One-body dynamical correlation function of Lieb-Liniger model at finite temperature

Song Cheng\textsuperscript{1,2,3}, Yang-Yang Chen\textsuperscript{2,4,5}, Xi-Wen Guan\textsuperscript{5,6,7}, Wen-Li Yang\textsuperscript{2,4,7}, and Hai-Qing Lin\textsuperscript{8,9}\textsuperscript{*}

\textsuperscript{1} Department of Physics, The University of Hong Kong, Hong Kong, China
\textsuperscript{2} Institute of Modern Physics, Northwest University, Xi’an 710069, China
\textsuperscript{3} Beijing Computational Science Research Center, Beijing 100193, China
\textsuperscript{4} Shaanxi Key Laboratory for Theoretical Physics Frontiers, Xi’an 710069, China
\textsuperscript{5} State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China
\textsuperscript{6} Department of Fundamental and Theoretical Physics, Research School of Physics, Australian National University, Canberra ACT 0200, Australia
\textsuperscript{7} Peng Huanwu Center for Fundamental Theory, Xi’an 710069, China and
\textsuperscript{8} School of Physics, Zhejiang University, Hangzhou 310058, China

The dynamical correlated properties of one-dimensional (1D) Bose gases provide profound understanding of novel physics emergent from collective excitations, for instance the breakdown of off-diagonal long-range order, and the establishment of Tomonaga-Luttinger liquid (TLL) theory. However, due to the non-perturbative nature of 1D many-body systems, the exact evaluation of correlation functions is notoriously difficult. Here by means of form factor approach based on algebraic Bethe ansatz and numerics, we present a thorough study on the one-body dynamical correlation function (1BDCF) of the Lieb-Liniger model at finite temperature. The influence of thermal fluctuation and interaction on the behavior of 1BDCF has been demonstrated and analyzed from various perspectives, including the spectral distribution, the line-shape at fixed momentum, and the corresponding static correlations.

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In the last two decades, a growing interest in low-dimensional quantum many-body systems has stimulated tremendous success in both theoretical and experimental developments of quantum physics \cite{1,2}. In contrast to Landau’s quasi-particles emergent from condensed matter problems of higher dimensions \cite{3,4}, the bosonic collective excitations \cite{5,6} take over the main role of low-energy physics for the one-dimensional (1D) strongly correlated systems. Consequently, significantly different phenomena away from the quasi-particle picture occur at low temperature in 1D interacting systems, such as the absence of true Bose-Einstein condensate (BEC) in homogeneous Bose gases \cite{7}, fractional spin and holon excitations \cite{8,9}, and spin-charge separation \cite{10,11}. Moreover, the presence of quantum integrability in 1D results in the breakdown of thermalization for quantum gases \cite{12,13}. The key to understanding such unique physics lies in the correlation functions of either ground state or finite temperatures, yet the non-perturbative nature brings with a big challenge on their exact evaluation \cite{14}. In this letter, making use of quantum integrable theory, we thoroughly study the finite temperature one-body dynamical correlation function (1BDCF) of the Lieb-Liniger model with an arbitrary interaction.

The Lieb-Liniger model describes $N$ spinless bosons confined in a line of length $L$ via contact interaction \cite{15}, and its Hamiltonian reads

$$
H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i>j}^{N} \delta (x_i - x_j),
$$

where $c > 0$ ($c < 0$) specifies the interaction strength of repulsion (attraction) and hereafter we only consider the repulsive case. The physics of this model is governed by two dimensionless parameters simultaneously, i.e., interaction strength $\gamma = c/n$ and temperature $\tau = T/T_d$. Here we denote the particle density $n = N/L$ and degenerate temperature $T_d = \hbar^2 n^2/(2mk_B)$, respectively. By tuning these parameters the system would vary across several different regimes, quasi-condensate, Tonks-Girardeau (TG) gas, degenerate regime, decoherence regime and quantum criticality etc \cite{16,17}. In the TG limit $\gamma \to \infty$, the one-body density matrix was derived at zero and finite temperatures by the trick of Bose-Fermi map \cite{18,19}, as well as in the presence of trap potential \cite{20,21}. Away from this limit, on basis of pseudopotential Hamiltonian and a combination of generalized Hartree-Fock approximation and random phase approximation, the dynamic structure factor (DSF) in strongly correlated region was obtained up to a correction of $1/\gamma$ order \cite{22}. While with the application of Hellmann-Feynman theorem, the pair correlation function was calculated \cite{23,24}, and a general expression for higher-order static correlation function in strongly correlated regime was found through the asymptotic Bethe ansatz solution \cite{25,26}. Besides, a variety of static correlated properties were studied through the Quantum Monte Carlo method \cite{27,28}, while the edge singularity of dynamical correlation functions was predicted by...
the nonlinear Tomonaga-Luttinger liquid (TLL) theory 3, 32.

