Evidence for ideal insulating or conducting state in a one-dimensional 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 nonintegrable cases. The integrable systems behave as ideal conductors in the metallic regime and as ideal insulators in the insulating one. The nonintegrable systems are, as expected, generic conductors in the metallic regime and activated ones in the insulating regime.

In classical integrable systems there is experimental[1] and theoretical evidence[2] that the existence of a macroscopic number of conservation laws has a profound consequence: dissipationless transport. The analogous effect in nontrivial *quantum* integrable systems has been studied only recently in a prototype model of dissipation.[3] 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 test 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 one-dimensional (1D) models as the Hubbard[4] or the spinless fermions with nearest-neighbor interaction model.[5]

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.[6] In this work, based on a recent reformulation of the finite temperature charge stiffness[3] and numerical methods,[7] we study the $T>0$ dynamical conductivity $\sigma(\omega)$ on finite-size systems. The results and arguments that will be presented below do not constitute a *proof* that integrable many-body systems are ideal conductors or insulators. However, motivated by (i) the coincidence of ideal conducting behavior with integrability in our model, (ii) analogous behavior in classical systems, and (iii) recent studies relating transport properties of quantum systems to level statistics[8] and level statistics to integrability,[9] we are led to conjecture that the observed ideal conducting behavior is related to the integrability of our model.

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

$$\sigma(\omega)=2\pi D\delta(\omega)+\sigma_{\rm reg}(\omega), \qquad (1)$$

$$\sigma_{\rm reg}(\omega)=\frac{1-e^{-\beta\omega}}{\omega}\frac{\pi}{L}\sum_{n,m\neq n} p_n|\langle n|\hat{j}|m\rangle|^2\delta(\omega-\epsilon_m+\epsilon_n), \qquad (2)$$

where $|n\rangle,\epsilon_n$ denote the eigenstates and eigenvalues of the Hamiltonian, p_n are the corresponding Boltzmann weights, $\hat{j}$ is 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:[10]

$$\int_{-\infty}^{\infty}\sigma(\omega)d\omega=\frac{\pi}{L}\langle-\hat{T}\rangle, \qquad (3)$$

where $\langle\hat{T}\rangle$ denotes the thermal expectation value of the kinetic energy. The sum rule (3) together with Eqs. (1,2) can be used for the evaluation of the stiffness $D(T)$.[11,3] It will be, however, more convenient to discuss the behavior of D at finite temperatures, with a generalization of the original Kohn's approach[11] for zero temperature, by relating $D(T)$ to the thermal average of curvatures of energy levels subject to a fictitious flux ϕ:[3]

$$D=\frac{1}{L}\sum_n p_nD_n=\frac{1}{L}\sum_n p_n\frac{1}{2}\frac{\partial^2\epsilon_n(\phi)}{\partial\phi^2}\Bigg|_{\phi\to 0}. \qquad (4)$$

At zero temperature $D(T=0)=D_0$ has been introduced[11] 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-neighbor 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.[7]

As we are interested mostly in differences in the *qualitative behavior* of integrable vs nonintegrable 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, to studying systems with mean free paths shorter than the lattice size.

Further, we present the integrated and normalized intensity

$$I(\omega)=D^*+\frac{2L}{\pi\langle-\hat{T}\rangle}\int_{0^+}^{\omega}d\omega'\sigma(\omega'),\quad D^*=\frac{2LD}{\langle-\hat{T}\rangle},\quad (5)$$

as it contains the relevant information in the conductance and avoids the smoothing procedure of the discrete $\sigma(\omega)$ spectra of finite-size systems.

The Hamiltonian we study is given by

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

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 $W=0$ (Ref. 5) and nonintegrable for $W\neq0$. 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.[7]

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 third-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 $1/L=0$).[12] We find that for $L\rightarrow\infty$ the extrapolated $D^*\neq0$. At the same time $\sigma_0=\sigma(\omega\rightarrow0)\rightarrow0$ 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^*_{∞} in the limit $T\rightarrow\infty$, depending on V/t and filling, as both D and $\langle-\hat{T}\rangle$ are proportional to β in this limit.

