Transport and conservation laws

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We study the effect of conservation laws on the finite-temperature transport properties in one-dimensional integrable quantum many-body systems. We show that the energy current is closely related to the first conservation law in these systems and therefore the *thermal* transport coefficients are anomalous. Using an inequality on the time decay of current correlations we show how the existence of conserved quantities implies a finite charge stiffness (weight of the zero-frequency component of the conductivity) and so ideal conductivity at finite temperatures. [S0163-1829(97)03318-3]

One-dimensional (1D) integrable quantum many-body (IQM) systems, such as the Heisenberg spin-1/2 chain, the Hubbard, or supersymmetric *t-J* model, are characterized by a macroscopic number of conservation laws.[1–4] We have recently proposed, based on analytical and numerical studies, that IQM systems show dissipationless finite-temperature conductivity.[5–7] It is natural to think that this anomalous transport behavior is related to the macroscopic number of conserved quantities characterizing these systems. 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, $[Q_n,H]=0$. The index n indicates that the operator Q_n is of the form $Q_n=\Sigma_{i=1}{}^{L}q_i^n$, where q_i^n are local operators involving n sites around site i, on a lattice of L sites.

Although rather formal procedures exist for the construction of these operators,[3,4] it is not clear how to study their physical content and even more how to take them into account in the analysis of transport properties. In this paper we show that, in different models of actual interest, the first nontrivial quantity Q_3 (Q_2 often denotes the Hamiltonian) has a simple physical significance: It is (or it is closely related to) the *energy current* operator. Further, we analyze how the coupling of the energy current or current operator to the conserved quantities results to time correlations not decaying to zero at long times. Thus, transport does not have a simple diffusive character and within the Kubo linear response theory[8] is described by diverging or ill-defined transport coefficients.

We can relate the time decay of correlations to the local conserved quantities in the Hamiltonian systems we discuss by using an inequality proposed by Mazur:[9]

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T\langle A(t)A\rangle dt\geqslant\sum_n\frac{\langle AQ_n\rangle^2}{\langle Q_n^2\rangle}. \tag{1}$$

Here $\langle\ \rangle$ denotes thermodynamic average, the sum is over a subset of conserved quantities Q_n, orthogonal to each other, $\langle Q_nQ_m\rangle=\langle Q_n^2\rangle\delta_{n,m}$, $A^\dagger=A$, and $\langle A\rangle=0$. In the following, we will only consider Q_3 in relation (1) so that the issue of orthogonality will not enter. Further, we can write $\langle A(t)A\rangle=C_{AA}+C(t)$ as the sum of a time-independent factor,

$$C_{AA}=\sum_a p_a\sum_{b(\epsilon_b=\epsilon_a)}|\langle a|A|b\rangle|^2, \tag{2}$$

and a time-dependent one,

$$C(t)=\sum_a p_a\sum_{b(\epsilon_b\neq\epsilon_a)}|\langle a|A|b\rangle|^2e^{i(\epsilon_a-\epsilon_b)t}. \tag{3}$$

Here $|a\rangle,|b\rangle$ are eigenstates of the Hamiltonian, $p_a=e^{-\beta\epsilon_a}/Z$ the corresponding Boltzmann weights, and β the inverse of the temperature. For time correlations $\langle A(t)A\rangle$ with nonsingular low-frequency behavior, the term $\lim_{T\to\infty}(1/T)\int_0^TC(t)dt$ goes to zero and so $C_{AA}=\lim_{t\to\infty}\langle A(t)A\rangle$,

$$C_{AA}\geqslant\sum_n\frac{\langle AQ_n\rangle^2}{\langle Q_n^2\rangle}. \tag{4}$$

In particular, we will use this inequality in the analysis of the real part of the conductivity, $\sigma'(\omega)=2\pi D(T)\delta(\omega)+\sigma_{\rm reg}(\omega)$, related within linear response theory to the current-current correlation $\langle J(t)J\rangle$. A finite value of the charge stiffness D, given also by $D=\frac{1}{2}\omega\sigma''(\omega)|_{\omega\to0}$, implies an ideally conducting system.[10,5] We will now argue that $D\simeq(\beta/2L)C_{JJ}$ and therefore the following inequality holds for the charge stiffness:

$$D\geqslant\left(\frac{\beta}{2L}\right)\sum_n\frac{\langle JQ_n\rangle^2}{\langle Q_n^2\rangle}. \tag{5}$$

In this derivation, we assume again that the regular part of the conductivity $\sigma_{\rm reg}(\omega)$ shows a nonsingular behavior at low frequencies so that the contribution from $C(t)$ in Eq. (1) vanishes. This is a very mild condition for the physical systems we consider; as numerical simulations indicate,[6,7] these IQM systems are characterized by a pseudogap and so a vanishing regular part $\sigma_{\rm reg}(\omega\to0)$.

