Spin Transport in the XXZ Chain at Finite Temperature and Momentum

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We investigate the role of momentum for the transport of magnetization in the spin-1/2 Heisenberg chain above the isotropic point at finite temperature and momentum. Using numerical and analytical approaches, we analyze the autocorrelations of density and current and observe a finite region of the Brillouin zone with diffusive dynamics below a cut-off momentum, and a diffusion constant independent of momentum and time, which scales inversely with anisotropy. Lowering the temperature over a wide range, starting from infinity, the diffusion constant is found to increase strongly while the cut-off momentum for diffusion decreases. Above the cut-off momentum diffusion breaks down completely.

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Understanding spin transport in quantum many-particle systems is a fundamental challenge to physics, of immediate relevance to future information technologies, and intimately related to timely issues of dynamics and thermalization in a more broader context. While conventional spin conductors like silicon, III-V semiconductors, carbon nanotubes, or graphene necessarily feature spins which are associated with itinerant charge carriers, insulating quantum magnets may open new perspectives for spin transport, with pure magnetization currents flowing solely by virtue of exchange interactions. Magnetic transport in one-dimensional (1D) quantum magnets has experienced an upsurge of interest in the last decade due to the discovery of very large magnetic heat conduction with mean free paths above 1µm. Genuine spin transport in quantum magnets remains yet to be observed experimentally, however long nuclear magnetic relaxation times have been established, which even allow for manipulation with magnetic fields.

Theoretically, significant attention has been devoted to spin transport in 1D quantum magnets, see Refs. [11] and [12] for reviews. The dissipation of spin currents is a key issue in this context and has been analyzed extensively at zero momentum and frequency in connection with the spin Drude weight. Spin current dynamics at finite momentum remains one of the open questions. In this Letter, we will address this question for the antiferromagnetic and anisotropic spin-1/2 Heisenberg (XXZ) chain

\[ H = J \sum_{r} (S_{r}^{x} S_{r+1}^{x} + S_{r}^{y} S_{r+1}^{y} + \Delta S_{r}^{z} S_{r+1}^{z}) \]  

where \( S_{r}^{i} \) (\( i = x, y, z \)) are the components of spin-1/2 operators at site \( r \), \( N \) denotes the number of sites, \( J > 0 \) represents the exchange coupling constant, and \( \Delta \) is the anisotropy. The XXZ chain is a fundamental model to describe magnetic properties of interacting electrons. It is relevant to the physics of low-dimensional quantum magnets, ultra-cold atoms, nanostructures, and – seemingly unrelated – fields such as string theory and quantum Hall systems.

Early analysis of the time-dependent correlation function of the local spin density has been performed in the high-temperature limit, \( T = \infty \), suggesting the absence of spin diffusion for \( 0 \leq \Delta \leq 1 \). Subsequent studies have concentrated on the spin Drude weight at zero momentum \( q = 0 \), allowing for no conclusions on diffusion laws at finite momentum. First low-temperature quantum Monte-Carlo studies at \( q \neq 0 \) found no evidence for spin diffusion; however, more recent results from bosonization and transfer-matrix renormalization group as well as quantum Monte-Carlo are consistent with finite-frequency spin diffusion in the small-momentum regime, at \( \Delta = 1 \) and for low temperatures \( T \ll J \), with a spin diffusion constant \( D \) which diverges \( \propto 1/T \ln T \). The physics at intermediate temperatures and arbitrary momenta remains undisclosed.

Therefore, in this Letter, we consider the transport of magnetization by analyzing autocorrelations of spin density and current at finite momenta, covering the complete Brillouin zone, and at intermediate temperatures \( 0.5J \leq T \leq \infty \) (\( \hbar = k_{B} = 1 \)). We focus on the case of finite anisotropy \( \Delta > 1 \), where Eq. [10] features a gapped ground state. Using a combination of exact diagonalization and perturbation theory, we uncover a regime of diffusive transport below a finite critical momentum \( q_{D} \). In this regime, density modes at fixed momentum \( q \) decay with a diffusion constant \( D_{q} \) and our analysis is consistent with \( D_{q} \) independent of momentum and inversely proportional to the anisotropy. As the temperature is lowered from \( T = \infty \), we observe a decrease of the critical momentum and an almost exponential increase of the diffusion constant. We provide evidence for a complete breakdown of diffusion above the critical momentum.

