefactor depends on the cut-off $\Lambda$ and it is reasonable to assume that the continuum theory over-estimates this prefactor. To summarize, the Drude weight of the spin ladder has three regimes: i) at very low temperatures, $T \ll \Delta$, we obtain the exponential behavior $\tilde{\kappa} \sim \exp(-\Delta/T)$; ii) for intermediate temperatures, $\Delta \ll T \ll J_{\parallel}$, we obtain the power-law behavior $\tilde{\kappa} \sim T^\gamma$; and iii) for $T \gg J_{\parallel}$, $\tilde{\kappa} \sim 1/T^2$.

Since $\tilde{\kappa}(T \to 0) = 0$, this implies the presence of at least one maximum in $\tilde{\kappa}$ at a finite temperature for a lattice model. We expect $\tilde{\kappa}$ to have a peak in the vicinity of $T \sim J_{\parallel}$ (cf. Fig. 45). We note that the numerical results for $\tilde{\kappa}(T)$ for the ladder presented in Ref. 15 confirm our picture.

To study the effect of an applied magnetic field $h$ on the thermal conductivity, we first note that the effect of the magnetic field is to alter the dispersion of the triplet. The degenerate triplet dispersion $\epsilon_1(k)$ now splits into three branches $\epsilon_1(k) + h, \epsilon_1(k)$ and $\epsilon_1(k) - h$ and the singlet dispersion $\epsilon_0(k)$ remains unaltered. The Drude weight in the presence of the field is now given by:

$$\tilde{\kappa} = \frac{1}{8T^2} \int_{-\Lambda}^{\Lambda} dk \left( \frac{\partial \epsilon_1(k)}{\partial k} \right)^2 \left\{ \frac{(\epsilon_1(k) - h)^2}{\cos^2 \left( \frac{\epsilon_1(k) - h}{2T} \right)} + \frac{(\epsilon_1(k) + h)^2}{\cos^2 \left( \frac{\epsilon_1(k) + h}{2T} \right)} + \frac{\epsilon_1(k)^2}{\cos^2 \left( \frac{\epsilon_1(k)}{2T} \right)} \right\} + \frac{1}{8T^2} \int_{-\Lambda}^{\Lambda} \frac{dk}{\cos^2 \left( \frac{\epsilon_0(k)}{2T} \right)}$$

(19)

There are now two regimes of interest: $h \ll \Delta$ and $h > \Delta$. In the former case, the effective gap $\Delta - h$ dominates the thermal conductivity and $\tilde{\kappa} \propto \exp(-\Delta(T)/h)$. The magnetic field leads to a sufficient enhancement of the low temperature thermal conductivity. The physical reason is that the increase of the number of triplet excitations with $S^z = +1$ strongly dominates the diminution of the number of excitations having $S^z = -1$. For $h \sim \Delta$, the dispersion of the Majorana fermions describing the $S_z = +1$ sector is no longer relativistic-like but quadratic, $\epsilon(k) \propto k^2$, resulting in $\tilde{\kappa} \sim T^3/2$. Finally, for $h > \Delta$, the gap in the spin ladder is closed [43], and the fermionic excitations have an effective linear dispersion, leading to $\tilde{\kappa}(T) = \frac{x^2T}{8} v(h)$, where the effective Fermi velocity $v(h) = v(1 - (\Delta/h)^2)$.

Let us note that the above results (17), (19) are also relevant for spin-1 chains. Indeed, spin-1 chains are also described at low energy by massive Majorana fermions, with a Hamiltonian similar to (12), except that the singlet mode $\xi^0$ is absent [44]. This mapping to massive Majorana fermions originally derived for a spin-1 chain with bi-quadratic interactions in the vicinity of the Takhtajan-Babujian point [45], is also expected to provide a qualitative description of the low energy properties of the Heisenberg spin-1 chain. Therefore, the thermal conductivity of the spin-1 chain is easily obtained by taking the limit $\epsilon_0 \to \infty$ in Eqs. (18) and (19). For the spin-1 chain, the low temperature behavior of the Drude weight in the thermal conductivity is still given by (13). The main difference between the ladder and the spin-1 chain stems from the fact that while in the former the gap to triplet excitations is small, in the latter the gap $\Delta$ is of the order of the Heisenberg exchange $J$ ($\Delta = 0.41J$). Consequently, the intermediate regime of linear temperature dependence of $\tilde{\kappa}$ can hardly be observed in the spin-1 chain. However, reasonably strong bi-quadratic interactions can reduce the gap appreciably rendering an observation of an intermediate linear regime possible. This predicted linear behavior might in fact be observable in the compound LiV$_2$GeO$_6$ which is expected to have sizeable bi-quadratic interactions [46].

D. Dimerized XY Chain

We consider a spin-\(\frac{1}{2}\) XY chain with alternating exchange in an external magnetic field $h$, described by the Hamiltonian:

$$H = \sum_n J_1 (S_{2n}^x S_{2n+1}^z + S_{2n+1}^y S_{2n}^z) + \sum_n J_2 (S_{2n}^x S_{2n-1}^z + S_{2n-1}^y S_{2n}^z) - h S_n^z$$

(20)

Using the Jordan-Wigner transformation [47],

$$S_n^+ = a_n^+ \cos \left( \sum_{m<n} a_m^+ a_m \right),$$

$$S_n^z = a_n^+ a_n - \frac{1}{2},$$

(21)

where the $a, a^\dagger$ are fermion annihilation and creation operators, the Hamiltonian (20) can be rewritten as:

$$H = J_1 \sum_n (a_{2n+1}^+ a_{2n} + \text{H.c.}) + J_2 \sum_n (a_{2n-1}^+ a_{2n} + \text{H.c.})$$

(22)

Diagonalizing the above Hamiltonian, we obtain

$$H = \sum_k [E(k) - h] a_{k+}^+ a_{k+} - [E(k) + h] a_{k-}^+ a_{k-},$$

(23)
where \( E(k) = \sqrt{(J_1 - J_2)^2 + 4J_1J_2 \cos^2 k} \). Clearly, the dimerization induces a gap in the dispersion. Using the results of the previous sections and Appendix B, the thermal Drude weight of this dimerized chain is

\[
\tilde{k}_{XY}(T, h) = \frac{1}{8T^2} \int_{-\pi}^{\pi} dk \left[ \frac{(E(k) - h)^2}{\cosh^2 \left( \frac{E(k) - h}{2T} \right)} + \frac{(E(k) + h)^2}{\cosh^2 \left( \frac{E(k) + h}{2T} \right)} \right] \left( \frac{\partial E(k)}{\partial k} \right)^2
\]

(24)