Being the simplest quantum integrable system 18, the
Lieb-Liniger model has been acting as a major subject of
textbook materials for quantum many-body physics 9,
32, 37. Nevertheless, the study of correlation functions
is still notoriously difficult due to complexity of many-
body eigenstates 37. Towards this end, much effort has
been devoted to finding the determinant representations
of various correlators through the algebraic Bethe ansatz
(ABA) technique 32, 31.

These tedious formulas represent a big challenge for
a full access to the correlated properties, and thus in-
trigue the numerical methods that counting in useful
eigenstates and calculating the determinant expressions
of form factors, such as ABACUS 12, 43, 47 and our
recent achievements 40, 48. This technique provides
theoretical benchmark for the cold-atom experiments on
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hand, by restricting the number of pairs of particle-hole
excitation, the DSF and spectral function were obtained
for the low density region by utilizing the thermodynamic
form factor 50. The quantum integrability technique en-
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Here we present a thorough study on 1BDCF of the
Lieb-Liniger model at zero and finite temperatures with
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approach on basis of ABA and numerics. The spectral
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This configuration of QNs is obviously symmetric. (d). shows an example of
'velative excitation' over the original reference state displayed in (c), giving birth to states responsible for the secondary
peak in Fig. 3.

where $\Psi(x,t) (\Psi^\dagger(x,t))$ is the bosonic field operator of
annihilation (creation) and $\langle \cdots \rangle_T$ stands for a statistical
expectation at finite temperature $T$. The standard treat-
ment for this ensemble average needs computation of the
partition function, which however is extremely hard to
conduct for a strongly correlated system. It turns out
this difficulty can be circumvented by means of quan-
tum integrability, namely by the thermodynamic Bethe
ansatz (TBA) equations 37, 44, 52. There it makes sense
to speak of an ensemble that solves the TBA equations.
These equations can be solved once the chemical potent-
ial, interaction strength and temperature are specified.
Meanwhile a thermodynamic equilibrium state consists of
a mixture of eigenstates sharing the same macroscopic
description correspondingly. Therefore it is crucial that
just finding one arbitrary eigenstate to represent all of
the states determined by the same TBA equations.
The problem now is simplified and similar to the ground state.
We will call this specified eigenstate henceforth 'reference
state' which comes from the generating process for ex-
cited states and we will discuss it later on. In principle,
the configuration of QNs for a reference state simultane-
ously depends on the interaction strength and tempera-
ture. For a given interaction strength $\gamma$, the higher tem-
perature will excite more p-h pairs over the Fermi sea in
a full access to the correlated properties, and thus in-
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we denote from solving the TBA equation. In the above equation, \( \langle \{|\lambda| T \rangle \} \) are the norm square of eigenstate, both of which can be numerically calculated through the determinants of system size \( N/L = 1 \), and \( \tau \) is the chemical potential. The left panel is for zero temperature and the right for finite temperature. The yellow- and red-dashed curves respectively stand for the Type-I and -II type dispersions. The sum rules (see Eq. 5) of (a)-(f) are 99.99 %, 99.83 %, 99.63 %, 97.63 %, 98.90 % and 98.99 % respectively.

In principle, the sum is taken over the whole Hilbert space, which is however impossible in practice. We therefore incorporate the states with significant contributions to the correlation function as many as possible until obtaining a satisfying result of sum rule. This exploring process is equal to reproducing excited states which of course can be fulfilled by generating 1-, 2-, \ldots, and \( m \)-pairs of p-h excitation over the ground state. Nevertheless, in the situation of finite temperature, this will be a waste of computation resource. To avoid this drawback, we start above generating process from an eigenstate derived from TBA equation instead, explaining the meaning of reference. Any configuration of QNs away from this reference state will be considered as ‘relative excitations’ since it needs not to be the ground state, see Fig. (d). More details can be found in Supplementary Materials. We then count states by manipulating such type of ‘relative excitations’. This thought comes from a naive observation that the most relevant states for the form factor of local observable should be of similar looking to the reference state from the viewpoint of configuration of QNs. For a dynamical correlation, there usually exists a sum rule that connects itself with a static quantity by integrating or summing out the frequency. This relation can be employed to check the validity of the dynamical correlation. Here for 1BDCF, the sum rule reads

\[
\sum_k n(k) = \frac{N}{L} \tag{5}
\]

where \( n(k) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} g_1(k,\omega) \) is the momentum distribution. In our setting, the density is \( n = N/L = 1 \), and thus the sum rule close to 1 indicates a faithful result, see Fig. 2 where the sum rule from (a) to (f) are respectively 99.99 %, 99.83 %, 99.63 %, 97.63 %, 98.90 % and 98.99 %.

