FINITE TEMPERATURE TRANSPORT IN INTEGRABLE QUANTUM MANY BODY SYSTEMS

X. ZOTOS, F. NAEF
Institut Romand de Recherche Numérique en Physique des Matériaux,
(EPFL-PPH) Ecublens, 1015 Lausanne, Switzerland

P. PRELOVSEK
Faculty of Mathematics and Physics,
and J. Stefan Institute, 1000 Ljubljana, Slovenia

Recent developments in the analysis of finite temperature dissipationless transport in integrable quantum many body problems are presented. In particular, we will discuss: (i) the role played by the conservation laws in systems as the spin 1/2 Heisenberg chain and the one-dimensional Hubbard model, (ii) exact results obtained using the Bethe ansatz method on the long time decay of current correlations.

1 Introduction

It has recently being proposed that integrable quantum many body systems show dissipationless transport at finite temperatures. This idea was motivated by analytical and numerical studies on a toy model and the fermionic version of the Heisenberg model. It is analogous to the well known effect of transport by solitons in classical nonlinear integrable systems. In this domain of classical physics, a part of the activity is already in the technological applications, for instance the propagation of solitons in optical fibers and in particular the robustness of dissipationless transport to perturbations.

In quantum many body systems, there is not yet clear experimental evidence for unusually high conductivity (close to ideal) at finite temperatures for a system described by a (nearly) integrable Hamiltonian. Perhaps the best candidates so far are quasi one dimensional spin 1/2 systems described by the Heisenberg model. In fact NMR studies on the SrCuO$_3$ compound showed an unusually high value of the diffusion constant, characteristic of ballistic rather than diffusive behavior.

Besides the magnetic compounds, systems characterized by strong short range electronic correlations (described by the integrable one dimensional Hubbard model) could be candidates for observing the predicted ballistic behavior, even more conspicuous at high temperatures, instead of the expected diffusive one due to electron-electron scattering. Nanotubes or artificially made nanostructures come to mind as possible experimental realizations.

From the experimental point of view, the most relevant question is the robustness of this dissipationless transport to perturbations, for instance impurities, 3d coupling, phonons. The same problem analyzed for classical systems, indicates relative insensitivity of the soliton propagation to disorder. From the theoretical perspective, an analytical solution of the dynamic properties of integrable systems should be expected, exactly due to the integrability of the models. On the other hand, the analysis of robustness might largely depend on numerical simulation studies, the same situation as in classical systems. We should also point out, that this problem is closely related to studies on dynamical systems, analyzing the conditions of appearance and stability of classical/quantum chaos.

The framework for discussing dynamic properties at finite temperatures/frequencies is the linear response theory (or Kubo formalism). In this formulation, using the fluctuation - dissipation theorem, the transport properties are related to the study of dynamic correlations at

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equilibrium. It might be objected that results drawn from this method for integrable systems are questionable. However, we can point out that transport properties derived by linear response theory for noninteracting systems (e.g. an harmonic crystal) or classical integrable systems are in accord with experimental observations and results from more sophisticated theoretical methods.

The basic way for characterizing the transport properties is by the dynamic current correlations $< j(t) j >$. As a criterion for dissipationless transport we will study the long time asymptotic value $C_{jj} = < j(t) j(0) >_{t \to \infty}$. If $C_{jj}$ is finite, the response is reactive and the system shows ideal conducting behavior. $C_{jj}$ is related to the Drude weight $D(T)$ in the real part of the conductivity as expressed in linear response theory:

$$\sigma(\omega) = 2\pi D(\omega) + \sigma_{\text{reg}}(\omega), \quad D = \frac{\beta}{2L} C_{jj}$$

It should be noted that a vanishing $D(T)$ does not necessarily imply diffusive behavior. If the current-current correlations decay too slowly then transport coefficients cannot be defined. In the analogous situation of one dimensional classical systems, different behaviors have been observed: typically if a system is integrable then $C_{jj} > 0$ and the system is an ideal conductor. If it is nonintegrable, then models have been found where correlations decay fast enough and a transport coefficient can be defined, but there are also models where the decay is too slow indicating anomalous low frequency conductivity. In quantum many body systems the situation is less clear, but we might similarly expect a variety of behaviors.