For \( T \ll |J_1 - J_2| \), and \( |J_1 - J_2| \ll \sqrt{J_1J_2} \) the physics is similar to that of the continuum model of the weakly coupled ladder discussed in Sec. I(1). The fact that the model is defined on a lattice allows us to verify that for \( h = 0 \) and at very high temperatures the thermal conductivity indeed decays as \( T^{-2/2} \). For \( T \gg \sqrt{J_1J_2} \), and \( h = 0 \), since the energy spectrum of the XY chain is bounded, one has:

\[
\tilde{k}_{XY}(T) = \frac{1}{4T^2} \int_{-\pi}^{\pi} dE(k)^2 \left( \frac{\partial E(k)}{\partial k} \right)^2
\]

(25)

This result is in fact more general. Since, at high temperatures, \( \langle J^2 \rangle \) is finite for a lattice model, we have the asymptotic behavior \( \tilde{k} \sim \langle J^2 \rangle_{T \to \infty}/T^2 \). Another interesting limit is when \( \sqrt{J_1J_2} \ll |J_1 - J_2| \), i.e. when the spin gap is much larger than the bandwidth of magnetic excitations. In this case, for \( \sqrt{J_1J_2} \ll T \ll |J_1 - J_2| \), replacing \( E(k) \) in (24) by \( |J_1 - J_2| = \Delta \) we obtain

\[
\tilde{k}(T) \simeq \frac{\pi J_1^2 J_2^2}{aT^2 \cosh^2 \left( \frac{\Delta}{2T} \right)}
\]

(26)

Note that the Drude weight can be recast in the form \( \tilde{k}(T) = \pi C_v(T) v_{\text{eff.}} \), where \( C_v(T) \) is the specific heat of a fermion that can occupy two levels separated by \( |J_1 - J_2| \) and with an effective velocity \( v_{\text{eff.}} \sim J_1J_2/|J_1 - J_2| \). However, this analogy cannot be extended systematically to other spin gapped systems.

Turning to the effect of the magnetic field, the Drude weight can again be rewritten as (see Eq. (A9)):

\[
\tilde{k}(T, h) = \int_{-\pi}^{\pi} dk [C_v(\epsilon(k) - h) + C_v(\epsilon(k) + h)] v^2(k)
\]

(27)

where \( C_v(\epsilon) \) is the specific heat of a single fermion of energy \( \epsilon \) and the velocity \( v(k) = \partial \epsilon / \partial k \). This form helps us derive a kind of sum rule for the thermal conductivity. For a free fermion, one has:

\[
\int_{0}^{\infty} \frac{C_v(T)}{T} dT = S(T = \infty) - S(T = 0) = k_B \ln 2,
\]

(28)

And thus:

\[
\int_{0}^{\infty} \frac{\tilde{k}(T, h)}{T} dT = k_B \ln 2 \int dk v^2(k).
\]

(29)

We note that the integral is independent of the magnetic field, so we have a kind of “sum rule”. Since in the presence of the magnetic field, it is easily seen that the low temperature thermal weight is enhanced by a factor \( e^{h/T} \), this necessarily implies that for higher temperatures, the thermal weight must decrease when a magnetic field is applied. This scenario is confirmed by Fig. 2.

FIG. 2: The field dependence of the thermal Drude weight \( \tilde{k}(T) \) for \( |J_1 - J_2| = 1 \), and \( \sqrt{J_1J_2} = 1 \).

Note that for high magnetic fields, a double peak structure appears in the thermal weight as seen in Fig. 3. The double peak results from the low temperature shift of the maximum of the contribution of the up spins, in a region in which the contribution of the down spins in negligible, and the high temperature shift of the maximum of the contribution of down spins. A similar double peak is also visible in the heat capacity. It would be interesting to investigate whether such a double peak is also present in other spin gap systems. It is known that a double peak is present in the specific heat of zig-zag spin ladder in a magnetic field. To summarize, the sum rule (29) for the thermal Drude weight, holds for all spin systems which can be described by an effective theory of non-interacting fermions.
E. The Massive Boson Model

We now consider the massive triplet boson model which was proposed as a phenomenological model for the spin-1 Heisenberg chain. This model can be obtained from the nonlinear sigma model\textsuperscript{[43]} that describes integer spin-$S$ chains in the limit $S \to \infty$ by softening the constraint on the $O(3)$ fields. More precisely, this model is characterized by a Hamiltonian density\textsuperscript{[43]}

$$\mathcal{H}(x) = \frac{u}{2} \sum_{\alpha=1}^{3} [\Pi_{x}^{2} + (\partial_{x} \phi_{\alpha})^{2}] + uV(\phi),$$

(30)

where $V(\phi) = \frac{\lambda}{2\alpha^{2}}\phi^{2} + \frac{1}{4}(\phi^{2})^{2}$, and $[\phi_{\alpha}(x), \Pi_{x}(x')] = i\delta(x-x')\delta_{\alpha,\beta}$. The energy current takes the simple form\textsuperscript{[3]}

$$j_{e}(x) = -u^{2} \sum_{\alpha=1}^{3} \Pi_{x} \partial_{x} \phi_{\alpha},$$

(31)

Note that this current is independent of the potential $V(\phi)$ and up to a prefactor, it is just the momentum density of the boson field\textsuperscript{[43]}. Consequently, translation invariance implies that the total thermal current $J_{e}$ is conserved. This allows us to use the Eq. (5) to obtain the thermal Drude weight. Since the bosons are weakly interacting, we can consider the case $\lambda = 0$, to obtain the Drude weight

$$\tilde{\kappa}(T) = \frac{3}{8T^{2}} \int_{-\Lambda}^{\Lambda} dk \frac{ue^{2}k^{2}}{\sinh^{2}\left(\frac{1}{2} \frac{u^{2}k^{2}}{\Lambda^{2} + \Delta^{2}}\right)}.$$ 

(32)

As before, the limit $T \ll \Delta$ again leads to the result \textsuperscript{[14]} for $\tilde{\kappa}(T)$ and for $T \gg \Delta$, we recover a linear weight $\kappa(T) = \pi^{2}uT$. Note that in the case of the Takhtajan-Babujian spin-$S$ chains (which are described by SU(2)$_{2S}$ WZNW models at low energy\textsuperscript{[14]}), the weight is given by:

$$\tilde{\kappa}(T) = \frac{\pi^{2}}{3} \frac{3S}{S+1} uT,$$

(33)

for $S \to \infty$, this weight is the same as the one of the triplet of bosons. This is consistent with the fact that the non-linear sigma model describes spin-$S$ chains in the limit $S \to \infty$.

