Effects of anisotropy on the dynamical and static spin conductivity of an anisotropic spin-1/2 two-leg ladder

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We address a detailed analysis of the dynamical spin conductivity of an anisotropic spin ladder in the direction of the legs by means of a quantum many-particle approach. Bond operator transformation has been employed in order to map the original spin model Hamiltonian to a bosonic one. This bosonic Hamiltonian should include an infinite hard-core repulsion to preserve the SU(2) algebra of the original model. Using a Green’s function approach, the energy spectrum of quasiparticle excitation has been obtained. Linear response theory has been implemented to obtain spin conductivity via calculation of time-ordered energy current correlation. The results show the spin conductivity possessing a nonzero value in a finite frequency interval. Increasing the rung-coupling exchange constant moved this frequency interval to higher frequencies. Also, the spin conductivity presents a small nonzero value at very low frequency for low rung-coupling constants. Furthermore, the effects of spin anisotropies on both leg and rung couplings are investigated. A tiny dependence of the spin transport on the anisotropy in the leg direction is observed in contrast to the strong one on the anisotropy along the rung direction, due to the direct effect of the triplet density. Additionally, the frequency behavior of the spin conductivity of the isotropic case has been studied due to the temperature effects. The temperature dependence of static spin conductivity has been found for various rung-coupling exchange constants and anisotropies in both coupling strengths.

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1. Introduction

The field of low-dimensional magnetism with small spins has attracted the interest of many researchers and is a successful example for fruitful interplay between theory and experiment [1,2]. In contrast to magnetic systems with classical long-range ferro or antiferromagnetic orders, novel ground state properties arise due to the existence of strong quantum fluctuations in reduced dimensions. In one dimension, magnetic ordering is often suppressed even at zero temperature, but rather spin liquid states are developed. Prominent examples are dimerized chains and spin ladders. This disordered phase is characterized by an energy gap in its magnetic excitations [3]. These $S = 1$ excitations, commonly called triplon, in the gapped ladders are topological excitations in the spin-1/2 Heisenberg chain. In spite of extensive study of low-dimensional quantum magnets, the transport properties still pose challenges for experimental and theoretical physicists [4–6]. The quasi-one-dimensional magnets such as the Sr$_2$CuO$_3$, SrCuO$_2$ chain or the Sr$_{14}$Cu$_{24}$O$_{41}$ ladder compounds [5] are electrically insulating compounds. The propagation of magnetic excitations along the chains...
(ladders) is attributed to the highly anisotropic spin and thermal conductivities. Finite temperature transport properties remain an exciting and active field of research. A more precise definition of ballistic transport can be given by introducing the spin Drude weight defined as the weight of the zero-frequency contribution to the real part of the conductivity [7]. The criterion for ballistic transport is the existence of a singularity at zero frequency of the real part of the spin conductivity. The appearance of a nonzero Drude weight is often ascribed to the influence of conservation laws on transport [8–10]. Also, fundamental questions have been raised, e.g. how the integrability of quasi-one-dimensional systems affects the ballistic property of spin conductivities [11–14].

As optical conductivity is the current response to a time-dependent electromagnetic vector potential, spin conductivity is conveniently derived as the spin current response to a long-wavelength, frequency-dependent magnetic field gradient [15].

Using an exact diagonalization method, the frequency dependence of the spin conductivity of dimerized spin-1/2 chains, with an energy gap in its spectrum, has been investigated [16]. This study shows that there is almost no weight in the regular part of \( \sigma(\omega) \) below a value of frequency beyond which the dominant peak is located. Turning on a magnetic field influences the curve drastically. The major portion of the weight still lies above the gap but is much smaller and without significant gap. Also, the results of this work indicate that going to higher temperatures results in a smooth curve due to thermal excitations, while the influence of the magnetic field is much weaker and only changes the numerical values without modifying the structure. The spin conductivity of Heisenberg chains has previously been studied within linear response theory in analogy to the Kubo formula for charge transport [17]. Also, spin transport properties in anisotropic Heisenberg antiferromagnets in two and three dimensions have been analysed within the Dyson–Maleev transformation [18–21] and interacting spin wave theory. Based on this study, the XXZ magnet in the ising regime is a spin insulator. In three dimensions the regular part of the spin conductivity vanishes linearly in the zero frequency limit, while \( d = 3 \) presents a finite zero frequency value [21]. In other theoretical work, finite temperature Drude weight and the regular part of spin conductivity are evaluated for the anisotropic spin-1/2 Heisenberg model using the exact diagonalization for small sizes [22]. The results of this numerical work show that spin Drude weight is found to scale to zero approaching the isotropic point. Unlike the isotropic case, anisotropy higher than two causes the Drude weight to be nearly exhausted with the overlap with conserved energy current. Also, the spin conductivity includes a peak which shifts as the inverse of system size for different anisotropy parameters [22].

For spin ladder systems the situation is more complex. Here, the magnon–magnon scattering, as well as magnon–phonon, suppress the ballistic spin conduction even though the coupling to acoustic phonons is weak [23]. Diffusive transport is a result of the interchain interactions, which break the integrability of the decoupled Heisenberg chains. Therefore, turning on the interchain interaction leads to zero value for spin Drude weight as well as the current correlations at long times. The spin ladder model Hamiltonian, as a nonintegrable model, is expected to have a vanishing Drude weight at infinite size with finite temperature; however, the regular part of the dynamical spin conductivity takes spectral weight at all frequencies. The zero frequency limit of spin conductivity is introduced by DC conductivity, which is a measure of dissipative transport. The finite value for DC spin conductivity without Drude weight addresses a normal metallic phase [24].

