PHYSICAL REVIEW B VOLUME 58, NUMBER 6 1 AUGUST 1998-II

Transport in the XXZ model

B. N. Narozhny
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey, 08855

A. J. Millis
Department of Physics and Astronomy, The Johns Hopkins University, 3400 North Charles Street, Baltimore, Maryland 21218

N. Andrei
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08855

(Received 4 May 1998)

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 diagonalization and finite size scaling we study both the stiffness and the level statistics. We show that the stiffness is nonzero at any temperature so that the transport is ballistic. Our results suggest that the nonzero stiffness arises because even in the presence of umklapp scattering a nonzero fraction of states remains degenerate in the thermodynamic limit. [S0163-1829(98)50630-3]

The problem of transport in a nondisordered 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 a gap in the excitation spectrum display diffusive behavior,[1] in reasonable agreement with theoretical work of Sachdev and Damle[2] relating diffusion to classical scattering of excitations near the gap edge. Reference 2 provided a detailed analysis indicating diffusive behavior for the $S=1$ chain and also gave arguments implying that for gapped systems in general the low-energy excitations display diffusive behavior. On the other hand, measurements on gapless $S=1/2$ chains[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 $D\sim J\sqrt{2\pi S(S+1)/3}$ expected from classical considerations.[4] We believe that the measured value for D in the $S=1/2$ system is so large that it implies that 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[5]) and prompts us to examine further the question of spin transport in gapless systems.

This question has been previously studied. An analysis based on a continuum limit Luttinger liquid representation[6] suggested that the diffusion constant was associated with umklapp operators and was finite but exponentially large in the umklapp gap. On the contrary, Zotos and collaborators have argued that integrable models exhibit ballistic transport while nonintegrable models are diffusive.[7] Recently Fabricius and McCoy[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 an XY anisotropy but not at the isotropic Heisenberg point. Very recently, Monte Carlo[9] and Bethe-ansatz[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 diagonalization and finite-size scaling to study the spin stiffness of the XXZ model and the behavior of the energy levels which leads to a nonzero stiffness.

The XXZ model is defined by the Hamiltonian

$$\hat{H}_{XXZ}=J\sum_{n}\,(S_i^xS_{i+1}^x+S_i^yS_{i+1}^y+\Delta S_i^zS_{i+1}^z). \tag{1}$$

At $T=0$ the gapless phase $-1<\Delta\leqslant 1$ of this model has a spin-current correlator which includes a term proportional to $\delta(\omega)$; the coefficient of this term defines the spin stiffness $\mathcal{D}_s$ (Ref. 11) (in the gapped phase $|\Delta|>1$ the $T=0$ stiffness is zero). The question of interest here is whether at $T>0$ the stiffness $\mathcal{D}_s$ remains nonzero, implying ballistic transport, or $\mathcal{D}_s$ vanishes, implying nonballistic (and perhaps diffusive) transport.

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

$$\hat{H}=\sum_n\left[-\frac{1}{2}(Jc_n^\dagger c_{n+1}+\text{H.c.})+J\Delta\left(c_n^\dagger c_n-\frac{1}{2}\right)\times\left(c_{n+1}^\dagger c_{n+1}-\frac{1}{2}\right)\right]. \tag{2}$$

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 $\sigma(\omega)$ may be written as

$$\text{Re}\sigma(\omega)=2\pi\mathcal{D}_c\delta(\omega)+\sigma_{reg}(\omega), \tag{3}$$

defining the charge stiffness $\mathcal{D}_c$, which is proportional to $\mathcal{D}_s$ of the original model. If $\mathcal{D}_c\neq 0$ the model has infinite conductivity whereas if $\mathcal{D}_c=0$ one has either a normal conductor $[\mathcal{D}_c=0,\ \sigma_{reg}(\omega\rightarrow 0)>0]$ with diffusive transport or an ideal insulator $[\mathcal{D}_c=0,\ \sigma_{reg}(\omega\rightarrow 0)=0]$.

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 ϕ, which modifies the hopping term in the Hamiltonian Eq. (2) by the usual Peierls phase factor $J\rightarrow J\ \exp(\imath\phi/L)$. For a system of size L, $\mathcal{D}_c=(L/2)\partial^2E_0/\partial\phi^2(\phi\rightarrow 0)$.