F. Discussion

In the preceding sections, we have seen that all the spin gap systems studied in this paper exhibit the same generic behavior for the thermal conductivity. The reason is that for gapped 1D systems that can be bosonized, the low energy theory is Lorenz invariant, and excitations are described by massive particles having relativistic-like dispersions $\epsilon_{\alpha}(p) = \sqrt{(vp)^{2} + m_{\alpha}^{2}}$, with the gap $\Delta$ being the mass of the lightest particle. When these excitations are spin triplets, the lowest excited state contains exactly one of these particles, and the total energy current is $\epsilon(p) \frac{d\epsilon}{dp}$ which then yields a weight:

$$\tilde{\kappa}(T) \sim \int dp \epsilon(p)^{2} \left(\frac{\partial\epsilon}{\partial p}\right)^{2} e^{-\epsilon(p)/T}$$

(34)

Since Lorentz invariance dictates that $\epsilon(p) \frac{d\epsilon}{dp} = p$, one obtains the same thermal weight as in (13) in the low-temperature regime. Examples of systems possessing this triplet branch are the alternating spin-$\frac{1}{2}$ chains\textsuperscript{[2]} and the two-leg spin ladder\textsuperscript{[44]} and the Heisenberg spin-1 chain\textsuperscript{[45]}. We therefore, expect that the above mentioned systems will exhibit a finite thermal Drude weight. However, this result could differ in the case of the zig-zag ladder or the frustrated spin-$\frac{1}{2}$ chain. This stems chiefly from the fact that though the zig-zag ladder has a gapful spectrum, the low energy excitations having a relativistic dispersion, are spinons\textsuperscript{[46]} carrying a spin $\frac{1}{2}$. Another example with spinonic excitations is the XXZ chain in the Ising phase\textsuperscript{[47]}. Since the total spin of the system can only vary by an integer, the spinons occur in pairs. Consequently, the interaction between these spinons has a strong influence on the thermal weight. In the case of the XXZ chain, since the spinons are non-interacting, the current of a given excited state is conserved, and one expects to recover a finite Drude weight. However, in the case of the zig-zag ladder or the frustrated spin-$\frac{1}{2}$ chain, the interaction between the spinons can lead to a non-conservation of the current of the two spinon states, resulting in the suppression of the thermal Drude weight\textsuperscript{[46]}.

It would be worthwhile to compare our predictions for the Drude weight for various systems with numerical simulations\textsuperscript{[17]} or with other analytical techniques on the lines of Ref.\textsuperscript{[21]} in the case of integrable models. However, in the former case, the extraction of the power law prefactor in the activated thermal Drude weight from numerical data might prove very difficult.

III. EFFECT OF IMPURITIES

We have seen in Sec. II that the thermal conductivity in clean systems has a Drude peak as a result of the translational invariance of the system. In a real system, we expect this Drude peak to be replaced by a finite thermal conductivity, due to the finite lifetime of eigenstates of the Hamiltonian induced by phonon or impurity scattering. In the present section, we study the effect of impurity scattering on the gapped systems we discussed in sections II C and II D. We will begin with a calculation of the conductance of the system with a single impurity, and then we will turn to a system with a nonzero concentration of impurities.
A. Single-impurity problem

The thermal conductivity of a system with a single-impurity can be calculated using the simple Landauer approach provided, the elementary excitations are non interacting. The basic idea is to consider two reservoirs at temperature $T_1$ and $T_2$ (with $T_1 > T_2$) in presence of a barrier (the impurity potential). Reservoir 1 emits a barrier (the impurity potential). Reservoir 1 emits a probability to traverse the barrier is given by the square of the transmission coefficient $|t(k)|^2$. The current flowing from reservoir 1 to reservoir 2 is:

$$J_{1\to2} = \int_0^\infty \frac{dk}{2\pi} n_1(k,T_1)|t(k)|^2\epsilon(k)\frac{\partial\epsilon(k)}{\partial k},$$

(35)

and similarly the current flowing from to reservoir 2 to 1 is:

$$J_{2\to1} = \int_0^\infty \frac{dk}{2\pi} n_2(k,T_2)|t(k)|^2\epsilon(k)\frac{\partial\epsilon(k)}{\partial k},$$

(36)

where $n_1,2(k,T_{1,2})$ are the fermion distribution functions at temperature $T_{1,2}$. In the limit $T_1 \simeq T_2$, the net current flowing through the barrier is:

$$J = J_{1\to2} - J_{2\to1} = \int_0^\infty \frac{dk}{2\pi} \frac{|t(k)|^2\epsilon(k)}{4T^2\cosh(\frac{\epsilon(k)}{2T})} \frac{\partial\epsilon(k)}{\partial k},$$

(37)

$$= K(T_1)(T_1 - T_2),$$

Hence a knowledge of the transmission probability $|t|^2$ permits us to obtain the thermal conductance

$$K(T) = \int_0^\infty \frac{dk}{2\pi} \frac{|t(k)|^2\epsilon(k)}{4T^2\cosh(\frac{\epsilon(k)}{2T})} \frac{\partial\epsilon(k)}{\partial k}.$$  

(38)

We now apply this general formula to two spin gap systems in which the elementary excitations are non-interacting.

1. Ladder with a defect

We consider a two leg spin 1/2 ladder with a defect on a rung, described by the Hamiltonian:

$$H = J_\parallel \sum_{p=1,2} S_{n,p}\cdot S_{n+1,p} + J_\perp \sum_{n\neq 0} S_{n,1}\cdot S_{n,2} + J_\perp' S_{0,1}\cdot S_{0,2}.$$  

(39)

This Hamiltonian can be fermionized following Ref. The perturbation to the ladder becomes:

$$(J_\perp' - J_\perp)\alpha^2 (J_1 + \mathbf{n}_1)(0) \cdot (J_2 + \mathbf{n}_2)(0),$$

(40)

where $J_{1,2}$ and $\mathbf{n}_{1,2}$ are the uniform and staggered spin densities, respectively, and the most relevant contribution is $(J_\perp' - J_\perp)\alpha^2 \mathbf{n}_1(0) \cdot \mathbf{n}_2(0)$. This contribution can be fermionized, so that the resulting low energy Hamiltonian of the ladder with a rung defect reads:

$$H = -\frac{i\nu}{2} \sum_{a=0}^4 \int dx \left( \xi_R^a \partial_x \xi_R^a - \xi_L^a \partial_x \xi_L^a \right)$$

$$+ i \int dx m(x) \left( \sum_{a=0}^3 \xi_R^a \xi_L^a - 3 \xi_R^a \xi_L^a \right),$$