The purpose of the present study is to sort out the effect of triplon–triplon scattering in limiting the spin conduction along the leg direction. A fictitious magnetic field can be applied to drive spin conductivity within linear response theory. According to this theory spin current is proportional to the magnetic field via a spin conductivity coefficient—i.e. the time-ordered energy current


correlation. We study the interchain and anisotropy dependence of spin conductivity as a function of frequency using the bond operator formalism [27,28] where the spin model is mapped to a bosonic one with hard-core triplon repulsion. The anisotropies account for the eventual effects of spin orbit coupling and the crystalline electric field. Although most ladder compounds are described with isotropic exchange interactions, the anisotropy plays an important role in some others, such as (CsH4)2CuBr4 [29] and CaCu2O3 [30]. We have implemented a Green’s function approach to calculate the current–current correlation function. Although the calculations are tedious and complex we have tried to elaborate the main steps in the following sections. In the last section we discuss and analyze our results to show how interchain interactions and anisotropies influence the dynamical spin transport. Moreover, the temperature dependence of DC conductivity of a spin ladder for various rung-coupling constants and both types of spin anisotropies has been investigated.

2. Bosonic representation of anisotropic spin Hamiltonian and its Green’s function

The Hamiltonian for the quasi-one-dimensional two-leg antiferromagnetic Heisenberg ladder with anisotropy of exchange coupling is defined as

\[ H = J_\perp \sum_i \left( S_i^x \tau_i^x + S_i^y \tau_i^y + \Delta S_i^z \tau_i^z \right) + J \sum_i \left( \tau_i^x \tau_{i+1}^x + \tau_i^y \tau_{i+1}^y + \delta \tau_i^z \tau_{i+1}^z \right) + J \sum_i \left( S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right). \]  

(1)

In Eq. (1), \( S \) and \( \tau \) denote the spin operators of different legs at position \( i \). \( J_\perp \) and \( J \) correspond to the exchange coupling between nearest-neighbor spins along legs and rungs, respectively. \( \Delta \) and \( \delta \) are the anisotropy parameters, where \( \Delta (\delta) \) refers to the strength of anisotropy on the rungs (legs).

The original model Hamiltonian (1) is transformed using the bond operator formalism [27,28] defined by the following transformations:

\[ S_{i,\alpha} = \frac{1}{2} \left( s_i^\dagger t_{i,\alpha} + t_{i,\alpha}^\dagger s_i - i \epsilon_{\alpha\beta\gamma} t_{i,\beta} t_{i,\gamma} \right), \]

\[ \tau_{i,\alpha} = \frac{1}{2} \left( -s_i^\dagger t_{i,\alpha} - t_{i,\alpha}^\dagger s_i - i \epsilon_{\alpha\beta\gamma} t_{i,\beta} t_{i,\gamma} \right), \]  

(2)

where \( s_i \) and \( t_{i,\alpha} \) are bond operators for the singlet and triplet states of each ladder rung. These operators have bosonic statistics, required to reproduce the SU(2) spin algebra. For this purpose they must also obey the local hard-core constraint \( s_i^\dagger s_i + \sum_{\alpha} t_{i,\alpha}^\dagger t_{i,\alpha} = 1 \) on each ladder rung. These operators are named hard-core bosons. In the bond operator representation, the Hamiltonian can be written in terms of a bilinear term and a quartic one. The bilinear part of the Hamiltonian of Eq. (1) (\( \mathcal{H}_{\text{bil}} \)) takes the form

\[ \mathcal{H}_{\text{bil}} = \mathcal{H}_{\text{local}} + \mathcal{H}_{\text{bil}}^{(2)}, \]

where \( \mathcal{H}_{\text{local}} \) and \( \mathcal{H}_{\text{bil}}^{(2)} \) are the local and intersite terms, respectively. These parts are given by

\[ \mathcal{H}_{\text{local}} = J_\perp \sum_{i,\alpha=x,y} \left[ \left( \frac{1 + \Delta}{2} \right) t_{i,\alpha}^\dagger t_{i,\alpha} + t_{i,z}^\dagger t_{i,z} \right], \]

\[ \mathcal{H}_{\text{bil}}^{(2)} = \frac{J}{2} \sum_{(i,j)} \sum_{\alpha=x,y} \left[ t_{i,\alpha} (t_{j,\alpha} + t_{j,\alpha}^\dagger) + \text{h.c.} \right] + \sum_k \frac{J_\delta}{2} \left[ t_{i,z} (t_{j,z} + t_{j,z}^\dagger) + \text{h.c.} \right]. \]  

(3)

It is worthwhile mentioning an important point in regards to the Hamiltonian obtained in Eq. (3). Here, we use the unconstrained case \( \langle s \rangle \approx 1 \), and in the present approach, we replace each singlet operator with its expectation value. In other words, the singlet operators are considered to be condensed. In fact, the occupation of singlet bosons at each site is much greater than the triplet ones and
the quantum fluctuation of singlet particles can be neglected. This is obviously justified in the strong coupling limit. However, as far as the Haldane phase is preserved for both strong and weak coupling limits, we consider the same approximation of $s \rightarrow \langle s_i \rangle \approx 1$ for both regimes.

There exists another part in the Hamiltonian, composed of quartic terms in the bosonic triplet operators. In the low-density limit of bosonic gas, we can neglect the effect of this term on the excitation spectrum of the model here. The hard-core constraint on bosonic gas can be implied by infinite on-site interaction between bosons:

$$H_U = U \sum_{\alpha=x,y,z} t_{i,\alpha}^{\dagger} t_{i,\beta}^{\dagger} t_{i,\beta} t_{i,\alpha}, \quad U \rightarrow \infty. \tag{4}$$

The bilinear part of the Hamiltonian in terms of the Fourier space representation of triplet operators can be rewritten

$$\mathcal{H}_{\text{bil}} = \sum_{k,\alpha=x,y,z} A_{k,\alpha} t_{k,\alpha}^{\dagger} t_{k,\alpha} + \sum_{k,\alpha=x,y,z} B_{k,\alpha} \left( t_{k,\alpha}^{\dagger} t_{-k,\alpha}^{\dagger} + \text{h.c.} \right). \tag{5}$$

The coefficients $A, B$ are given by

$$A_{k,x} = A_{k,y} = J_\perp \left( \frac{1 + \Delta}{2} \right) + J \cos(k), \quad A_{k,z} = J_\perp + \delta J \cos(k),$$
$$B_k = -J \cos(k_x), \quad B_{k,z} = J \delta \cos(k). \tag{6}$$

