Breakdown of Luttinger liquid state in a one-dimensional frustrated spinless fermion model

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The Haldane hypothesis about the universality of the Luttinger liquid (LL) behavior in conducting one-dimensional fermion systems is checked numerically for the spinless fermion model with next-nearest-neighbor interactions. It is shown that for the large enough interactions the ground state can be gapless due to frustrations but at the same time might not belong to the same universality class as a simple LL. The exponents of the correlation functions for this unusual conducting state are found numerically by a finite-size method.

One-dimensional (1D) Fermi systems have a number of peculiarities that distinguish them drastically from three-dimensional (3D) ones (for review, see Ref. 1). In particular, gapless (metallic) 1D systems of the interacting fermions never behave as a normal Fermi liquid. Haldane[2] has proposed another class of universality which is called the Luttinger liquid (LL) state. In this state the low-energy excitation spectrum consists of three branches, namely, (i) the density fluctuation boson mode, (ii) current, and (iii) charge excitations with the velocities v_S, v_J, and v_N, correspondingly.

The first one is connected with the variation of the total energy E of the system under the variation of the total momentum P, $v_S=\delta E/\delta P$; the second one (v_J), with the variation of the energy under a shift of all the particles in momenta space, which can be done physically by the application of magnetic flux to the system closed as a ring; and the third one, with the variation of the chemical potential μ under the change of the total number of particles N, $v_N=(L/\pi)\delta\mu/\delta N$, where L is the length of the system. In the LL state there is an exact relation between the velocities

$$\chi\equiv v_J v_N/v_S^2=1, \tag{1}$$

which is the criterion of LL. The only dimensionless parameter that determines all the infrared properties of the system (e.g., time and space asymptotics of fermionic Green functions and susceptibilities) is the ratio

$$e^{-2\varphi}=v_N/v_S=v_S/v_J. \tag{2}$$

Original arguments by Haldane were based on the exact Bethe-Ansatz solutions as well as on the perturbation theory for weakly interacting systems. The set of models that fall into the LL universality class incorporates all the ''common'' short-ranged 1D models, such as the spinless fermion and the Hubbard models with the nearest-neighbor interactions, but there is no rigorous proof that *all* the possible 1D models should belong to this class, too. For the discussion in terms of the conformal field theory, see, e.g., Ref. 3 and references therein. All the known analytical and numerical results about 1D fermion systems confirm the Haldane hypothesis,[4,5] at least for fermions without internal degrees of freedom. Otherwise, the modification of the LL state which is known as the multicomponent LL state[6] can take place.

Anderson[7] has supposed that some two-dimensional (2D) systems such as the copper-oxide superconductors belong to the class of LL also. This fact made the concept of the Luttinger liquid one of the most ''fashionable'' in the contemporary many-particle physics. Therefore the investigation of a status of the Haldane hypothesis seems to be important. Here we present a counterexample to this hypothesis based on exact numerical results for the spinless fermion model.

We proceed with the Hamiltonian

$$H=-t\sum_{i=1}^{L}(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i)+V\sum_{i=1}^{L}n_i n_{i+1}+V'\sum_{i=1}^{L}n_i n_{i+2}, \tag{3}$$

where $c_i^\dagger$, c_i are Fermi creation and annihilation operators on a site i, $n_i=c_i^\dagger c_i$. We investigated a phase diagram of this model, and the results are presented in Ref. 8. In particular, it has been shown that for a half-occupied case, $\rho=N/L=1/2$ and arbitrarily small t the ground state turns out to be gapless (metallic) along the line $V=2V'$. It is the consequence of frustrations which lead to the macroscopically large degeneracy (finite entropy per a site) of the ground state at the Ising limit $t=0$. A similar result has been obtained also in Ref. 9. It is important that, according to our calculations, the metallic region has nonzero width in the (V,V') plane. One can assert that the gap is zero at $(V/2)-0.6t\leqslant V'\leqslant(V/2)$, and that the ground state is insulating at $|(V/2)-V'|>t$. To check the Haldane hypothesis we restrict ourselves by the consideration of the straight line $V=2V'$ where the system is definitely metallic. According to our calculations some deviations from the LL behavior exist in a whole domain along this line; however, the obtained results are not sufficient to determine its exact boundaries at the phase diagram.

