Spin Transport Properties in Heisenberg Antiferromagnetic Spin Chains: Spin Current induced by Twisted Boundary Magnetic Fields

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Spin transport properties of the one-dimensional Heisenberg antiferromagnetic spin systems for both \(S = 1/2\) and \(S = 1\) are studied by applying twisted boundary magnetic field. The spin current displays significantly different behavior of the spin transport properties between \(S = 1/2\) and \(S = 1\) cases. For the spin-half case, a London equation for the current and the detection of an alternating electric field are proposed for the linear response regime. The correlation functions reveal the spiral nature of spin configuration for both ground state and the spinon excitations. For the spin-one chain otherwise, a kink is generated in the ground state for the size is larger than the correlation length, leading to an exponential dependence of spin current with respect to the chains length. The midgap state emerges from the degenerate ground state even for small boundary fields.

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A significant amount of experimental and theoretical efforts has been focused on the controlling of spin degree of freedom in recent years. For the most part the research effort has been concentrated on the dilute magnetic semiconductors as well as the spin Hall effect emerging from the spin-orbital coupling in two dimensions. However, spin transport properties in pure spin systems, such as the Heisenberg system, is also of great interests because many of the novel concepts associated with spin conduction can be tested without the interference of charge degrees of freedom. For instance, ballistic transport characterized by a finite Drude weight or spin stiffness has been found for both the integrable systems and certain class of Luttinger liquids. Recently, Meier and Loss studied the magnetization transport properties in a finite spin-half Heisenberg chain linked to two bulk magnets. They obtained a finite spin conductivity for a confined antiferromagnetic chain and predicted that a magnetization current produces an electric field. Alternatively, Schütz et al. investigated a mesoscopic spin ring in the inhomogeneous magnetic field to search for persistent spin current for different spins. On the experimental front, mean free paths of several hundred nanometers were found to suggest a quasi-ballistic transport of one dimensional elementary spin excitations in \(\text{Sr}_2\text{CuO}_3\) and \(\text{SrCuO}_2\) samples.

In the present work, we study the spin transport properties of one-dimensional (1D) Heisenberg antiferromagnetic (HAF) spin models. It is well known that the integer-spin HAF chain is distinguished by a finite gap in spectrum from the half-integer spin one. As expected that the spin transport is diffusive for the integer spin case, experimental NMR and thermal conductivity measurements have indicated finite spin diffusion and thermal diffusion constants in \(\text{AgVP}_2\text{S}_6\). On the other hand, Fujimoto based on the integrability of the nonlinear \(\sigma\)-model suggested that the spin transport is ballistic in the perfect 1D spin one system. Therefore, a general criteria on ballistic spin transport are yet to be established generally for either homogenous spin chains with different spins or mesoscopic (quasi-)one dimensional Heisenberg systems with an inhomogeneous magnetic field. This motivates us to devise a simplified case in which twisted magnetic fields are applied to both ends of a finite HAF chain with both \(S = 1/2\) and \(S = 1\). Whether the twisted boundary magnetic fields, breaking the translational as well as SU(2) symmetry, can properly drives the spin to flow through the chains alternatively presents distinguishable transport nature between the spin half and one cases.

The Hamiltonian we will consider reads:

\[
\hat{H} = J \sum_{i=1}^{N-1} \hat{S}_i \cdot \hat{S}_{i+1} - h_1 \cdot \hat{S}_1 - h_2 \cdot \hat{S}_N, \tag{1}
\]

where \(\hat{S}_i\) is the spin operator for either \(S = 1/2\) or \(1\) at the \(i\)th site, respectively. \(h_1\) and \(h_N\) are the magnetic fields applied to the spins \(\hat{S}_1\) and \(\hat{S}_N\). For convenience, we set \(J = 1\) and \(|h_1| = |h_N| = h\) unless specified, take \(h_1 = (0, 0, h)\) and \(h_N = (h \sin \theta, 0, h \cos \theta)\) where \(\theta\) is the angle between \(h_1\) and \(h_N\) and in \([0, \pi]\). We note that such a system can be realized experimentally by attaching two magnetic leads on two ends of the chains.

We employ the density matrix renormalization group (DMRG) method to study the present twisted magnetic field effects. In our computations, we use both the infinite and the finite size algorithm. The maximum number of sweeps is five and the number of states is kept up to 400. The efficiency of computations is not reduced.
significantly by the absence of the conserved $S^z_{\text{total}}$. The truncation errors are about $10^{-12}$ and the relative errors maintained below one percent as examined by increasing more kept states and sweeps. The computations are performed up to 100 sites usually and 400 sites for the proper extrapolations needed for thermodynamics limit.

