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LETTER TO THE EDITOR

Spin and energy correlations in the one dimensional spin-$\frac{1}{2}$ Heisenberg model

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Abstract. In this paper, we study the spin and energy dynamic correlations of the one-dimensional spin-$\frac{1}{2}$ Heisenberg model, using mostly exact diagonalization numerical techniques. In particular, observing that the uniform spin and energy currents decay to finite values at long times, we argue for the absence of spin and energy diffusion in the easy plane anisotropic Heisenberg model.

1. Introduction

Recently there has been a renewed interest in the finite temperature dynamics of the one-dimensional spin-$\frac{1}{2}$ Heisenberg model, especially on the question of diffusive spin transport [1–4]. In particular, it was argued that the integrability of the model implies pathological spin dynamics and presumably the absence of spin diffusion [5, 6]. The role of conservation laws was pointed out in [7], where it was shown that in several quantum integrable models the uniform ($q = 0$) current correlations do not decay to zero at long times. This result, established using the Mazur inequality [8], suggests pathological finite temperature dynamics.

As far as the Heisenberg model is concerned, the analysis of conservation laws has shown that the energy current operator commutes with the Hamiltonian, suggesting anomalous finite-(q, ω) energy density correlations. However, for zero magnetic field, this method turned out to be inadequate for describing the decay of the uniform spin current correlations. This case is closely related to the behaviour of the finite temperature conductivity in the one-dimensional model of spinless fermions at half-filling interacting with a nearest neighbour interaction (the 't–V' model [7]).

In this work, we address the issues raised above by the numerical diagonalization of the Hamiltonian matrix on finite size lattices. More precisely, we study the implications of the energy current conservation on the (q, ω) energy density correlations, and as an alternative route to the analysis of spin diffusion, we investigate the decay of the uniform ($q = 0$) spin current correlations.

The letter is organized as follows: in section 2, we recall the Heisenberg Hamiltonian and define the various quantities studied below. In section 3 we briefly summarize the phenomenological picture of diffusion. There, we also argue that the decay of the uniform spin current correlations to a finite value is incompatible with a diffusive behaviour, *assuming* continuity in the wave vector q of the correlations at $q = 0$. Next, we test these ideas in section 4 in the XY limit, where results can be obtained analytically. Turning to the numerical results, in section 5.1 we present the energy density correlations at infinite temperature for the case of the isotropic Heisenberg model. A simple ansatz for the observed behaviour suggests a logarithmic dependence at low frequencies for the energy autocorrelation function. As far as the spin dynamics are concerned, numerous studies of the (q, ω) spin density correlations exist [1–3]. Therefore, in section 5.2, we restrict ourselves to the decay of the uniform spin current correlations for various temperatures and values of the anisotropy parameter Δ. Interestingly, it turns out that these do not decay to zero for $\Delta < 1$. According to the argument given in section 3, this result implies non-diffusive spin transport. Section 6 contains a short discussion on experimental relevance of these findings and open questions.

2. The model

The anisotropic Heisenberg Hamiltonian for a chain of L sites with periodic boundary conditions is given by

$$H = \sum_{l=1}^{L} h_l = J \sum_{l=1}^{L} (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \Delta S_l^z S_{l+1}^z) \tag{1}$$

where $S_l^\alpha = \frac{1}{2}\sigma_l^\alpha$, σ_l^α are the Pauli spin operators with components $\alpha = x, y, z$ at site l.

For a conserved quantity $A = \sum_{l=1}^{L} a_l$, $[A, H] = 0$, the continuity equation in q-space defines the current j_q:

$$\frac{\partial a_q(t)}{\partial t} = 2\mathrm{i}\sin(q/2)\, j_q \tag{2}$$

with

$$a_q = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{\mathrm{i}ql} a_l \qquad j_q = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} \mathrm{e}^{\mathrm{i}ql} j_l \tag{3}$$

and $a_q(t) = \mathrm{e}^{\mathrm{i}Ht} a_q \mathrm{e}^{-\mathrm{i}Ht}$.

