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

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(November 10, 2001)

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^2 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.

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 70s [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.

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 [9,10] constitutes a strongly correlated system dual to a free Fermi gas. In experiments with one-dimensional atomic gases [11,12] the one-body momentum distribution of the gas, along with the density profiles [13] and phase fluctuations [14–16], 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 [3,17–19]. 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

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

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\[
E/N = \frac{\hbar^2}{2m} n^2 e(\gamma), \tag{3}
\]

where \(e(\gamma)\) is inversely proportional to the one-dimensional gas parameter \(n|a_{1D}|\), \(n\) is the one-dimensional number density of particles, \(a_{1D} = -2\hbar^2/m g_{1D}\) is the one-dimensional scattering length introduced in [17], and the function \(e(\gamma)\) is given by the solution of Lieb-Liniger system of equations [1]: it is tabulated in [20]. Note the asymptotic behavior of \(e(\gamma)\) (first computed in [1]):

\[
e(\gamma) \approx \frac{1}{3\pi^2} \left( \frac{\gamma}{\gamma + 2} \right)^2, \tag{4}
\]

where \(\gamma \to 0\) corresponds to the mean-field or Thomas-Fermi regime, whereas \(\gamma \to \infty\) 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 [21]:

\[
\]
\[ \Psi(z_1, \ldots, z_i, \ldots, z_j, \ldots, z_N) = \Psi(z_1, \ldots, Z_{ji}, \ldots, Z_{ji}, \ldots, z_N) \]
\[ \times \{1 - |z_j|/a_{1D} + \varepsilon(|z_j|; \{Z_{ji}\})\} \]
\[ \varepsilon(|z_j|; \{Z_{ji}\}) = O(|z_j|^2), \]
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 \( \{Z_{ji}\} = \{Z_{ji}, z_1, \ldots, z_{j-1}, z_{j+i}, \ldots, z_{j-1}, z_{j+1}, \ldots, z_N\} \) 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 \( \alpha \neq 0, 2, 4 \ldots \). Then the leading term in the asymptotics of the Fourier transform of \( f \) reads [22]
\[ \int_{-L/2}^{+L/2} dz e^{-ikz} f(z) \]
\[ \approx 2 \cos \left( \frac{\pi}{2}(\alpha + 1) \right) \Gamma(\alpha + 1)e^{-ikz_0} F(z_0) \frac{1}{|k|^\alpha+1}, \]
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 (6).

Let us evaluate, using (5) and (6), the momentum representation of the ground state wavefunction of the Hamiltonian (1) with respect to the first particle:
\[ \Psi(p_1, z_2, \ldots, z_N) = L^{-\frac{\gamma}{2}} \int_{-L/2}^{+L/2} dz_1 e^{-ip_1z_1/\hbar} \Psi(z_1, z_2, \ldots, z_N) \]
\[ \times \{1 - |z_1|/a_{1D} + \varepsilon(|z_1|; \{Z_{ji}\})\} \]
\[ \varepsilon(|z_1|; \{Z_{ji}\}) = O(|z_1|^2), \]
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 \( \sum_{|p| = \infty} w(2\pi\hbar s/L) = 1 \).

The expression (8) 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 [15], who derived it using the Hellmann-Feynman theorem [24]: \( L^2 \rho_2(0, 0, 0, 0) = c'(\gamma) \). 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 \( \delta \)-interacting bosons in a box with periodic boundary conditions:
\[ W(p) \mid_{|p| = \infty} = \frac{1}{2\pi} \frac{\pi^2 e^\gamma}{\hbar} \left( \frac{\hbar n}{p} \right)^4, \]
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 \( \gamma \). (Note that for \( \gamma \to \infty \), this law was predicted in [19].) Formula (9) 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: \( \sigma(z, z') \approx \frac{2 L^2}{\gamma} \sigma_{u}(z - z')/n((z + z')/2) \), 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, \( l \) is the typical length on which the density changes. (Tested against the exact results on correlation function of the trapped Tonks-Giradeau gas [25] 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 (9) over the density profile of the atomic cloud. The density profiles themselves can also be obtained using LDA ( [13], Eqs. 21 and 22, where the governing parameter \( \eta \) should be replaced by \( 2/\gamma_{TF} \), see below), and this is the method we used. The final result is presented in Fig.1. There the dimensionless coefficient \( \Omega = \lim_{|p|\to\infty} W(p)p^4/(\hbar n^3) \) in front of the high-\( p \) asymptotics of the momentum distribution is plotted as
a function of the interaction strength parameter $\gamma^0$ in the center of the cloud; $\gamma^0$ in turn depends on of the experimental parameters, such as the number of particles $N$, the coupling constant $g_{1D}$, and the longitudinal trap frequency $\omega$, through a system of implicit equations [13]. Here $n^0$ is the density in the center of the trap. To establish a link to the experimental parameters we also present a plot for the Thomas-Fermi (weak interactions) prediction for $\gamma$ in the center of the atomic cloud, $\gamma_{TF}^{\alpha} = (8/3^2/3)(Nma^2\omega/h)^{-2/3}$, as a function of $\gamma^0$.

