

Short-Distance Correlation Properties of the Lieb-Liniger System and Momentum Distributions of Trapped One-Dimensional Atomic Gases

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We derive exact closed-form expressions for the first few terms of the short-distance Taylor expansion of the one-body correlation function of the Lieb-Liniger gas. As an intermediate result, we obtain the high- p asymptotics of the momentum distribution of both free and harmonically trapped atoms and show that it obeys a universal $1/p^4$ law for *all* values of the interaction strength. We discuss the ways to observe the predicted momentum distributions experimentally, regarding them as a sensitive identifier for the Tonks-Girardeau regime of strong correlations.

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Introduction.—Even though the correlation functions for the Lieb-Liniger gas of δ -interacting one-dimensional bosons [1] have been an object of intense research in the integrable systems community since the late 1970s [2], the full closed-form expressions are known only in the Tonks-Girardeau limit of infinitely strong interactions [3]. While the scaling properties of the long-range [4] asymptotics of the correlation functions can be derived from Haldane's theory of quantum liquids [5], conformal field theory [6], and quantum inverse scattering method [2,7], *virtually nothing* is known about short-range one-body correlations at finite coupling strength [8]. One of the goals of this paper is to extend the existing knowledge in this direction.

The interest to the correlation functions of the Lieb-Liniger gas has been significantly revived over the past two years. The few-body local correlation functions for both weak and strong interactions were computed via new methods [9–11]. Relevant to the current experiments, research on correlation functions of a harmonically trapped gas has been performed in [9,12–14].

It is known that, while for weak interactions the Lieb-Liniger system is well described by the mean-field theory, the opposite, Tonks-Girardeau regime of infinitely strong interactions [15,16] constitutes a strongly correlated system dual to a free Fermi gas. In experiments with one-dimensional atomic gases [17,18], the one-body momentum distribution of the gas, along with the density profiles [19] and phase fluctuations [9,20,21], can readily help to distinguish between the two quantum regimes. In the Tonks-Girardeau limit, the momentum distribution for both free and harmonically confined gases was investigated by several authors [3,22–24]. In this paper, we address the question of the momentum distribution in the intermediate, in between mean-field and Tonks-Girardeau, regime, as more realistic from the experimental point of view.

System of interest.—Consider a one-dimensional gas of N δ -interacting bosons confined in a length L box with

periodic boundary conditions. The Hamiltonian of the system reads

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{j=1}^N \frac{\partial^2}{\partial z_j^2} + g_{1D} \sum_{i=1}^N \sum_{j=i+1}^N \delta(z_i - z_j) \quad (1)$$

$$= \int_{-L/2}^{+L/2} \frac{\hbar^2}{2m} \partial_z \hat{\Psi}^\dagger \partial_z \hat{\Psi} + \frac{g_{1D}}{2} \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}, \quad (2)$$

where m is the atomic mass, and g_{1D} is the one-dimensional coupling constant, whose expression for real atomic traps is given in [22]. This Hamiltonian can be diagonalized via Bethe ansatz [1]. At zero temperature, the energy of the system is given through $E/N = [\hbar^2/(2m)]n^2 e(\gamma)$, where the dimensionless parameter $\gamma = 2/n|a_{1D}|$ is inversely proportional to the one-dimensional gas parameter $n|a_{1D}|$, n is the one-dimensional number density of particles, $a_{1D} = -2\hbar^2/mg_{1D}$ is the one-dimensional scattering length introduced in [22], and the function $e(\gamma)$ is given by the solution of Lieb-Liniger system of equations [1]: It is tabulated in [25]. Note the asymptotic behavior of $e(\gamma)$ (first computed in [1]): $e(\gamma) \stackrel{\gamma \rightarrow 0}{\approx} \gamma$ and $e(\gamma) \stackrel{\gamma \rightarrow \infty}{\approx} \frac{1}{3} \pi^2 (\frac{\gamma}{\gamma+2})^2$, where $\gamma \rightarrow 0$ corresponds to the mean-field or Thomas-Fermi regime, whereas $\gamma \rightarrow \infty$ corresponds to the Tonks-Girardeau regime.