Kohn's result has been recently generalized to finite temperatures,[7]

$$\mathcal{D}_c=\frac{L}{2\mathcal{Z}}\sum_n \frac{1}{2}\frac{\partial^2 E_n}{\partial\phi^2}e^{-\beta E_n}, \tag{4}$$

where $\mathcal{Z}$ is the partition function of the system and n labels exact eigenstates.

We further rewrite Eq. (4) as $\mathcal{D}_c=\mathcal{D}_1+\mathcal{D}_2$, with

$$\mathcal{D}_1=-\frac{L}{2\beta}\frac{1}{\mathcal{Z}}\frac{\partial^2\mathcal{Z}}{\partial\phi^2} \tag{5}$$

and

$$\mathcal{D}_2=\frac{\beta L}{2}\frac{1}{\mathcal{Z}}\sum_n\left(\frac{\partial E_n}{\partial\phi}\right)^2 e^{-\beta E_n}. \tag{6}$$

The advantage of this representation is that it separates $\mathcal{D}_c$ into a thermodynamic part (depending only on derivatives of $\mathcal{Z}$) and a *positive* part, depending on current-carrying $(j_{nn}\sim\partial E_n/\partial\phi)$ states. $\mathcal{D}_1$ gives no contribution to the charge stiffness at $T>0$ and $L\rightarrow\infty$;[13] for example, for $T\ll J$

$$\mathcal{D}_1(T\gg 2\pi/vRL)=LT\ \exp\left(-\frac{2\pi LT}{vR}\right), \tag{7}$$

with $R^2=[1-(1/\pi)\cos^{-1}\Delta]/2\pi$. Thus at $T>0$ any nonzero $\mathcal{D}_c$ must be due to $\mathcal{D}_2$ which essentially counts the number of thermally accessible current carrying states.

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

For any finite-size chain the Heisenberg Hamiltonian Eq. (1) is a Hermitian matrix. We construct this matrix for $\phi=1\times10^{-4}$, 2×10^{-4}, 3×10^{-4}, 4×10^{-4} and use the standard QL routine from the Numerical Recipes package[14] to calculate the eigenvalues (with accuracy given by machine precision). We then fit ϕ dependence of the eigenvalues to obtain derivatives. Our choices of ϕ lead to $\sim10^{-6}$ accuracy for the derivative values. The size of matrices that could be diagonalized by the routine is limited by computer memory; for an $N\times N$ matrix it requires $\approx 8N^2$ bytes of storage space. With computer memory of about 360 MB available to us we can diagonalize matrices up to $N=7000$, corresponding 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 nonzero. At small temperatures the value of $\mathcal{D}_2$ 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 $\mathcal{D}_2$ decreases with the system size, but appears to tend to a nonzero limit as $L\rightarrow\infty$.

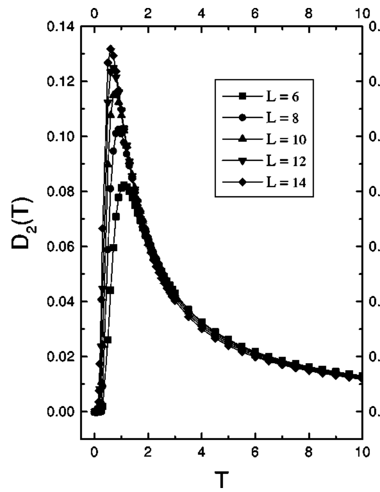

FIG. 1. $D_2(T)$ for different system sizes for $\Delta=0.4$.

To investigate the finite-size scaling in Fig. 2 we plot $(D_2T)_\infty=\lim_{T\rightarrow\infty}D_2T$ 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 $(D_2T)_\infty(L)=A+B/L+\cdots$ with A,B depending on the interaction, but with A always positive for $\Delta\leq 1$. For small Δ the best-fit line is flat and the fit using four largest sizes is excellent (least-squares 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 $(D_2T)_\infty(L)=C/L^\theta$ lead to even larger errors, so the hypothesis $(D_2T)(L\rightarrow\infty)\rightarrow 0$ is inconsistent with our data.