The wave vectors $k$ are considered in the first Brillouin zone of the ladder ($-\pi < k < \pi$). The effect of hard-core repulsion ($U \rightarrow \infty$) of the interacting Hamiltonian, Eq. (4), is dominant over the remaining quartic terms (which have not been presented here). Thus, it is sufficient to take into account the effect of hard-core repulsion on the triplon spectrum and neglect the remaining quartic terms. Under the unitary Bogoliubov transformation introduced by $t_{k,\alpha} = u_{k,\alpha} \tilde{t}_{k,\alpha} - v_{k,\alpha} \tilde{t}_{-k,\alpha}^{\dagger}$, the bilinear Hamiltonian readily takes the diagonalized form

$$\mathcal{H}_{\text{bil}} = \sum_{k,\alpha} \omega_{k,\alpha} t_{k,\alpha}^{\dagger} t_{k,\alpha},$$
$$\omega_{k,\alpha} = \sqrt{A_{k,\alpha}^2 - B_{k,\alpha}^2}, \tag{7}$$

where $\omega_{k,\alpha}$ is the quasi-particle excitation spectrum. Furthermore, the Bogoliubov coefficients are

$$u_{k,\alpha}^2 (v_{k,\alpha}^2) = \frac{A_{k,\alpha}}{2 \left( \sqrt{A_{k,\alpha}^2 - B_{k,\alpha}^2} \right)} \tag{8}.$$

The Fourier transforms of the noninteracting normal and anomalous Green’s functions are written in the following form:

$$G_{n,\alpha}^{(0)}(k, i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} \langle T(t_{k,\alpha}(\tau) t_{k,\alpha}^{\dagger}(0)) \rangle = \frac{u_{k,\alpha}^2}{i\omega_n - \omega_{k,\alpha}} - \frac{v_{k,\alpha}^2}{i\omega_n + \omega_{k,\alpha}}, \tag{9}$$
$$G_{d,\alpha}^{(0)}(k, i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} \langle T(t_{k,\alpha}(\tau) t_{-k,\alpha}^{\dagger}(0)) \rangle = \frac{u_{k,\alpha} v_{k,\alpha}}{i\omega_n - \omega_{k,\alpha}} - \frac{u_{k,\alpha} v_{k,\alpha}}{i\omega_n + \omega_{k,\alpha}}.$$
component of the triplet bosons), the single-particle retarded Green’s function is obtained in the low-energy limit of retarded self-energy:

\[ G^\alpha_{n,a}(k, \omega) = g_n(k, i\omega_n \rightarrow \omega + i0^+) = \frac{Z_{k,a}U^2_{k,a}}{\omega - \Omega_{k,a} + i0^+} - \frac{Z_{k,a}V^2_{k,a}}{\omega + \Omega_{k,a} + i0^+}. \] (10)

More explanations of the detailed calculations can be found in our previous works [34–36]. The renormalized excitation spectrum and renormalized single particle weight are given by

\[ \Omega_{k,a} = Z_{k,a} \sqrt{[A_{k,a} + \text{Re}(\Sigma^\text{Ret}_{n,a}(k,0))]^2 - [B_{k,a} + \text{Re}(\Sigma^\text{Ret}_{\alpha,\alpha}(k,0))]^2}, \]

\[ Z_{k,a}^{-1} = 1 - \left( \frac{\partial \text{Re}(\Sigma^\text{Ret}_{n,a})}{\partial \omega} \right)_{\omega=0}, \]

\[ U^2_{k,a}(V^2_{k,a}) = (-\frac{1}{2}) + \frac{Z_{k,a}[A_{k,a} + \text{Re}(\Sigma^\text{Ret}_{n,a}(k,0))]}{2\Omega_{k,a}}. \] (11)

The renormalized weight constant is the residue of the single-particle pole of the Green’s function. In the next step we will take into account the effect of hard-core repulsion on the magnon spectrum.

3. Effect of hard-core repulsion on triplon excitation

The interacting part of the Hamiltonian in terms of the Fourier transform of bosonic operators is given by

\[ \mathcal{H}_U = U \sum_{k,k',q,a=x,y,z} t^\dagger_{k+q,a} t^\dagger_{k'-q,b} t_{k',b} t_{k,a}. \] (12)

In this section we intend to obtain the effect of above hard-core Hamiltonian on the Green’s function of the bilinear Hamiltonian in Eq. (5). The density of the triplons for each polarization component can be easily obtained by using the normal Green’s functions

\[ n_{i,a} = \langle t^\dagger_{i,a} t_{i,a} \rangle = \frac{1}{L} \sum_k \{1 + 2n_B(\omega_{k,a})|v^2_{k,a} + n_B(\omega_{k,a}) \}, \] (13)

where \( L \) is the number of rungs on the ladder and \( n_B \) is the bosonic distribution function. Since the Hamiltonian \( \mathcal{H}_U \) in Eq. (12) is short-ranged and \( U \) is large, the Brueckner approach (ladder diagram summation) [32,33] can be employed for the low density limit of bosonic gas and for low temperature, \( T < J_\perp, J \). The interacting normal Green’s function is obtained by imposing the hard-core boson repulsion, \( U \rightarrow \infty \). First, the scattering amplitude (t-matrix) \( \Gamma(p_1, p_2; p_3, p_4) \) of magnons is introduced, where \( k_i \equiv (p, (p_0)) \). The basic approximation made in the derivation of \( \Gamma(K \equiv p_1 + p_2) \) is that we neglect all anomalous scattering vertices, which are present in the theory due to the existence of anomalous Green’s functions. According to the Feynman rules [32,33], in momentum space at finite temperature and after taking limit \( U \rightarrow \infty \), the scattering amplitude is calculated (see Fig. 1 of Refs. [35,36]).

By replacing the noninteracting normal Green’s function in the Bethe–Salpeter equation and taking the limit \( U \rightarrow \infty \), the scattering matrix is obtained in the following form:

\[ \Gamma_{\alpha\beta,a\beta}(K, i\omega_n) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} dQ \left[ u^2_{Q,a} u^2_{K-Q,\beta} \left( \frac{n_B(\omega_{Q,a})}{i\omega_n - \omega_{Q,a} - \omega_{K-Q,\beta}} - \frac{n_B(-\omega_{K-Q,\beta})}{i\omega_n - \omega_{K-Q,\beta} - \omega_{Q,a}} \right) \right]. \]
Fig. 1. Dynamical spin conductivity of the isotropic spin ladder ($\Delta = \delta = 1$) along leg direction versus $\omega/J$ for different values of $J_\perp/J$ and for $kT/J = 0.5$.