It is natural to first examine the twisted magnetic field effects on the correlation function

$$C_{zz}(r) = (-1)^r \left\langle \hat{S}_i^z \hat{S}_{i+r}^z \right\rangle$$

for the spin $z$-component and its alternative form

$$G_{zz}(r) = C_{zz}(r) - (-1)^r \left\langle \hat{S}_i^z \right\rangle \left\langle \hat{S}_{i+r}^z \right\rangle.$$  

Figure 1 shows the correlation function $C_{zz}(r)$ with respect to the distance $r$ for the chain length $L = 100$ and various angles at $h = 1$. We found that $C_{zz}(r)$ is nonzero almost for all $r$ and $\theta$ for the $S = 1/2$, while $C_{zz}(r)$ is finite only when $r$ is nearby both ends of the chain owing to gapful excitation for the $S = 1$ case. This is intrinsically associated with their algebraic and the exponent behaviors at $h = 0$ for $S = 1/2$ and 1, respectively. As expected, $C_{zz}(r, \theta) + C_{zz}(r, \pi - \theta) = 2C_{zz}(r, \frac{\pi}{2})$. In addition, the insets demonstrate that $G_{zz}(r)$ decays toward zero very rapidly, surprisingly independent of the magnitude of spins and angle $\theta$.

On the other hand, the twisted magnetic fields can directly alter spin configurations in the ground state, which in principle reflects intrinsic properties in the different spin case. We thus analyze how the direction of spin polarization changes with site-$i$ by introducing a classic polarized angle defined as

$$\alpha_i = \tan^{-1} \left\langle \hat{S}_i^z \right\rangle / \left\langle \hat{S}_i^z \right\rangle$$

which essentially measures the deviation of the spin polarization at Figure 2 shows $\alpha_i$ with three different values of $\theta$ at $h = 1$. For $S = 1/2$, we found that

$$\alpha_i = \alpha_{res} - \frac{i - 1}{N}(\pi - \theta) + \pi \mod (i - 1, 2)$$

where $\alpha_{res}$ is a residual angle which is two orders smaller than $\alpha_i$ but depends on $i$, $\mathbf{h}_1$ and $\mathbf{h}_N$. One can see that $\alpha_i$ depends almost linearly on $i$, implying that ground state configuration displays a perfect classical spiral structure in spite of strong quantum fluctuations. The present ground state is just the superposition of some originally lowest-lying states whose energy is the order of the edge excitation energy and depends also weakly on the magnetic field. Since arbitrary boundary fields do not change the integrability of the Hamiltonian (1) for $S = 1/2$, there may still be spinon-like topological excitations.[21] However, for $\theta \neq 0$ or $\pi$, the total spin and its $z$-component are no longer good quantum numbers, and the spinon essentially does not carry definite spin in contrast to the $\theta = 0$ case where the spinon possesses a spin of one half. This implies that the spinon propagates through some kind of spiral path in response to twisted magnetic fields. Nevertheless, since the integrability of the system ensures the spiral spinon is dissipationless, it is unclear what the topological charge of the spiral spinon is and what kind of conservation law accounts for the topological charge of the spiral spinon, which is beyond the current studies.

![FIG. 1: Spin correlation function $C_{zz}(r)$ for both $S = 1/2$ (left penal) and $S = 1$ (right penal) for six angles $\theta = 0$, $\pi/6$, $\pi/3$, $\pi/2$, $2\pi/3$ and $\pi$ with $h = 1$. The insets show $G_{zz}(r)$.](image_url)

![FIG. 2: The spin polarization angle $\alpha_i$ as a function $i$ with various twisted angle $\theta$ at $h = 1$. In the figure, $\alpha_i$ are explicitly displayed with odd $i$ only, while the results for even $i$ are obtained from shifting those for odd $i$ upwards by $\pi$. The solid curves on the right panel fit Eq. (6).](image_url)
large $N$. However, it depends on the value of $\theta$ and independent of the magnitude of external fields as we have checked for $h = 0.1$ and 10 cases. $\xi_{\theta,N} = 2.9, 3.6$ and 4.0 for $\theta = \pi/3, \pi/2$ and $2\pi/3$. The kink can be interpreted as a consequence of the soliton-like nature of the magnon excitation owing to the presence of the gap for $S = 1$.

For the quantum spin-1 HAF chain, there exists the $Z_2 \times Z_2$ hidden symmetry, which makes its excitations unstable against disturbances. It has been found that an open boundary can result in four-fold degeneracy with $S = 0, 1$ in the thermodynamic limit, while the magnetic doping causes a midgap state \[24, 25\]. In the present case, the boundary field simply lifts the degeneracy and induces subsequently a midgap. Figure 3 shows that a midgap energy emerges linearly in $h$ for small $h$ and enters the continuum when $h \gtrsim 0.5$. Therefore, the boundary field can be devised as a tuning parameter to manipulate such a macroscopic quantum state, which is detectable in neutron scattering measurements 24.

Now we turn to the intrinsic transport properties associated with above findings. We notice that the twisted magnetic fields essentially impose a “spin voltage” between two ends of spin chains 11. For $S = 1/2$, the spin spiral polarization homogeneously extends over the whole chain, resulting in a spin current which does not depend on the chain length (see below). This supports the conjecture of Zotos and coworkers on an ideal metallic spin chain with $S = 1/2$ 5, resulting from the integrability. In this sense, the correlation function $C_{zz}(r)$ in the bulk shown in Fig. 4 properly reflects the quasi-long range character and the edge effects near the end of the chain. However, for the $S = 1$ case, the kink prevents the propagation of the magnon over characteristic distance $2\xi_{\theta,N}$. One can observe the spin current only when the size is the order of $2\xi_{\theta,N}$ or smaller. This is consistent with the conjecture on the persist spin current on a ring proposed in Ref. 12. $C_{zz}(r)$ in Fig. 4 indeed displays a short-range correlation for the spin-1 chain, while the tails confined nearby $r \sim N$ unveils the fact that edge spins are indeed asymptotically free due to the breaking of the hidden $Z_2 \times Z_2$ symmetry.