In the strongly degenerate regime (\( \tau \ll 1 \)), it is reasonable to assume 1BDCF to be similar to its zero temperature situation, merely differing with a temperature-dependent perturbation. In a weakly interacting regime (\( \tau \ll \gamma \ll 1 \) or \( \gamma \ll \tau \ll \sqrt{\tau} \)), the Gross-Pitaevskii equation provides a way to understand the quantum correlation functions. Away from this limit, increasing temperature gradually destroys the phase coherence and thus the system eventually arrives at the decoherent regime. Here we focus on the regime \( \tau \sim \sqrt{\tau} \sim 1 \), where the competition between thermal fluctuation and interaction recovers the correlated properties.

The frequency-momentum resolved 1BDCF is demonstrated in Fig. 2 with system size \( N = L = 60 \). Thus the Fermi momentum \( k_F = \pi n = \pi \), the momentum and energy are expressed in units of Fermi momentum and Fermi energy respectively. \( h \) is the chemical potential. The left panel shows that at zero temperature, in the situation of weak interaction, spectral weights mostly focus on the Type-I dispersion represented by the yellow dashed curves; while away from the weakly interacting region, the spectral weights mostly concentrate on the Type-II dispersion represented by the red-dashed curves, and spread across the Type-I dispersion. The latter (former) dispersion corresponds to adding a particle (hole) outside (inside) of the Fermi sea. In the right panel of finite temperature case, immediate differences are observed with the non-vanishing spectral distribution in the
half-plane of negative energy. This is easy to understand from the perspective of p-h excitation as being given in Fig. 1. In Fig. 1 (c), the reference state at finite temperature indicates a melted Fermi sea. Besides the normal ‘relative excitations’ whose absolute values of particle QN increase, there exists such case that the absolute value of particle QN decrease. A typical example of such an ‘excitation’ is depicted by the red arrow in Fig. 1 (d), which generates the states bearing non-vanishing spectral contribution while possessing lower energy than the reference state. In quantum degenerate regime, the reference state contains very few holes lying almost on the Fermi points, which leaves no further room for above type of ‘excitations’. This in consequence suppresses the spectral distribution to negative energy plane.

In Fig. 3 the line-shape of 1BDCF with a given momentum is displayed by taking the intermediate interaction strength \( \gamma = 4 \). At zero temperature, there is an analog of Fermi edge singularity lying on the Type-II dispersion \([35, 43, 46]\), which is smeared for finite temperature by the thermal fluctuation. Although the spectral weight in Fig. 3 at the given momenta shrink, comparing with the counterpart in ground state, the percentage of spectral weight occupied by the multi-pairs of p-h excitation become prominent. Accompanied with this process is the re-distribution of spectral weight on the energetic axis, as is shown in Fig. 2. Along with an increase of the temperature, a secondary peak emerges in the plane of negative energy gradually. Like what is discussed before, its emergence arises from the states produced by the relative excitation which decreasing the absolute values of QN. Besides, the main peak is lowered in this process, whose loss of spectral weight is compensated partly by the secondary peak. In fact, this double-peak phenomenon is exactly the reflection of detailed balancing relation for the dynamic correlation functions \([54]\),

\[
g_1(k, \omega) = e^{i(kx - \omega t)}/2 \langle \Psi(0,0)\Psi(0,0)\rangle_T.
\]

Similar phenomenon is observed for DSF as well \([55, 56]\). Fig. 4 (a) explicitly shows this relation for the line-shape of 1BDCF with \( \gamma = 4 \) and \( \tau = 1.25 \) of system size \( N = L = 60 \). The green and red curves indicate \( g_1(k, 0.3k_F, \omega) \) and \( g_1(k, 0.3k_F, -\omega) \) respectively, and the blue one is obtained by utilizing detailed balancing relation, in accordance with that of 1BDCF. We briefly show the finite-size effect through Fig. 4 (b), where the 1BDCF of different system sizes are compared. It is shown that the results of \( N = L = 60 \) and 80 basically agree with each other, with slight difference from that of \( N = L = 40 \). Hence it is convincing to make use of the system size \( N = L = 60 \).