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

$$
W(p) \approx \begin{cases} 
\frac{1}{p_{HO}} \frac{2 \cdot 3}{5 \pi} N^2 \left( \frac{a_{HO}}{a_{1D}} \right) \left( \frac{p_{HO}}{p} \right)^4 & \text{for } |p| \rightarrow \infty, \gamma \rightarrow 0 \\
\frac{1}{p_{HO}} \frac{\sqrt{2} \cdot 128}{45 \pi^3} N^2 \left( \frac{p_{HO}}{p} \right)^4 & \text{for } |p| \rightarrow \infty, \gamma \rightarrow \infty 
\end{cases}
$$

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

In the limit of infinitely strong interactions $\gamma \rightarrow \infty$, this expansion is known to all orders [3]:

$$
c_1^{TG} = 0; \quad c_2^{TG} = -\frac{\pi^2}{6}; \quad c_3^{TG} = \frac{\pi^2}{9}; \quad c_4^{TG} = \frac{\pi^4}{120}; \ldots \quad (13)
$$

Our goal now is to obtain the first few (through the order $|z|^3$) coefficients of the expansion (12) for an arbitrary interaction strength $\gamma$.

The knowledge of the momentum distribution (9) 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 theformer is simply the Fourier transform of the latter: $W(p) = (2\pi \hbar n)^{-1} \int_{-\infty}^{\infty} dz e^{-ipz/h} g_1(z)$. Since the leading term in the asymptotics of $W(p)$ is $1/p^4$ we may conclude, using the Fourier analysis theorem (6), 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:

$$
c_1 = 0. \quad (14)
$$

Furthermore, the theorem (6) allows one to deduce the coefficient $c_3$ from the momentum distribution (9):

$$
c_3 = \frac{1}{12} \gamma^2 e'(\gamma) . \quad (15)
$$

To obtain the coefficient $c_2$, we employ the Hellmann-Feynman theorem [24] 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 $\kappa$ and differentiate the Hamiltonian (2) with respect to $\kappa$. According to the Hellmann-Feynman theorem, we get

$$
\frac{1}{2} \int_{-L/2}^{+L/2} dz \left( \partial^2 / \partial \kappa \partial^2 / \partial \kappa \right) \langle \hat{\Psi}^\dagger(z) \hat{\Psi}(z) \rangle = -L \partial^2 / \partial \kappa \langle \hat{\Psi}^\dagger(z) \hat{\Psi}(z) \rangle |_{z=0} = dE/\kappa, \quad (16)
$$

where we have used the known expression for the energy (3).

Note that, as expected, our expressions for the coefficients $c_1\ldots c_3$ converge, in the limit $\gamma \rightarrow \infty$, to the known results for the impenetrable bosons (13). This can be easily verified using the $\gamma \rightarrow \infty$ expansion for the function $e(\gamma)$ (4).

Expressions (14), (16), and (15) constitute the second principal result obtained in our paper.

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

(a) First of all, we would like to discuss the momentum range where the $1/p^4$ tail should be looked for experimentally. Relying on the $\gamma \to \infty$ results [2] and an analysis of the predicted-by-Bogoliubov’s-theory momentum distribution (corresponding to $\gamma \to 0$), we conjecture that in the whole range of the interaction strength $\gamma$, the high-$p$ asymptotics of the momentum distribution corresponds to the range of momenta given by $p \gg (m\mu/\hbar^2)^{1/2}$ for all $\gamma$, where $\mu$ is the chemical potential of the system. For the case of a harmonically confined gas at $\gamma \gtrsim 1$ this leads to

$$p \gg \sqrt{N} \rho_{HO} \quad \text{for} \quad \gamma \gtrsim 1. \quad (17)$$

(b) Our zero-temperature results are valid as long as the temperature does not exceed the chemical potential, $k_B T \ll \mu$ (for all $\gamma$), or, for the Tonks-Giradeau case,

$$k_B T \ll N \hbar \omega \quad \text{for} \quad \gamma \gtrsim 1. \quad (18)$$

For temperatures comparable to the chemical potential, the $1/p^4$ law should persist within the range (17), but the prefactor is not yet known and it is a subject of future research.

(c) Experimentally, the momentum distribution of the Tonks-Girardeau gas can be detected either \textit{in situ} [26] or via a ballistic expansion [27]. The latter option requires some caution, especially in the Tonks-Girardeau ($\gamma \to \infty$) case. If only the longitudinal confinement is released, the interactions will modify the momentum distribution during the expansion, and, as follows from the Bose-Fermi mapping [10], the detected momentum distribution will correspond to a free Fermi gas. Instead one should release both longitudinal and transverse confinements simultaneously. In this case rapid transverse ballistic expansion will lead to a quick drop-off of the density, making the interactions negligible.

(d) We believe that the coefficient in front of the high-$p$ tail of the momentum distribution (Fig.1) may provide a \textit{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 [11], 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 [28].

\textbf{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 $\delta$-interacting Bose gas (see Eqns. 12, 14, 16, and 15). We compute the leading term in the high-$p$ asymptotics of the momentum distribution for both free (Eqn. 9) 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.

