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

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(October 15, 2018)

Haldane hypothesis about the universality of Luttinger liquid (LL) behavior in conducting one-dimensional (1D) fermion systems is checked numerically for spinless fermion model with next-nearest-neighbor interactions. It is shown that for large enough interactions the ground state can be gapless (metallic) due to frustrations but not be LL. The exponents of correlation functions for this unusual conducting state are found numerically by finite-size method.

PACS: 71.10.Pm, 71.10.Fd

One-dimensional (1D) Fermi systems have a number of peculiarities which distinguish them drastically from 3D ones (for review, see [1]). In particular, gapless (metallic) 1D systems of interacting fermions never behave as normal Fermi-liquid. Haldane [2] have proposed another class of universality Luttinger liquid (LL) state, namely. It is characterized by the existence of three branches of low-lying Bose excitations, density, current, and 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 of the system $E$ 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 the shift of all the particles in momenta space, that 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 $\mu$ at the change of the total number of particles $N$, $v_N = (L/\pi)\delta \mu/\delta N$, with $L$ being the length of the system. In LL state there are an exact relation between the velocities

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

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

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

Original arguments by Haldane were based on exact Bethe Ansatz solutions as well as on the perturbation theory for weakly interacting systems. There are no general and rigorous proof of this assumption but all the known analytical and numerical results about 1D fermion systems confirm Haldane hypothesis [3,4]. Anderson [5] proposed that some 2D systems such as copper-oxide superconductors also belong to the class of LL which made the concept of Luttinger liquid one of the most “fashionable” in contemporary many-particle physics. Therefore the investigation of the status of Haldane hypothesis seems to be of importance. Here we present a counterexample to this hypothesis basing on exact numerical results for spinless fermion model.

We proceed with the Hamiltonian

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

(3)

where $c_i^{\dagger}, c_i$ are Fermi creation and annihilation operators on site $i, n_i = c_i^{\dagger}c_i$. Phase creation of this model has been investigated by us in [6]. In particular, it has been shown that for 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 site) of the ground state at the Ising limit $t = 0$. A similar result has been obtained also in Ref. [7]. It is important that, according to our calculations, the metallic region has non-zero width in $(V, V')$ plane. One can say with certainty that the gap is zero at $(V/2) - 0.6t \leq V' \leq (V/2)$. One can show also with certainty that the ground state is insulating at $|(V/2) - V'| > 1$. To check the Haldane hypothesis we restrict ourselves by the consideration of the straight line $V = 2V'$ where the system is definitely metallic. Similarly, we have the 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 metallic state with strong interactions and it seems to be interesting to check the Haldane assumptions for this unusual case. As it 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 “unusual” character of metallic state at $\rho = 1/2, V \approx 2V'$ has been mentioned in [3] but without specification what this state is.

We have carried out the calculations of the ground state of the model (3) by Lanczos method for finite clusters with the consequent extrapolation to $L \to \infty$ (for details, see [8]). Velocities of low-lying excitations has been calculated as [9].
\[ v_S = \frac{L}{2\pi} [E_{1p}(L, N) - E_0(L, N)] \]
\[ v_J = \frac{L}{2\pi} [E_a(L, N) - E_0(L, N)] \]
\[ v_N = \frac{L}{\pi} [E_0(L, N + 1) - 2E_0(L, N) + E_0(L, N - 1)] \]

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 ground state energy for antiperiodic boundary conditions (transition to the antiperiodic conditions corresponds to magnetic flux \( \Phi = 1/2 \) of the flux quantum), \( E_{1p}(L, N) \) is the ground state energy for minimal nonzero total momentum \( P = 2\pi/L \). Then we have verified the criterion of LL \( \chi = 1 \) using Eq. (1).

The results of the testing calculations for the case \( \rho = 1/2, V' = 0, 0 \leq V < 2t \) where the system has to be LL [2] are shown in Fig.1 (open circles and triangles). We also present in the same figure the calculated values of \( \chi \) along the line \( V = 2V' \). One can see that at \( V \leq 10t \) we have, within the accuracy of the computations, \( \chi \approx 1 \), in agreement with Haldane hypothesis. However, for \( V > 30t \) the values of \( \chi \) is definitely less than unity, that is obvious even without extrapolation to \( L \to \infty \) 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 LL picture is caused by the competitions of nearest-neighbor and next-nearest-neighbor interactions (i.e. frustrations) which allow the system to be metallic in the limit of strong interactions. A schematic phase diagram is shown in Fig.2. The question is still open whether the transition from insulating state to non-LL conducting state is the direct one or there exists intermediate conducting LL phase. At the same time, our calculations demonstrate that for \( \rho = 2/3 \) the relation [5] takes place with the accuracy of calculations for any values of parameters under consideration even along the lines \( V = 0 \) or \( V' = 0 \). It would be very interesting to understand analytically the reason for the difference between these two cases with strong frustrations.