In the following we will discuss two recent developments for analyzing the transport properties in integrable systems: the first, it is the way in which the conservation laws characterizing these systems affect their long time current correlations; the second, it is a procedure based on the Bethe ansatz method for calculating analytically $D(T)$.

2 The role of conservation laws

Integrable many body systems are characterized by a macroscopic number of conserved quantities. A set of conservation laws is represented by local involutive operators $Q_n$, commuting with each other $[Q_n, Q_m] = 0$ and with the Hamiltonian, $[Q_n, H] = 0$. We can relate the time decay of correlations to local conserved quantities in Hamiltonian systems by using an inequality proposed by Mazur:

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T < A(t) A > dt \geq \sum_{n} \frac{< A Q_n >^2}{< Q_n^2 >}$$

Here <> denotes thermodynamic average, the sum is over a subset of conserved quantities $Q_n$, orthogonal to each other $< Q_n Q_m >= < Q_n^2 > \delta_{n,m}$, $A^\dagger = A$ and $< A >= 0$. Applying this inequality to current-current correlations we obtain:

$$D \geq \frac{\beta}{2L} \sum_{n} \frac{< j Q_n >^2}{< Q_n^2 >}$$

We will now discuss two applications of this inequality, the decay of spin currents in the Heisenberg model and the electrical conductivity in the Hubbard model.

2.1 $s=1/2$ Heisenberg model

It is described by the Hamiltonian:

$$H = \sum_{l=1}^{L} (J_x S_x^l S_x^{l+1} + J_y S_y^l S_y^{l+1} + J_z S_z^l S_z^{l+1})$$

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by a Jordan-Wigner transformation the Heisenberg model is equivalent to a model of spinless fermions interacting with a nearest-neighbor interaction $(t - V)$ model).

This model is characterized by a macroscopic number of conservation laws. It is worth to note that the first nontrivial conservation law $Q_3$ is related to a physical quantity, it coincides with the energy current $j^E$:

$$Q_3 = j^E = \sum_{l=1}^{L} J_x J_y (S_{l-1}^x S_{l+1}^x + S_{l-1}^y S_{l+1}^y) + (x, y, z).$$  

(5)

This is particularly interesting and of actual experimental relevance as it implies ideal thermal conductivity (energy currents do not decay at all, $< j^E(t) j^E > = \text{const.}$). It should also be taken into account in the analysis of the quasielastic peak in Raman experiments where the local dynamic energy correlations enter.

Regarding the spin current correlations, for $J_x = J_y = 1, J_z = \Delta$ we find that:

$$D = \beta \frac{2L}{C_{j^z j^z}} \geq \frac{\beta}{2L} \frac{< j^z Q_3 >^2}{< Q_3^2 >},$$  

where $j^z = \text{spin current} = \sum_{l=1}^{L} (S_{l}^y S_{l+1}^y - S_{l}^x S_{l+1}^x)$, implying ideal spin conductivity and the absence of spin diffusion. We can analytically calculate the right hand size of this inequality in the $\beta \to 0$ limit,

$$D \geq \beta \frac{8 \Delta^2 m^2 (1/4 - m^2)}{2L (1 + 8 \Delta^2 (1/4 + m^2))}, \quad m = \langle S_l^z \rangle$$  

(7)

From this result we notice that we obtain a positive bound only for a finite magnetization $m$, when the system is in a magnetic field. For $m = 0$ this inequality does not provide a useful bound although, as we will show below using the Bethe ansatz method, $D(T)$ is still positive.