The scaling of D_2 can be expressed in terms of the size

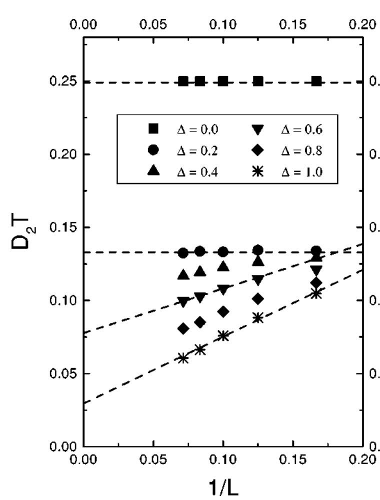

FIG. 2. (D_2T) plotted against inverse system size at $T=50$.

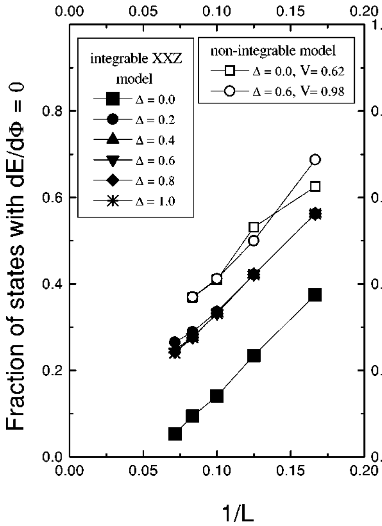

FIG. 3. Fraction of states with zero current.

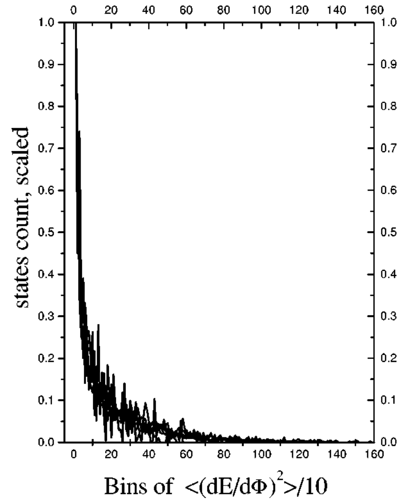

FIG. 4. Histogram of current values; lines for different Δ are indistinguishable.

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 nonzero current $\partial E_n/\partial\phi\sim 1/\sqrt{L}$. 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, 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 state changing the value of the total current carried. To analyze these effects we plot in Fig. 3 the fraction of states with $\partial E_n/\partial\phi(\phi\rightarrow 0)=0$ as a function of system size for the *XXZ* model with varying interaction strength Δ (solid symbols). One sees that adding an interaction sharply increases the fraction of noncurrent-carrying states, but this fraction remains small and decreases with system size.

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 Δ. For each Δ 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 into 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 Δ 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 $V\Sigma_i S_i^z S_{i+2}^z$ 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 nonintegrable interaction is mostly to reduce the values of the current carried by the remaining degenerate states as is illustrated in Fig. 5. At least for large V, $(D_2T)(L\rightarrow\infty)\rightarrow 0$, implying that the current carried by a typical state, although not 0, is much less than $1/\sqrt{L}$ and is presumably $o(1/L)$. Interestingly, the effect seems not to occur for $V<\Delta$. For $\Delta=0$ Fig. 5 shows clearly that even $V=0.02$ leads to D_2T which vanishes as $L\rightarrow\infty$, whereas for $\Delta=0.2$ large $V=0.62$ leads to a vanishing $(D_2T)(L\rightarrow\infty)$, while the effect of $V=0.02$ is much smaller than for $\Delta=0$ and our data are consistent with a nonzero $(D_2T)(L\rightarrow\infty)$. Our system sizes are too small to allow us to make a definite statement about $(D_2T)(L\rightarrow\infty)$ for $V<\Delta$, but clearly the relative size of the effect of the nonintegrable interaction depends strongly on the ratio V/Δ.

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 $\mathcal{D}_2$ is greater than zero and

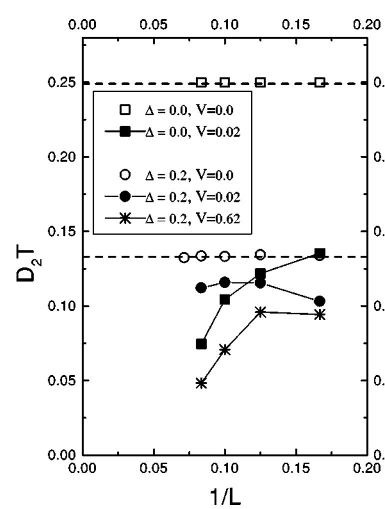

FIG. 5. $D_2T(1/L)$ comparing integrable and nonintegrable cases; the lines are guides to the eye.

extrapolates to a nonzero value in the thermodynamic limit in agreement with previous work.[5,7] At small Δ this extrapolation seems unambiguous in agreement with the perturbation theory results,[5] which are valid for small Δ where the umklapp is irrelevant in the renormalization group sense. For larger Δ the data seems to slowly decrease with size extrapolating to some small but nonzero 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 operator becomes marginal at this point, but our results seem inconsistent with vanishing $\mathcal{D}_c$ obtained in Ref. 8.