(41)

where $m(x) = m + g\delta(x)$, with $m = J_\perp/(2\pi)$ and $g = (J_\perp' - J_\perp)a/(2\pi)$. Clearly, each Majorana mode is scattered independently from the barrier, so that their contributions to the thermal conductivity is additive. As discussed in in the preceding sections and in App. A we use the correspondence between the Majorana and Dirac fermions to calculate the thermal conductivity with the barrier. The First Quantized Hamiltonian for the Dirac fermions reads:

$$H = -\nu\sigma_3 \partial_x + m(x)\sigma_2,$$

(42)

where $\sigma_i$ are Pauli matrices. Solving the Schrödinger equation with appropriate boundary conditions for the wavefunction at the barrier, we obtain the transmission probability

$$|t(k)|^2 = \cos^2 \psi \frac{k^2}{k^2 + K^2},$$

(43)

where $K = m/v \sin \psi$ and $\tan(\psi/2) = \frac{\nu}{k} = (J_\perp' - J_\perp)/(2\nu^2J_\parallel)$, Eq. (38) becomes:

$$K(T) = \int_0^\infty \frac{dk}{2\pi} \frac{\cos^2 \psi}{k^2 + K^2} \frac{k^2}{2T^2} \cosh(\sqrt{(vk)^2 + m^2}/2T) - \frac{(vk)}{\sqrt{(vk)^2 + m^2}}.$$  

(44)

where we have used $\epsilon(k) = \sqrt{(vk)^2 + m^2}$. In the limit $T \to 0$, the transmission probability is dominated by momentum $k \ll K$ for which $|t(k)|^2 \sim k^2/K^2$ i.e. the barrier is a strong scatterer, and

$$K(T) = \frac{3m}{2\pi} e^{-m/T \cot^2 \psi},$$

(45)

where we have taken into account the triplet of Majorana modes. One can obtain an estimate of the temperature $T^*$ below which this result is valid by noting that for $T \ll m$, one has $(\langle v\rangle k)^2 = mT$, so that the criterion for low temperature is $mT \ll m^2\sin^2 \psi$, i.e. $T \ll T^* = J_\perp (J_\perp' - J_\perp)^2/J_\parallel^2$. This temperature is clearly much smaller than the gap $m$. For higher temperatures, $T^* \ll T < m$, the thermal conductance is obtained by making the approximation $|t(k)|^2 \sim \cos^2 \psi$, leading to:

$$K(T) = \frac{3\cos^2 \psi}{4\pi} T \int_{m/T}^\infty dx \left( \frac{x/2}{\sinh(x/2)} \right)^2$$

$$+ \frac{\cos^2 \psi}{4\pi} T \int_{3m/T}^\infty dx \left( \frac{x/2}{\sinh(x/2)} \right)^2.$$  

(46)
For $T^* \ll T \ll m$, one finds $K(T) \sim \frac{3m^2}{2T^2}e^{-m/T}$, and for $T \gg m$, $K(T) = \frac{2m}{T^2}\cos^2\psi$. Contrary to the result for the pure ladder, the thermal conductance for $T \ll T^*$ is purely activated without any $T$ dependent prefactor. Therefore, the Drude weight in the thermal conductivity for the pure system is not an accurate indication on the behavior of the thermal conductivity in a system with impurities. The reason for that is clear from the Appendix C, namely low energy modes experience much stronger impurity scattering than the high-energy ones. It is only in the high temperature limit $T \gg m$ that the replacement $\delta(\omega) \rightarrow \tau$ is justified. We will see in the following section that this result is not restricted to the spin ladder.

2. XY chain with a defect

We consider again the XY-chain with alternating exchange of Sec. [11]. We now suppose that the bond strength $J_i$ between the sites 0 and 1 is replaced by $J'_i$. This bond acts as a barrier and using the results of Appendix C, the transmission probability across this barrier is given by

$$|t(k)|^2 = \frac{4J_i^2(J'_i)^2\sin^2\phi_k}{(J_i^2 - (J'_i)^2)^2 + 4J_i^2(J'_i)^2\sin^2\phi_k}$$

(47)

In particular, we can show that when $k \approx \pi/2$ we have:

$$|t(k)|^2 = \frac{16J_i^2(J'_i)^2J_i^2(k - \pi/2)^2}{(J_i^2 - (J'_i)^2)^2(J_i - J'_i)^2 + 16J_i^2(J'_i)^2J_i^2(k - \pi/2)^2}$$

(48)

which indicates that for low temperatures $T \ll \sqrt{J_iJ'_i}$, the behavior of the thermal conductivity in the XY chain with a bond defect is identical to the behavior of the thermal conductivity in the ladder discussed in Sec. [11A1].

For high temperatures, $T \gg \sqrt{J_iJ'_i}$, we can neglect the variation of the transmission coefficient with the energy, and assume that all states have the same probability of occupation. Then, the thermal conductance reads:

$$K(T) = T \int_{(J_i - J'_i)/T}^{(J_i + J'_i)/T} \frac{d\omega}{2\pi} |t(\omega)|^2 \sim 1/T^2$$

(49)

B. Many impurities case

In this section, we consider the effect of a finite concentration of impurities on the thermal conductivity of the ladder. As before, the disorder we consider is a random rung coupling. The Hamiltonian of the disordered ladder reads:

$$H = J_{\parallel} \sum_{p=1,2} S_{i,p} \cdot S_{i+1,p} + \sum_i J_{\perp}^i S_{i,1} \cdot S_{i,2},$$

(50)

where $J_{\perp}^i = J_{\perp} + \eta_i$. We have $|\eta_i| < J_{\perp}$, so that all rung interactions remain antiferromagnetic. This Hamiltonian can be analyzed by mapping onto a random mass Majorana fermions model [28].

$$H = -\sum_{a=1}^4 \int dx \frac{i\omega}{2} \left[ \xi^a_R(x)\partial_x \xi^a_R(x) - \xi^a_L(x)\partial_x \xi^a_L(x) \right.$$ 

$$+ im^a(x)\xi^a_R(x)\xi^a_L(x) \right],$$

(51)

with $m^{1,2,3}(x) = m(x)$ for the triplet magnetic excitation, $m^0 = -3|m|/x$ for the singlet excitation and $m(x) = m + \eta(x)$ where $\eta(x)\eta(x') = D\delta(x - x')$. We note that disorder does not mix the different flavors of Majorana fermions. Consequently, the contribution of the Majorana modes to the thermal conductivity remains additive. As before, to calculate the disorder induced self-energy, it is useful to recast the above problem in terms of Dirac Fermions.

$$H = -iv \int dx (\psi^+_R \partial_x \psi_R - \psi^+_L \partial_x \psi_L)$$

$$+ m(x) \int dx (\psi^+_R \psi_L + \psi^+_L \psi_R),$$

(52)