Similarly, we have a metallic state for $\rho=2/3$ at $V'=0$ and arbitrarily large V or, vice versa, at $V=0$ and arbitrarily large V'. There are rare examples of a metallic state with strong interactions and it seems to be interesting to check the Haldane assumptions for this unusual case. As was already mentioned the original Haldane hypothesis is based, on the one hand, on the consideration of exactly integrable systems and, on the other hand, on the perturbation treatment of systems with weak correlations. Therefore, its validity in the case under consideration is not obvious. Note that the ''un-

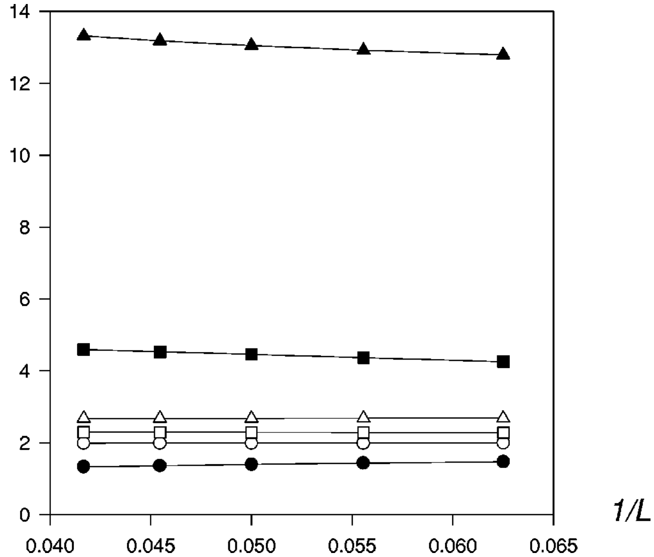

FIG. 1. The dependence of the velocities [Eq. (4), in t units] on the inverse size of the cluster; empty symbols correspond to $V=0.5t$, $V'=0$, black symbols correspond to $V=200t$, $V'=100t$ (circles: v_J; squares: v_S; triangles: v_N).

usual'' character of a metallic state at $\rho=1/2$, $V\approx 2V'$ has been mentioned in Ref. 9 but the detail description of this state has not been presented.

We have carried out the calculations of a ground state of the model (3) by the Lanczos method for finite clusters with the consequent extrapolation to $L\rightarrow\infty$ (for details, see Ref. 8). Velocities of low-lying excitations have been calculated as[5,10]

$$v_S=\frac{L}{2\pi}[E_{1p}(L,N)-E_0(L,N)],$$

$$v_J=\frac{L}{2\pi}[E_a(L,N)-E_0(L,N)], \tag{4}$$

$$v_N=\frac{L}{\pi}[E_0(L,N+1)-2E_0(L,N)+E_0(L,N-1)].$$

Here $E_0(L,N)$ is the ground-state energy of the cluster with L sites for periodic boundary conditions and N particles, $E_a(L,N)$ is the ground-state energy for antiperiodic boundary conditions (transition to the antiperiodic conditions corresponds to magnetic flux $\Phi=1/2$ of the flux quantum), and $E_{1p}(L,N)$ is the ground-state energy for the minimal nonzero total momentum $P=2\pi/L$. The corresponding results for different cluster lengths are shown in Fig. 1. One can see that the cluster sizes in our calculations are sufficient to consider in a rather reliable way the limit of the infinite chain. Then we have verified the criterion of the LL $\chi=1$ using Eq. (1).

