Evidence for ideal insulating/conducting state in a 1D integrable system

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Using numerical diagonalization techniques we analyze the finite temperature/frequency conductance of a one dimensional model of interacting spinless fermions. Depending on the interaction, the observed finite temperature charge stiffness and low frequency conductance indicate a fundamental difference between integrable and non-integrable cases. The integrable systems behave as ideal conductors in the metallic regime and as ideal insulators in the insulating one. The non-integrable systems are, as expected, generic conductors in the metallic regime and activated ones in the insulating regime.

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In classical integrable systems the existence of a macroscopic number of conservation laws has a profound consequence, dissipationless transport \[1\]. The analogous effect in nontrivial quantum integrable systems has been studied only recently in a prototype model of dissipation \[2\]. In this model, describing a particle interacting with a fermionic bath in one dimension, we found that the tagged particle shows ideal mobility even at finite temperatures, \(T > 0\), when the system is integrable. It is desirable to extend these ideas to homogeneous many-body models, which are at present of particular interest in connection with strongly correlated electrons. In this field, most analytical findings are on integrable 1D models as the Hubbard \[3\] or the spinless fermions with nearest neighbor interaction model \[4\].

Progress in the study of dynamical response at \(T > 0\) is hindered by the lack of reliable methods. The only attempts, which however might obscure the role of integrability, start from a Luttinger liquid effective Hamiltonian description \[5\].

In this work, based on a recent reformulation of the finite temperature charge stiffness \[2\] and numerical methods for calculating \(T > 0\) dynamical conductivities \(\sigma(\omega)\) \[6\] on finite size systems, we present evidence of the importance of integrability for transport properties.

From linear response theory, the real part of the conductance \(\sigma(\omega)\) at frequency \(\omega\) is given by:

\[
\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{reg}(\omega),
\]

\[
\sigma_{reg}(\omega) = \frac{1 - e^{-\beta\omega}}{\omega} \sum_{n,m \neq n} p_n \langle n \mid \hat{j} \mid m \rangle^2 \delta(\omega - \epsilon_m + \epsilon_n),
\]

where \(| n \rangle, \epsilon_n\) denote the eigenstates and eigenvalues of the Hamiltonian, \(p_n\) the corresponding Boltzmann weights, \(\hat{j}\) the current operator and \(\beta = 1/k_BT\). We will consider 1D tight-binding models of \(L\) sites \((k_B = \hbar = e = 1)\).

\(\sigma(\omega)\) satisfies the optical sum rule \[7\]:

\[
\int_{-\infty}^{\infty} \sigma(\omega) d\omega = \frac{\pi}{L} \langle \hat{T} \rangle,
\]

where \(\langle \hat{T} \rangle\) denotes the thermal expectation value of the kinetic energy. The sum rule \[7\] together with Eqs.\(1,2\) can be used for the evaluation of the stiffness \(D(T)\) \[8\]. It will be however more convenient to discuss the behavior of \(D\) at finite temperatures, with a generalization of the original Kohn’s approach \[8\] for zero temperature, by relating \(D(T)\) to the thermal average of curvatures of energy levels subject to a fictitious flux \(\phi\) \[2\] :

\[
D = \frac{1}{L} \sum_n p_n D_n = \frac{1}{L} \sum_n \left( p_n \frac{1}{2} \frac{\partial^2 \epsilon_n(\phi)}{\partial \phi^2} \right)_{\phi \rightarrow 0}.
\]

At zero temperature \(D(T = 0) = D_0\) has been introduced \[8\] to distinguish an ideal conductor with \(D_0 > 0\) from an insulator with \(D_0 = 0\). Our aim here is to analyze the transport behavior at finite temperatures. For orientation,
at $T > 0$, a conductor can develop either to a normal conductor (resistor) with $D(T) = 0$ but $\sigma_0 = \sigma(\omega \to 0) > 0$, or remain an ideal conductor characterized by $D(T) > 0$. An insulator might develop to a normal conductor (conducting by thermally activated transport) with $D(T) = 0$, $\sigma_0(T) > 0$, remain an ideal insulator with $D(T) = 0$, $\sigma_0(T) = 0$ or even become an ideal conductor with $D(T) > 0$.

Below we present results for $\sigma(\omega)$ for the prototype 1D tight-binding model of interacting spinless fermions with nearest and next-nearest neighbor interaction. For systems with Hilbert space dimension less than typically 1000 states (after implementation of translational symmetry) we calculate $\sigma(\omega)$ directly from Eq. (2) by finding all eigenstates and evaluating current matrix elements; for systems with larger basis dimensions we use a $T > 0$ Lanczos-based numerical technique [6].