Fig. 2. Dynamical spin conductivity versus normalized frequency ($\omega/J$) for different anisotropies in the rung coupling ($\Delta$) and for $J_\perp/J = 2.5$ and $\delta = 0.0$, $kT/J = 0.5$. A strong dependence on $\Delta$ is clear.

The low density limit of bosonic gas implies that we can neglect the terms including the coefficients $v_\alpha$. According to Fig. 2 of Ref. [34], the normal self-energy is obtained by using the vertex function obtained in Eq. (14). After performing integration on the internal energy ($p_0$), the normal
self-energy is obtained in the following form:

\[
\Sigma_{xx}^{U}(k, \omega_{n}) = \frac{3}{2\pi} \int dp (u_{p,x}^{2} n_{B}(\omega_{p,x}) \Gamma_{xx,xx}(p + k, \omega_{p,x} + i\omega_{n}) - v_{p,x}^{2} n_{B}(-\omega_{p,x}) \Gamma_{xx,xx}(p + k, -\omega_{p,x} + i\omega_{n}))
+ \frac{1}{2\pi} \int dp (u_{p,z}^{2} n_{B}(\omega_{p,z}) \Gamma_{xz,xz}(p + k, \omega_{p,z} + i\omega_{n}) - v_{p,z}^{2} n_{B}(-\omega_{p,z}) \Gamma_{xz,xz}(p + k, -\omega_{p,z} + i\omega_{n})).
\]

(15)

The other components of self-energy are found in a similar way. In addition to the normal self-energy presented in Eq. (15), there are anomalous self-energy diagrams which are formally at most linear in the density of bosonic gas. In the dilute gas approximation, the contributions of such terms are numerically smaller than Eq. (15).

4. Spin conductivity and spin diffusion constant

In order to obtain the spin conductivity, we add a fictitious Zeeman Hamiltonian term described as a coupled external space- and time-dependent magnetic field with spins to the original spin model Hamiltonian. Therefore, the time-dependent model Hamiltonian becomes

\[
H(t) = H - g\mu_{B} \sum_{i} \left( S_{z}^{i}(i) + \tau_{z}^{i}(i) \right) B(t)(i, t),
\]

(16)

where \(g\) is the gyromagnetic constant and \(\mu_{B}\) denotes the Bohr magneton constant. \(H\) is the model Hamiltonian of the spin ladder presented in Eq. (1). The spin current density operator for the \(z\) component of magnetization \((j_{xz}(i))\) which transposes along the spatial direction \((x)\) axis satisfies the continuity equation

\[
\partial_{t}(S_{z}^{i}(i) + \tau_{z}^{i}(i)) + \partial_{x} j_{xz}(i) = 0.
\]

(17)

Here, \(\partial_{x} j_{xz}(i)\) implies the lattice divergence of the local spin current density at site \(i\). The spin current can be derived by using an auxiliary operator which is defined as

\[
R_{i} = \sum_{j} R_{j}(S_{z}^{j} + \tau_{z}^{j}),
\]

(18)

where \(R_{i} = (ia, 0, 0)\) implies the position of \(i\)th spin dimer along the \(x\) direction and the lattice constant, \(a\), is set to one. According to Eq. (17), the spin current density operator along the \(x\) direction for the \(z\) component of spin \((j_{xz}(i) = j_{x}(i))\) can be obtained from the Heisenberg equation of motion, \(\partial_{t} S_{z}^{i} = i[H, S_{z}^{i}]\), as

\[
\frac{dR_{i}^{z}}{dt} = i[H, R_{i}^{z}] = \frac{iJ}{2} (S_{i+1}^{-} S_{i+1}^{+} - S_{i}^{-} S_{i+1}^{+} + \tau_{i+1}^{+} \tau_{i+1}^{+} - \tau_{i}^{+} \tau_{i}^{+}).
\]

(19)

In the above equation, \(i + x\) denotes the nearest-neighbor spin dimer of spin dimer \(i\) in the positive \(x\) direction. The Fourier transform of the spin current operator in terms of spin operators can be written as

\[
j_{x}(q) = \frac{ij}{2N} \sum_{k} (S_{k}^{+} S_{q-k}^{-} - S_{k}^{-} S_{q-k}^{+} + \tau_{k}^{+} \tau_{q-k}^{-} - \tau_{k}^{-} \tau_{q-k}^{+}) e^{i(q-k)a},
\]

(20)

where \(N\) is the number of dimer spins. The spin conductivity of spin chains was previously investigated using linear response theory in a similar way to the Kubo formula for charge transport [17].
longitudinal spin conductivity coefficient along the $x$ direction, $\sigma_{xx}(\omega)$, connects the magnetization current to the long wavelength and frequency-dependent magnetic field and is given by

$$j_{m,x}(q, \omega) = g \mu_B j_x(q, \omega) = \sigma_{xx}(q, \omega) i q q_B^2 (q, \omega). \quad (21)$$

The Kubo formula has been implemented in order to obtain dynamical spin conductivity as \([12,13,21]\)

$$\sigma_{xx}(q, \omega) = -(g \mu_B)^2 \frac{(-\chi_{xx}(\omega) - \chi_{\omega}(\omega))}{i(\omega + i 0^+)} , \quad (22)$$

where $\chi_{xx}(\omega)$ is defined as the longitudinal retarded current–current correlation function \([12,13]\) and is given by

$$\chi_{xx}(\omega) = \frac{1}{hN} \int_0^\infty \mathrm{d}\tau e^{i(\omega + i 0^+ )\tau} \langle [J_x(q=0, t), J_x(-q=0, 0)] \rangle \ . \quad (23)$$

Now, the real part of the spin conductivity is usually decomposed as

$$\Re \sigma_{xx}(\omega) = D_s(T) \delta(\omega) + \sigma_{xx}^{\text{reg}}(\omega) . \quad (24)$$