We begin by introducing the generalized diffusion coefficient as a quantity suitable to describe the evolution of a harmonic spin density profile close to equilibrium, i.e., in the linear response regime. To this end, the central quantities we analyze are the autocorrela-
tion functions $C_{S,q}(t) = \text{Re}(S^z_q(t) S^z_{-q})/N$ and $C_{J,q}(t) = \text{Re}(J^z_q(t) J^z_{-q})/N$ of the spin density $S^z_q$ and the spin current $J^z_q = \sum e^{iqr} (S^x_q S^y_{q+1} - S^y_q S^x_{q+1})$ at momentum $q = 2\pi k/N$ \cite{23}, where $\text{Re}$ indicates the real part, (...) denotes the canonical equilibrium average at the inverse temperature $\beta = 1/T$, and $t$ represents the time. Since the density $S^z_q$ and the current $J^z_q$ are connected by the lattice continuity equation $\partial_t S^z_q = (1 - e^{iq}) J^z_q$, the autocorrelations are related by $\partial_t^2 C_{S,q}(t) = -q^2 C_{J,q}(t)$ with the abbreviation $q^2 = 2(1 - \cos q)$. The generalized, time- and momentum-dependent diffusion coefficient is defined via

$$D_q(t) = \frac{\partial_t C_{S,q}(t)}{q^2 C_{S,q}(t)} = \frac{I^1_q(t)}{C_{S,q}(0) - q^2 I^2_q(t)}. \quad (2)$$

To arrive at the right-hand expression in Eq. (2), we integrate the continuity equation twice, using $\partial_t C_{S,q}(t)|_{t=0} = 0$ and introducing the two integrals $I^1_q(t) = \int_0^t dt' C_{J,q}(t')$ and $I^2_q(t) = \int_0^t dt' I^1_q(t')$.

The left-hand expression in Eq. (2) identifies the quantity $q^2 D_q(t)$ with the instantaneous decay rate, at time $t$, of a spin density profile with wave vector $q$ close to equilibrium. Fick’s law corresponds to the case of $D_q(t) = \text{const}$. The main goal of this Letter is to analyze the time- and momentum-dependence of this quantity versus temperature. We emphasize that a complete knowledge of this dependence allows to propagate arbitrarily shaped spin density profiles in time. This does not only share a common interest with time-dependent density-matrix renormalization group studies \cite{24}, yet confined to zero temperature, but even more so may be of relevance to laser pulse induced time-dependent transport measurements, including recently proposed time-offlight and thermal imaging techniques \cite{25}.

Qualitatively, the variation of $D_q(t)$ versus $t$ can be understood from a standard relaxation-time ansatz, in which the current autocorrelation $C_{J,q}(t) = \exp(-t/t_q) C_{J,q}(0)$ decays exponentially. For short times, $t \ll t_q$, Eq. (2) then yields $D_q(t) \sim 1 - e^{-t/t_q}$, which starts with a linear increase, $D_q(t) \propto t$, and turns into a ‘plateau’ $D_q(t) \approx \text{const}$, starting at $t = \tau_q \gg t_q$. This plateau marks the hydrodynamic regime. Namely, proceeding to the long-time limit, i.e. for $t \gg t_q$, and to the long-wavelength limit, i.e. for $q^2(t - t_q) D_q \ll 1$, Eq. (2) leads to a time-independent diffusion constant $D_q(t) = D_0 + O(q^2)$, where $D_0 = t_q C_{J,q}(0)/C_{S,q}(0)$, which is equivalent to Einstein’s relation \cite{24}, and $D_0 = D_{q=0}$.

In principle, partial conservation of currents at $q = 0$, i.e. the impact of a finite Drude weight at zero frequency \cite{13}, can also be included into this qualitative picture. For that case the exponential decay of $C_{J,0}(t)$ has to be leveled off into $C_{J,0}(t \to \infty) = \text{const.} > 0$. This leads to a linear increase $D_q(t \to \infty) \propto t$. However, the Drude weight will not be an issue in this Letter. In fact, there is no zero-frequency contribution of currents at $q \neq 0$, which follows directly from the continuity equation.