As we are interested mostly in differences in the qualitative behavior of integrable vs. non-integrable systems we can restrict our study to high temperatures thus minimizing spurious effects due to the sparse low energy level spectrum in finite size systems. It corresponds, in normal conductors, studying systems with mean free paths shorter than the lattice size.

Further, we present results for $\sigma(\omega)$ for the prototype 1D tight-binding model of interacting spinless fermions with nearest and next-nearest neighbor interaction. For systems with Hilbert space dimension less than typically 1000 states (after implementation of translational symmetry) we calculate $\sigma(\omega)$ directly from Eq. (2) by finding all eigenstates and evaluating current matrix elements; for systems with larger basis dimensions we use a $T > 0$ Lanczos-based numerical technique [6].

The Hamiltonian we study is given by:

$$\hat{H} = -t \sum_{i=1}^{L} (e^{i\phi}c_{i+1}^\dagger c_i + H.c.) + V \sum_{i=1}^{L} n_i n_{i+1} + W \sum_{i=1}^{L} n_i n_{i+2}$$  \quad (6)

where $c_i(c_i^\dagger)$ are annihilation (creation) operators of a spinless fermion at site $i$, $n_i = c_i^\dagger c_i$. This Hamiltonian is integrable using the Bethe ansatz method for $W = 0$ and non-integrable for $W \neq 0$. For $W = 0$ and $V < 2t$ the ground state is metallic, while for $V > 2t$ a charge gap opens and the system is an insulator.

We study numerically various size systems with periodic boundary conditions and $M = L/2$ fermions (half-filling). The results for $L = 8, 12, 16$ are obtained by the complete diagonalization of the Hamiltonian, while for $L = 20, 24$ the Lanczos method is employed. It should be mentioned that in the latter cases results, e.g. for $D^*$, are subject to small statistical error due to finite random sampling [6].

**Metallic state:** In Fig. 1 we show the finite temperature conductance for an integrable case. To study the finite size dependence of the charge stiffness, we plot in the inset $D^*$ as a function of $1/L$; the dashed lines indicate a $3^{rd}$ order polynomial extrapolation based on the $L = 8, 12, 16$ site systems, suggested by the very good agreement obtained with the $T = 0$ analytical result (square at $1/L = 0$) [6]. We find that for $L \to \infty$ the extrapolated $D^* \neq 0$. At the same time $\sigma_0 = \sigma(\omega \to 0) \to 0$ as $I(\omega)$ seems to approach $\omega = 0$ with zero slope ($\sigma(\omega)$ is the derivative of $I(\omega)$). This behavior is reminiscent of a pseudogap. These two results indicate that the integrable system behaves as an ideal conductor at $T > 0$. Moreover we find that the normalized $D^*$ approaches a nontrivial finite value $D^*_\infty$ in the limit $T \to \infty$, depending on $V/t$ and filling, as both $D$ and $\langle -T \rangle$ are proportional to $a_0^2$ in this limit.

In Fig. 2 we show $I(\omega)$ and $D^*$ for a non-integrable case. Here, as expected for a generic metallic conductor (resistor), we find that $D^*$ scales to zero, probably exponentially with system size, and $\sigma_0 > 0$ if $I(\omega)$ approaches $\omega = 0$ with a finite slope. These two results imply that the non-integrable system behaves as a normal conductor at $T > 0$.

To further point out the particularity of integrable systems, we investigate the behavior of the conductance on approaching the integrable point $W = 0$. In Fig. 3 we present $I(\omega)$ scanning the parameter $W$. We clearly recognize a continuous transfer of the $\delta$–function weight $I(\omega = 0) = D^*$ at $W = 0$ to low frequencies, both for $W > 0$ and $W < 0$. From a calculation of the second frequency moment of the conductance at infinite temperature, we estimate the frequency range of $\sigma(\omega) > 0$ proportional to $(V - W)^2 + W^2/2t^2$. Due to remaining finite size effects we are not attempting yet to make more quantitative statements about the critical behavior of the low frequency conductance.

These numerical results on the finite temperature charge stiffness, although not conclusive, strongly suggest a qualitative difference between integrable and nonintegrable systems. We can argue about this difference by considering the expression for $D$ as a thermal average of the curvatures of levels subject to a fictitious flux. The integrable systems, as they are characterized by absence of repulsion between levels, they allow larger fluctuations in the level response to a flux and thus plausibly a finite charge stiffness.