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

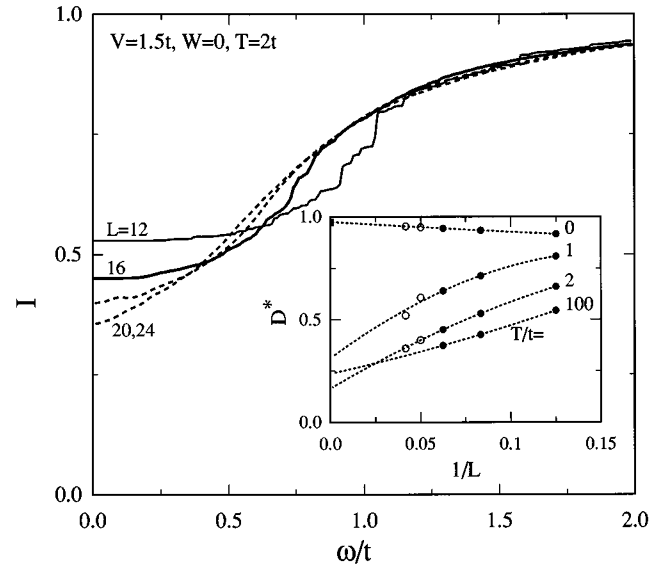

FIG. 1. Integrated conductance $I(\omega)$ for $V=1.5t,W=0,T=2t$, for $L=12-16$ (exact diagonalization, full fines) and $L=20,24$ (Lanczos method, dotted lines). Inset shows normalized charge stiffness D^* vs $1/L$: exact diagonalization (closed circles), $T>0$ Lanczos method (open circles), analytical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

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 δ-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.

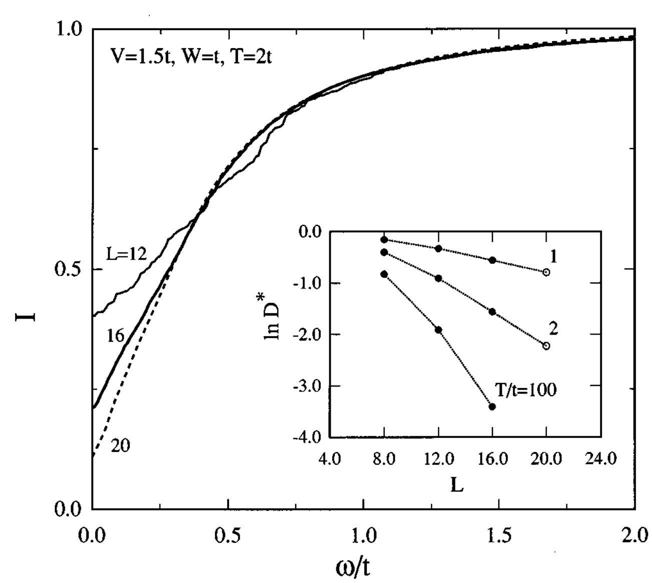

FIG. 2. Integrated conductance $I(\omega)$ for $V=1.5t,W=t,T=2t$, for $L=12-20$. In the inset $\ln D^*$ vs L is plotted. Notation is as in Fig. 1.

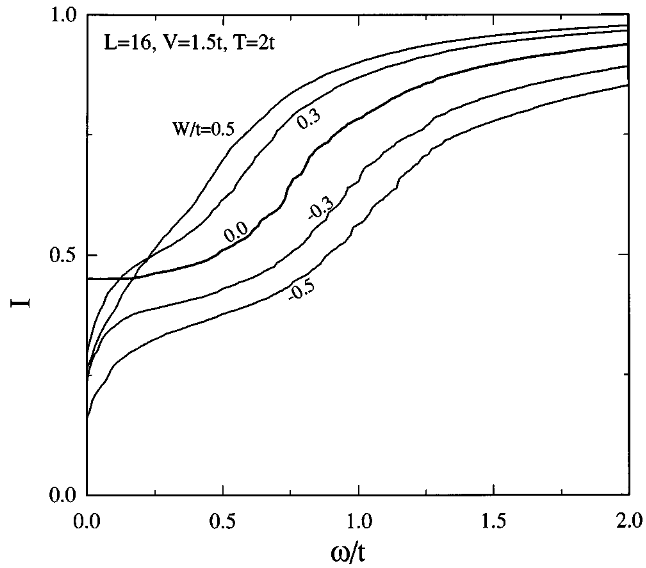

FIG. 3. $I(\omega)$ for $L=16, V=1.5t, T=2t$, and $W/t=-0.5,-0.3,0.0,0.3,0.5$.