The first part is singular at zero frequency and is a measure of ballistic transport. The second part, $\sigma_{xx}^{\text{reg}}(\omega)$, shows no divergence in the zero frequency limit and thus introduces the regular part of $\sigma(\omega)$. The prefactor $D_s(T)$ of the delta function $\delta(\omega)$ is the so-called spin Drude weight \([25,26]\), which measures the conserved part of the current and is given by

$$D_s = \pi (g \mu_B)^2 [(-\chi_{xx}) - \Re(\chi_{xx}(\omega \to 0))] , \quad (25)$$

and the regular part takes the following expression:

$$\sigma_{xx}^{\text{reg}}(\omega) = \frac{\Im(\chi_{xx}(\omega))}{\omega} . \quad (26)$$

The physical retarded linear response function can be obtained readily via calculating the correlation function of two current operators ($\Pi_{xx}(i \omega_n)$) in the Matsubara representation. This representation is given as

$$\Pi_{xx}(i \omega_n) = \frac{1}{hN} \int_0^\infty \mathrm{d}\tau e^{i\omega_n \tau} \langle T(J_x(q, \tau) J_x(-q, 0)) \rangle \ , \quad (27)$$

where $\omega_n = 2n \pi k_BT$ is the bosonic Matsubara frequency. The correlation function in Eq. (27) can be calculated by implementing Wich’s theorem. Substituting Eq. (20) into Eq. (27) leads to following equation for $\Pi_{xx}(\tau)$:

$$\Pi_{xx}(\tau) \equiv \langle T_r(J_x(q=0, \tau) J_x(q=0, 0)) \rangle = \frac{J^2}{4N^2} \sum_{k,k'} \sum_{\alpha \beta} e^{-i(k+k')a}$$

$$\times \langle T(S_{-k}^+(\tau) S_{-k}^-(-\tau) - S_{-k}^-(-\tau) S_{-k}^+(\tau) + \tau_{-k}^-(\tau) \tau_{-k}^+(\tau) - \tau_{-k}^+(\tau) \tau_{-k}^-(\tau))$$

$$\times (S_{k}^+(0) S_{-k}^-(0) - S_{k}^-(0) S_{-k}^+(0) + \tau_{k}^+(0) \tau_{-k}^-(-\tau) - \tau_{k}^-(-\tau) \tau_{-k}^+(0)) \rangle . \quad (28)$$

The above equation can be written in terms of the different forms of transverse spin susceptibilities. For this purpose, we introduce the different forms of the correlation functions of the components of spin operators as

$$\chi_{ss}^{\tau}(k, \tau) = -\langle T(S_x^+(k, \tau) S_x^-(\tau, 0))\rangle$$

$$\chi_{xx}^{\tau}(k, \tau) = -\langle T(S_x^+(k, \tau) S_x^-(\tau, 0))\rangle$$

$$\chi_{xx}^{\tau}(k, \tau) = -\langle T(S_x^+(k, \tau) S_x^-(\tau, 0))\rangle . \quad (29)$$

According to the bond operator transformation in Eq. (2), the relations $\chi_{ss}^{\tau} = \chi_{xx}^{\tau} = \chi_{xx}^{\tau}$ follow immediately. Now, one can rewrite the correlation function between the spin currents in
Eq. (28) as the multiplication of the two dynamical spin susceptibilities introduced in Eq. (29) in the form

\[
(T_x(J_x(q = 0, \tau)J_x(q = 0, 0)))
\]

\[
= \frac{J^2}{N} \sum_k (e^{2ika} - 1)(\chi_{++}^{ss}(k, \tau)\chi_{-+}^{ss}(-k, \tau) + \chi_{++}^{st}(k, \tau)\chi_{-+}^{st}(-k, \tau)).
\]

(30)

Combining Eq. (30) with Eq. (27), \(\Pi_{xx}(\tau)\) can be obtained as

\[
\Pi_{xx}(i\omega_n) = \frac{J^2}{N\beta} \sum_{k,m} (e^{2ik} - 1)
\]

\[
\times \left( \chi_{++}^{ss}(k, i\omega_m)\chi_{-+}^{ss}(-k, i\omega_n - i\omega_m) + \chi_{++}^{st}(k, i\omega_m)\chi_{-+}^{st}(-k, i\omega_n - i\omega_m) \right),
\]

(31)

where \(\omega_n(\omega_m)\) are the bosonic Matsubara frequencies. Based on the definition of ladder component of spin operators in terms of \(x\) and \(y\) components of spin as \(\chi_{++}^{ss(\tau)} = \chi_{xx}^{ss(\tau)} + \chi_{yy}^{ss(\tau)} = 2\chi_{xx}^{ss(\tau)}\), the \(x\) component of dynamical spin susceptibility (\(\chi\)) is obtained by bond operator transformation (Eq. (2)) and is given by

\[
\chi_{xx}^{ss}(k, i\omega_n) = -\int_0^\beta d\tau e^{i\omega_n \tau} (T(S_x(k, \tau)S_x(-k, 0))) = -\frac{1}{4} \int_0^\beta d\tau e^{i\omega_n \tau}
\]

\[
\times \left( T \left( t_{-k,x}(\tau) + \frac{i}{v} t_{k,x}(\tau) + \sum_q \left( -it_{k+q,y}^{\dagger}(\tau) t_{q,z}(\tau) + it_{k+q,z}^{\dagger}(\tau) t_{q,y}(\tau) \right) \right) \right.
\]

\[
\times \left. \left( \frac{1}{2} t_{-k,x}(0) + \frac{i}{v} t_{k,x}(0) + \sum_q \left( it_{k,q,y}^{\dagger}(0) t_{q,z}(0) + it_{k,q,z}^{\dagger}(0) t_{q,y}(0) \right) \right) \right). \quad (32)
\]