2.2 Hubbard model

Finally, for the Hubbard model described by the Hamiltonian,

$$H = (-t) \sum_{\sigma, i=1}^{L} (c_{i\sigma}^\dagger c_{i+1\sigma} + h.c.) + U \sum_{i=1}^{L} (n_{i\uparrow} - \frac{1}{2})(n_{i\downarrow} - \frac{1}{2})$$  

(8)

considering $Q_3$ given by:

$$Q_3 = \sum_{\sigma} (-t)^2 (i c_{i+1\sigma}^\dagger c_{i-1\sigma} + h.c.) - U (j_{i-1,i,\sigma} + j_{i,i+1,\sigma})(n_{i,-\sigma} - \frac{1}{2})$$  

(9)

we obtain for the decay of current correlations in the $\beta \to 0$ limit,

$$D \geq \beta \frac{2L}{U \sum_{\sigma} 2 \rho_{\sigma} (1 - \rho_{\sigma}) (2 \rho_{-\sigma} - 1)}$$  

$$D \geq \frac{\beta}{2} \frac{[U \sum_{\sigma} 2 \rho_{\sigma} (1 - \rho_{\sigma}) (2 \rho_{-\sigma} - 1)]^2}{\sum_{\sigma} 2 \rho_{\sigma} (1 - \rho_{\sigma}) [1 + U^2 (2 \rho_{-\sigma}^2 - 2 \rho_{-\sigma} + 1)]}$$  

(10)

Again, we obtain a finite value for $D(T)$ and so ideal conducting behavior for a system out of half-filling. Bethe ansatz analysis by Fujimoto and Kawakami confirm this result (the system at half-filling has also been analyzed).
3 Bethe ansatz analysis for the Heisenberg model

Recently a new procedure was proposed for analytically calculating $D(T)$ using the Bethe ansatz method. The application to the Heisenberg spin 1/2 model, that we will now sketch, is based on a series of assumptions and developments.

First, the structure of the solutions of the Bethe ansatz equations for $0 \leq \Delta \leq 1$ conjectured by Takahashi and Suzuki is used. Parametrizing the anisotropy coupling by $\Delta = \cos \theta$, $\theta = \frac{\pi}{\nu}$, $\nu$ integer, and the pseudomomenta $k_\alpha$ by the rapidities $x_\alpha = \cot(\frac{k_\alpha}{2}) = \cot(\frac{\theta}{2}) \tanh(\frac{\theta x_\alpha}{2})$, the solutions are organized into a finite number of allowed strings $n = 1, 2, ..., \nu - 1$.

\[
x^{n,k}_{\alpha,+} = x^n_\alpha + (n + 1 - 2k)i + O(e^{-\delta N}); \quad k = 1, 2, ...n
\]

\[
x^{n,k}_{\alpha,-} = x^n_\alpha + i\nu + O(e^{-\delta N}), \quad \delta > 0.
\]

Next, finite size corrections on the positions of the strings are expressed by introducing the functions $g_{1j}$ and $g_{2j}$:

\[
x^j_N = x^j_\infty + \frac{g_{1j}}{N} + \frac{g_{2j}}{N^2}
\]

where $x^j_N(x^j_\infty)$ are the rapidities for a system of size $N(\infty)$.

Finally introducing excitation and hole densities $\rho_j$ and $\rho^h_j$ as in the standard thermodynamic Bethe Ansatz and expanding the Bethe ansatz equations to $O\left(\frac{1}{N}\right)$ and $O\left(\frac{1}{N^2}\right)$ we obtain:

\[
D = \frac{1}{2} \beta \sum_j \int_{-\infty}^{+\infty} dx (\rho_j + \rho^h_j) < n_j > (1 - < n_j >) \left( \frac{\partial \epsilon_j}{\partial x} \frac{\partial g_{1j}}{\partial \phi} \right)_{\phi \rightarrow 0}
\]

where $< n_j > = 1/(1 + e^{\beta \epsilon_j})$ and $\epsilon_j = (1/\beta) \ln(\rho^h_j/\rho_j)$. This expression looks formally analogous to that for free fermions:

\[
D = \frac{\beta}{2N} \sum_\mu < n_\mu > (1 - < n_\mu >) \left( \frac{\partial \epsilon_\mu}{\partial \phi} \right)^2_{\phi \rightarrow 0}
\]

where $< n_\mu >$ is the Fermi-Dirac distribution and $\epsilon_\mu$ are single particle energies.