We note that the Hamiltonian (52) can also be derived from a dimerized XY chain with bond defects [28]. We define the $2 \times 2$ matrix disordered averaged Green’s function $G$ by its components,

$$G_{\alpha\beta}(x, \tau) = -(T, \psi_{\alpha}(x, \tau)\psi^\dagger_{\beta}(0, 0)),$$

(53)

where $\alpha, \beta \in \{R, L\}$. The Hamiltonian (52) can be rewritten in matrix form as:

$$H = \int dx \Psi^\dagger(x)[-i v \tau_3 \partial_x + m(x) \tau_1] \Psi(x),$$

(54)

where $\tau_{1,3}$ are Pauli matrices. The impurity self-energy matrix $\Sigma$ can be calculated within the Self Consistent Born Approximation (SCBA) [23] and satisfies the Dyson equation for the disorder averaged Green’s function:

$$(i\omega_n - v k \tau_3 - m \tau_1 - \Sigma)G = 1,$$

(55)

In this approximation, the self-energy is independent of momentum and is determined self-consistently by

$$\Sigma(i\omega_n) = D \int \frac{dk}{2\pi} \tau_1 [i\omega_n - v k \tau_3 - m \tau_1 - \Sigma(i\omega_n)]^{-1} \tau_1$$

(56)

Clearly, the self-energy possesses the following structure, $\Sigma(i\omega_n) = i\sigma(i\omega_n) + V(i\omega_n)\tau_1$ leading to the following self-consistent equations for $\sigma$ and $V$:

$$\sigma(i\omega_n) = \frac{D}{2v} \frac{\sigma(i\omega_n) - \omega_n}{\sqrt{(\sigma(i\omega_n) - \omega_n)^2 + (m + V(i\omega_n))^2}}$$

$$V(i\omega_n) = \frac{D}{2v} \frac{V(i\omega_n) - m}{\sqrt{(V(i\omega_n) - m)^2 + (m + V(i\omega_n))^2}}$$

(57)

Introducing the dimensionless variables: $s = i\sigma/m$, $t = V/m$, $x = i\omega_n/m$ and $\lambda = D/(2vm)$ the above self-consistent equations simplify to:

$$t = -\frac{s}{x - 2s},$$

(58)

$$s^4 - s^3x - s^2\left(\frac{1}{4} - \frac{x^2}{4} - \lambda^2\right) - \lambda^2sx + \frac{\lambda^2}{4}x^2 = 0,$$

(59)
 FIG. 4: The imaginary part of the self energy in units of $m$ calculated from Eq. (3) for various values of the scaled impurity strength $\lambda$. Note that the effective gap decreases with increasing $\lambda$.

This quartic equation can be solved numerically. Some sample curves are shown in Fig. 4. We find that the disorder renormalizes the gap in the spectrum and a sufficiently strong disorder ($\lambda = 0.5$) closes the gap indicating a disorder induced phase transition within the SCBA. A plot of the renormalized gap $\omega_c$ as a function of disorder strength is shown on Fig. 3. In the ensuing calculation, we only consider disorder strengths for which the renormalized gap is

FIG. 5: The effective gap in units of $m$ as a function of the scaled impurity strength $\lambda$.

Using the results of the previous sections, the thermal conductivity for the disordered ladder can be rewritten as

$$
\kappa(T) = \frac{1}{T} \int \frac{d\omega}{2\pi} \left[ \frac{\partial n_P}{\partial \omega} \right] [P(\omega-i0, \omega+i0) - \text{Re}P(\omega+i0, \omega+i0)],
$$

where:

$$
P(\omega, \omega') = \int \frac{dk}{2\pi} (v^2 k)^2 \text{Tr} [G(k, \omega) G(k, \omega')],
$$

Vertex corrections to (60) are negligible in the weak disorder limit. Contrary to the suggestion in Ref. 20 that

$\text{Re}P(\epsilon + i0, \epsilon + i0)$ in Eq. (60) can be neglected, we find that this term is indeed crucial to take into account the presence of a gap in the energy spectrum. To proceed with the calculation of $\kappa$, we first note that for weak disorder i.e., $D \ll \nu m$, since the off-diagonal self-energy $V$ always occurs in the combination $m + V$ (63), it is reasonable to neglect $V$ in the Green’s function $G$ which can then be approximated as

$$
G(k, \omega) = \frac{\omega - \sigma(\omega) + vk\sigma_3 + m\sigma_1}{(\omega - \sigma(\omega))^2 - \epsilon(k)^2},
$$

where $\epsilon(k) = \sqrt{v^2 k^2 + m^2}$. This yields

$$
G(k, \omega + i0) = \frac{1}{2} \left[ 1 + \frac{vk\sigma_3 + m\sigma_1}{2\epsilon(k)} \right] \frac{1}{\omega - \sigma(\omega) - \epsilon(k)}
$$

$$
+ \left[ 1 - \frac{vk\sigma_3 + m\sigma_1}{2\epsilon(k)} \right] \frac{1}{\omega - \sigma(\omega) + \epsilon(k)},
$$

$$
G(k, \omega - i0) = \frac{1}{2} \left[ 1 + \frac{vk\sigma_3 + m\sigma_1}{2\epsilon(k)} \right] \frac{1}{\omega - \sigma^*(\omega) - \epsilon(k)}
$$

$$
+ \left[ 1 - \frac{vk\sigma_3 + m\sigma_1}{2\epsilon(k)} \right] \frac{1}{\omega - \sigma^*(\omega) + \epsilon(k)}.
$$

Substituting the above in (63), we obtain

$$
P(\omega+i0, \omega-i0) - \text{Re}P(\omega+i0, \omega+i0) = \int \frac{dk}{2\pi} (v^2 k)^2 K(\omega, k)
$$

where

$$
K(\omega, k) = \frac{\text{Im}^{\sigma(\omega)}(\omega)}{[\omega - \epsilon(k) - \text{Re}^\sigma(\omega)]^2 + (\text{Im}^{\sigma(\omega)}(\omega))^2}
$$

$$
+ \frac{\text{Im}^{\sigma(\omega)}(\omega)}{[\omega + \epsilon(k) - \text{Re}^\sigma(\omega)]^2 + (\text{Im}^{\sigma(\omega)}(\omega))^2}
$$

This expression can now be used in (60) to obtain the thermal conductivity. At low temperatures, the derivative of the Fermi function in (60) decays exponentially as exp $-\omega/T$ indicating that frequencies much larger than $T$ can be neglected in the integral for the thermal conductivity $\kappa(T)$. Consequently, the low temperature behavior of $\kappa(T)$ is completely dictated by the low frequency behavior of $K(\omega, k)$. We now analyze the behavior of $K$. Firstly, since the diagonal self energy $\text{Im}^{\sigma(\omega)} = 0$, for $\omega < \omega_c$ i.e., for frequencies smaller than the disorder renormalized gap, $K(\omega, k)$ is identically zero for all $\omega < \omega_c$. A typical plot of $K$ as a function of $\omega$ for two different values of $k$ is shown on figure 3.

