Low temperature transport in the XXZ model

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We present evidence suggesting that spin transport in the gapless phase of the $S=1/2$ XXZ model is ballistic rather than diffusive. We map the model onto a spinless fermion model whose charge stiffness determines the spin transport of the original model. By means of exact numerical diagonalisation and finite size scaling we study both the stiffness and the level statistics. We show that the stiffness is non-zero at low temperatures so that the transport is ballistic. Our results suggest that the non-zero stiffness is due to the fact that even in the presence of Umklapp scattering a non-zero fraction of states remain degenerate in the thermodynamic limit.

The problem of transport in a non-disordered interacting many particle system is one of the oldest unsolved problems in solid state physics. A particular case which has attracted recent attention is spin diffusion in one dimensional spin systems. Recent experiments indicated that $S=1$ chains with the gap in the excitation spectrum display diffusive behavior \cite{1}, in reasonable agreement with theoretical work \cite{2} relating diffusion to classical scattering of excitations near the gap edge. On the other hand, measurements on gapless $S=1/2$ chains \cite{3} show a different behavior. The authors fit their data with a diffusion constant which is much larger than either the value found experimentally for the $S=1$ chains or the value $D_s \sim J / (2 \pi S(S + 1) / 3)$ expected from classical considerations \cite{4}. We believe that the measured value for $D_s$ in the $S=1/2$ system is so large that it implies that the diffusion is not an intrinsic property of an $S=1/2$ spin system but is due to a weak coupling to other degrees of freedom (for example to phonons \cite{5}).

A theoretical analysis based on a continuum limit Luttinger liquid representation \cite{6} suggested that the diffusion constant was associated with Umklapp operators and was finite but exponentially large in the Umklapp gap. Damle and Sachdev \cite{2} provided a detailed analysis indicating diffusive behavior for the $S=1$ chain, however, their work suggests that in general low energy excitations of gapped systems display diffusive behavior even if the effective low energy theory describing these excitations is integrable. On the contrary, Zotos and collaborators have argued that integrable models exhibit ballistic transport while non-integrable models are diffusive \cite{7}. Recently Fabricius and McCoy \cite{8} have shown that numerical computations of the long time behavior of the correlation functions of the $S=1/2$ XXZ chain in the $T = \infty$ limit are consistent with ballistic transport if the model has a XY anisotropy but suggest that at the isotropic Heisenberg point the transport is not ballistic. Very recently, Monte Carlo \cite{9} and Bethe-ansatz \cite{10} analyses of the stiffness of related models have appeared, reporting similar conclusions.

In this paper we approach the question in a different way. We use exact numerical diagonalisation and finite size scaling to study the spin stiffness of the XXZ model and the behavior of the energy levels which leads to a non-zero stiffness.

The XXZ model is defined by the Hamiltonian

\begin{equation}
\hat{H}_{XXZ} = J \sum_n (S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + \Delta S^z_i S^z_{i+1}).
\end{equation}

At $T = 0$ the gapless phase $-1 < \Delta \leq 1$ of this model is characterized by a non-zero spin stiffness $D_s$ \cite{11} (in the gapped phase $|\Delta| > 1$ the stiffness is zero). The question of interest here is whether at $T > 0$ the stiffness $D_s$ remains non-zero, implying ballistic transport, or $D_s$ vanishes, implying non-ballistic (and perhaps diffusive) transport.

The XXZ model is equivalent via the Jordan-Wigner transformation to the spinless fermion model,

\begin{equation}
\hat{H} = J \sum_n \left[ -\frac{1}{2} (c^+_n c_{n+1} + h.c.) + \Delta \left( (c^+_n c_n - \frac{1}{2}) (c^+_{n+1} c_{n+1} - \frac{1}{2}) \right) \right].
\end{equation}

In this mapping the fermion density-density correlation function represents the $S^z - S^z$ correlator and therefore the description of fermion transport directly translates into the spin language. In particular the real part of the frequency dependent conductivity may be written as

\begin{equation}
\text{Re} \sigma(\omega) = 2 \pi D_c \delta(\omega) + \sigma_{reg}(\omega),
\end{equation}

defining the charge stiffness $D_c$. If $D_c \neq 0$ the model has infinite conductivity whereas if $D_c = 0$ one has either a normal conductor ($D_c = 0, \sigma_{reg}(\omega \rightarrow 0) > 0$) with diffusive transport or an ideal insulator ($D_c = 0, \sigma_{reg}(\omega \rightarrow 0) = 0$). In the spin language $D_c$ becomes the spin stiffness, which, if non-zero, corresponds to ballistic spin transport, whereas if it is equal to zero then the long time relaxation at finite temperatures is expected to be diffusive.
As was first noted by Kohn \[12\], in systems with periodic boundary conditions the stiffness at $T = 0$ can be related to the response of the ground state energy $E_0$ to a magnetic flux $\phi$, which modifies the hopping term in the Hamiltonian Eq. (3) by the usual Peierls phase factor $t \to t \exp(\pm i\phi/L)$, so that $D_c = (L/2)\partial^2 E_0/\partial \phi^2 (\phi \to 0)$, where $L$ is the system size. This phase factor can be absorbed into twisted boundary conditions for the wave functions.