High- p momentum distribution.—Our first object of interest is the high- p asymptotics of the one-body momentum distribution in the ground state. To evaluate it, we need two mathematical facts, (a) and (b).

(a) The presence of the delta-function interactions in the Hamiltonian (1) implies that its eigenfunctions undergo, at the point of contact of any two particles i and j , a kink in the derivative proportional to the value of the eigenfunction at this point [26]:

$$\Psi(z_1, \dots, z_i, \dots, z_j, \dots, z_N) = \Psi(z_1, \dots, Z_{ji}, \dots, Z_{ji}, \dots, z_N) \\ \times \{1 - |z_{ji}|/a_{1D} + \varepsilon(|z_{ji}|; \{Z_{ji}\})\} \\ \varepsilon(|z_{ji}|; \{Z_{ji}\}) = \mathcal{O}(|z_{ji}|^2), \quad (3)$$

where $Z_{ji} = (z_i + z_j)/2$ and $z_{ji} = z_j - z_i$ are the center-of-mass and relative coordinates of the ij pair of particles, respectively, and $\{Z_{ji}\} = \{Z_{ji}, z_1, \dots, z_{i-1}, z_{i+1}, \dots, z_{j-1}, z_{j+1}, \dots, z_N\}$ denotes a set consisting of the center-of-mass coordinate of the i th and j th particles and the coordinates of all the other particles.

(b) Imagine that a periodic function $f(z)$, defined on the interval $[-L/2, +L/2]$, has a singularity of the form $f(z) = |z - z_0|^\alpha F(z)$, where $F(z)$ is a regular function, $\alpha > -1$ and $\alpha \neq 0, 2, 4, \dots$; then the leading term in the asymptotics of the Fourier transform of f reads [27]

$$\int_{-L/2}^{+L/2} dz e^{-ikz} f(z) \stackrel{|k| \rightarrow \infty}{\approx} 2 \cos\left(\frac{\pi}{2}(\alpha + 1)\right) \Gamma(\alpha + 1) e^{-ikz_0} F(z_0) \frac{1}{|k|^{\alpha+1}} + \mathcal{O}\left(\frac{1}{|k|^{\alpha+2}}\right), \quad (4)$$

where $k = (2\pi/L)s$ and s is an integer. For multiple singular points of the same order, the full asymptotics is the sum of the corresponding partial asymptotics of the form (4).

Let us evaluate, using (3) and (4), the momentum representation of the ground state wave function of the Hamiltonian (1) with respect to the first particle:

$$\begin{aligned} \Psi(p_1, z_2, \dots, z_N) &= L^{-1/2} \int_{-L/2}^{+L/2} dz_1 e^{-p_1 z_1/\hbar} \Psi(z_1, z_2, \dots, z_N) \stackrel{\forall i: 2 \leq i \leq N}{\approx} L^{-1/2} \int_{-L/2}^{+L/2} dz_1 e^{-ip_1 z_1/\hbar} \\ &\quad \times \Psi(z_1 = Z_{1i}, \dots, z_i = Z_{1i}, \dots, z_N) \times \{1 - |z_{1i}|/a_{1D} + \dots\} \\ &\quad \stackrel{|p_1| \rightarrow \infty}{\approx} \sum_{i=2}^N (2L^{-1/2}/a_{1D}) e^{-ip_1 z_i/\hbar} \times \Psi(z_1 = z_i, \dots, z_i, \dots, z_N) \frac{1}{(p_1/\hbar)^2}. \end{aligned} \quad (5)$$

Here $p_1 = (2\pi\hbar/L)s$, where s is an integer.