To relate D to C_{JJ}, it is convenient to use a generalization of Kohn's approach[10,5] to finite temperatures. In this formulation $D(T)$ can be expressed as the thermal average of curvatures of energy levels in a Hamiltonian describing a system on a ring pierced by a fictitious flux ϕ, $D=(1/2L)\Sigma_a p_a(\partial^2\epsilon_a/\partial\phi^2)|_{\phi\to 0}$. Evaluating the second derivative of the free energy F as a function of the flux ϕ we find

$$\frac{\partial^2 F}{\partial \phi^2}=2LD-\beta\sum_a p_a\left(\frac{\partial \epsilon_a}{\partial \phi}\right)^2+\beta\left(\sum_a p_a\frac{\partial \epsilon_a}{\partial \phi}\right)^2. \qquad (6)$$

In the models we will discuss, the third term on the right-hand side (RHS) vanishes by symmetry (summing over k and $-k$ subspaces). Further, these systems show no persistent currents at finite temperatures in the thermodynamic limit; therefore, $\partial^2F/\partial\phi^2|_{\phi\to 0}\to 0$ in this limit. We have numerically verified that this is indeed the case for temperatures larger than the level spacing; at zero temperature, there is no contradiction with Kohn's formula for D as the second term on the RHS vanishes in a ground state with zero current. Finally, as $\partial\epsilon_a/\partial\phi|_{\phi\to 0}=\langle a|j|a\rangle$ and degenerate levels contribute a vanishing weight in Eq. (2), we arrive at relation (5). This inequality provides a lower bound for the charge stiffness D which, if not zero, implies ideal conductivity at finite temperatures.

In general, it is difficult to evaluate the right-hand side of the inequality (4) involving the ''overlap'' $\langle AQ_n\rangle$. However, we will give some examples below, this correlation can easily be evaluated in the case of a grand canonical trace over states, in the thermodynamic limit and for $\beta\to 0$. We thus obtain the charge stiffness in leading order in β.

Before studying concrete models, we construct the energy current operator as follows: We consider Hamiltonians defined on a 1D lattice with L sites and periodic boundary conditions $h_{L,L+1}=h_{L,1}$ of the form

$$H=\sum_{i=1}^{L} h_{i,i+1}. \qquad (7)$$

Because the energy is a conserved quantity, the time evolution of the local energy operator $h_{i,i+1}(t)$ can be written as the discrete divergence of the energy current operator $J^E=\Sigma_{i=1}^L j_i^E$:

$$\frac{\partial h_{i,i+1}(t)}{\partial t}=i[H,h_{i,i+1}(t)]=-[j_{i+1}^E(t)-j_i^E(t)], \qquad (8)$$

where $h_{i,i+1}(t)=e^{iHt}h_{i,i+1}e^{-iHt}$ and $j_i^E=-i[h_{i-1,i},h_{i,i+1}]$. Now, by direct evaluation for some IQM systems, we will see that the energy current J^E is closely related to a conserved quantity.

(i) *Heisenberg model*. The general anisotropic Heisenberg Hamiltonian is given by

$$H=\sum_{i=1}^{L} h_{i,i+1}=\sum_{i=1}^{L}(J_xS_i^xS_{i+1}^x+J_yS_i^yS_{i+1}^y+J_zS_i^zS_{i+1}^z), \qquad (9)$$

where $S_i^\alpha=\frac{1}{2}\sigma_i^\alpha$, σ_i^α are Pauli spin operators with components $\alpha=x,y,z$ at site i. The local energy current operator j_i^E is

$$j_i^E=J_xJ_y(S_{i-1}^xS_i^zS_{i+1}^y-S_{i-1}^yS_i^zS_{i+1}^x)$$
$$+\text{cyclic permutations of }(x,y,z). \qquad (10)$$

Now it is straigthforward to verify that the global energy current operator J^E commutes with the Hamiltonian (9). Further, J^E coincides with the first nontrivial conserved quantity Q_3 as obtained from an expansion of the transfer matrix in the algebraic Bethe ansatz method.[1,4] In agreement with the notation Q_2 for the Hamiltonian, the local energy operator $h_{i,i+1}$ involves two sites $(i,i+1)$, while the local energy current operator $q_i^3=j_i^E$ involves three sites $(i-1,i,i+1)$.