Both one- and two-particle Green’s functions contribute to the spin susceptibility. Since the anomalous Green’s function is negligible compared to the normal Green’s function, we only consider bubble diagrams that include the normal Green’s function. The details of the calculation of spin susceptibility via the Green’s function of triplet gas can be found in Ref. [35]. After some calculations, the \(x\) component of susceptibility takes form of the following Fourier transformation:

\[
\chi_{xx}^{ss}(k, i\omega_n) = \frac{1}{4} \left[ u_{k,x}^2 \left( \frac{1}{i\omega_n - \omega_{k,x}} - \frac{1}{i\omega_n + \omega_{k,x}} \right) \right.
\]

\[
- \left. \sum_q u_{q,z}^2 u_{k+q,x}^2 \frac{n_B(\omega_{q,z}) - n_B(\omega_{k+q,z})}{i\omega_n - \omega_{k+q,z} + \omega_{q,z}} \right]. \quad (33)
\]

In a similar way, the final result for \(\chi_{xx}^{st}(k, i\omega_n)\) is obtained as

\[
\chi_{xx}^{st}(k, i\omega_n) = \frac{1}{4} \left[ -u_{k,x}^2 \left( \frac{1}{i\omega_n - \omega_{k,x}} - \frac{1}{i\omega_n + \omega_{k,x}} \right) \right.
\]

\[
- \left. \sum_q u_{q,z}^2 u_{k+q,x}^2 \frac{n_B(\omega_{q,z}) - n_B(\omega_{k+q,z})}{i\omega_n - \omega_{k+q,z} + \omega_{q,z}} \right]. \quad (34)
\]

In the low density limit of the triplet bosons, the terms being proportional to the fourth order of \(u\) give dominant contribution to the spin susceptibilities in Eqs. (33), (34). Furthermore, \(u\) is close to 1 since \(u^2 = 1 + v^2\) and \(v^2\) is proportional to the triplet boson density. Once the relation for the
The static spin conductivity takes the following form:

\[
\Pi_{xx}(\omega_n) = \frac{J^2}{4N} \sum_k u_{k,x}^4 \left[ (\cos(2k) - 1) \left( \frac{n_B(\omega_{k,x}) - n_B(-\omega_{k,x})}{i\omega_n - 2\omega_{k,x}} + \frac{n_B(-\omega_{k,x}) - n_B(\omega_{k,x})}{i\omega_n + 2\omega_{k,x}} \right) \right]
+ \frac{J^2}{4N} \sum_{k,q,q'} u_{q,z}^2 u_{k+q,x}^2 u_{q',z}^2 u_{k+q',x}^2 (\cos(2k) - 1)
\times \left( n_B(\omega_{q,z}) - n_B(\omega_{k+q,x}) \right) \left( n_B(\omega_{q',z}) - n_B(\omega_{k+q',x}) \right)
\times \frac{n_B(-\omega_{q,z} + \omega_{k+q,x}) - n_B(\omega_{q',z} - \omega_{k+q',x})}{i\omega_n + \omega_{q',z} + \omega_{q,z} - \omega_{k+q,x} - \omega_{k+q',x}}
+ \frac{n_B(\omega_{q,z}) - n_B(\omega_{k+q,x})}{i\omega_n + \omega_{q',z} + \omega_{q,z} - \omega_{k+q,x} - \omega_{k+q',z}}
+ \frac{n_B(-\omega_{q,z} + \omega_{k+q,x}) - n_B(\omega_{q',z} - \omega_{k+q',x})}{i\omega_n + \omega_{q',z} + \omega_{q,z} - \omega_{k+q,x} - \omega_{k+q',z}}
\right). 
\]  

(35)

This retarded representation of conductivity is related to the Matsubara one which was introduced in Eqs. (18), (27) via a straightforward analytical continuation as \( \Pi_{xx}(\omega) = \Pi_{xx}(i\omega_n \rightarrow \omega + i0^+) \). Afterwards, the dynamical spin conductivity along the rung direction, \( \sigma_{\text{DC}}(\omega) \), is found using Eq. (26). The other interesting quantity, being a measure of dissipative transport, is the static spin conductivity \( \sigma_{\text{DC}} = \lim_{\omega \rightarrow 0} \omega \sigma_{\text{reg}}(\omega) \). After a little algebraic calculation, the final result for the static spin conductivity takes the following form:

\[
\sigma_{\text{DC}}(T) = \lim_{\omega \rightarrow 0} \frac{\text{Im} \Pi_{xx}(i\omega_n \rightarrow \omega + i0^+)}{\omega}
= \frac{J^2}{4N} \sum_k u_{k,x}^4 (\cos(2k) - 1) (n'_B(-\omega_{k,x}) + n'_B(\omega_{k,x}))
+ \frac{J^2}{4N} \sum_{k,q,q'} u_{q,z}^2 u_{k+q,x}^2 u_{q',z}^2 u_{k+q',x}^2 (\cos(2k) - 1)
\times \left( n_B(\omega_{q,z}) - n_B(\omega_{k+q,x}) \right) \left( n_B(\omega_{q',z}) - n_B(\omega_{k+q',x}) \right) \times n'_B(\omega_{q',z} - \omega_{k+q',x})
+ \frac{n_B(\omega_{q,z}) - n_B(\omega_{k+q,x})}{i\omega_n + \omega_{q',z} + \omega_{q,z} - \omega_{k+q,x} - \omega_{k+q',z}}
+ \frac{n_B(\omega_{q,z}) - n_B(\omega_{k+q,x})}{i\omega_n + \omega_{q',z} + \omega_{q,z} - \omega_{k+q,x} - \omega_{k+q',z}}
\right). 
\]  

(36)

where \( n'_B(E) \) implies differentiation of the Bose population function with respect to \( E \).