Setting $a_l = S_l^z, h_l$ we find the following spin and energy currents respectively

$$j_l^z = J(S_l^y S_{l+1}^x - S_l^x S_{l+1}^y) \tag{4}$$

$$j_l^H = J^2(S_{l-1}^x S_l^z S_{l+1}^y - S_{l-1}^y S_l^z S_{l+1}^x) + J^2\Delta(S_{l-1}^y S_l^x S_{l+1}^z - S_{l-1}^z S_l^x S_{l+1}^y) + J^2\Delta(S_{l-1}^z S_l^y S_{l+1}^x - S_{l-1}^x S_l^y S_{l+1}^z). \tag{5}$$

For the discussion of dynamic correlations at finite temperatures, we chose to analyse the anticommutator form

$$S_{AA}(q, t - t') = \tfrac{1}{2}\langle\{a_q(t), a_{-q}(t')\}\rangle \tag{6}$$

where $\langle\ \rangle$ is the thermal average at temperature $T = 1/\beta$ over a complete set of states. Further, the frequency dependent correlation function defined by

$$S_{AA}(q, \omega) = \int_{-\infty}^{+\infty} \mathrm{d}\omega \mathrm{e}^{\mathrm{i}\omega t} S_{AA}(q, t) \tag{7}$$

is symmetric in frequency, $S_{AA}(q, \omega) = S_{AA}(q, -\omega)$.

A central point in our approach is the relation between the dynamic correlations of a quantity A and its corresponding current correlations, which we obtain by using the continuity equation (2):

$$\omega^2 S_{AA}(q, \omega) = 4\sin^2(q/2) S_{j^A j^A}(q, \omega). \tag{8}$$

In particular, we will discuss the asymptotic value of the current correlations

$$C_{j^A j^A} = \lim_{t\to\infty} \frac{S_{j^A j^A}(q=0,t)}{S_{j^A j^A}(q=0,t=0)}. \tag{9}$$

A finite value of $C_{j^A j^A}$ translates to a $\delta(\omega)$ peak in $S_{j^A j^A}(q=0,\omega)$ and as we will discuss below, implies restrictions in the behaviour of $S_{AA}(q,\omega)$.

An important observation is that the energy current j^H of the Heisenberg model commutes with the Hamiltonian [7], so that $C_{j^H j^H} = 1$, whereas the spin current does not. However, it will turn out that $C_{j^z j^z} > 0$ for $\Delta < 1$, meaning that the spin current and energy current correlations are similar in the sense that in their frequency representation, they both exhibit a finite weight $\delta(\omega)$ function.

3. Diffusive behaviour

When we consider the (q,ω)-dependent correlations of a conserved quantity A such as the magnetization, it is usually assumed, largely on phenomenological grounds, that they exhibit a diffusive behaviour in the long-time $|t-t'| \to \infty$, short wavelength $q \to 0$ regime [9]:

$$S_{AA}(q,t-t') \sim \mathrm{e}^{-D_A q^2 |t-t'|} \tag{10}$$

where D_A is the corresponding diffusion constant, or

$$S_{AA}(q,\omega) \sim \frac{2D_A q^2}{(D_A q^2)^2 + \omega^2} \tag{11}$$

for $\omega \to 0$.

This Lorentzian form correctly reduces to a $\delta(\omega)$ function in the limit $q \to 0$, as implied by $[A,H]=0$. Further, using the continuity equation (8) for $q \to 0$, we obtain

$$S_{j^A j^A}(q,\omega) \sim \frac{2D_A \omega^2}{(D_A q^2)^2 + \omega^2} \tag{12}$$

which gives the diffusion constant D_A when first, the limit $q \to 0$ and then, $\omega \to 0$ are taken. On the other hand, if the current correlations for $q=0$ do not decay to zero at long times, $C_{j^A j^A} > 0$ and $S_{j^A j^A}(q,\omega)$ has a finite weight $\delta(\omega)$ component which is incompatible with the diffusive form (12). In this reasoning, we must assume a regular behaviour of the correlation functions in the q variable.

To summarize the argument, if a quantity A is conserved ($[A,H]=0$) and its current j^A is either conserved ($[j^A,H]=0$), or $C_{j^A j^A} > 0$, then continuity in q at $q=0$ excludes a diffusive form (10) for the corresponding correlation $S_{AA}(q,t-t')$.