Let us now turn to the one-body momentum distribution *per se*. After a lengthy but straightforward calculation, it takes the form

$$w(p) \equiv \int_{-L/2}^{+L/2} dz_2 \dots \int_{-L/2}^{+L/2} dz_N |\Psi(p, z_2, \dots, z_N)|^2 \stackrel{|p| \rightarrow \infty}{\approx} \frac{4(N-1)\rho_2(0, 0, 0, 0)}{a_{1D}^2} \frac{1}{(p/\hbar)^4}, \quad (6)$$

where $\rho_2(z_1, z_2; z'_1, z'_2)$ is the two-body density matrix, normalized as $\int_{-L/2}^{+L/2} dz_1 \int_{-L/2}^{+L/2} dz_2 \rho_2(z_1, z_2; z_1, z_2) = 1$, and $w(p)$ is the momentum distribution, normalized as $\sum_{s=-\infty}^{+\infty} w(2\pi\hbar s/L) = 1$.

The expression (6) involves the two-body density matrix whose form is unknown for a finite system. However, an elegant thermodynamic limit formula for $\rho_2(0, 0, 0, 0)$ does exist due to Gangardt and Shlyapnikov [9], who derived it using the Hellmann-Feynman theorem [28]: $L^2 \rho_2(0, 0, 0, 0) = e'(\gamma)$. We are now ready to give a closed-form thermodynamic limit expression for the high- p asymptotics of the one-body momentum distribution for one-dimensional δ -interacting bosons in a box with periodic boundary conditions:

$$W(p) \stackrel{|p| \rightarrow \infty}{\approx} \frac{1}{\hbar n} \frac{\gamma^2 e'(\gamma)}{2\pi} \left(\frac{\hbar n}{p}\right)^4, \quad (7)$$

where $W(p) = (L/2\pi\hbar)w(p)$ is normalized as $\int_{-\infty}^{+\infty} dp W(p) = 1$. Notice that this asymptotics is *universally* described by a $1/p^4$ law for all values of the coupling strength γ . (Note that, for $\gamma \rightarrow \infty$, this law was predicted in [24].) Formula (7) is *the first of the two principal results of our paper*.

Harmonically trapped 1D gas: momentum distribution.—To evaluate the high- p asymptotics of the momentum distribution of atoms confined in a harmonic oscillator potential, we are going to employ the local density approximation (LDA). It is based on an intuitive, but hard to justify rigorously, assumption that in

the thermodynamic limit the short-range correlation properties of a trapped gas are indistinct from the ones of a uniform gas of the same local density: $\sigma(z, z') \stackrel{z, z' \ll l}{\approx} \sigma_u(z - z' | n[(z + z')/2])$, where $\sigma(z, z')$ and $\sigma_u(z - z' | n)$ are one-body density matrix of the trapped gas and one-body density matrix of a density n uniform gas, respectively, both normalized to the respective number of particles, $n(z)$ is the density profile of the trapped gas, and l is the typical length on which the density changes. [Tested against the exact results on correlation function of the trapped Tonks-Girardeau gas [13], this assumption can be shown to lead to an exact prediction for the value of the coefficient in front of the $(z - z')^2$ term in the Taylor expansion around $z' = -z \approx 0$.] From this ansatz, it immediately follows that the high- p asymptotics of the momentum distribution (sensitive to the short-range correlations only) is given by the *spatial average* of the uniform case expression (7) over the density profile of the atomic cloud. The density profiles themselves can also be obtained using LDA [[19], Eqs. 21 and 22, where the governing parameter η should be replaced by $2/\gamma_{TF}^0$, see below], and this is the method we used. The final result is presented in Fig. 1. There the dimensionless coefficient $\Omega_{HO} = \lim_{|p| \rightarrow \infty} W(p)p^4/(\hbar n^0)^3$ in front of the high- p asymptotics of the momentum distribution is plotted as a function of the interaction strength parameter γ^0 in the center of the cloud; γ^0 in turn depends on of the experimental