Kohn’s method has been recently generalized to finite temperatures \[9\],

$$D_c = \frac{L}{2Z} \sum_n \frac{1}{2} \frac{\partial^2 E_n}{\partial \phi^2} e^{-\beta E_n}$$

(4)

where $Z$ is the partition function of the system and $n$ labels exact eigenstates.

We further rewrite Eq. (4) as $D_c = D_1 + D_2$, with

$$D_1 = -\frac{L}{2Z} \sum_n \left( \frac{\partial E_n}{\partial \phi} \right)^2 e^{-\beta E_n}$$

(5)

and

$$D_2 = \frac{\beta L}{2} \sum_n \left( \frac{\partial E_n}{\partial \phi} \right)^2 e^{-\beta E_n}.$$  

(6)

The advantage of this representation is that it separates $D_c$ into a thermodynamic part (depending only on derivatives of $Z$) and a positive part, depending on current-carrying ($\langle j_n \sim \partial E_n/\partial \phi \rangle$) states. The thermodynamic part may be seen to give no contribution to the charge stiffness at $T > 0$ \[13\]: for example at low temperatures $T \ll J$

$$D_1(T \gg 2\pi/vRL) = LT \exp(-\frac{2\pi LT}{vR}).$$  

(7)

with $R^2 = (1 - (1/\pi) \cos^{-1} \Delta)/2\pi$. Thus at $T > 0$ any non-zero $D_c$ must be due to $D_2$ which essentially counts the number of thermally accessible current carrying states.

Time reversal invariance implies that for a non-degenerate state $\partial E_n/\partial \phi (\phi \to 0) = 0$. Current carrying states occur in degenerate pairs which which are split by the application of magnetic flux. A sufficient condition for a non-vanishing $D_c$ is to have a non-zero fraction of current carrying states with $\partial E_n/\partial \phi \sim 1/L^{1/2}$. In what follows, we investigate $D_c$ and the statistics of the current carrying states numerically.

To compute the eigenvalues we notice that for any finite size chain the Heisenberg Hamiltonian Eq. (1) is just a hermitian matrix. Our strategy is to construct this matrix for $\phi = 1 \times 10^{-4}, 2 \times 10^{-4}, 3 \times 10^{-4}, 4 \times 10^{-4}$ and use the exact diagonalisation to obtain the eigenvalues and compute the derivatives. We use the standard QL routine from the Numerical Recipes package \[14\] which calculates the eigenvalues through a series of orthogonal transformations with accuracy given by machine precision. Our choices of $\phi$ lead to $\sim 10^{-6}$ accuracy for the derivative values. The size of matrices that could be diagonalised by the routine is limited by computer memory; for a $N \times N$ matrix it requires $\approx 8N^2$ bytes of storage space. With the available computer memory of about 360 MB we can diagonalise matrices up to $N = 7000$ which limited us to chain sizes $L \leq 14$.

The result of the calculation is presented in Fig. 1. For all system sizes we found $D_2$ to be non-zero. At small temperatures the value of $D_2$ appears to grow with system size (especially the peak value). At large temperatures all eigenvalues become involved in the sum Eq. (6) and the temperature dependence is defined by the prefactor $1/T$, while the value of $D_2$ decreases with the system size.

To investigate the finite size scaling in Fig. 2 we plot $(D_2T)_\infty = \lim_{T \to \infty} D_2T$ versus the inverse system size for different values of the interaction. The symbols represent the actual data points and the best fit lines are continued to the infinite size ($1/L = 0$). We are unaware of theoretical results for the large $L$ behavior of $(D_2T)_\infty$: our numerical results are consistent with the ansatz $(D_2T)_\infty \propto A + B/L + ...$ with $A, B$ depending on the interaction, but with $A$ always positive for $\Delta \leq 1$. For small $\Delta$ the best fit line is flat and the fit using four largest sizes is excellent (error estimate for parameter $A$ is 0.7%). For $\Delta = 0.6$ we find $A \approx 0.076, B \approx 0.32$ with 3.6% error. At the isotropic point $\Delta = 1$ the best straight line fit yields $A \approx 0.029, B \approx 0.46$ but with rather larger 11% error leading us to question whether we have assumed the correct functional form. We note, however, that fits to the form $(D_2T)_\infty(L) = C/L^p$ lead to even larger errors, so the hypothesis $(D_2T)(L \to \infty) \to 0$ is inconsistent with our data.
The scaling of $D_2$ can be expressed in terms of the size dependence of the current carried by a typical excited state. For the free case a typical state contains a total number $P \sim L$ of fermions excited above both left and right Fermi points and has a $\sqrt{P}$ imbalance between the left and right movers, producing a non-zero current $\partial E_n/\partial \phi \sim 1/\sqrt{L}$.

Fig. 2. $(D_2 T)$ plotted against inverse system size at $T = 50$.

