Spin and energy correlations in the one dimensional spin 1/2 Heisenberg model

F Naef and X Zotos
Institut Romand de Recherche Numérique en Physique des Matériaux (IRRMA), EPFL-PPH, CH-1015 Lausanne, Switzerland

Abstract. In this paper, we study the spin and energy dynamic correlations of the one dimensional spin 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.

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1. Introduction

Recently there has been a renewed interest in the finite temperature dynamics of the
dimensional spin 1/2 Heisenberg model, especially on the question of diffusive spin
transport[1, 2, 3, 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 reference[7] were 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-($q, \omega$) energy density correlations. However, for zero magnetic field,
this method turned out to be insufficient for deciding about the decay of the uniform spin
current correlations. This case is closely related to the behavior of the finite temperature
conductivity in the one dimensional model of spinless fermions at half-filling interacting
with a nearest neighbor 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 ($q, \omega$) 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 paper 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 behavior,
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 behavior suggests a logarithmic dependence at low frequencies for the
energy autocorrelation function. As far as the spin dynamics is concerned, numerous
studies of the ($q, \omega$) spin density correlations exist[1, 2, 3]. Therefore, in section 5.2,
we restrict ourselves to the decay of the uniform spin current correlations for various
values of the anisotropy parameter $\Delta$ and temperatures. 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:

\[
H = \sum_{l=1}^{L} h_l = J \sum_{l=1}^{L} (S_{l}^{x} S_{l+1}^{x} + S_{l}^{y} S_{l+1}^{y} + \Delta S_{l}^{z} S_{l+1}^{z}),
\]

(1)

where \( S_{l}^{\alpha} = \frac{1}{2} \sigma_{l}^{\alpha}, \) \( \sigma_{l}^{\alpha} \) 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 \( j_{q} \):

\[
\frac{\partial a_{q}(t)}{\partial t} = 2i \sin(q/2) j_{q}
\]

(2)

with

\[
a_{q} = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{iql} a_{l}, \quad j_{q} = \frac{1}{\sqrt{L}} \sum_{l=1}^{L} e^{iql} j_{l}
\]

(3)

and \( a_{q}(t) = e^{iHt} a_{q} e^{-iHt} \).

Setting \( a_{l} = S_{l}^{z}, h_{l} \) we find the following spin and energy currents respectively:

\[
j_{l}^{z} = J (S_{l}^{y} S_{l+1}^{x} - S_{l}^{x} S_{l+1}^{y})
\]

(4)

\[
j_{l}^{H} = J^{2} (S_{l-1}^{x} S_{l}^{z} S_{l+1}^{y} - S_{l-1}^{y} S_{l}^{z} S_{l+1}^{x})
+ J^{2} \Delta (S_{l-1}^{y} S_{l}^{x} S_{l+1}^{z} - S_{l-1}^{x} S_{l}^{z} S_{l+1}^{y})
+ J^{2} \Delta (S_{l-1}^{z} S_{l}^{y} S_{l+1}^{x} - S_{l-1}^{x} S_{l}^{y} S_{l+1}^{z})
\]

(5)

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

\[
S_{AA}(q, t - t') = \frac{1}{2} \langle \{a_{q}(t), a_{-q}(t')\} \rangle
\]

(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:

\[
S_{AA}(q, \omega) = \int_{-\infty}^{+\infty} d\omega e^{i\omega t} S_{AA}(q, t)
\]

(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):

\[
\omega^{2} S_{AA}(q, \omega) = 4 \sin^{2}(q/2) S_{j_{A},j_{A}}(q, \omega)
\]

(8)
In particular, we will discuss the asymptotic value of the current correlations

$$C_{j^A j^A} = \lim_{t \to \infty} \frac{S_{j^A j^A}(q = 0, t)}{S_{j^A j^A}(q = 0, t = 0)}.$$  \hfill (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 behavior of $S_{A A}(q, \omega)$.

