Presence of Energy Flux in Quantum Spin Chains: An Experimental Signature

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Using the *XXZ* model for the description of one-dimensional magnetic materials we show that an energy flux, j_E, produces a shift, $\delta k \sim \sqrt{j_E}$, in the characteristic wavenumber of the spin-spin correlations. We estimate δk for a realistic experimental setup and find that it is measurable in inelastic neutron scattering experiments.

1. INTRODUCTION

The problem of thermal transport in one-dimensional systems has been much investigated, the main goal being to derive Fourier's heat law. Analytical and numerical studies of a number of classical lattice-dynamical models indicate that the condition for Fourier's law to hold is the presence of strong nonlinearities i.e., nonintegrability (chaoticity) of the dynamics.[1] Although quantum systems have been less studied, it appears that similar considerations apply to quantum spin chains as well.[2]

Integrable systems, on the other hand, show anomalous thermal transport. No internal thermal gradient is formed in a harmonic crystal[3] or in a transverse Ising chain[2] and, as a consequence, the energy (heat) flux is not proportional to the temperature gradient inside the sample. The origin of this anomaly may be the fact that the energy current in integrable systems often emerges as an integral of motion which automatically yields anomalous thermal transport coefficients.[4]

The flat temperature profile in the presence of energy current is an intriguing feature of integrable systems. In effect, it points to the existence

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of a homogeneous state carrying finite energy current. In this paper, we shall explore the experimentally measurable properties of such a state by studying the XXZ spin chain in the presence of an energy current. The most spectacular feature of such a state is the incommensurability of magnetic excitations. Namely, in the presense of energy flow j_E, the characteristic wave vector is shifted from its antiferromagnetic value π by the amount $\delta k \sim \sqrt{j_E}$. Since there are quite a few well established realizations of quasi-one-dimensional Heisenberg chains[5] (e.g., KCuF$_3$,[6] Cs$_2$COCl$_4$,[7] Copper Benzoate,[8] Sr$_2$CuO$_3$, Cs$_2$CuCl$_4$[9]), we believe that the predicted changes in the dynamical correlation functions bear direct experimental relevance.

The basic problem of constructing a state which carries an energy current is the nonequilibrium nature of that state. Even if we assume that the flat temperature profile means the existence of equilibrium, we still face a problem that the value of the established temperature is not known.[10] We shall avoid this problem by restricting our calculation to zero temperature $(T = 0)$ and assuming that the ground state correlations are robust enough to survive at low temperatures.

The construction of a homogeneous state with energy current at $T = 0$ can be done by adding the energy current with a Lagrange multiplier to the XXZ Hamiltonian and then finding the ground state. Similar calculations have been carried out already for the transverse Ising and XX chains[11, 12] and, in a different context, for the XXZ model.[13, 14] The new result we report is the calculation of an experimentally accessible parameter, namely the shift, δk, of the characteristic wavenumber in the spin-spin correlations as a function of the energy current, j_E.

Once we have $\delta k(j_E)$, we turn to a realistic experimental setup and estimate j_E flowing through a single spin chain which gives an estimate of δk. Our result shows that δk is in the accessible range of an inelastic neutron scattering experiment.

2. THE MODEL AND THE CHARACTERISTIC WAVE NUMBER

The model we study is the spin-1/2 XXZ chain defined by the Hamiltonian

$$\hat{H}_{XXZ} = \mathscr{J} \sum_{\ell} \left[\sigma_{\ell}^x \sigma_{\ell+1}^x + \sigma_{\ell}^y \sigma_{\ell+1}^y + \Delta \sigma_{\ell}^z \sigma_{\ell+1}^z \right] \tag{1}$$

where the spins σ_{ℓ}^{α} ($\alpha = x, y, z$) are Pauli spin matrices at sites $\ell = 1, 2,..., N$ of a one-dimensional periodic chain ($\sigma_{N+1}^{\alpha} = s_1^{\alpha}$). We shall use the parametrization $\Delta = \cos \gamma$ and consider only the "antiferromagnetic" region