The vanishing commutator $[J^E,H]=0$ implies that the energy current time correlations are independent of time:

$$\langle J^E(t)J^E\rangle=\sum_a p_a j_{Ea}^2, \qquad (11)$$

where j_{Ea} are the eigenvalues of J^E, $J^E|a\rangle=j_{Ea}|a\rangle$. The nondecaying of the energy current leads to a *diverging thermal conductivity* related to the $\langle J^E(t)J^E\rangle$ correlation.[8]

As for the conductivity, it is more relevant to discuss the fermionic version of the Heisenberg model, defined through the Jordan-Wigner transformation, the so-called t-V model:

$$H=(-t)\sum_{i=1}^{L}(c_i^\dagger c_{i+1}+\text{H.c.})+V\sum_{i=1}^{L}(n_i-\tfrac{1}{2})(n_{i+1}-\tfrac{1}{2}), \qquad (12)$$

where $c_i(c_i^\dagger)$ denote annihilation (creation) operators of spinless fermions at site i and $n_i=c_i^\dagger c_i$.

In this case, the corresponding energy current operator that commutes with the Hamiltonian (12) is given by

$$J^E=\sum_i (-t)^2(ic_{i+1}^\dagger c_{i-1}+\text{H.c.})+Vj_{i,i+1}(n_{i-1}+n_{i+2}-1), \qquad (13)$$

where $j_{i,i+1}=(-t)(-ic_{i+1}^\dagger c_i+\text{H.c.})$ is the particle current. Therefore, for this fermionic model, we find that the $\langle J^E(t)J^E\rangle$ as well as the $\langle J^E(t)J\rangle$ correlations are time independent, implying a diverging thermal conductivity and ill-defined thermopower, respectively.

Regarding the charge stiffness D, we can evaluate analytically $\langle JQ_3\rangle^2/\langle Q_3^2\rangle$ for $\beta\to 0$ and in the thermodynamic limit, obtaining from Eq. (5),

$$D\geqslant\frac{\beta}{2}\,\frac{2V^2\rho(1-\rho)(2\rho-1)^2}{1+V^2(2\rho^2-2\rho+1)}, \qquad (14)$$

where ρ is the fermion density $t=1$. We note that for $\rho\neq 1/2$, D is finite, implying ideal conductivity as we have suggested before.[6] For $\rho=1/2$, this inequality is, however, insufficient for proving that D is nonzero. Due to electron-hole symmetry, this remains true even if we consider all the higher-order conserved quantities Q_n. The reason is that, for the Heisenberg model, all Q_n's can be generated[3,4] by a recursive relation $[B,Q_n]\sim Q_{n+1}$ where B is a ''boost'' operator given by $B=\Sigma_n n h_{n,n+1}$. Then by the electron-hole transformation $c_i=(-1)^i\tilde{c}_i^\dagger$, we see that $J\to -J$ but $Q_n\to Q_n$ and therefore for $\rho=1/2$, $\langle JQ_n\rangle=0$. The eventual nonorthogonality of the Q_n's is not important as we can see by

TABLE I. $(\langle JQ_3\rangle^2/\langle Q_3^2\rangle)/C_{JJ}$ as a function of filling ρ and V/t.

V/t	$\rho=1/3$	$\rho=1/4$
0.0	0.0	0.0
1.0	0.11	0.23
2.0	0.50	0.58
4.0	0.83	0.89
8.0	0.96	0.98
∞	1.0	1.0

considering new orthogonal conserved quantities constructed using, for instance, a Gram-Schmidt orthogonalization procedure.

In Table I, we present some indicative numerical results comparing C_{JJ} with $\langle JQ_3\rangle^2/\langle Q_3^2\rangle$ for a couple of ρ values and $\beta\to 0$. The results for C_{JJ} were obtained by exact diagonalization of the Hamiltonian matrix on finite-size lattices (L up to 20 sites), followed by finite-size scaling using a second-order polynomial in $1/L$. From this table we see that (i) the smaller the density, the more the inequality (5) is exhausted by just considering the contribution from Q_3; (ii) for $V/t\to\infty$, the overlap $\langle JQ_3\rangle$ gives the total weight of C_{JJ}; indeed, studying the higher-order local conserved quantities we can see that they only contribute terms in powers of $1/V$. Nevertheless, it is not clear why the inequality (4) is exhausted and no other, e.g., nonlocal, conserved quantities contribute.