5. Results and discussions

Both static and dynamical spin conductivities of the two-leg spin-1/2 antiferromagnetic ladder along the leg direction have been obtained in the presence of both rung (\( \Delta \)) and leg (\( \delta \)) anisotropies. Using a bosonic representation for the spin ladder, each rung is represented by bosonic bond operators, i.e. a singlet and three flavor triplets. To avoid double occupation of bosons at each lattice site, a hard-core repulsion constraint is added to the bosonic model. In the limit \( J_\perp/J \rightarrow \infty \), the spin ladder has a spin liquid ground state which is a direct product of singlet states where a finite energy gap exists to the lowest excited state. The energy gap is robust and remains finite even for small values of \( J_\perp/J \), which defines the energy scale of the quasi-particles which are called triplons. A Green's
function approach has been implemented to obtain the single particle excitations of the bosonic model. Eventually, the spin conductivity is obtained by calculating the spin current correlation function. The spin excitations of the ladder should be found from a self-consistent solution of Eqs. (15), (14), and (11) with the substitutions \( u_{k,\alpha} \rightarrow \sqrt{Z_{k,\alpha}} U_{k,\alpha}, v_{k,\alpha} \rightarrow \sqrt{Z_{k,\alpha}} V_{k,\alpha}, \omega_{\alpha}(k) \rightarrow \Omega_{k,\alpha} \) into the corresponding equations. The process is started with an initial guess for \( Z_{k,\alpha}, \Sigma_{\alpha}(k,0) \), and by using Eq. (11) we find the corrected excitation energy and the renormalized Bogoliubov coefficients. (The effects of finite relaxation time, corresponding to the hard-core repulsion between triplet bosons, on the calculation of spin conductivity in Eqs. (33), (34), (35), and (36) are accounted for within the substitutions \( u_{k,\alpha} \rightarrow \sqrt{Z_{k,\alpha}} U_{k,\alpha}, v_{k,\alpha} \rightarrow \sqrt{Z_{k,\alpha}} V_{k,\alpha}, \omega_{k,\alpha} \rightarrow \Omega_{k,\alpha} \) into Eqs. (33), (35), and (36)).

Using the final values for energy gap, renormalization constants, and Bogoliubov coefficients, we can calculate the static and dynamical spin conductivities by Eqs. (35) and (36).

Figure 1 presents the dynamical spin conductivity \( (\sigma_{\text{reg}}(\omega)) \) of the isotropic ladder \( (\Delta = \delta = 1) \) versus normalized external magnetic field frequency \( (\omega/J; k \text{ is the Boltzmann constant}) \) for different values of rung coupling \( (J_{\perp}/J) \) and for fixed normalized temperature \( KT/J = 0.5 \). Two features are pronounced in this figure. For normalized coupling constants above 1.5, there is a finite frequency region for which spin conductivity takes zero values; however, the results show that \( \sigma_{\text{reg}}(\omega) \) takes small nonzero values for \( J_{\perp}/J < 1.5 \). The width of this frequency region increases with enhancement of \( J_{\perp}/J \) and spin conductivity reduces with rung exchange coupling. Increased rung exchange coupling enhances the energy gap between the singlet and triplet states on each rung which consequently reduces the number of triplons that participate in spin transport and results in lower spin conductivity. According to Fig. 1, we find spectral weight for \( \sigma_{\text{reg}}(\omega) \) at small frequencies for \( J_{\perp}/J < 1.5 \). Also, the zero frequency limit of dynamical spin conductivity takes a nonzero value for decreasing \( J_{\perp}/J \). The frequency region where \( \sigma_{\text{reg}}(\omega) \) gets the considerable values broadens with \( J_{\perp}/J \) according to Fig. (1). Furthermore, the position of peaks in the spin conductivity moves to higher frequencies with increase of rung exchange coupling constant parameter \( J_{\perp}/J \). This behavior addresses this point that exciting the triplons requires the higher magnetic field frequency with raising parameter \( J_{\perp}/J \).

We have also studied the effect of rung anisotropies on the spin conductivity of the spin ladder for \( kT/J = 0.5 \) and for fixed rung-exchange coupling \( J_{\perp}/J = 2.5 \). We have plotted the frequency dependence of the spin conductivity for different values of anisotropies on the rung Hamiltonian, namely \( \Delta = 0.6, 0.8, \) and \( 1.0, \) for \( J_{\perp}/J = 2.5 \) and \( \delta = 0.0 \) according to Fig. 2. This plot shows a strong dependence on \( \Delta \) for the whole frequency range. This can be understood from the fact that the singlet–triplet gap depends on the rung anisotropy \( (\delta) \). The increase of the gap in spin conductivity with the anisotropy parameter \( \Delta \) is a significant property of Fig. 2. Increasing \( \Delta \) raises the triplon gap which gives lower conductivity at a given temperature. Moreover, lower values of \( \Delta \) mean weaker interactions on the rungs which consequently improve the spin conductivity. As with the other results, one can point to the shift of the peak to higher frequencies and decrease of spin conductivity with \( \Delta \). The increase of the frequency gap in the spin conductivity is in agreement with a theoretical study on the spin conductivity of the anisotropic XXZ Heisenberg antiferromagnet in which the anisotropy parameter causes the energy gap in the excitation spectrum [21]. However, the situation is different for the leg anisotropy \( (\delta) \). Figure 3 shows the behavior of spin conductivity versus normalized frequency for different values of anisotropies on the leg Hamiltonian, namely \( \delta = 0.2, 0.4, 0.6, \) and \( 0.8 \) for \( J_{\perp}/J = 2.5 \). This plot indicates a weak dependence on \( \delta \) in the frequency region \( 5.0 < \omega/J < 6.0 \). This can be understood from the fact that the singlet–triplet gap is practically independent of the
Fig. 3. Dynamical spin conductivity versus normalized frequency ($\omega/J$) for different anisotropies in the leg coupling ($\Delta$), $J_{\perp}/J = 2.5$ and $\Delta = 1.0, kT/J = 0.5$. A weak dependence on $\Delta$ is clear.

Fig. 4. The regular part of the dynamical spin conductivity $\sigma_{\text{reg}}(\omega)$ as a function of normalized frequency ($\omega/J$) for different normalized temperatures in the isotropic spin ladder ($\delta = \Delta = 1$) with $J_{\perp}/J = 2.5$. An increase in the frequency gap with temperature is readily seen.

The leg anisotropy ($\delta$) and thus the triplon density and the spin transport are unaffected. All the plots presented in Fig. 3 show no dependence on the leg anisotropy. In particular, the width of the frequency region where spin conductivity takes nonzero values is clearly independent of $\delta$. Moreover, the values of the frequency gap for all values of $\delta$ are obviously the same.