$0 < \gamma < \pi/2$. In order to impose a fixed energy current j_E in the ground state, we add the current operator to the Hamiltonian with a Lagrange multiplier

$$\hat{H} = \hat{H}_{XXZ} + \lambda \hat{j}_E \tag{2}$$

where

$$\hat{j}_E = \frac{\mathscr{J}^2}{h} \sum_\ell \sigma_\ell^z [\sigma_{\ell-1}^y \sigma_{\ell+1}^x - \sigma_{\ell-1}^x \sigma_{\ell+1}^y$$

$$+ \Delta(\sigma_{\ell-2}^x \sigma_{\ell-1}^y - \sigma_{\ell-2}^y \sigma_{\ell-1}^x + \sigma_{\ell+1}^x \sigma_{\ell+2}^y - \sigma_{\ell+1}^y \sigma_{\ell+2}^x)] \tag{3}$$

Importantly, $\hat{j}_E$ is an integral of motion, $[\hat{j}_E, \hat{H}] = 0$, thus indicating that (i) the transport of energy is singular in this system[4] and (ii) the states carrying fixed energy current can be obtained as stationary states of $\hat{H}_{XXZ}$.

The XXZ model can be described in terms of interacting fermions and has been solved using the Bethe Ansatz method. The same approach works in the presence of the driving term, $\lambda \hat{j}_E$, as well, and the solution has been given in refs. 13 and 14. An interesting feature of the solution is that the system displays rigidity against the drive, namely the ground state supports a nonzero energy current, $\langle \hat{j}_E \rangle \equiv j_E \neq 0$, only if the coupling λ exceeds some critical value $\lambda_c(\gamma)$. As we are interested in fixed energy currents, we simply choose sufficiently large values of λ. Furthermore, since in realistic situations j_E turns out to be small, we concentrate on the region $\lambda \approx \lambda_c(\gamma)$, in which case $j_E \propto (\lambda - \lambda_c)$.

Once the energy current flows, an important restructuring takes place in the ground state. The single Fermi sea characterizing the ground state without current splits into *two* Fermi seas as shown in Fig. 1 for the simple case of the XX limit ($\Delta = 0$) where a free-fermion description applies. There are now four Fermi wave vectors, $\pm \pi/2$ and $\pi/2 \pm \delta k$, and the structure of the ground state immediately implies that there will be gapless excitations at wave vectors 0, δk, $2\delta k$, $\pi - \delta k$, π and $\pi + \delta k$, which is readily confirmed by the exact solution at arbitrary Δ.

Thus an incommensurability characterized by δk appears in the system. This can be seen readily in the ground-state correlations. Indeed, it has been shown[12, 15] that, in the XX limit, the longitudinal correlations for small $j_E \neq 0$ can be expressed in a scaling form

$$\frac{\langle \sigma_\ell^x \sigma_{\ell+n}^x \rangle_{j_E \neq 0}}{\langle \sigma_\ell^x \sigma_{\ell+n}^x \rangle_{j_E = 0}} = \Phi(\delta k n) \tag{4}$$
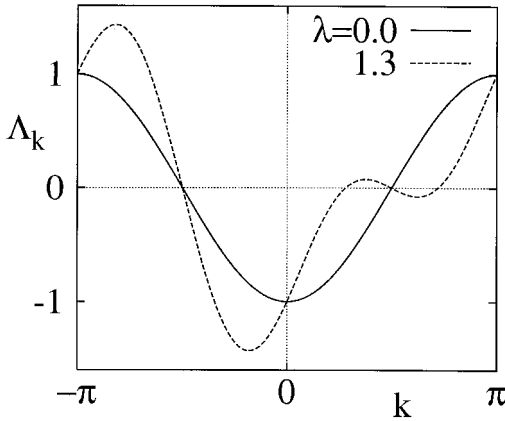
Fig. 1. Single-particle fermionic spectrum in the XX limit ($\Delta = 0$) of the $\hat{H}_{XXZ} + \lambda \hat{j}_E$ hamiltonian with and without energy current in the ground state (dashed line, $\lambda = 1.3$ and solid line, $\lambda = 0$, respectively). The energy is measured in units of $\mathscr{J}$ while the wave number, k, is given in units of the inverse lattice spacing. The Fermi energy is zero independently of λ.