The results of the test calculations for the case $\rho=1/2$, $V'=0$, $0\leqslant V<2t$ where the system is in the LL state definitely[2] are shown in Fig. 2 (open circles and triangles). We also present in the same figure the calculated values of χ along the line $V=2V'$. One can see that at $V\leqslant 10t$ we have, within the accuracy of the computations, $\chi\approx 1$, in an agreement with the Haldane hypothesis. However, for $V\geqslant 30t$ the

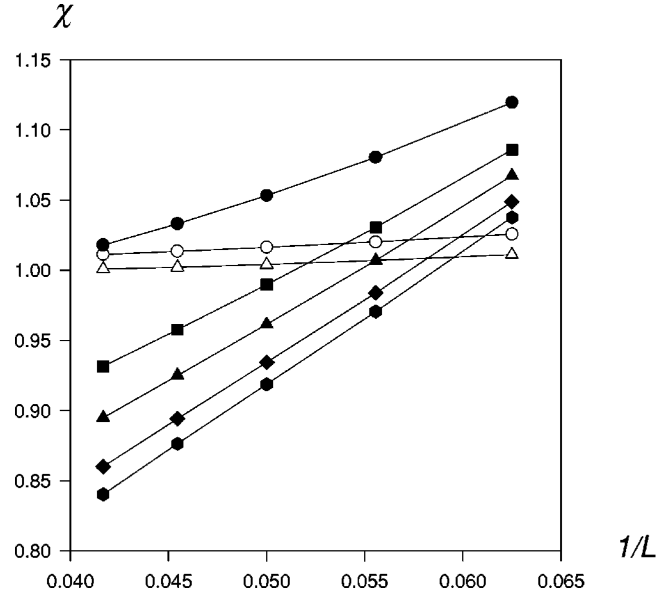

FIG. 2. The dependence of the ratio χ [Eq. (1)] on the inverse size of the cluster; empty symbols correspond to $V'=0$ (circles: $V=0.5t$; triangles: $V=1.5t$); black symbols correspond to $V=2V'$ (circles: $V=10t$; squares: $V=30t$; triangles: $V=50t$; diamonds: $V=100t$; hexagons: $V=200t$).

values of χ is definitely less than unity, which is obvious even without extrapolation to $L\rightarrow\infty$, since $\chi(L)<1$ for finite L and diminishes with L increase. Therefore we have demonstrated that there are one-dimensional conducting systems of interacting fermions which *are not* LL. The breakdown of the LL picture is caused by the competition of nearest-neighbor and next-nearest-neighbor interactions (i.e., frustration) which allows the system to be metallic in the limit of strong interactions. A schematic phase diagram is shown in Fig. 3. The question is still open whether the transition from insulating state to the non-LL conducting state is the direct one or an intermediate conducting LL phase exists. At the same time, our calculations demonstrate that for $\rho=2/3$ the relation (1) takes place with the accuracy of calculations for any values of parameters under consideration even along the

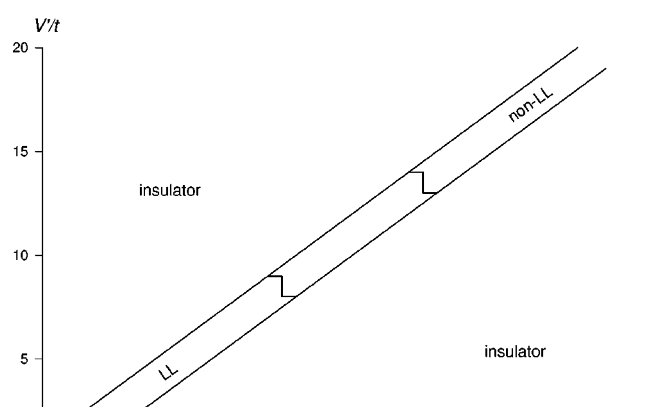

FIG. 3. The phase diagram of the model. The boundary between conducting LL and non-LL phases is shown schematically by zigzags.