Clearly, the dominant contribution to $\kappa$ for temperatures $T < \omega_c$ comes from the behavior of $K(\omega, k)$ in the vicinity of $\omega_c$. This behavior has been analyzed numerically, and we find that for all $k$, $K$ can be developed as a series in $\omega - \omega_c$:

$$
K(\omega, k) = \alpha(k)(\omega - \omega_c) + \beta(k)(\omega - \omega_c)^2 + \ldots
$$
We find that $\alpha, \beta$ are fast decreasing functions of $|k|$, such that $\int dk^2 \alpha(k) < \infty$ and $\int dk^2 \beta(k) < \infty$. Substituting (65) in (60), we obtain

$$\kappa(T) = \frac{1}{4T^2} \int dk \int d\omega k^2 e^{-\omega/T} \Theta(\omega - \omega_c) \left[ \alpha(k)(\omega - \omega_c) + \beta(k)(\omega - \omega_c)^2 + \ldots \right]$$

leading to,

$$\kappa(T) \sim \tilde{\alpha} e^{-\omega_c/T} + \tilde{\beta} T e^{-\omega_c/T} + o(T e^{-\omega_c/T})$$

(67)

$\tilde{\alpha}, \tilde{\beta}$ are temperature independent constants. We find that the results are similar to those for a single impurity case with the difference that a finite concentration of impurities renormalizes the gap. At very high temperatures one recovers the usual $T^{-2}$ decrease of the thermal conductivity. It would be interesting to obtain the crossover behavior from the low to high temperature regimes. However, the rather complicated form of the self energies makes analytical calculations very difficult for these intermediate temperatures and this is left for future work. For small magnetic fields $h \ll \omega_c$ the same result holds with the substitution $\omega_c \rightarrow \omega_c - h$.

IV. DISCUSSION

We now highlight the connection between our approach and that of the Boltzmann equation. A Boltzmann like equation for the thermal conductivity can be recovered from the SCBA in the limit of small self energies. For $\sigma(\omega) \ll m$, the function $K$ defined by (64), takes the simpler form

$$K(\omega, k) = \pi [\delta(\omega - \epsilon(k)) + \delta(\omega - \epsilon(k))] (\text{Im} \sigma(\omega))^{-1}$$

(68)

Inserting the above result in (60), we obtain:

$$\kappa(T) = \frac{1}{T} \int \frac{dk}{2\pi} \left( \epsilon(k) \frac{\partial \epsilon(k)}{\partial k} \right)^2 \left( -\frac{\partial n_F}{\partial \epsilon} \right) (\epsilon(k)) (\text{Im} \sigma(\epsilon(k)))^{-1}$$

(69)

We see that in the limit of very small self energies, we recover the Boltzmann equation result for the thermal conductivity. Comparing (65) with (6) and (17), we see that if $\text{Im} \sigma(\epsilon(k)) = \tau^{-1}$ where $\tau$ is a constant independent of $\epsilon$, the thermal conductivity can be written as a product of the Drude weight in the absence of impurities and the mean relaxation time $\tau$ as was proposed in Ref. [3]. The underlying assumption there, was that all the eigenstates of the system have the same lifetime $\tau$ independent of the energy of the eigenstate. As shown above, the explicit energy dependence of the self energy found in Sec. II, i.e., the fact that the low energy spin excitations are much more scattered by impurities than high energy excitations, shows that any assumption of energy independent lifetime is invalid even for the simplest models. As a result, the thermal Drude weight can at most yield a heuristic behavior of the thermal conductance in a real system in which spin excitations are interacting with impurities and/or phonons due to the different extrinsic lifetimes of current carrying states.

We present a brief comparison of our results with experiments. Since disorder is ubiquitous in real systems, it is reasonable to compare our results for the two leg ladder with impurities with experimental measurements. One of the systems studied extensively is the spin gap compound Sr$_{14-x}$(La,Ca)$_x$Cu$_2$O$_{41}$ [41]. In the insulating phase, these systems can be well described by an array of two-leg spin ladders. In this system, the phonon subtracted thermal conductivity was shown to have an exclusive spin contribution. At low temperatures, a fit for spin thermal conductivity yielded a $\kappa(T) \sim e^{-\Delta/T}$. This low temperature fit is in good accord with our prediction of $\kappa(T) \sim e^{-\omega_c/T}$. However, a full quantitative comparison requires an understanding of the effect of the disorder in the material on the spins, the effect of spin-phonon interactions and other exchange interactions in the ladder.

V. CONCLUSION

In the present paper, we have calculated the thermal conductivity of gapless spin chains and spin gap systems including the two-leg spin-1/2 ladder and the dimerized XY spin-1/2 chain. In the absence of disorder, the thermal Drude weight of gapless spin chains vanishes linearly with temperature. On the other hand, for the ladder and the XY chain, which can both be represented as free fermions, we find that the thermal Drude weight $\tilde{\kappa} \sim T^{-1/2} e^{-m/T}$, where $m$ is the gap to the lowest triplet excitation. For intermediate temperatures, $\tilde{\kappa} \propto T$ and decays as $T^{-2}$ at very high temperatures. We argue that this behaviour is generic to all quasi-one dimensional spin gapped systems having low energy triplet excitations with a relativistic-like dispersion. We have also considered the effect of a magnetic field which results in a substantial enhancement of the low temperature thermal conductivity. Furthermore, in the case of dimerized
XY chains, a double peak can be obtained in the thermal conductivity for large enough fields. We have also studied the effect of impurities on spin gap systems like the ladder and the XY chain. Impurities destroy the Drude peak resulting in a finite thermal conductivity at zero frequency. This thermal conductivity has a generic form $e^{-\tilde{m}/T}$ at low temperatures where, $\tilde{m}$ is the effective gap of the system. It would be interesting to include the effects of magnetic impurities and also scattering from phonons. These and other questions are left for future work.