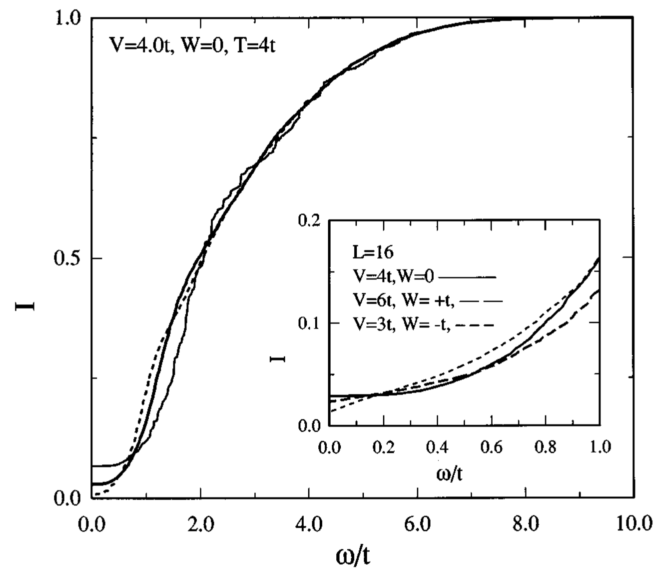

FIG. 4. $I(\omega)$ for $V=4t, W=0, T=4t$, for $L=12,16$ (full lines with increasing line thickness, exact diagonalization) and $L=20$ (Lanczos method, dotted line). Inset: $I(\omega)$ for $L=16$, $T=4t$.

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, 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 $e^{-\alpha L}$, inversely proportional to 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 Gaussian orthogonal ensemble (GOE) statistics.[9]

As for σ_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 σ_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 $\Delta_0\simeq t$.[13] 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 $L=16$), nonintegrable 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_s of soliton-antisoliton $(s\bar{s})$ pairs, solitons corresponding to nearest-neighbor occupied sites, and 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 therefore grouped in characteristic sequences of solitons and antisolitons.

To analyze the flux ϕ 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 ϕ dependence of the hopping matrix elements can be removed by a redefinition of the phase of the states. A nontrivial ϕ 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 $N_s t$, but the energy levels are independent of the flux ϕ 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 σ_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. 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 σ_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 σ_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.

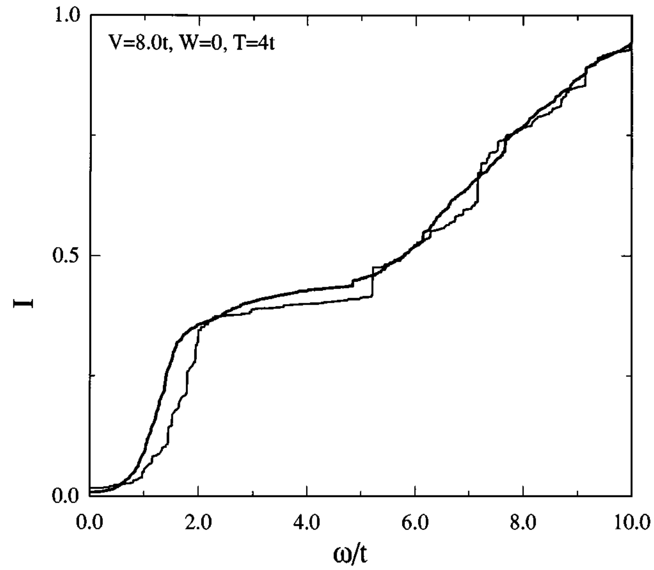

FIG. 5. $I(\omega)$ for $V=8t, W=0, T=4t$, for $L=12,16$, with the notation as in Fig. 4.

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 (6), analogous conclusions should apply for the spin stiffness and spin diffusion at $T>0$. Furthermore, we have numerical evidence (to be presented elsewhere) that the integrable 1D Hubbard model also exhibits the same features found for the prototype model (6). 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 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, a problem similar to the stability of classical soliton systems.

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