On the other hand in the nonintegrable systems, because of level repulsion, the motion of levels with flux is constrained within a characteristic level spacing that is proportional to $e^{-\alpha L}$, the density of states, and thus to a vanishing charge stiffness with increasing system size.
We have also verified that in our integrable system the absence of level repulsion leads to Poisson statistics of the level spacings while in the integrable one the level repulsion leads to GOE statistics \[10\].

As for \(\sigma_0\), it is more difficult to ascertain its behavior in the infinite size limit from numerical results in finite size systems. For the nonintegrable systems we find, as expected, a finite value for \(\sigma_0\). For the finite size integrable systems that we can study, although \(I(\omega)\) seems to approach \(\omega = 0\) with a zero slope, we cannot really exclude a finite slope for \(L \to \infty\). However, from the physical point of view, even in this case one can expect ideal conductance provided the charge stiffness remains finite. It is indicative of a free accelerating system similar in the spirit of a two fluid model.

**Insulating state:** In Fig. 4 we show \(I(\omega)\) for the integrable case \(V = 4t, W = 0\). At this value of \(V > 2t\) the ground state is insulating characterized by \(D_0 = 0\) and a charge gap \(\Delta_0 \simeq t\) \[11\]. We find that, at finite temperatures, \(D^*(T > 0) = I(\omega = 0)\) seems also to decrease exponentially with the system size scaling to zero for \(L \to \infty\). This precludes a possibility for ideal conductance at \(T > 0\). Furthermore \(I(\omega)\) seems to approach \(\omega = 0\) with zero slope, showing a depletion of weight within a low frequency region of order \(\omega < t\). These are characteristics of an ideal insulator, not conducting even at high temperatures \(T \gg \Delta_0\).

In contrast, as shown in the inset of Fig. 4 (for \(L = 16\)), non-integrable systems of roughly the same charge gap exhibit a qualitatively different behavior. \(I(\omega)\) approaches \(\omega = 0\) with finite (although small) slope, consistent with a small static conductance \(\sigma_0 > 0\). As expected, conductance here is of a thermally activated character, since appreciable \(\sigma_0 > 0\) appears only at elevated \(T \gg t\).

To discuss the behavior of the conductance in the insulating regime, it is a good starting point to think about the large \(V/t\) limit. In this limit the energy spectrum splits in "Hubbard" bands with a fixed number \(N_0\) of soliton-antisoliton \((s\bar{s})\) pairs, solitons corresponding to nearest neighbor occupied sites while antisolitons to nearest neighbor empty sites. In the \(V = \infty\) limit solitons and antisolitons are impenetrable. Crossing can only occur by annihilation and creation of a pair which corresponds to mixing with other "Hubbard" bands and it has an amplitude of order \(t^2/V\). The states are grouped in characteristic sequences of solitons and antisolitons and the energies of the eigenstates are the same as those of a gas of \(2N_0\) impenetrable particles.

To analyze the flux \(\phi\) dependence of the energy we note that the phase associated with the hopping of a soliton in a given direction is opposite to the phase picked by an antisoliton; so solitons and antisolitons carry opposite charge. It follows that, in this \(V = \infty\) limit, the flux \(\phi\) dependence of the hopping matrix elements can be removed by a redefinition of the phase of the states. A nontrivial \(\phi\) dependence would have appeared if by successively applying the Hamiltonian on a given \(s\bar{s}\) state we could bring it to an equivalent one but with an accumulation of a nonzero phase factor. This process, which corresponds to a uniform translation of fermions, is not possible provided we do not allow for soliton-antisoliton crossing.

Therefore, as we have also numerically verified, the width of the "Hubbard" band is of the order of \(N_0t\) but the energy levels are independent of the flux \(\phi\) and \(D\) is strictly zero. At the same time it is reasonable to argue that a static electric field acting on impenetrable particles of opposite charge cannot produce a uniform current and the static conductance \(\sigma_0\) should also be zero. Thus, in this \(V = \infty\) limit, we find an ideal insulator at any temperature independently of the integrability of the system.

Now, allowing crossing of solitons and antisolitons leads to a \(D \neq 0\) in a finite size system. However our numerical results above suggest that \(D\) scales again to zero exponentially with the system size. To estimate the dependence of the energies in the flux \(\phi\) due to \(s\bar{s}\) crossing we can argue in terms of ordinary perturbation theory. As above, a \(\phi\) dependence will appear if by applying the Hamiltonian on a \(s\bar{s}\) state we can bring it to an equivalent one but with an accumulation of a nonzero phase factor. This process, that is now possible, necessitates the successive creation and annihilation of \(N_0\) \(s\bar{s}\) pairs and will appear in the \(\sim N_0\) order in perturbation expansion. As it involves \(N_0\) intermediate states with energy difference \(V\) it is an exponentially small contribution.