The static correlation function corresponding to 1BDCF (i.e. the momentum distribution) is obtained by integrating out the frequency, whose Fourier transformation is the one-body density matrix. In Fig. 5 (a) we compare the momentum distribution at zero and finite temperatures based on the data from Fig. 2. Despite no BEC in the Lieb-Liniger model, the weak interaction still results in a prominent zero-momentum occupation than the larger interactions do. A direct comparison shows obvious discrepancies between the curves of zero and finite temperatures with the same interaction strength, which is simply a result of disturbance from the thermal fluctuation on particles of small momentum. It is also evidenced by Fig. 5 (b) where the height of secondary peaks can be thought of as a measure to the influence of thermal fluctuation. Therein at the same temperature, the
FIG. 5. (a). The momentum distributions at different temperature $\tau$ and interaction strength $\gamma$. All data come from Fig. 2. For the sake of a clear visibility, we take a logarithmic scale for the momentum distribution. The dotted and solid curves stand for the situations at zero and finite temperatures, respectively. (b). The one-body density matrix with different temperature $\tau$ and interaction strength $\gamma$. The solid and dotted lines respectively correspond to the TLL predictions and our results derived from form factor approach (FFA). The parameters of $(\gamma, \tau)$ for red, green and blue curves are $(0.5, 0.55)$, $(4, 1.25)$, and $(16, 1.5)$. The TLL prediction does not work in above parameter setting since the thermal fluctuation is strong enough to break down its validity.

curves at small momentum have higher secondary peaks, implying the stronger influence. Besides, it is seen that the interaction strength affects the discrepancy between results of zero and finite temperatures, i.e. the curves of larger interaction show less discrepancy. The one-body density matrix is shown in Fig. 5 (b) by comparing our results and the TLL prediction. The TLL prediction does not work because the temperature considered here is beyond its validity, see Part E of Supplementary Material.

In conclusion, a detailed study on the finite temperature 1BDCF of the Lieb-Liniger model with variable repulsive interaction strengths has been presented by using the determinant expression of form factor and numerics. In particular, we have considered the regime far away from the GP and TG limit [1]. By comparing the situations of the 1BDCF at zero and finite temperatures, the results of spectral distribution, line-shape, the momentum distribution and one-body density matrix have demonstrated the subtle competition between thermal fluctuation and quantum interaction. The thermal fluctuation destroys the sharp edge singularity behaviour of single particle spectrum, especially removing the singularity at the hole-induced edge i.e. Type-II type dispersion relation. It drives the distribution of spectral weight spread in the negative energy plane, clearly reflected by the line-shape of 1BDCF. The double-peaks structure of 1BDCF can be explained by a series of ‘relative excitation’ over the reference state, as well as by the perspective of the detailed balancing relation. Our results of the one-body density matrix manifests the intensity of thermal fluctuation in the region considered is strong enough to break down the validity of TLL, demonstrating a broadly applicable range of our method. It is worth to emphasizing that our method can be further generalized into the realistic experimental setting, the gases of cold atoms are trapped in a harmonic potential. This problem can be treated as a uniform case together with local density approximation. The capability of our method for dealing with arbitrary interaction strength and a wide range of temperatures promises a reliable benchmark for the cutting-edge cold atom experiments. Moreover, our method can be employed in the study of dynamical fermionization and interaction quench.

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Note Added. After the release of this work on arXiv: 2211.00282, we notice recently another paper discusses the improvements on ABACUS, and the difficulty in evaluating 1BDCF at finite temperatures.

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See Eq. (1.4.29) of Ref. 37 for more explanation.

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\[
n(k, T) \approx \left(\frac{2K}{\pi}\right)^{1/3} \left(\frac{nL_\theta}{K}\right)^{1-1/3} \Gamma \left(1 - \frac{1}{2K}\right) \\
\cdot \text{Re} \left[ \frac{\Gamma(\frac{1}{2K} + i\frac{\pi}{2\Gamma})}{\Gamma(1 - \frac{1}{2K} + i\frac{\pi}{2\Gamma})} \right]
\]

where \(m\) is the particle mass, \(K\) the Luttinger parameter, and \(L_\theta = \hbar^2 / (mk_\theta T)\) is the phase correlation length.

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