Figure 4 presents the effect of temperature on the frequency behavior of the spin conductivity of an isotropic spin ladder for fixed $J_{\perp}/J = 2.5$. The temperature influences the spin conductivity in two ways. First, temperature increases the energy gap which consequently reduces the triplon population that participates in spin transport and results in lower spin conductivity. To be more explicit, the temperature dependence of the energy gap in the excitation spectrum of bosonic gas has been plotted in...
Fig. 5. The energy gap of the isotropic spin ladder as a function of normalized temperature $kT/J$ for $J_{\perp}/J = 2.5$. A monotonic increase versus temperature is clearly observed for temperatures higher than 0.5.

Fig. 5. For temperatures $kT/J > 0.5$, an increasing behavior for the energy gap is clearly observed. Moreover, a numerical study using quantum Monte Carlo simulations for a double layer Heisenberg antiferromagnet justifies an increasing behavior for temperature dependence of the energy gap in the excitation spectrum of this model [37]. Second, raising the temperature causes more scattering of triplons which reduces the spin conductivity. As Fig. 4 shows, the increase of frequency gap with temperature enhances the spin conductivity and consequently the peak moves to higher frequencies. The other novel property of Fig. 5 is that the broadening of the peaks in the spin conductivity has no variation with increase of temperature. The frequency region where spin conductivity takes finite nonzero values is expected to be connected to the band width of the spin excitation spectrum. According to our method, this spectrum corresponds to one-particle excitation energies of bosonic gas, namely triplet states. As long as the frequency of the magnetic field is less than the energy gap between the singlet state and the first excited triplet state, no triplon boson is excited. As a result, spin conductivity takes tiny values for frequencies below the energy gap. Since temperature increases the energy gap, one can expect to enhance the width of the frequency gap in the conductivity. When the frequency of the magnetic field takes values higher than the energy gap in the spectrum of bosonic gas, the conductivity takes finite values because bosons can excite to triplet states. It should be mentioned that the excitation states, i.e. triplet levels, broaden in wave vector space. In other words, we deal with band state for triplet states. As a result, one can point out that the band width of the triplon spectrum does not show any considerable change when temperature varies. As we mentioned, the energy gap is affected due to temperature variation. This result can be understood from the fact that interaction effects between bosons rise with temperature. On the other hand, the band width of triplon states are not noticeably affected when temperature increases. Although the intensity of the spin conductivity reduces with temperature, the width of the peak in spin conductivity is not affected.

The DC spin conductivity is given by the $\omega \rightarrow 0$ limit of the regular part of the dynamical conductivity. When the frequency tends to zero, a nonzero value for conductivity is found at different values of $J_{\perp}/J$. A nonzero value of $\sigma_{\text{DC}}$ is an indicator of a nonideal spin conductor. The static spin conductivity for the isotropic spin ladder model versus $kT/J$ and for various $J_{\perp}/J$ has been plotted.
The DC conductivity of the isotropic spin ladder versus temperature \( (kT/J) \) for different values of coupling constant ratios \( J_\perp/J \). Each plot clearly includes a peak.

Each curve shows an exponential decay at low temperatures which manifests the presence of a finite energy gap. However, DC conductivity for the case \( J_\perp/J = 0.5 \) behaves linearly in the low temperature region. Larger values of \( J_\perp/J \) show more rapid decay corresponding to the larger energy gap. There is also a peak around \( \omega/J \approx 0.9 \) in the static conductivity for \( J_\perp/J = 0.2 \). This peak moves to higher temperatures with increasing \( J_\perp/J \). Since the energy gap is robust and remains finite even for small values of rung coupling \( (J_\perp/J) \), the enhancement of temperature leads to the transition of more triplons to excited states, which consequently results in higher static spin conductivity. Therefore, below the temperature for which DC conductivity attains its maximum value, an increasing behavior for \( \sigma_{DC} \) is seen in Fig. 6. As temperature continues to increase, the triplons suffer from scattering by each other which reduces the spin conductivity. In fact, the peak in each curve is due to competition between two phenomena: the scattering of triplon particles and their transition from ground state to the excited state. The former case is dominant at high temperatures while the latter has significance at low ones. The movement of the peak in the spin conductivity can be understood based on the energy gap in the excitation spectrum of the model Hamiltonian. Enhancement of the rung exchange coupling \( J_\perp/J \) leads to an increase in the energy gap. Therefore, the increase in temperature causes the population of excited triplons to increase, which improves the spin conductivity up to the characteristic temperature of the peak. For temperatures higher than the peak, scattering leads to a decrease in conductivity. In addition, at a fixed value of temperature, a lower value of rung coupling \( (J_\perp/J) \) causes a greater population of triplons and spin conductivity gets higher values.

Figure 7 plots the results of static spin conductivity \( (\sigma_{DC}) \) versus temperature for different values of anisotropies on the rung Hamiltonian, namely \( \Delta = 0.2, 0.4, 0.6, 0.8, \) and \( 1.0 \) for \( J_\perp/J = 2.5 \) by setting \( \delta = 0.0 \). This figure shows that the peak in static spin conductivity moves to higher temperatures with increase of the anisotropy parameter \( \Delta \). Since the increase of rung anisotropy enhances the triplon gap, the static spin conductivity shows increasing behavior up to higher temperatures and consequently the position of the peak shifts to higher temperatures. Figure 8 presents the results of static spin conductivity of a spin ladder in the presence of anisotropy along the leg direction. This plot indicates that the static conductivity is independent of \( \delta \) over the whole temperature range. This can
Fig. 7. The DC conductivity of the anisotropic spin ladder versus temperature \((kT/J)\) for different anisotropies in the rung direction \(\Delta\) and \(\delta = 0.0\). The exchange coupling is assumed to be \(J_\perp/J = 2.5\). The strong dependence on anisotropy is evident.

Fig. 8. The DC conductivity of the anisotropic spin ladder versus temperature \((kT/J)\) for different anisotropies in the leg direction \(\delta\) and \(\Delta = 1.0\). The exchange coupling is assumed to be \(J_\perp/J = 2.5\). A weak dependence on \(\delta\) is clearly observed over the whole temperature range.

be justified from the fact that the singlet–triplet gap is practically independent of the leg anisotropy and thus the triplon density and the spin conductivity are unaffected.

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