While the gross feature of the preceding relaxation-time ansatz can serve as a guideline to interpret the results of unbiased exact diagonalization data, on which we will report later, it is not justified a priori. Therefore, and to gain a deeper insight into the high-temperature current dynamics generated by the Heisenberg model, we will first turn to a quantitative discussion using an analytical method. This method employs the projection operator perturbation theory (POPT) of Ref. \cite{27}, which allows to derive a rate equation $\partial_t C_{J,[S,q]}(t) = -\gamma_{J,[S,q]}(t) C_{J,[S,q]}(t)$ for the current/density autocorrelation. This rate equation gives access to $D_q(t)$ through the right-hand [central] expression in Eq. (2). The POPT yields a short-time expansion for the decay rate $\gamma_{J,[S,q]}(t)$, the terms of which can be evaluated from a decomposition $H = H_0 + H_I$, if the observable of the autocorrelation $C_{J,[S,q]}(t)$ is a conserved quantity for the unperturbed Hamiltonian $H_0$. For the current, we choose the XY model for $H_0$, in which $J_q$ is conserved only at $q = 0$. For the density, we choose the Ising model for $H_0$, in which $S_q$ is conserved for all $q$. Then for short times we obtain approximately:

$$\gamma_{J,0}(t) \approx \langle J(t) \rangle^3/24 + O((\langle J(t) \rangle^3)^2), \quad t J \lesssim 1.5 \quad (3)$$

$$\gamma_{S,q}(t) \approx \langle q \rangle J(t)^3/24 + O((\langle q \rangle J(t)^3)^2), \quad t J \lesssim 2 \Delta \quad (4)$$

For the full quantitative evaluation of $D_q(t)$ we determine the leading-order term in Eqs. (3) and (4) numerically exact, following the scheme in Ref. \cite{27}, which leads to small changes only. We note that for a complete integration of

![Figure 1](image-url)
For the remainder of this Letter we refer to the satutative short times, set by Eq. (4). The resulting quantitate $D_q$ as in this Letter, the current relaxation time from Eq. (3) is $D_q(t) \propto q \tau_0$, as in Eq. (3) for $D_q(t)$ for $D_q(t) \propto q \tau_0$. Therefore for $\Delta = 1.5$ or $2.0$, we find no indications of diffusion for $q \geq 0.22 \pi \Delta = \omega D$. Instead, $D_q > q \omega(t)$ displays divergent behavior due to oscillations of $C_S(q,t)$ with time, preventing diffusive behavior to occur. These oscillations have already been reported in Ref. 24 for smaller $\Delta$.

We emphasize that ED results for the spectra $C_{t,0}(q,\omega)$ at small $q$ versus frequency $\omega$ agree with our interpretation from the time domain. E.g., focusing on $\Delta = 1.5$, Fig. 2 (a) shows that the spectrum $C_{t,0}(q,\omega) / C_S(q,0)$ is consistent with a Gaussian of height $D_0 \omega J \approx 0.59$, as predicted by the POPT at $q = 0$. The low-frequency behavior is still governed by finite-size effects and deviations from the Gaussian occur at a frequency scale $\omega \Delta$.
decreases. At 
observe two effects. First, as the temperature is lowered, 
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marizes our findings for  \( \Delta = 1 \) from 0 to  
for diffusive density decay. 
can be determined with a precision of 20% (error bars).

Now we turn to the effects of temperature by increasing  
\( \beta > 0 \) for  \( \Delta = 1.5 \) and  \( N = 18 \) (curves). Thick arrows mark the approximate locations of the current decay time  \( \tau_q \). (d) The resulting diffusion constant  \( D_0 \) versus  \( \beta \) for  \( \Delta = 1.5 \) (squares) and  \( \Delta = 2.0 \) (circles), which can be determined with a precision of 20% (error bars).

\( \omega/J < 1 \), which is independent of  \( q \). This agrees with the  \( q \)-independent time scale in Fig. 2 where finite-size effects set in. Similar spectra of  \( C_{S,0}(\omega) \) have been obtained in Ref. 31 for  \( q = 0 \). Note that the (finite size)  \( q = 0 \) Drude weight at  \( \omega = 0 \) is not shown in Fig. 3 (a).

Figure 3 (b) shows that  \( C_{S,0}(\omega) \) is consistent with a Lorentzian of width  \( \tilde{q}^2 D_0 \) again  \( D_0 J \approx 0.59 \), as expected for diffusive density decay.