FIG. 3: The midgap energy versus $h$ with various $\theta$ for the $S = 1$ case. The horizontal line indicates the Haldane gap.

Following Shen 21, we introduce a spin current:

$$I_s = \langle S_i \times S_{i+1} \rangle.$$  

which is site-independent. As the twisted magnetic field is applied on the $xz$ plane for both $i$ and $N$, only $y$-component is non-zero. Figure 4 shows $N I_s$ as a function of the chain length $N$ for both $S = 1/2$ and $S = 1$. When $N$ increases, it increases for small $h$ or unchanged for large $h$ for $S = 1/2$, but it always decreases for $S = 1$. The results for $S = 1/2$ indicate again an ideal magnetic metal for the spin-half HAF chain, while generally an insulator for $S = 1$ except for small size systems where the spin current is observable 12. As far as the spin dissipation is concerned in the $S = 1$ case, we found that $I_s \sim Ae^{-N/\xi}$ with $A = 0.39$ and $\xi = 6.04$ apart from a weak $\theta$-dependence. $\xi$ is in very good agreement with the correlation length of the ordinary $S = 1$ HAF chain 22.

Since the $S = 1$ chain is an insulator, we focus on the $S = 1/2$ case below. We notice that the spin current is very sensitive to the twisted angle $\theta$ as shown in Fig. 5(a) and (b). On the other hand, as seen from Fig. 5(c), the spin current rapidly increases with increasing $h$ and reaches a maximum at about $h = 1$ which is the critical value of the uniform field to saturate the uniform magnetization. When $h$ is further increased, $I_s$ saturates. For very small $h_1$ and $h_N$, the system lies in the linear response regime. In this case, we found that the spin current is proportional to the vector $h_1 \times h_2$ which precisely follows $\sin \theta$ as demonstrated in Fig. 5(b). Therefore, we can naturally devise a “spin voltage” in a form of

$$V_s = h_1 \times h_2,$$  

a “spin-vector potential” for Eq. (1). Then we obtain the spin current as follows:

$$I_s = D \cdot V_s.$$  

FIG. 4: The spin current multiplied by $N$ shows a significantly different size-dependence for both $S = 1/2$ and 1. $h$ equals to one for various cases and is explicitly indicated otherwise.
FIG. 5: The spin current and the spin conductance for $S = 1/2$. (a) For various $h$ and $\theta$; (b) For the linear response regime with different $h_1$ and $h_N$. Solid curves draw $\sin \theta$, which indicate that $I_s$ is proportional to $h_1 \times h_2$; (c) $I_s$ as a function of $h$ with $\theta = \pi/2$. (d) The same size-dependence of the spin conductance with all $h$ as the same as in (b).

which is one kind of the London equation with $D$ being the spin conductance. Since both sides of the above equation are time-reversal invariant so that the spin current is dissipationless. The spin conductivity characterizing the bulk properties described by Eq. (1) is given by $\sigma = DN$. We calculated the spin conductance $D$ for various $h_1$ and $h_N$ with different chain length $N$ as explicitly demonstrated in Fig. 5(d) and found that it is linearly scaled to zero $1/N$. With making extrapolation for the thermodynamic limit, we obtain $\sigma = 10.0$ for the Heisenberg antiferromagnetic spin-half chain, which is expected in connection with the Drude weight studied by Zotos with the finite temperature.

Is the spin current discussed here observable? The system discussed here is implementable experimentally as a two leads spin systems introduced recently in Ref. 11. A spin current generates an electric field. By measuring the electric voltage difference between two points in the vicinity of the spin chain, one can detect the spin current. We propose another way of detecting the spin current in a spin half chain. With a fixed $h_1$ and a rotating $h_2$, an alternating spin current is generated and an alternating electric field is subsequently observable nearby the spin chain. Measurement of the ac voltage of a given point close to the chain and the reference point (ground) reveals the spin current.

In conclusion, we study the spin transport properties of the Heisenberg spin chains for $S = 1/2$ as well as $S = 1$ via applying twisted boundary magnetic fields. Although the boundary conditions generally do not affect bulk of a sufficiently large system, the twisted boundary fields indeed change entirely spin orientation for the chains in the thermodynamic limit, allowing to detect the spin transport properties. The significantly different transport properties are found for $S = 1/2$ and $S = 1$ chains. The former is spin-metallic and has spiral spinon excitation, while the later is spin-insulator which involves a static kink and unveils a midgap state lift from the degenerate ground state by the external field. A London-type equation for spin current with the spin voltage and the detection of an alternating electric field are proposed for the spin-metallic case in the linear response regime.

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