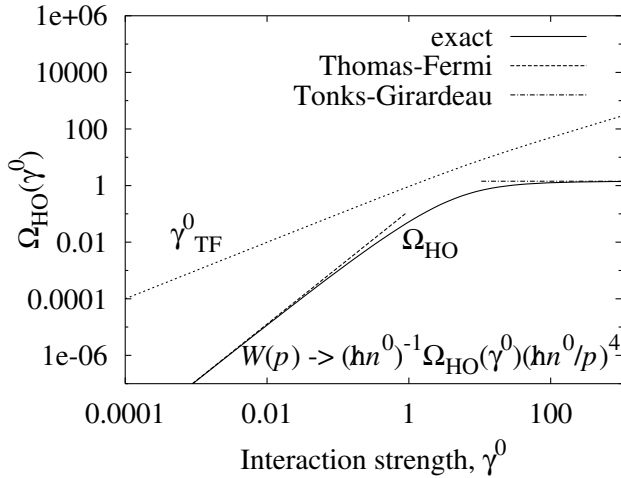


FIG. 1. Dimensionless coefficient $\Omega_{\text{HO}}(\gamma^0)$ in front of the leading term of the high- p asymptotics of the momentum distribution of *harmonically* trapped atoms, as a function of the interaction strength γ^0 in the center of the cloud. Also shown is the directly related to the experimental parameters Thomas-Fermi estimate $\gamma_{\text{TF}}^0 = (8/3^{2/3})(Nma_{\text{1D}}^2\omega/\hbar)^{-2/3}$ for the interaction strength in the center, as a function of γ^0 . Both momentum and momentum distribution are measured in units related to the density in the center n^0 , that can be expressed through γ^0 using $\gamma^0 = 2/n^0 a_{\text{1D}}$.

parameters, such as the number of particles N , the coupling constant g_{1D} , and the longitudinal trap frequency ω , through a system of implicit equations [19]. Here n^0 is the density in the center of the trap, and HO stands for the “harmonic oscillator.” To establish a link to the experimental parameters, we also present a plot for the Thomas-Fermi (weak interactions) prediction for γ in the center of the atomic cloud, $\gamma_{\text{TF}}^0 = (8/3^{2/3})(Nma^2\omega/\hbar)^{-2/3}$, as a function of γ^0 .

In the limiting, Thomas-Fermi and Tonks-Girardeau regimes, the momentum distribution is given by

$$W(p) \stackrel{|p| \rightarrow \infty, \gamma \rightarrow 0}{\approx} \frac{1}{p_{\text{HO}}} \frac{2 \times 3^{2/3}}{5\pi} N^{2/3} \left(\frac{a_{\text{HO}}}{|a_{\text{1D}}|} \right)^{5/2} \left(\frac{p_{\text{HO}}}{p} \right)^4,$$

$$W(p) \stackrel{|p| \rightarrow \infty, \gamma \rightarrow \infty}{\approx} \frac{1}{p_{\text{HO}}} \frac{\sqrt{2} \times 128}{45\pi^3} N^{3/2} \left(\frac{p_{\text{HO}}}{p} \right)^4, \quad (8)$$

where $a_{\text{HO}} = (\hbar/m\omega)^{1/2}$ and $p_{\text{HO}} = \hbar/a_{\text{HO}}$.

Short-range expansion for the correlation function.—Let us now redirect our attention to the ground state one-body correlation function,

$$g_1(z) = \langle \hat{\Psi}^\dagger(z) \hat{\Psi}(0) \rangle, \quad (9)$$

and, in particular, to its Taylor expansion around zero:

$$g_1(z)/n = 1 + \sum_{i=1}^{\infty} c_i |nz|^i. \quad (10)$$

In the limit of infinitely strong interactions $\gamma \rightarrow \infty$, this expansion is known to all orders [3]: $c_1^{\text{TG}} = 0$; $c_2^{\text{TG}} = -(\pi^2/6)$; $c_3^{\text{TG}} = \pi^2/9$; $c_4^{\text{TG}} = \pi^4/120$; Our goal

now is to obtain the first few (through the order $|z|^3$) coefficients of the expansion (10) for an *arbitrary* interaction strength γ .