Now we turn to the effects of temperature by increasing  \( \beta \) from 0 to  \( \beta J = 2 \). Since the POPT is not applicable at  \( \beta \neq 0 \), we focus on the ED results. Figure 4 (a)–(c) summarizes our findings for  \( \Delta = 1.5 \) and  \( \beta J = 0.5, 1, 2 \). We observe two effects. First, as the temperature is lowered, the number of momenta with diffusive density dynamics decreases. At  \( \beta J = 0.5 \) and 1 the mode with  \( q = 0.11 \pi \) still decays diffusively but for  \( \beta J = 2 \) only the  \( q = 0 \) mode displays diffusion. Second, as the temperature is lowered,  \( D_q \) and  \( \tau_q \) increase significantly. For  \( q = 0 \) this increase can be followed up to  \( \beta J = 2 \). Figure 4 (d) displays  \( D_0 \) versus  \( \beta \) in a semi-logarithmic plot for  \( \Delta = 1.5 \) and 2.0. From this plot, one might be tempted to speculate on an exponential increase of  \( D_0 \) with  \( \beta \) beyond the temperature window depicted, see a related claim in Ref. 32. However, in view of the hydrodynamic relation  \( D_0 = t_0 C_{S,0}(0)/C_{S,0}(0) \) this is a subtle issue. From our numerical analysis, we find  \( C_{S,0}(0) \) to be the dominant source of  \( D_0 \)’s  \( T \)-dependence for  \( 0 < \beta J < 2 \). But  \( C_{S,0}(0) \) is not \( \propto \exp(\epsilon c^2) \) for all  \( \beta \) \cite{33}. An exponential increase of  \( D_0 \) must further break down as  \( \beta \to \infty \) due to the finite spin gap for  \( \Delta > 1 \). We also mention that, for  \( \Delta = 1 \) and  \( \beta J \gg 1 \), the dominant  \( T \)-dependence of  \( D_0 \) stems from  \( t_0 \propto 1/(T \ln T) \) \cite{21,22}, which is not exponential.

Finally, we turn to a more detailed discussion of the temperature dependence of the critical momentum  \( q_D \).

To this end, we first collect all momenta  \( q \lesssim q_D \) in Fig. 5. Then, to rationalize this, we invoke the standard hydrodynamics criterion that the relaxation time  \( 1/(\tilde{q}^2 D_0) \) of a diffusive density mode should be larger than the decay time  \( \tau_q \) of the current, or equivalently, that a diffusive density spectrum should be narrower than the current spectrum, see Fig. 3. Therefore, breakdown of diffusion occurs at  \( \tilde{q}^2 D_0 \tau_q \sim 1 \), where we may set  \( D_q = D_0 \) and  \( \tau_q = \tau_0 \), due to the weak  \( \beta \)-dependence of these quantities in our case. Based on our ED results for  \( D_0 \) and  \( \tau_0 \), Fig. 5 displays the lines  \( \tilde{q}^2 D_0 \tau_0 = 1 \) versus  \( \beta \) for both  \( \Delta = 1.5 \) and 2.0 (solid curves). The obvious agreement between these lines and the boundaries for the collected values of  \( q \lesssim q_D \) is a convincing consistency check of our approach. Apparently, as  \( \beta \) increases,  \( q_D \) decreases. In view of the temperature dependence of  \( D_0 \) and  \( \tau_0 \), this decrease is also approximately exponential for  \( 0 \leq \beta J \lesssim 2 \). To assess the relevance of finite size effects, Fig. 5 contains a comparison between the lines  \( \tilde{q}^2 D_0 \tau_0 = 1 \) and the observed diffusive modes for  \( N = 16 \) and 18 (symbols). Given the limited resolution of the  \( q \)-grid, the agreement with these two system sizes is remarkably good.

In summary we have investigated magnetization transport in the spin-1/2 XXZ chain above the isotropic point at finite temperature and momentum. We found an extended momentum-space region of spin-diffusion with an approximately time and momentum independent diffusion constant. The diffusion cut-off wave vector (diffusion constant) was found to scale approximately linear with the (inverse) anisotropy and to decrease (increase) strongly with the inverse temperature.

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