The functions $\rho_j$, $\rho^h_j$, $g_{1j}$, $g_{2j}$ are determined numerically by iteration. Using this procedure we obtain $D(T)$ for all temperatures and couplings $0 \leq \Delta \leq 1$ as is shown in Fig. 1.

![Figure 1](image.png)  

Figure 1: $D(\Delta)$ evaluated at the points $\nu = 3, ..., 16$ and various temperatures. The continuous line is the high temperature proportionality constant $C_{jj} = D/\beta$. The $\diamond$ indicate exact diagonalization results from ref. (17)
In particular, we recover the known $T = 0$ value $D_0$ with a characteristic power law behavior:

$$D(T) = D_0 - \text{const.}T^\alpha, \quad \alpha = \frac{2}{(\nu - 1)},$$

and we obtain good agreement with numerical simulations for $\beta = 0$ (diamonds), a result that lends support both to the Bethe ansatz procedure and the string assumption.

Particularly interesting is the vanishing of $D(T)$ for $\Delta = 1$ at any finite temperature. This result suggests that for $\Delta \geq 1$ the Heisenberg model does not show ideal conducting behavior and the isotropic model is a borderline case. If the conjecture, born out of a numerical study of absence of weight in the conductivity at low frequencies proves valid in the thermodynamic limit, then we would have a realization of an exotic ideal insulating phase. Finally, from the results presented, it is not unreasonable to expect anomalous low frequency spin dynamics for the isotropic Heisenberg model, hopefully observable in experiments.

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References

1. X. Zotos, H. Castella and P. Prelovšek, in Proceedings of the XXXI Rencontres de Moriond, ed. T. Martin et al, (Editions Frontières, 1996).
2. H. Castella, X. Zotos, P. Prelovšek, Phys. Rev. Lett. 74, 972 (1995).
3. X. Zotos and P. Prelovšek, Phys. Rev. B53, 983 (1996).
4. see e.g. L.F. Mollenauer, in Optical Solitons - Theory and Experiment, ed. J.R. Taylor (Cambridge Studies in Modern Optics, 1992), p.30.
5. M. Takigawa, N. Motoyama, H. Eisaki and S. Uchida, Phys. Rev. Lett. 24, 4612 (1996).
6. G. J. Lasinio and C. Presilla, Phys. Rev. Lett. 77, 4322 (1996).
7. T. Prosen, Phys. Rev. Lett. 80, 1808 (1998).
8. Z. Rieder, J.L. Lebowitz and E. Lieb, J. Math. Phys. 8, 1073 (1967).
9. H. Beck, in Dynamical properties of solids, vol.2, 205 (North-Holland, Amsterdam, Netherlands, 1975)
10. S. Lepri, R. Livi and A. Politi, Europh. Lett. 43, 271 (1998).
11. X. Zotos, F. Naef and P. Prelovšek, Phys. Rev. B55 11029 (1997).
12. S. Fujimoto and N. Kawakami, J. Phys. A. 31, 465 (1998).
13. M. Lüscher, Nucl. Phys. B117, 475 (1976).
14. P. Mazur, Physica 43, 533 (1969).
15. A.N. Vasil’ev et al, Phys. Rev. Lett., 81, 1949 (1998).
16. H. Kuroe et al, Phys. Rev. B55, 409 (1997).
17. F. Naef and X. Zotos, J. Phys. C10, L183 (1998).
18. X. Zotos, Phys. Rev. Lett. 82, 1764 (1999).
19. M. Takahashi and M. Suzuki, Prog. Theor. Phys. 48 2187 (1972).
20. M. Fowler and X. Zotos, Phys. Rev. 24,2634 (1981).
21. A. Berkovits and N. G. Murthy, J. Phys. A21, 3703 (1988).
22. B.S. Shastry and B. Sutherland, Phys. Rev. Lett. 65, 243 (1990).