An important observation is that the energy current $j^H$ of the Heisenberg model commutes with the Hamiltonian, 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 behavior

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

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

where $D_A$ is the corresponding diffusion constant, or

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

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:

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

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 behavior 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:\[^{10}\]  

\[
S_{S^z S^z}(q, \omega) = \frac{1}{2} \left( \frac{4 J^2 \sin^2(\frac{q}{2}) - \omega^2}{\omega} \right)^{1/2} \theta(|2J \sin(\frac{q}{2})| - |\omega|) 
\]

\[
S_{H H}(q, \omega) = \frac{(4 J^2 \sin^2(\frac{q}{2}) - \omega^2)^{1/2}}{8 \sin^2(\frac{q}{2})} \theta(|2J \sin(\frac{q}{2})| - |\omega|) 
\]

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,

\[
\langle S^z_i(t)S^z_i \rangle = \frac{1}{4} J^2_0(Jt) 
\]

\[
\langle h_i(t)h_i \rangle = \frac{J^2}{8} \left( J^2_0(Jt) + J^2_1(Jt) \right) 
\]

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 commutes with the Hamiltonian for all values of the parameter $\Delta$. Therefore, the time correlations do not decay at all ($C_{jjj} = 1$) 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 $S_{H H}(q, \omega)$ 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 $S_{H H}(q, \omega)$ for $\Delta = 1$, which is experimenenally the most interesting point as it describes isotropic quasi one-dimensional antiferromagnets. We study the high 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 $0.06\omega/J$, all the frequencies which fall into one interval are summed up. The inset shows the normalized, integrated (prior to summing nearby frequencies) quantity

$$I_{HH}(q, \omega) = \frac{\int_0^\omega d\omega' S_{HH}(q, \omega')}{\int_0^\infty d\omega' S_{HH}(q, \omega')}$$

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

The simplest way to describe this behavior is by means of “plateaus” given by the following ansatz:

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

which satisfy the first $\int d\omega S_{HH}(q, \omega) = 3\pi J^2/8$ and the second $\int d\omega' \omega^2 S_{HH}(q, \omega) = 3\pi J^4(1 - \cos(q))/8$ 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 $\omega$

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

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 $q$):

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

a logarithmic behavior 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 $S_{S_zS_z}(q, \omega)$ 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 $\delta-$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 behavior of $S_{j^z,j^z}(q = 0, \omega)$ depending on the anisotropy parameter $\Delta$. In figure 2, we show

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

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 $\delta$-function at $\omega = 0$. In contrast, for neighboring 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 behavior of this special $\Delta$ 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 $\Delta$.

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 $\Delta \geq 1$. In this regime, according to our previous argument, we expect a non-diffusive behavior.

Deciding about the behavior of $C_{j^z,j^z}$ for $\Delta \geq 1$ 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 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 of spin dynamics in quasi-one dimensional materials such as CuGeO$_3$ and Sr$_2$CuO$_3$. Particular attention should be paid to the unusually high value of the diffusion constant found in NMR experiments on Sr$_2$CuO$_3$, perhaps related to the integrability of the Heisenberg model as discussed above. Furthermore, our results on the behavior of energy density correlations are of interest in the interpretation of the quasi-elastic Raman scattering, related to magnetic energy fluctuations. We should emphasize that no diffusion form should be expected for the energy density correlations in the isotropic Heisenberg model with only nearest neighbor interaction. An eventual diffusive behavior should be attributed to next-nearest neighbor 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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Figure captions

**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 $J_2' = 0.2J$.

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

**Figure 3.** Values of $C_{j^zj^z}$ as function of $\Delta$ and $\beta$ 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 $\Delta = 1.0, 1.1, 1.5$. 
$S_{HH}(q, \omega)$

$q = \pi/8, J_2 = 0$
$q = \pi/4, J_2 = 0$
$q = \pi/8, J_2 = 0.2 J$
$q = \pi/4, J_2 = 0.2 J$

$N=16, \Delta=1, \beta=0$