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APPENDIX A: CALCULATION OF THE THERMAL CONDUCTIVITY FOR MAJORANA FERMIONS

1. Thermal conductivity of Dirac fermions

We consider massive Dirac fermions with the following Hamiltonian density:

$$\mathcal{H}(x) = -\frac{i}{2} \sum_{k,L} \left( \bar{\psi}_{k,L} \frac{1}{2} \left( \begin{array}{c} 0 \\ \psi_{k,L} \end{array} \right) + (\bar{\psi}_{k,L}) \right) + m \left( \frac{1}{2} \Omega \psi_{k,L}^\dagger \psi_{k,L} + e^{-i\phi} \psi_{k,L}\psi_{k,L} \right)$$

(A1)

In this case, the energy current reads:

$$j_e(x) = -i \sum_{k,L} \left( \bar{\psi}_{k,L} \psi_{k,L} \right) \frac{1}{2} \left( \begin{array}{c} 0 \\ \psi_{k,L} \end{array} \right) + \frac{1}{2} \Omega \psi_{k,L}^\dagger \psi_{k,L} - \frac{1}{2} \Omega \bar{\psi}_{k,L} \psi_{k,L}$$

(A2)

We note that using the transformation $\psi_{k,L} \rightarrow e^{i\phi} \psi_{k,L}$ we can reduce the Hamiltonian (A1) to the case $\phi = 0$, while leaving the current (A2) invariant. Therefore, for the purpose of calculating the thermal transport we can without loss of generality restrict to the case $\phi = 0$ in (A1).

Using the Fourier decomposition

$$\psi_{k,L}(x) = \frac{1}{\sqrt{L}} \sum_k c_k e^{ikx}$$

(A3)

the Dirac Hamiltonian $H = \int dx \mathcal{H}(x)$ can be diagonalized to obtain

$$H = \sum_k \epsilon(k) \left( c_{k,+}^\dagger c_{k,+} + c_{k,-}^\dagger c_{k,-} \right)$$

(A4)

where the fermionic operators $c_{k,\pm}$ are linear combinations of the $c_{k,R/L}$ such that $c_{k,+} = c_{k,R}^\dagger + c_{k,L}^\dagger$ and $c_{k,-} = c_{k,R}^\dagger c_{k,L}$ and $\epsilon(k) = \sqrt{(vk)^2 + m^2}$. This allows us to rewrite the total energy current $J_e = \int dx j_e(x) = \sum_k v^2 k (c_{k,R}^\dagger c_{k,R} + c_{k,L}^\dagger c_{k,L} - 1)$ as:

$$J_e = \sum_k v^2 k (c_{k,+}^\dagger c_{k,+} + c_{k,-}^\dagger c_{k,-} - 1).$$

(A5)

Using (A4), one easily obtains

$$\langle J_e^2 \rangle = 2 \sum_k v^2 k^2 (n_+ + 1)$$

(A6)

where the Fermi distribution function $\langle n_+ \rangle = (e^{\beta \epsilon(k)} + 1)^{-1}$. From (B), the thermal conductivity $\kappa(\omega, T) = \tilde{\kappa}(\omega)$ with a Drude weight

$$\tilde{\kappa}(T) = \frac{1}{4 \pi^2} \int_{-\infty}^{\infty} dk \frac{v^2 k^2}{\cosh^2 \left( \frac{\epsilon(k)}{2T} \right)}$$

(A7)

The above result has a simple interpretation in terms of kinetic theory. Consider the expression for the specific heat:

$$C_v(T) = \frac{1}{T^2} \int \frac{dk}{2\pi} \frac{\epsilon(k)^2}{\cosh^2 \left( \frac{\epsilon(k)}{2T} \right)} = \frac{1}{T^2} \int dk c_v(k, T),$$

(A8)

i.e., a mode of momentum $k$ contributes $c_v(k)$ to the specific heat. Such a mode has a velocity $v(k) = v^2 k / \epsilon(k)$. This now permits us to rewrite (16) as:

$$\tilde{\kappa} = \int \frac{dk}{2\pi} c_v(k, T) v^2(k),$$

(A9)

i.e., the contribution of each mode $k$ to the Drude weight is just the product of its specific heat and square of the velocity. This is similar to the kinetic theory result that the thermal Drude weight is given by the product of the specific heat and the square of the velocity of the free modes.

2. Majorana fermions

It is well known that the Dirac Hamiltonian (A1) can be re-expressed in terms of two Majorana fermions fields defined by $\psi_{k,L} = (c_{k,L}^\dagger + i c_{k,R}^\dagger) / \sqrt{2}$. The Hamiltonian can be written as a sum of two Majorana Hamiltonians

$$H_{\text{Dirac}} = H_M [\psi_1^\dagger] + H_M [\psi_2^\dagger]$$

(A10)

Similarly, the energy current (A2) can be written as the sum of two energy currents, each associated with one Majorana field: $j^1_e(x) = j^1_e(x) + j^2_e(x)$. The thermal conductivity of the Dirac Hamiltonian can then be written as the sum of the conductivities associated with the two Majorana field i.e., $\kappa_{\text{Dirac}}(\omega, T) = \kappa_1(\omega, T) + \kappa_2(\omega, T)$. The expression of the currents and the Hamiltonian being identical for the two species of Majorana fermions, it
is clear that \( \kappa^1(\omega, T) = \kappa^2(\omega, T) \). Thus, one obtains the generic result that
\[
\kappa_{\text{Majorana}}(\omega, T) = \kappa_{\text{Dirac}}(\omega, T)/2.
\]
This result shows that it suffices to calculate the thermal conductivity of the corresponding Dirac Hamiltonian to obtain the Majorana thermal conductivity. This correspondence holds provided there are no interactions between the various species of Majorana fermions.

**APPENDIX B: THERMAL CURRENT IN THE PRESENCE OF AN APPLIED MAGNETIC FIELD**

In the presence of an applied magnetic field, the Hamiltonian density is \( \mathcal{H}(x) = \mathcal{H}(x) + \mathbf{h} \cdot \mathbf{m}(x) \), where \( \mathbf{m}(x) \) is the magnetization density and \( \mathbf{h} \) is the external magnetic field. Using the continuity equation for the Hamiltonian density and the equation of conservation of the moment \( \partial_t \mathbf{m} + \mathbf{J}_s = 0 \), the thermal current is now given by
\[
\mathbf{j}_\text{th.}(x) = \mathbf{j}_e(x) - \mathbf{h} \cdot \mathbf{J}_s(x),
\]
where \( \mathbf{j}_e \) is the energy current for \( \mathbf{h} = 0 \) and \( \mathbf{J}_s(x) \) is the magnetization current.