The knowledge of the momentum distribution (7) is crucial for determining the c_1 and c_3 coefficients. Let us look at the relation between the momentum distribution and the correlation function, where the former is simply the Fourier transform of the latter: $W(p) = (2\pi\hbar n)^{-1} \int_{-\infty}^{\infty} dz e^{-ipz/\hbar} g_1(z)$. Since the leading term in the asymptotics of $W(p)$ is $1/p^4$, we may conclude, using the Fourier analysis theorem (4), that the lowest *odd* power in the short-range expansion of the correlation function $g_1(z)$ is $|z|^3$, and therefore the $|z|$ term is absent from the expansion:

$$c_1 = 0. \quad (11)$$

Furthermore, the theorem (4) allows one to deduce the coefficient c_3 from the momentum distribution (7):

$$c_3 = \frac{1}{12} \gamma^2 e'(\gamma). \quad (12)$$

To obtain the coefficient c_2 , we employ the Hellmann-Feynman theorem [28] again. Let a Hamiltonian $\hat{H}(w)$ depend on a parameter w . Let $E(w)$ be an eigenvalue of this Hamiltonian. Then the mean value of the derivative of the Hamiltonian with respect to the parameter can be expressed through the derivative of the eigenvalue: $\langle \Psi_E(w) | \frac{d}{dw} \hat{H}(w) | \Psi_E(w) \rangle = \frac{d}{dw} E(w)$. Let us now denote the fraction \hbar^2/m as κ and differentiate the Hamiltonian (2) with respect to κ . According to the Hellmann-Feynman theorem, we get $\frac{1}{2} \int_{-L/2}^{+L/2} dz (\partial^2/\partial z^2) \langle \hat{\Psi}^\dagger(z) \hat{\Psi}(z') \rangle|_{z'=z} = dE/d\kappa$. Now, using $\langle \hat{\Psi}^\dagger(z) \hat{\Psi}(z') \rangle = \langle \hat{\Psi}^\dagger(z-z') \hat{\Psi}(0) \rangle$, we obtain $-\frac{1}{2} L [(d^2/dz^2) g_1(z)]|_{z=0} = dE/d\kappa$, and, finally,

$$c_2 = -\frac{1}{2} \{e(\gamma) - \gamma e'(\gamma)\}, \quad (13)$$

where we have used the known expression for the energy given above.

Note that, as expected, our expressions for the coefficients c_{1-3} converge, in the limit $\gamma \rightarrow \infty$, to the known [3] listed above results for the impenetrable bosons. This can be easily verified using the $\gamma \rightarrow \infty$ expansion for the function $e(\gamma)$ given above.

Expressions (11)–(13) constitute the *second principal result obtained in our paper*.

Concluding remarks.—Below, we present a discussion on empirical observation of and application for the $1/p^4$ momentum distribution tails, in experiments with *harmonically trapped* atomic gases.

We would like to note that the $1/p^4$ law predicted in our paper corresponds to the values of momentum large as compared to the inverse correlation length $p \gg (m\mu/\hbar^2)^{1/2}$, where μ is the chemical potential. The law should persist at finite temperatures, but the prefactor given above will be valid only for small temperature:

For higher temperatures, the value of prefactor can be corrected via methods developed in [10].

We believe that the coefficient in front of the high- p tail of the momentum distribution (Fig. 1) may provide a *robust* experimental identifier of the quantum regime of the gas of interest, and, in particular, serve to detect the Tonks-Girardeau regime. (i) The high- p tail is not sensitive to the finite temperature corrections to the correlation function, which appear predominantly in the low- p (long-range) domain. (ii) In experiments with 2D optical lattices, where a single cigar-shaped trap is replaced by an array of traps [17], the effect of the residual 3D mean-field pressure acting during the expansion becomes relevant: The high- p part of the momentum distribution is far less sensitive to this effect as compared to the low- p part. (iii) The theoretical interpretation of the experimental results is simpler in the high- p case thanks to the applicability of the LDA. In the opposite low- p case, the LDA leads to entirely wrong predictions [29].

Summary.—In this paper, we present a short-range Taylor expansion (up to the order $|z|^3$) for the zero-temperature correlation function $g_1(z)$ of a one-dimensional δ -interacting Bose gas [see Eqs. (10)–(13)]. We compute the leading term in the high- p asymptotics of the momentum distribution for both free [Eq. (7)] and harmonically trapped (Fig. 1) atoms. We regard the high- p tail of the momentum distribution as an efficient tool for identification of the Tonks-Girardeau regime in experiments with dilute trapped atomic gases.

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