Further, taking the point of view that the large \(V/t\) limit is the fixed point of the insulating behavior, we can argue against the scenario of an insulator at zero temperature developing to an ideal conductor at finite temperatures.

The next point to discuss is the possibility of an integrable insulating system developing into a normal conductor (resistor) at finite temperatures. Unfortunately this point can only be settled after clarifying the exact connection between the static conductance, \(\sigma_0\), and integrability. However, consistently with our conjecture, we have found from independent spectral analysis that whenever the insulating system is integrable, the level spacing distribution is Poisson and \(\sigma_0\) seems to vanish, while when the system is nonintegrable, the statistics is GOE and \(\sigma_0 \neq 0\).

Finally, in order to visualize the above picture of the insulating state, we present in Fig. 5 calculations in the large \(V/t\) limit. For \(V = 8t\) the system is characterized by a much larger charge gap \(\Delta_0 \sim 6t\). Indeed we see a region of finite conductance in the frequency region \(0 < \omega < 4t\) corresponding to excitations within the first, one soliton-antisoliton pair, "Hubbard" band. The weight in this region is increasing exponentially with temperature, a sign of activated transport. It is followed by a vanishing conductance up to \(\omega \sim 6t\), when transitions from the ground state to the first Hubbard band start.

**Comments:** Our conclusions should hold for other integrable systems as well. Since the anisotropic (and isotropic)
spin-1/2 Heisenberg model is equivalent to the integrable \((W = 0)\) model, analogous conclusions should apply for the spin stiffness and spin diffusion at \(T > 0\). Furthermore, we have numerical evidence (to be presented elsewhere) that also the integrable 1D Hubbard model, exhibits the same features found for the prototype model \((W = 0)\). Namely, out of half filling, the system seems to be an ideal conductor, while at half-filling results are consistent with an ideal insulator with \(\sigma_0(T > 0) = 0\), for any strength of the repulsive interaction.

We should stress that the above results are only indicative of a relation between integrability and finite temperature conductance and our arguments are far from rigorous. Further analytical and numerical studies are necessary to prove the validity of our conclusions. However, taking into account present limitations on the size of the systems that can be numerically studied and the absence of analytical work, we think that the results presented here are qualitatively clear enough to warrant further work on this novel idea. Furthermore, an experimental effort is necessary to observe this unusual conductance enhancement. Finally the stability of this effect to deviations from integrability should be studied, similarly to the problem of stability of classical soliton systems.

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FIG. 1. Integrated conductance \(I(\omega)\) for \(V = 1.5t, W = 0, T = 2t\), for \(L = 12 - 16\) (exact diagonalization - full lines) and \(L = 20, 24\) (Lanczos method - dotted lines). Inset shows normalized charge stiffness \(D^*\) vs. \(1/L\): exact diagonalization (disks), analytical result (square) and 3\(^{rd}\) order polynomial extrapolation from \(L = 8, 12, 16\) (dotted line).

FIG. 2. Integrated conductance \(I(\omega)\) for \(V = 1.5t, W = t, T = 2t\), for \(L = 12 - 20\). In the inset \(\ln D^*\) vs. \(L\) is plotted. Notation is as in Fig. 1.

FIG. 3. \(I(\omega)\) for \(L = 16, V = 1.5t, T = 2t\), and \(W/t = -0.5, -0.3, 0.0, 0.3, 0.5\).

FIG. 4. \(I(\omega)\) for \(V = 4t, W = 0, T = 4t\), for \(L = 12, 16\) (full lines with increasing line thickness-exact diagonalization) and \(L = 20\) (Lanczos method-dotted line). Inset: \(I(\omega)\) for \(L = 16, T = 4t\).

FIG. 5. \(I(\omega)\) for \(V = 8t, W = 0, T = 4t\), for \(L = 12, 16\) with the notation as in Fig. 4.
$I = 1.5t, W=0, T=2t$

$\frac{1}{L}$

$D^*$

$\frac{T}{t} = 1, 2, 100$

fig. 1 X. Zotos, P. Prelovsek
$V = 1.5t, W = t, T = 2t$

Fig. 2 X. Zotos, P. Prelovsek
fig. 3  
X. Zotos, P. Prelovsek
\( V = 4.0t, \ W = 0, \ T = 4t \)

\[ L = 16 \]

\( V = 4t, \ W = 0 \]
\( V = 6t, \ W = +t \]
\( V = 3t, \ W = -t \]

fig. 4  
X. Zotos, P. Prelovsek
V=8.0t, W=0, T=4t

fig. 5 X. Zotos, P. Prelovsek