We also have calculated the static correlation functions
\[ G(R) = \langle c_R^\dagger c_0 \rangle \]
\[ K(R) = \langle \delta n_R \delta n_0 \rangle \]
where brackets mean the averaging over the ground state, \( \delta n_k = n_k - \rho \). In LL the following asymptotics have to be valid at \( R \gg 1 \) [4]
\[ G(R) \sim \sum_{m=0}^{\infty} C_m \sin [(2m+1)k_F R] R^{-\eta_m} \]
\[ K(R) \sim \sum_{m=0}^{\infty} D_m \cos (2mk_F R) R^{-\theta_m} \]
where \( \eta_m = \frac{1}{2} e^{-2\nu} + 2 (m+\frac{1}{2})^2 e^{2\nu}, \theta_m = 2m^2 e^{2\nu} (m > 0), k_F = \rho/2 \) is the Fermi momentum. The most important exponent \( \alpha \) determines the behavior of one-particle distribution function \( n(k) \) near the Fermi surface
\[ n(k) \approx \frac{n(k_F) - C \text{sign}(k-k_F)|k-k_F|^\alpha}{(k-k_F)^2} \]
where \( \alpha = \eta_0 - 1 \).

However we cannot use these expressions \textit{a priori} since for the model under consideration the system is not always LL. We have found the asymptotics of the correlation functions by direct computation. It is known (see, e.g., [6]) that it is very difficult to find the correlation exponents from the calculations for a given \( L \), even as large as \( L \approx 32 \). Therefore we use the finite size scaling technique [4]. Specifically we use the following procedure.

Our aim is to find the function \( \varphi(R) \equiv \langle \phi(0) \phi(R) \rangle \) for the 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
\[ \lim_{L \to \infty} r(R,L) = R. \]

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 [8] we have \( \lim_{L \to \infty} r'(\lambda, L) = \lambda \). Also the function \( r' \) satisfies the condition \( r'(1, \lambda, L) \). For small \( \lambda \) one has \( r'(\lambda, L) \approx \lambda \). To satisfy all these requirements we try the function \( r' \) as a Fourier series
\[ r'(\lambda) = \sum_{n=1}^{\infty} \frac{\sin(\pi\lambda) + a_3 \sin(3\pi\lambda) + a_5 \sin(5\pi\lambda) + \ldots}{\pi(1 + a_3 + a_5 + \ldots)} \]
Using the asymptotic expression similar to [4] for the dependence \( f(R,L) = \varphi(Lr'(\lambda, L)) \) at finite \( L \) and optimizing the result with respect to both \( a_n \) and the correlation exponents we can find the latter with high enough accuracy. At least the results for the exponents appeared to be accurate enough for the clusters with \( 14 \leq L \leq 26 \) 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 Haldane formula [5] 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 [4] and have to restrict ourselves only by the consideration of the leading terms in the asymptotics of correlation functions which are tried in the following form
\[ G(R) \sim \left( C_1 + C_2 \sin(\frac{2\pi R}{L}) \right)/R^\gamma \]
\[ K(R) \sim \left( D_1 + D_2 (-1)^R \right)/R^\delta \]
(we consider the case $\rho = 1/2$). To diminish the number of states in the Gilbert space under consideration we use only the states which has the same (minimal) energy for $V = 2V'$ and $t = 0$ which corresponds to the consideration of the case $V/t \to \infty, V'/t \to \infty, V/V' = 2$. It allows us to consider as large clusters as $L = 32$. The results of the calculations for the correlation functions are shown in Figs.3,4. We have found by the technique described above $\gamma = 2.009 \div 2.013$ and $\delta = 1.80 \div 1.83$. Note that the envelope of the function $K(R)$ turns out to be non-monotonous in non-LL regime (see the black circles for $R = 2, 4, 6$ in Fig.4.

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

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CAPTIONS TO FIGURES

Fig.1. The dependence of the ratio $\chi$ (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: $V = 200t$).

Fig.2. Phase diagram of the model. The boundary between conducting LL and non-LL phases is shown schematically by zigzags.

Fig.3. 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.4. The same as in Fig.3, for $K(R)$ (Eq.(5)).