The interaction affects current carrying states in two ways. As we noted above these states come in degenerate pairs. If the momentum of two degenerate states differs exactly by a reciprocal lattice vector, the these states will be mixed by the Umklapp interaction term which will destroy the degeneracy. Consequently these states will no longer carry current. On the other hand if two degenerate states differ by a momentum which is incommensurate with a reciprocal lattice vector, they cannot be mixed by the Umklapp interaction. The interaction can mix a given current-carrying state with another current-carrying states changing the value of the total current carried. To analyse these effects we plot in Fig. 3 the fraction of states with $\partial E_n/\partial \phi(\phi \to 0) = 0$ as a function of system size for the XXZ model with varying interaction strength $\Delta$ (solid symbols). One sees that adding an interaction sharply increases the fraction of non-current-carrying states, but this fraction remains small and decreases with system size.

Fig 3. Fraction of states with zero current

Fig. 4. Histogram of current values; lines for different $\Delta$ are indistinguishable

We now consider the statistical distribution of the currents carried by the eigenstates. We show in Fig. 4 a histogram of $(\partial E_n/\partial \phi)^2$ values for $L = 14$ and all previously considered values of $\Delta$. For each $\Delta$ the $x$-axis has been scaled so $x = 10$ corresponds to $(\partial E_n/\partial \phi)^2$ equal to the average value. The data have been grouped in to bins of width 0.1 of the average $(\partial E_n/\partial \phi)^2$ and the $y$-axis has been scaled so that $y = 1$ represents the number of states in bin 1. With this choice of scaling the distributions for different $\Delta$ are indistinguishable: the interaction does not change the shape of the distribution, but merely reduces the average value of $(\partial E_n/\partial \phi)^2$.

We now consider the effect of an interaction that spoils the integrability of the XXZ model by adding the next-nearest neighbor interaction $V \sum_i S_i^z S_{i+2}^z$ to the Hamiltonian Eq. (1). As shown in Fig. 3 this term lifts more degeneracies, so that more states carry zero current. However the relative change in the fraction of these states is small and the size dependence is similar to the integrable case.

The effect of the non-integrable interaction is mostly to reduce the values of the current carried by the remaining degenerate states as is illustrated on Fig. 5. At least
for large $V$, $(D_2 T)(L \to \infty) \to 0$, implying that the current carried by a typical state, although not 0, is much less than $1/\sqrt{L}$ and is presumably $o(1/L)$. Interesting, the effect seems not to occur for $V < \Delta$. For $\Delta = 0$ Fig. 5 shows clearly that even $V = 0.02$ leads to $D_2 T$ which vanishes as $L \to \infty$, whereas for $\Delta = 0.2$ large $V = 0.62$ leads to a vanishing $(D_2 T)(L \to \infty)$, while the effect of $V = 0.02$ is much smaller than for $\Delta = 0$ and our data are consistent with a non-zero $(D_2 T)(L \to \infty)$. Our system sizes are too small to allow us to make a definite statement about $(D_2 T)(L \to \infty)$ for $V < \Delta$, but clearly the relative size of the effect of the non-integrable interaction depends strongly on the ratio $V/\Delta$.

Fig 5. $D_2 T(1/L)$ comparing integrable and non-integrable cases; the lines are guides to the eye.

In conclusion we have studied the spin transport in the Heisenberg model by calculating the finite temperature stiffness for small system sizes. The data presented in Fig. 2 show that for the available sizes $D_2$ is greater than zero and extrapolates to a non-zero value in the thermodynamic limit. At small $\Delta$ this extrapolation seems unambiguous in agreement with the perturbation theory results [4], which are valid for small $\Delta$ where the Umklapp is irrelevant in the renormalisation group sense. For larger $\Delta$ the data seems to slowly decrease with size extrapolating to some small but non-zero value as $1/L \to 0$. For the isotropic Heisenberg point ($\Delta = 1$) the considered sizes are too small to make conclusive predictions about the thermodynamic limit behavior perhaps because the Umklapp becomes marginal at this point.

The non-zero stiffness at $T > 0$ means that the model possess a macroscopic fraction of current carrying states. These states come in degenerate pairs, so the stiffness essentially is a measure of non-trivial degeneracy of the energy eigenvalues. We argue that this degeneracy is the underlying physical reason for the ballistic transport in the XXZ model. However, the degeneracy of the XXZ model is due to its integrability and it was earlier argued [4] that the anomalous transport is due to the large number of conservation laws which characterise an integrable model. We believe that among all those conservation laws there should be only one that is responsible for the degeneracies and therefore for the anomalous transport. Based on our results for the non-integrable model with the next-nearest neighbor interaction we infer that this conservation law is probably not specific to integrable models. The next-nearest neighbor interaction destroys the integrability but still leaves a macroscopic fraction of degenerate (current-carrying) states. In the integrable models (except possibly for $\Delta = 1$) and possibly in the non-integrable models (for $V < \Delta$) the typical current carried by these states is $\sim 1/\sqrt{L}$ leading to non-zero stiffness as $L \to \infty$. For $V > \Delta$ we see the typical current is much smaller, leading to vanishing stiffness and speculate that there is a length scale $\xi(V, \Delta)$ such that for system sizes $L < \xi$ the current carried by a typical state scales as $1/\sqrt{L}$ but that for $L > \xi$ the current scales as $\xi^{-1/2}/L$.

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