where $\Phi(x \to 0) = 1$ and the large argument asymptotics of the scaling function is given by

$$\lim_{x \to \infty} \Phi(x) \sim \frac{1}{\sqrt{x}} (1 + \cos x) \tag{5}$$

Since $\langle \sigma_\ell^x \sigma_{\ell+n}^x \rangle_{j_E = 0} \sim (-1)^n / \sqrt{n}$ Eqs. (4), (5) imply that, as the current is switched on, the static structure factor develops additional peaks at $k = \pi \pm \delta k$ (as it will turn out, δk is small thus it is better to speak about the $k = \pi$ peak developing shoulders for $j_E \neq 0$).

In order to connect δk to the current one determines both j_E and δk through λ and then eliminates the Lagrange multiplier. The expressions are simple for the XX limit[12]

$$j_E = \frac{\mathscr{J}^2}{2\pi h} \left(1 - \frac{1}{\lambda^2} \right), \qquad \cos \delta k = \lambda^{-1} \tag{6}$$

and, for small currents ($\lambda \gtrsim \lambda_c = 1$), they yield

$$\delta k = \sqrt{\frac{j_E}{j_E^{(1)}}} \tag{7}$$

where a "natural unit" of the current, $j_E^{(1)} = \mathscr{J}^2/h$, has been introduced.

The above calculation can be carried out for any $0 \leqslant \Delta < 1$ and the result for δk differs only in a prefactor of order unity[16]

$$\delta k = \frac{2\gamma}{\pi \sin \gamma} \sqrt{\frac{j_E}{j_E^{(1)}}} \tag{8}$$

As one can see, the largest δk is obtained in the XX limit ($\gamma \to \pi/2$).

In principle, if δk is large enough then the extra peaks at $\pi \pm \delta k$ should be observable as Bragg peaks in an elastic neutron scattering experiment. In practice, however, the incommensurate modulations of distinct spin chains are not correlated and, as a consequence, the delta function of the Bragg peak would spread out into a plain and the effect would be unobservable.

3. STRUCTURE FACTOR AND AN EXPERIMENTAL SETUP

It is more promising to look for an experimental signature in an inelastic neutron scattering experiment where the excitations of the system are measured and no coherence among the chains is needed. Taking into account the facts that, for $j_E = 0$, most of the spectral weight is concentrated on the region around the antiferromagnetic wave vector π, and furthermore that, for $j_E \neq 0$, there are gapless excitations at wave vectors $\pi \pm \delta k$, we expect that the presence of the current manifests itself via the emergence of *additional* inelastic peaks at wave vector $\pi \pm \delta k$. This expectation can be put on a more solid base by calculating the dynamic structure factor and examining the relative weights at wave vectors π and $\pi \pm \delta k$.

The simplest case is again the XX limit where the calculation of the time-dependent transverse correlation function, $\langle \sigma_n^z(t) \sigma_0^z(0) \rangle$, is straightforward. There is, however, a principal problem at the outset of the calculation. Namely, it is not clear whether the time-evolution of $\sigma_n^z(t)$ is governed by $\hat{H}_{XX}$ or by $\hat{H}_{XX} - \lambda \hat{j}^E$. We shall take the view that in reality the current-carrying state is formed as a result of boundary conditions. Thus the local perturbation caused by an incoming neutron evolves by the local hamiltonian i.e., by $\hat{H}_{XX}$.[17] Once $\langle \sigma_n^z(t) \sigma_0^z(0) \rangle$ is known its Fourier transform in time and space gives the structure factor $S_{zz}(k, \omega)$ as shown in Fig. 2.