4. XY limit

A simple model for testing these ideas is the XY limit ($\Delta = 0$), of the Heisenberg model. In this case, both the energy current j^H and the spin current j^z commute with the Hamiltonian. The model can be mapped to a free spinless fermion model by using a Jordan–Wigner transformation which allows us also to evaluate explicitly the spin and energy dynamic correlations at $\beta = 0$. In the spin case, these are well known results [10]:

$$S_{S^z S^z}(q,\omega) = \frac{1}{2\,(4\,J^2\,\sin^2(q/2) - \omega^2)^{1/2}}\,\theta(|2\,J\,\sin(q/2)| - |\omega|) \tag{13}$$

$$S_{HH}(q,\omega) = \frac{(4\,J^2\,\sin^2(q/2) - \omega^2)^{1/2}}{8\,\sin^2(q/2)}\,\theta(|2\,J\,\sin(q/2)| - |\omega|). \tag{14}$$

These forms are indeed consistent with the conservation of both spin (energy) and spin current (energy current) as they reduce to a $\delta(\omega)$ function when the limits $q \to 0$, $\omega \to 0$ are taken. Further, the time decay of the autocorrelations at $\beta = 0$ is not of the form $1/\sqrt{t}$, as predicted by the diffusion hypothesis. Indeed,

$$\langle S_l^z(t) S_l^z \rangle = \frac{1}{4} J_0^2(Jt) \tag{15}$$

$$\langle h_l(t) h_l \rangle = \frac{J^2}{8} \left(J_0^2(Jt) + J_1^2(Jt) \right) \tag{16}$$

which both behave as $1/t$ for $t \to \infty$.

5. Anisotropic Heisenberg model

5.1. Energy correlations

As we mentioned earlier, the energy current j^H associated with the anisotropic Heisenberg model (1) commutes with the Hamiltonian for all values of the parameter Δ. Therefore, the time correlations do not decay at all ($C_{j^H j^H} = 1$) and according to the argument explained in section 3, no diffusive energy transport occurs. However, the conservation of j^H does not provide us with any details about the shape of $S_{HH}(q, \omega)$ at finite q. In the absence of an analytical solution, we investigate this quantity by numerical diagonalization of the Hamiltonian matrix on a ring of 16 sites.

In figure 1, we show $S_{HH}(q, \omega)$ for $\Delta = 1$, which is experimenally the most interesting point as it describes isotropic quasi one-dimensional antiferromagnets. We study the high

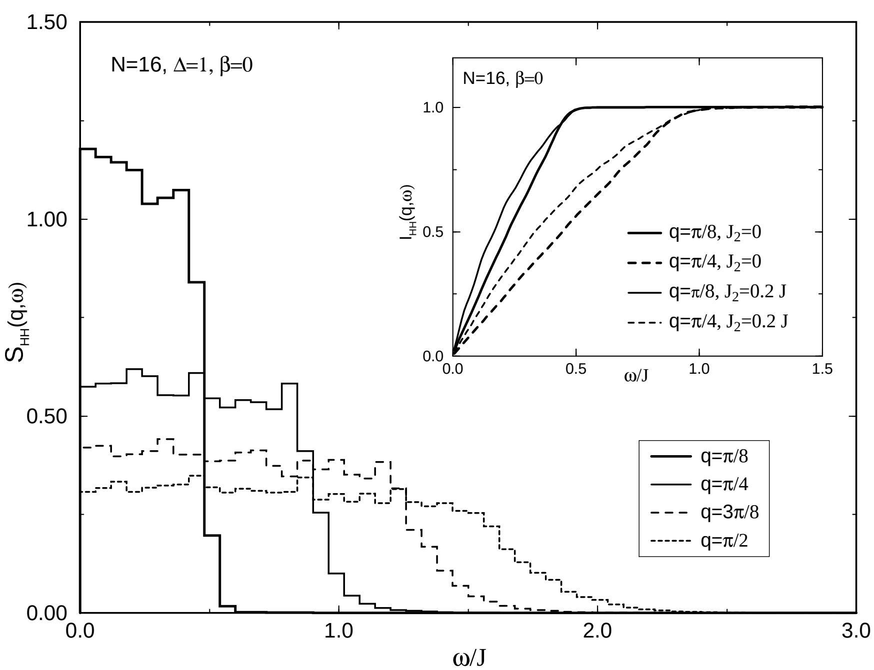

Figure 1. Energy density correlation function $S_{HH}(q, \omega)$ at $\beta = 0$ for $\Delta = 1$, $q = (2\pi/16)n$, $n = 1, \ldots, 4$. The inset shows the normalized, integrated quantity $I_{HH}(q, \omega)$ for $\Delta = 1$, $J_2 = 0$ and $J_2 = 0.2J$.