Finally, returning to the Heisenberg model, we note that the bound (14) implies anomalous spin transport at finite magnetization, as the particle current maps to the spin current and the density ρ to the magnetization (half-filling $\rho=1/2$ corresponding to zero magnetization).

(ii) *Hubbard model*. It describes a system of interacting fermions on a lattice with Hamiltonian given by

$$H=(-t)\sum_{\sigma,i=1}^{L}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})+U\sum_{i=1}^{L}(n_{i\uparrow}-\tfrac{1}{2})(n_{i\downarrow}-\tfrac{1}{2}), \tag{15}$$

where $c_{i\sigma}(c_{i\sigma}^{\dagger})$ are annihilation (creation) operators of fermions with spin $\sigma=\uparrow,\downarrow$ at site i and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$.

Similarly as above, we can define a local energy operator by

$$h_{i,i+1}=(-t)\sum_{\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})+\frac{U}{2}[(n_{i\uparrow}-\tfrac{1}{2})(n_{i\downarrow}-\tfrac{1}{2})+(n_{i+1\uparrow}-\tfrac{1}{2})(n_{i+1\downarrow}-\tfrac{1}{2})]. \tag{16}$$

From the time evolution of $h_{i,i+1}$ we find the local energy current operator j_i^E involving sites $(i-1,i,i+1)$:

$$j_i^E=\sum_{\sigma}(-t)^2(ic_{i+1\sigma}^{\dagger}c_{i-1\sigma}+\text{H.c.})-\frac{U}{2}(j_{i-1,i,\sigma}+j_{i,i+1,\sigma})\times(n_{i,-\sigma}-\tfrac{1}{2}), \tag{17}$$

where $j_{i,i+1\sigma}=(-t)(-ic_{i+1\sigma}^{\dagger}c_{i\sigma}+\text{H.c.})$ is the particle current. By comparing this expression for the energy current to the conserved quantity[2,4] Q_3, we find that they coincide when the factor $U/2$ in Eq. (17) is replaced by U. So the energy current $J^E=\Sigma_{i=1}^{L}j_i^E$ does not commute with the Hamiltonian. However, as J^E has a finite overlap $\langle J^EQ_3\rangle$, with the conserved quantity Q_3 we still find that the energy current correlations decay to a finite value at long times so that the thermal transport coefficients are anomalous. We can find a lower bound for the decay by using Eq. (1) for $\beta\to 0$ and in the thermodynamic limit ($t=1$)

$$\lim_{t\to\infty}\langle J^E(t)J^E\rangle=C_{J^EJ^E}\geqslant\frac{\langle J^EQ_3\rangle^2}{\langle Q_3^2\rangle}, \tag{18}$$

$$\frac{\langle J^EQ_3\rangle^2}{\langle Q_3^2\rangle}=L\sum_{\sigma}2\rho_\sigma(1-\rho_\sigma)+\frac{U^4}{4}\frac{[\Sigma_\sigma 2\rho_\sigma(1-\rho_\sigma)(2\rho_{-\sigma}^2-2\rho_{-\sigma}+1)]^2}{\Sigma_\sigma 2\rho_\sigma(1-\rho_\sigma)[1+U^2(2\rho_{-\sigma}^2-2\rho_{-\sigma}+1)]}. \tag{19}$$

As for the charge stiffness D, we can again evaluate analytically $\langle JQ_3\rangle^2/\langle Q_3^2\rangle$ for $\beta\to 0$ and in the thermodynamic limit, obtaining, from Eq. (5),

$$D\geqslant\frac{\beta}{2}\frac{[U\Sigma_\sigma 2\rho_\sigma(1-\rho_\sigma)(2\rho_{-\sigma}-1)]^2}{\Sigma_\sigma 2\rho_\sigma(1-\rho_\sigma)[1+U^2(2\rho_{-\sigma}^2-2\rho_{-\sigma}+1)]}, \tag{20}$$

where ρ_σ are the densities of $\sigma=\uparrow,\downarrow$ fermions, $t=1$. For $\rho_\sigma=1/2$, the right-hand side of Eq. (20) vanishes, although a general proof involving all higher conserved quantities is not possible as a boost operator for the Hubbard model is not known.