As we can see, a large part of the weight of the $j_E = 0$ peak of the structure factor at π shifts to $\pi \pm \delta k$ for $j_E \neq 0$. Thus one can expect that even if δk is small, the presence of a small energy current will result in a *broadening* by $2\delta k$ of the inelastic peak centered at wavevector π. It is this broadening that we propose as an experimental signature for the current-carrying state. The remaining question now is how to estimate δk.
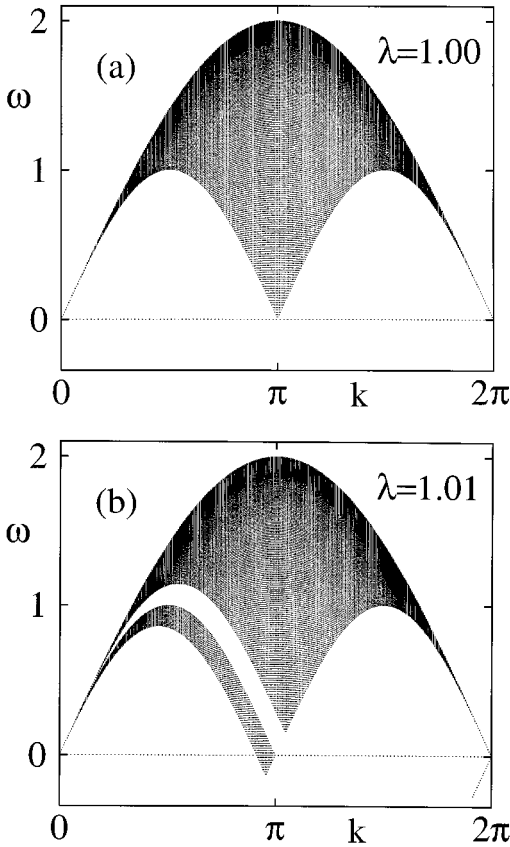
Fig. 2.   The structure factors $S_{zz}(k, \omega)$ displayed on the wavenumber-frequency $(k - \omega)$ plane for cases of (a) $\lambda = 1.00$ (no flux) and (b) $\lambda = 1.01$. The unit of ω is $\mathcal{J}/h$ while k is measured in units of the inverse lattice spacing. The darkness of the shading is proportional to $S_{zz}(k, \omega)$.

As we can see from (8), an estimate of δk requires the value of the energy current, j_E. Thus we should, in principle, calculate j_E in a spin chain where the two ends are kept at different temperatures. We are unable to do this for any reasonable size system, and so we shall treat the energy flux as a parameter taken from experiments $(j_E \equiv j_E^{\text{exp}})$. Then a thermodynamic measurement of j_E^{exp} can be used to estimate the value of δk in an independent neutron-scattering experiment. Below we shall show how to estimate j_E^{exp} using parameters from a realistic experimental setup.

Let the sample be a cube of side $l = 10^{-2}$ m and let the spin chains be along x direction with the distance between the neighboring chains being $d = 10^{-9}$ m. Furthermore, let the sides of the cube perpendicular to the chains be at temperatures T and $T + \delta T$ (see Fig. 3). The temperature

should be chosen to be low in order to minimize the phonon contribution to j_E^{exp}. However, T cannot be too small since then the small coupling between the chains makes the system three-dimensional. The value of δT should be, in principle, chosen large but the limitations of cryogenics of a realistic setup restrict the steady-state temperature-differences to $\delta T \leqslant 0.1 T$. From the above considerations we arrive at the following ranges for the possible temperatures and temperature-differences

$$T = (1-10)^\circ \text{K}; \qquad \delta T = 0.1 T = (0.1-1)^\circ \text{K} \tag{9}$$