temperature limit $\beta = 0$, which is the most convenient for a numerical study as it involves the full excitation spectrum, but is also relevant experimentally for spin systems as the magnitude of J can be of the order of T. The plot is represented as histograms of width $0.06\omega/J$. The inset shows the normalized, integrated (prior to summing nearby frequencies) quantity

$$I_{HH}(q,\omega) = \frac{\int_{0+}^{\omega} \mathrm{d}\omega' S_{HH}(q,\omega')}{\int_{0+}^{\infty} \mathrm{d}\omega' S_{HH}(q,\omega')} \tag{17}$$

which has the advantage of smoothing out the finite size discontinuities. To point out the practically linear integrated behaviour of the pure Heisenberg model, we also show the same quantity for a more generic case obtained by adding a next-next neighbour (non-integrable) interaction J_2.

The simplest way to describe this behaviour is by means of 'plateaus' given by the ansatz:

$$S_{HH}(q,\omega) = \frac{\sqrt{3}\pi J}{16\sqrt{1-\cos(q)}}\,\theta(|\omega| - J\sqrt{3(1-\cos(q))}) \tag{18}$$

which satisfy the first $\int \mathrm{d}\omega\, S_{HH}(q,\omega) = 3\pi J^2/8$ and the second $\int \mathrm{d}\omega\, \omega^2 S_{HH}(q,\omega) = 3\pi J^4(1-\cos(q))/8$ exact moments for $\beta = 0$. Further, this ansatz is compatible with the limit $S_{HH}(q \to 0,\omega) \to \delta(\omega)$ as implied by the conservation of energy. Using the continuity equation (8), we obtain for small q and ω

$$S_{j^H j^H}(q,\omega) = \frac{\sqrt{6}\pi J}{16}\,\frac{\omega^2}{q^3}\,\theta(|\omega| - \sqrt{\frac{3}{2}}J|q|) \tag{19}$$

which correctly reduces to a $\delta(\omega)$-function for $q \to 0$, in agreement with the conservation of the energy current $[j^H, H] = 0$.

Using this ansatz we find for the energy autocorrelation function (obtained by integration over q)

$$\int_{-\infty}^{+\infty} \langle h_l(t) h_l\rangle\, \mathrm{e}^{\mathrm{i}\omega t}\, dt = C_0 - C_1 \ln(\omega/J) + O(\omega^2) \qquad C_0, C_1 > 0 \tag{20}$$

a logarithmic behaviour at low frequencies, in contrast to the diffusion form $1/\sqrt{\omega}$.

We should stress that these results are only *indicative*, as they are obtained from small size lattices which can provide reliable information only for correspondingly high frequencies and large wave vectors. Nevertheless, the consistency of these results with the arguments presented above against a diffusion form are encouraging.

5.2. *Spin correlations*

The spin density dynamic correlations $S_{S^z S^z}(q,\omega)$ have been the subject of many studies which have not been able to answer the question of spin diffusion unambiguously. Here, we revisit this problem by investigating the compatibility between spin density and spin current correlations, which requires that we calculate $C_{j^z j^z}$. In contrast to the energy current, the spin current j^z does not commute with the Hamiltonian, so that $S_{j^z j^z}(q = 0,\omega)$ is different from a pure $\delta(\omega)$ function. Nevertheless, if $C_{j^z j^z} > 0$, which means that $S_{j^z j^z}(q = 0,\omega)$ has a finite weight δ-function at $\omega = 0$, our previous arguments against diffusion still hold.