(iii) ''*t-J*'' *model*. It belongs to a class of multicomponent quantum systems[11] describing interacting particles of different species, singly occupying each site. The Hamiltonian acts on each bond $(i,i+1)$ by the operator $P_{i,i+1}$ which permutes neighboring particles, independently of their type:

$$H=\sum_{i=1}^{L}P_{i,i+1}. \tag{21}$$

For this generic model we can directly verify that the energy current operator

$$J^E=-i\sum_{i=1}^{L}[P_{i-1,i},P_{i,i+1}] \tag{22}$$

coincides with a conserved quantity[12] and so commutes with the Hamiltonian.

Now considering three types of particles, corresponding to empty sites, up spins, and down spins, we recover the t-J model[12] for special values of J/t. This model describes a system of interacting fermions subject to a constraint of no double occupancy, with the Hamiltonian given by

$$H=-t\sum_{\sigma,i=1}^{L} P(c_{i\sigma}^{\dagger}c_{i+1\sigma}+\text{H.c.})P + J\sum_{i=1}^{L}(\vec{S}_i\vec{S}_{i+1}-n_in_{i+1}/4)+2N-L, \quad (23)$$

where $c_{i\sigma}$ ($c_{i\sigma}^{\dagger}$) are annihilation (creation) operators of a fermion on site i with spin $\sigma=\uparrow,\downarrow$. $P=\Pi_{i=1}^{L}(1-n_{i\uparrow}n_{i\downarrow})$ is a projection operator on sites with no double occupancy, $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$, $N=\Sigma_{i=1,\sigma}^{L}n_{i\sigma}$.

This model is integrable for $J/t=0$, corresponding to the $U/t\rightarrow\infty$ limit of the Hubbard model or to the model (21) where permutations act only on bonds with ''empty-up spin'' or ''empty-down'' configurations. For this case, we found that the corresponding energy current commutes with the Hamiltonian, as is also known for the particle current.[13] Finally, for $J=2t$, the ''supersymmetric'' model (23) is also integrable and the energy current coincides with the conserved quantity Q_3 as is presented in Ref. 12. Therefore the transport coefficients of the supersymmetric t-J model are also anomalous.

The above results imply that, at least, certain quantities related to transport coefficients in IQM systems are nonergodic (see, however, Ref. 14 for the recent notion of ''quantum mixing''). Within linear response theory, this translates to ideal conducting behavior at finite temperatures, the charge stiffness D being a measure of nonergodicity. We also expect that the noise spectrum, described by the current-current correlations, shows anomalous behavior characteristic of a ballistic rather than a diffusive system. This behavior is to be contrasted to the normal dissipative behavior we found[6,7] for similar nonintegrable systems with no conservation laws.

In conclusion, IQM systems open the possibility of studying a new kind of (nearly) dissipationless finite-temperature transport in quantum many-body systems. The observability of these effects will depend on the robustness of ideal conducting behavior for systems close to integrability, an issue very similar to the one in classical near-integrable nonlinear systems.

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[1] M. Lüscher, Nucl. Phys. B **117**, 475 (1976).
[2] B. S. Shastry, Phys. Rev. Lett. **56**, 1529 (1986); E. Olmedilla and M. Wadati, Phys. Rev. Lett. **60**, 1595 (1988).
[3] M. G. Tetel'man, Sov. Phys. JETP **55**, 306 (1982); H. B. Thacker, Physica D **18**, 348 (1986).
[4] M. P. Grabowski and P. Mathieu, Ann. Phys. (N.Y.) **243**, 299 (1996).
[5] H. Castella, X. Zotos, and P. Prelovšek, Phys. Rev. Lett. **74**, 972 (1995).
[6] X. Zotos and P. Prelovšek, Phys. Rev. B **53**, 983 (1996).
[7] H. Castella and X. Zotos, Phys. Rev. B **54**, 4375 (1996).
[8] R. Kubo, J. Phys. Soc. Jpn. **12**, 570 (1957).
[9] P. Mazur, Physica **43**, 533 (1969); M. Suzuki, *ibid.* **51**, 277 (1971).
[10] W. Kohn, Phys. Rev. **133**, 171 (1964).
[11] B. Sutherland, Phys. Rev. B **12**, 3795 (1975); P. P. Kulish and N. Yu. Reshetikhin, Sov. Phys. JETP **53**, 108 (1981).
[12] F. H. L. Essler and V. E. Korepin, Phys. Rev. B **46**, 9147 (1992).
[13] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[14] G. Jona-Lasinio and C. Presilla, Phys. Rev. Lett. **77**, 4322 (1996).