The total current of heat across the sample can now be estimated as

$$j_E^{\text{total}} = \kappa l^2 \frac{\delta T}{l} \tag{10}$$

provided we know the heat conductivity, κ. We note here that the finiteness of the experimental κ is not in contradiction with the singular nature ($\kappa^{\text{int}} = \infty$) of the heat conductivity of integrable spin chains. A macroscopic sample consist of spin chains of characteristic length $\ell \approx 10^{-4}$ cm and the energy must also be transported between chains. This leads to the loss of ideal conductivity and results in a finite κ. Consequently, the estimate of energy flux using the experimental κ does give an estimate of the energy flux through the chains provided the spin chains are the main channels of energy transport.
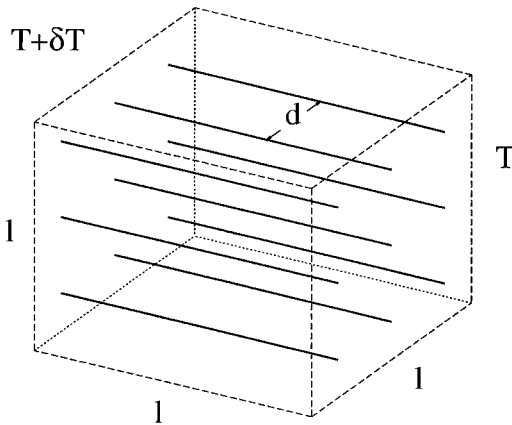

Fig. 3. Experimental setup for measuring the effect of energy flux. The solid lines represent the spin chains in a cubic sample of volume l^3 with d being the distance between the chains. The energy flux is generated by keeping the two ends of the chains at temperatures T and $T + \delta T$, respectively.

Unfortunately, κ, is not available for the materials we have in mind,[6–9] and another problematic issue is how much of the conductivity comes from the spin-chains. Since measurements of the magnetothermal conductivity of magnetic materials[18, 19] indicate that spin waves provide a significant fraction of the low-temperature thermal conductivity, we shall assume that an order of magnitude estimate of the energy current through the spin chains is given by j_E^{total}. Furthermore, we shall assume that, as a value of κ, we can take a characteristic value of this parameter in crystalline magnetic materials in the temperature range $T = (1-10)^{\circ}$K:[20]

$$\kappa \approx (1-10) \cdot \frac{W}{m \cdot {}^{\circ}\text{K}} \tag{11}$$

We can then estimate $j_E^{\text{total}} \approx (10^{-3} - 10^{-1})\, W$ and, since the number of spin-chains in the sample is $\mathcal{N} = l^2/d^2 = (10^{-2}/10^{-9})^2 = 10^{14}$, we obtain the energy flux per chain, j_E^{exp}, as

$$j_E^{\text{exp}} \approx \frac{j_E^{\text{total}}}{\mathcal{N}} = (10^{-17} - 10^{-15})\, W \tag{12}$$

As we have seen (7) the natural unit of energy current in a spin chain is $j_E^{(1)} = J^2/h$. Using a characteristic value of $J = (1-10)^{\circ}$K for the spin coupling we find $j_E^{(1)} \approx (10^{-12} - 10^{-10})\, W$ and obtain the following estimate for the shift of the wavenumber

$$\delta k \sim \sqrt{\frac{j_E^{\text{exp}}}{j_E^{(1)}}} \sim 10^{-4} - 10^{-2} \tag{13}$$

This is our central result. Since $\delta k \sim 10^{-2}$ is accessible in an inelastic neutron scattering experiment, the effect of shift in the wavenumber should be observable.

In summary, we have studied an integrable system which doesn't obey Fourier's law. We proposed that, under some simplifying assumptions, one can explore states of this system which carry current of energy and, furthermore, one can derive theoretical results verifiable in experiments.

ACKNOWLEDGMENTS

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