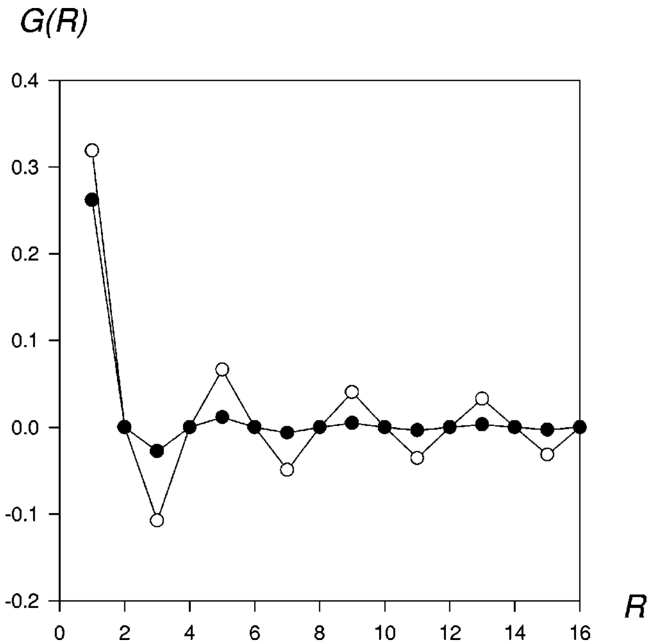

FIG. 4. The dependence of the correlation functions $G(R)$ [Eq. (5)] for $L=32$; open circles correspond to $V=V'=0$, black ones correspond to $V=2V', V\to\infty$.

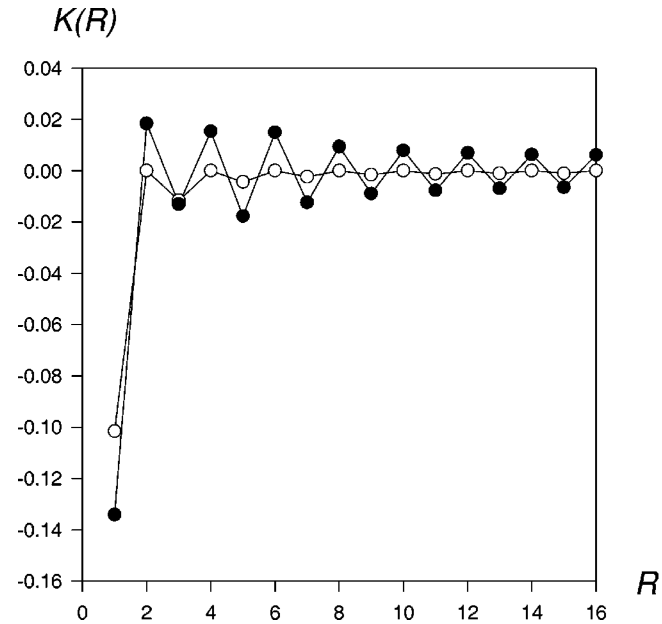

FIG. 5. The same as in Fig. 4, for $K(R)$ [Eq. (5)].

lines $V=0$ or $V'=0$. It would be very interesting to understand the reason for the difference between these two cases with strong frustrations.

We also have calculated the static correlation functions

$$G(R)=\langle c_R^\dagger c_0\rangle, \tag{5}$$

$$K(R)=\langle \delta n_R \delta n_0\rangle,$$

where angular brackets mean the averaging over the ground state, $\delta n_i = n_i - \rho$. In LL the following asymptotics have to be valid at $R \gg 1$ (Ref. 2),

$$G(R)\sim \sum_{m=0}^{\infty} C_m \sin[(2m+1)k_F R] R^{-\eta_m}, \tag{6}$$

$$K(R)\sim \sum_{m=0}^{\infty} D_m \cos(2mk_F R) R^{-\theta_m},$$

where $\eta_m = \frac{1}{2}e^{-2\varphi}+2(m+\frac{1}{2})^2 e^{2\varphi}$, $\theta_m = 2m^2 e^{2\varphi}$ $(m>0)$, $k_F=\rho/2$ is the Fermi momentum. The most important exponent α determines the behavior of the one-particle distribution function $n(k)$ near Fermi surface

$$n(k)\approx n(k_F) - C\,\text{sign}(k-k_F)|k-k_F|^{\alpha}, \tag{7}$$

where $\alpha=\eta_0 - 1$.