In determining $C_{j^z j^z}$, we noticed a peculiar difference in the low frequency behaviour of $S_{j^z j^z}(q = 0,\omega)$ depending on the anisotropy parameter Δ. In figure 2, we show

$$I_{j^z j^z}(\omega) = C_{j^z j^z} + 2\int_{0+}^{\omega} \mathrm{d}\omega' S_{j^z j^z}(q = 0,\omega') \tag{21}$$

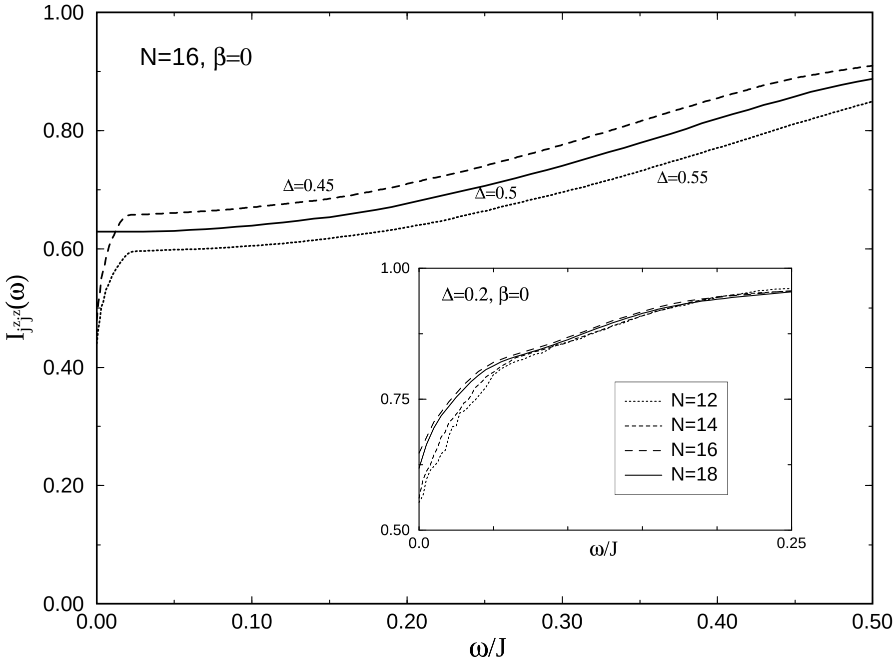

Figure 2. Integrated $q = 0$ energy current correlations $I_{j^z j^z}(\omega)$ for $N = 16$, $\beta = 0$ and $\Delta = 0.45$, 0.5 and 0.55. The inset displays $I_{j^z j^z}(\omega)$ for $L = 12$, 14, 16, 18 at inverse temperature $\beta = 0$ and $\Delta = 0.2$.

the corresponding integrated, normalized quantity. We see that for $\Delta = \cos(\pi/n)$, $n = 3, 4, \ldots$ ($n = 3$ in the figure) all the low frequency weight of $S_{j^z j^z}(q = 0, \omega)$ is concentrated in the δ-function at $\omega = 0$. In contrast, for neighbouring values such as $\Delta = 0.45$ or 0.55, we observe a shift of weight to a low frequency region whose size decreases as the system grows (inset) and eventually vanishes as $L \to \infty$. We believe that the behaviour of these special Δ points is related to the existence of finite length strings (bound states) as they appear in the formulation of the thermodynamics of the Heisenberg model, within the Bethe ansatz method [11]. It seems that in order to determine $C_{j^z j^z}$ from finite size systems for $\Delta \neq \cos(\pi/n)$, we should include the weight from these low frequency regions. As an example, doing so for $\Delta = 0.45$ gives us a value of $C_{j^z j^z} = 0.66$ for $L = 16$ (figure 2). Having discussed this technical issue, we can then determine $C_{j^z j^z}$ for different size systems, as a function of temperature and Δ. By extrapolating our finite size results to the thermodynamic limit using second order polynomials in $1/L$ for $L = 8, \ldots, 18$, we obtain the results shown in figure 3. Their striking feature is that for $T > J$, $C_{j^z j^z}$ is finite in the $\Delta < 1$ region, and practically zero when $\Delta \geqslant 1$. In this regime, according to our previous argument, we expect a non-diffusive behaviour.