Our results provide a new perspective on the origin of the nonzero stiffness at $T > 0$. One necessary condition for a nonzero stiffness is *degeneracy*: current carrying states come in degenerate pairs related by time reversal. It is tempting to argue that for integrable models such as the XXZ model the large number of conserved quantities arising from integrability ''protects the degeneracy'' and thus ensures a nonzero stiffness; indeed a connection between the large number of conservation laws and ballistic transport has previously been noted.[7] However, our results suggest that this is not the whole story. We see from Fig. 4 the existence of a large number of degenerate states is not specific to integrable models. The next-nearest-neighbor interaction destroys the integrability but still leaves a macroscopic fraction of degenerate (current carrying) states. A more important difference is this: in the integrable models (except possibly for $\Delta = 1$) and possibly in the nonintegrable models (for $V < \Delta$) the typical current carried by these states is $\sim 1/\sqrt{L}$ leading to nonzero stiffness as $L \to \infty$, whereas for $V > \Delta$ we see the typical current is much smaller, presumably $\sim 1/L$. Thus the crucial issue is the size of the current carried by each state, not the number of current carrying states.

Finally our results seem to indicate a difference in behavior between $V < \Delta$ and $V > \Delta$ in the nonintegrable model. A scenario involving critical value of V separating ballistic and diffusive behavior seems to us unlikely; we speculate that for all $V \neq 0$ $\mathcal{D}_c \to 0$ in the thermodynamic limit, but that there is a length scale $\xi(V,\Delta)$ diverging as $V \to 0$ 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 $\xi^{-1/2}/L$; our system sizes are too small to allow definite conclusions.

We are grateful to Lev Ioffe for stimulating our interest in the problem and for helpful discussions and to Ian Affleck for pointing out an error in an earlier draft of this paper. A.J.M. thanks the Physics Department of Rutgers University for hospitality and NSF Grant No. DMR 9707701 for support.

[1] M. Takigawa, T. Asano, Y. Ajiro, M. Mekata, and Y. J. Uemura, Phys. Rev. Lett. **76**, 2173 (1996).
[2] S. Sachdev and K. Damle, Phys. Rev. Lett. **78**, 943 (1997).
[3] M. Takigawa, N. Motoyama, H. Eisaki, and S. Uchida, Phys. Rev. Lett. **76**, 4612 (1996).
[4] R. M. White, *Quantum Theory of Magnetism* (Springer-Verlag, New York, 1983).
[5] B. N. Narozhny, Phys. Rev. B **54**, 3311 (1996).
[6] T. Giamarchi and A. J. Millis, Phys. Rev. B **46**, 9325 (1992).
[7] X. Zotos and P. Prelovsek, Phys. Rev. B **53**, 983 (1996); H. Castella, X. Zotos, and P. Prelovsek, Phys. Rev. Lett. **74**, 972 (1995).
[8] K. Fabricius and B. M. McCoy, Phys. Rev. B **57**, 8340 (1998).
[9] S. Kirchner, H. G. Everts, and W. Hanke, cond-mat/9804148 (unpunblished).
[10] N. M. R. Peres, P. D. Sacramento, D. K. Campbell, and J. M. P. Carmelo, cond-mat/9804169 (unpublished).
[11] B. S. Shastry and B. Sutherland, Phys. Rev. Lett. **65**, 243 (1990).
[12] W. Kohn, Phys. Rev. **133**, A171 (1964).
[13] P. Ginsparg, in *Fields, Strings and Critical Phenomena* (North-Holland, Amsterdam, 1990); we thank I. Affleck and S. Lukyanov for clarifying this issue.
[14] W. H. Press, B. P. Flannery, S. A. Teukolsky, and W. T. Vetterling, *Numerical Recipes* (Cambridge University Press Cambridge, England, 1986).