For the specific case of the ladder with a magnetic field along the \( z \) direction, the Pauli coupling is
\[
H_{\text{mag.}} = -i\hbar \int dx (\xi_{\mathcal{R}}^1 \xi_{\mathcal{L}}^2 + \xi_{\mathcal{L}}^1 \xi_{\mathcal{R}}^2) \quad (B2)
\]
Note that the contribution to the thermal conductivity arising from the \( \xi_{\mathcal{R},L}^0, \xi_{\mathcal{R},L}^3 \) is not changed by the application of the magnetic field. To obtain the thermal conductivity coming from the modes \( \xi_{\mathcal{R},L}^{1,2} \) it is convenient to turn to the Dirac Fermions. For \( \psi_{\nu,s} = (\xi_{\nu} + i\xi_{\nu}^2)/\sqrt{2} \). Then, one can rewrite \( H_{\text{mag.}} \) as:
\[
H_{\text{mag.}} = -\hbar \int dx (\psi_{\nu,s}^\dagger \psi_{\nu,s} + \psi_{\nu,s}^\dagger \psi_{\nu,s}) \quad (B3)
\]
The expression of the total thermal current then reads:
\[
J_e = \sum_k \left[ (\epsilon(k) - \hbar) \frac{\partial \epsilon}{\partial k} (c_{k,+}^\dagger c_{k,+} - \langle c_{k,+}^\dagger c_{k,+} \rangle) \\
- (\epsilon(k) + \hbar) \frac{\partial \epsilon}{\partial k} (c_{k,-}^\dagger c_{k,-} - \langle c_{k,-}^\dagger c_{k,-} \rangle) \right] \quad (B4)
\]
The contribution of the \( \xi_{\mathcal{R},L}^{1,2} \) modes to the Drude weight in the thermal conductivity is then calculated to be
\[
\kappa^1(T, h) + \kappa^2(T, h) = \frac{1}{8T^2} \int dk \left[ \frac{(\epsilon(k) - \hbar)^2}{\cosh \left( \frac{\epsilon(k) - \hbar}{2T} \right)} \\
+ \frac{(\epsilon(k) + \hbar)^2}{\cosh \left( \frac{\epsilon(k) + \hbar}{2T} \right)} \right] \quad (B5)
\]

**APPENDIX C: EIGENVALUES AND EIGENSTATES OF THE FERMIONIZED XY CHAIN**

1. **Translational Invariant Case**

The eigenstates of the Hamiltonian (22) are obtained by solving the equations:
\[
J_1 A_{2n} + J_2 A_{2n+2} = EA_{2n+1} \quad (C1)
\]
\[
J_2 A_{2n-1} + J_1 A_{2n+1} = EA_{2n} \quad (C2)
\]
One finds positive energy solutions:
\[
\begin{pmatrix} A_{2n} \\ A_{2n+1} \end{pmatrix} = e^{2i\kappa_n} \begin{pmatrix} e^{-i\phi_k/2} \\ e^{i\phi_k/2} \end{pmatrix} \quad (C3)
\]
with \( E(k) = \sqrt{(J_1 - J_2)^2 + 4J_1 J_2 \cos^2 k} \) and \( J_1 + J_2 e^{2i\kappa} = E(k) e^i\phi_k \), and negative energy solutions:
\[
\begin{pmatrix} A_{2n} \\ A_{2n+1} \end{pmatrix} = e^{2i\kappa_n} \begin{pmatrix} -e^{-i\phi_k/2} \\ e^{i\phi_k/2} \end{pmatrix} \quad (C4)
\]
with \( E(k) = -\sqrt{(J_1 - J_2)^2 + 4J_1 J_2 \cos^2 k} \) and \( J_1 + J_2 e^{2i\kappa} = |E(k)| e^i\phi_k \).

2. **Single impurity case**

Clearly, the solutions with momentum \( k \) and \(-k \) are degenerate in energy, thus we search the solution as a linear combination of these solutions. The system of equations to solve reads:
\[
J_1 A_{2n} + J_2 A_{2n+2} = EA_{2n+1} (n \neq 0) \quad (C5)
\]
\[
J_2 A_{2n-1} + J_1 A_{2n+1} = EA_{2n} (n \neq 0) \quad (C6)
\]
\[
J'_1 A_0 + J_2 A_2 = EA_1 (n = 0) \quad (C7)
\]
\[
J_2 A_{-1} + J'_1 A_1 = EA_0 (n = 0) \quad (C8)
\]
We search for solutions of the form:
\[
\begin{pmatrix} A_{2n} \\ A_{2n+1} \end{pmatrix} = e^{2i\kappa_n} \begin{pmatrix} e^{-i\phi_k/2} \\ e^{i\phi_k/2} \end{pmatrix} + r(k) e^{-2i\kappa_n} \begin{pmatrix} e^{i\phi_k/2} \\ e^{-i\phi_k/2} \end{pmatrix} \quad (C9)
\]
for \( n \leq -1 \) and:
\[
\begin{pmatrix} A_{2n} \\ A_{2n+1} \end{pmatrix} = t(k) e^{2i\kappa_n} \begin{pmatrix} e^{-i\phi_k/2} \\ e^{i\phi_k/2} \end{pmatrix} \quad (C10)
\]
for \( n \geq 1 \). Applying equations (C3) for \( n = -1 \) and (C6) for \( n = 1 \) we obtain respectively:
\[
A_0 = e^{-i\phi_k/2} + r(k) e^{i\phi_k/2} \quad (C11)
\]
\[
A_1 = t(k) e^{i\phi_k/2} \quad (C11)
\]
The equations that determine \( t, r \) are obtained from (C7) and (C8). They read:
\[
J_2(e^{-2i\kappa} e^{i\phi_k/2} + r(k) e^{2i\kappa} e^{-i\phi_k/2} + J_1 t(k) e^{i\phi_k/2} = E(e^{-i\phi_k/2} + r(k) e^{i\phi_k/2} + J_2(e^{-2i\kappa} e^{i\phi_k/2} + r(k) e^{2i\kappa} e^{-i\phi_k/2} = E t(k) e^{i\phi_k/2})
\]
Using the relation $J_1 + J_2 e^{2ik} = E(k) e^{i\phi_k}$ these equations are simplified as follows:

$$- J_1 e^{-i\phi_k} r(k) + J'_1 e^{i\phi_k} t(k) = J_1 e^{i\phi_k} / 2 \quad (C14)$$

$$J'_1 e^{i\phi_k} r(k) - J_1 e^{-i\phi_k} t(k) = -J'_1 e^{-i\phi_k} / 2 \quad (C15)$$

We obtain the transmission amplitude $t(k)$ and the reflection amplitude $r(k)$ as:

$$r(k) = \frac{(J'_1)^2 - J_1^2}{J'_1 e^{-i\phi_k} - (J'_1)^2 e^{i\phi_k}} \quad (C16)$$

$$t(k) = \frac{-2iJ_1J'_1 \sin \phi_k}{J'_1 e^{-i\phi_k} - (J'_1)^2 e^{i\phi_k}} \quad (C17)$$