\textbf{Acknowledgments.} Authors are grateful to M. Girardeau, D.M. Gangardt and C. Menotti for enlightening discussions on the subject. M. O. would like to acknowledge the hospitality of the European Centre for Theoretical Studies in Nuclear Physics and Related areas (ECT*) during the 2002 BEC Summer Program, where the presented work was initiated. This work was supported by the NSF grant PHY-0070333 and ONR grant N000140310427. Authors appreciate financial support by NSF through the grant for Institute for Theoretical Atomic and Molecular Physics, Harvard Smithsonian Center for Astrophysics.

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[1] Elliott H. Lieb and Werner Liniger, Phys. Rev. 130, 1605 (1963)

[2] V. E. Korepin, N. M. Bogoliubov, and A. G. Izergin, \textit{Quantum Inverse Scattering Method and Correlation Functions} (Cambridge University Press, Cambridge, 1993)

[3] T. D. Schultz, J. Math. Phys. 1, 666 (1963); A. Lenard, J. Math. Phys. 5, 930 (1964); H. G. Vaidya and C. A. Tracy, Phys. Rev. Lett., 42, 3 (1979); a corrected version of the Vaidya-Tracy expansions can be found in M. Jimbo, T. Miwa, Y. Mori, and M. Sato, Physica 1D, 80 (1980)

[4] The boarder between short and long range is given by the correlation length $\xi_c \sim \hbar/\sqrt{m\mu}$, $\mu$ being the chemical potential.

[5] F.D.M. Haldane, Phys. Rev. Lett. 47, 1840 (1981); F. D. M. Haldane, Phys. Lett. 81A, 153 (1981)

[6] A. Berkovich and G. Murthy, Physics Letters A, 142, 121 (1989)

[7] V. Korepin V and N. Slavnov, Phys. Lett. A 236, 201 (1997)

[8] The first few terms of the $1/\gamma$ expansion of the short-range correlation function can be deduced from the results of Dennis B. Creamer, H. B. Thacker, David Wilkinson, Phys. Rev. D 23, 3081 (1981); Michio Jimbo and Tetsuji Miwa, Phys. Rev. D 24, 3169 (1981)

[9] L. Tonks, Phys. Rev. 50, 955 (1936)

[10] M. Girardeau, J. Math. Phys., 1, 516 (1960)

[11] M. Greiner, O. Mandel, T. Esslinger, T.W. Hänsch, and I. Bloch, Nature 415, 39 (2002).
[12] A. Görlich, J. M. Vogels, A. E. Leanhardt, C. Raman, T. L. Gustavson, J. R. Abo-Shaeer, A. P. Chikkatur, S. Gupta, S. Inouye, T. Rosenband, and W. Ketterle, Phys. Rev. Lett. 87, 130402 (2001); F. Schreck, L. Khaykovich, K. L. Corwin, G. Ferrari, T. Bourdel, J. Cubizolles, and C. Salomon, Phys. Rev. Lett. 87, 080403 (2001); Kevin E. Strecker, Guthrie B. Partridge, Andrew G. Truscott, Randall G. Hulet, Nature, 417, 150 (2002); S. Burger, K. Bongs, S. Dettmer, W. Ertmer, K. Sengstock, A. Sanpera, G. V. Shlyapnikov, and M. Lewenstein, Phys. Rev. Lett. 83, 5198 (1999)

[13] Vanja Dunjko, Vincent Lorent, and Maxim Olshanii, Phys. Rev. Lett. 86, 5413 (2001)

[14] D. S. Petrov, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. Lett. 85, 3745 (2000)

[15] D.M. Gangardt and G.V. Shlyapnikov, ⟨cond-mat/0207338⟩

[16] J. O. Andersen, U. Al Khawaja, and H. T. C. Stoof, Phys. Rev. Lett. 88, 070407 (2002)

[17] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998)

[18] M. D. Girardeau, E. M. Wright, and J. M. Triscari, Phys. Rev. A 63, 033601 (2001)

[19] A. Minguzzi, P. Vignolo, M. P. Tosi, Phys. Lett. A 294, 222 (2002)

[20] The numerically tabulated function $e(\gamma)$ can be downloaded from http://physics.usc.edu/~olshanii/DIST/

[21] See for example [2], p. 7

[22] N. Bleistein and R. Handelsman, Asymptotic Expansions of Integrals, (Dover Publications, Inc., Mineola, N.Y., 1986)

[23] The double sum over particles involved in the computation can be split into a diagonal part (proportional to the two-body density matrix) and an off-diagonal part involving Fourier transforms of the three-body density matrix. The latter can be shown to decay faster than $1/p^4$ and thus does not contribute to the final result.

[24] H. Hellmann, Z. Physik. 85, 180 (1933); R.P. Feynman, Phys. Rev. 56, 340 (1939)

[25] T. Papenbrock, Phys. Rev. A 67, 041601(R) (2003)

[26] M. D. Girardeau and E. M. Wright, Phys. Rev. Lett. 87, 050403 (2001)

[27] M. Greiner and I. Bloch, private communication

[28] C. Menotti, private communication