However, we cannot use these expressions *a priori* because the system under consideration is not always LL. We have found the asymptotics of the correlation functions by direct computation. It is known (see, e.g., Ref. 11) that it is very difficult to find the correlation exponents from the calculations for a given L, even if L is as large as 32. Therefore we use the finite-size scaling technique.[12]

Specifically we use the following procedure. Our aim is to find the function $\varphi(R)\equiv\langle\phi(0)\phi(R)\rangle_\infty$ for an infinite chain. Direct calculations give us the functions $f(R,L) \equiv\langle\phi(0)\phi(R)\rangle_L$ for $R<L$. From the symmetry considerations we have $f(R,L)=f(L-R,L)$. Let us introduce the function $r(R,L)$ to have, by definition, $\varphi[r(R,L)]=f(R,L)$. Therefore

$$\lim_{L\to\infty} r(R,L)=R. \tag{8}$$

Then we introduce the new variable $\lambda\equiv R/L$ so that $r(R,L)=L\cdot r'(\lambda,L)$ where $r'(\lambda,L)$ is a new unknown function. To provide Eq. (8) we have $\lim_{L\to\infty} r'(\lambda,L)=\lambda$. Also the function r' satisfies the condition $r'(\lambda,L)=r'(1-\lambda,L)$. For small λ one has $r'(\lambda)\approx\lambda$. To satisfy all these requirements we try the function r' as Fourier series

$$r'(\lambda)=\frac{\sin(\pi\lambda)+a_3\sin(3\pi\lambda)+a_5\sin(5\pi\lambda)+\cdots}{\pi(1+3a_3+5a_5+\cdots)}. \tag{9}$$

Using the asymptotic expression similar to Eq. (6) for the dependence $f(R,L)=\varphi[Lr'(\lambda)]$ at finite L and optimizing the result with respect to both a_n and the correlation exponents we can find the latter ones with high enough accuracy. At least the results for the exponents appeared to be accurate enough for the clusters with $14\leqslant L\leqslant 26$ used in our calculations. For the testing case $V'=0$, $0<V<2t$ where the system is definitely LL the results for the correlation exponents coincide with that from the Haldane formula (6) with the accuracy of 0.5% for the function $G(R)$ and 8% for the function $K(R)$.

In the most interesting case $\chi\neq 1$ we cannot use the expression (6) and have to restrict ourselves only by the consideration of the leading terms in the asymptotics of the correlation functions which are tried in the following form:

$$G(R)\sim\left[C_1+C_2\sin\left(\frac{\pi}{2}R\right)\right]\Big/ R^{\gamma}, \tag{10}$$

$$K(R)\sim[D_1+D_2(-1)^R]/R^{\delta}$$

(we consider the case $\rho=1/2$). To diminish the number of states in the Gilbert space under consideration we use only the states that have the same (minimal) energy for $V=2V'$ and $t=0$ which corresponds to the case $V/t\rightarrow\infty$, $V'/t\rightarrow\infty$, $V/V'=2$. It allows us to consider clusters as large as $L=32$. The results of the calculations for the correlation functions are shown in Figs. 3 and 4. We have found by the technique described above $\gamma=2.009-2.013$ and $\delta=1.80-1.83$. Note that the envelope of the function $K(R)$ turns out to be nonmonotonous in the non-LL regime (see the black circles for $R=3,5,7$ in Fig. 5.)

The results of computer simulation demonstrating possible violation of the Haldane hypothesis seem to be rather unexpected. In particular, we cannot see any simple cause for the difference between two frustrated cases: $\rho=1/2$, $V=2V'\rightarrow\infty$ (non-LL behavior) and $\rho=2/3$, $V'=0$, $V\rightarrow\infty$ (LL behavior). It would be very important to understand these numerical results by regular field-theoretical methods.

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