Describing the behaviour of $C_{j^z j^z}$ for $\Delta \geqslant 1$ at finite temperatures is rather subtle. The reason is that in the Heisenberg model, $\Delta = 1$ corresponds to a point of change of symmetry, from easy plane to easy axis, accompanied by the opening of a gap. In the fermionic version of the model, the 't–V' model, it corresponds to a metal–insulator Mott–Hubbard type transition, with the charge stiffness changing discontinuously [12] at zero temperature. We should note that this discontinuity is difficult to reproduce by numerical simulations on small finite size lattices, as the transition corresponds to the divergence of

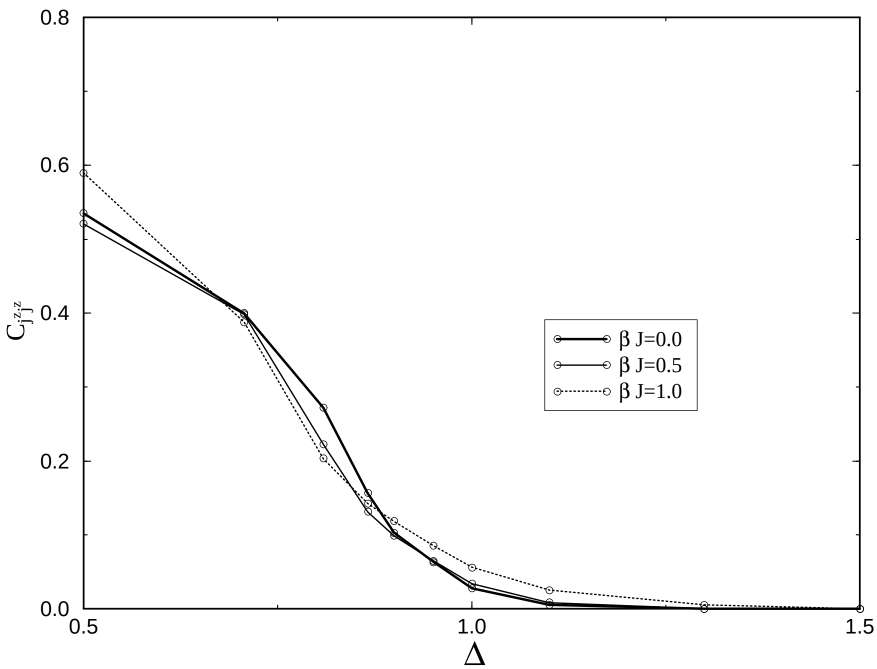

Figure 3. Values of $C_{j^z j^z}$ as function of Δ and β obtained by extrapolating second order polynomials in $1/L$ from results on systems of sizes $L = 8, \ldots, 18$. Calculations were done for $\Delta = \cos(\pi/n)$, $n = 3, 4, 5, 6, 7, 10$ and $\Delta = 1.0, 1.1, 1.5$.

the localization length. Considering that at high temperature, $C_{j^z j^z}$ behaves similarly to the charge stiffness in the 't–V' model [7] we understand why it is difficult to decide whether $C_{j^z j^z}$ is greater than zero in the region $\Delta \gtrsim 1$ and $T < \infty$. For the same reason, we cannot exclude that $C_{j^z j^z}$ behaves discontinuously at $\Delta = 1$. Nevertheless, it seems unambiguous that $C_{j^z j^z} \simeq 0$ for $\Delta > 1.5$ and $T > J$.

6. Discussion

The results presented are of interest in recent experimental studies [13] of spin dynamics in quasi-one-dimensional materials such as $CuGeO_3$ and Sr_2CuO_3. Particular attention should be paid to the unusually high value of the diffusion constant found in NMR experiments on Sr_2CuO_3 [13], perhaps related to the integrability of the Heisenberg model as discussed above. Furthermore, our results on the behaviour of energy density correlations are of interest in the interpretation of the quasi-elastic Raman scattering, related to magnetic energy fluctuations [14, 15]. We should emphasize that no diffusion form should be expected for the energy density correlations in the isotropic Heisenberg model with only nearest neighbour interaction. An eventual diffusive behaviour should be attributed to next-nearest neighbour coupling, interaction with phonons or deviations from one dimensionality. Finally, the main unresolved issue in this work is a better understanding of the finite temperature spin dynamics at the isotropic point.

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