Pair Correlations in a Finite-Temperature 1D Bose Gas

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We calculate the two-particle local correlation for an interacting 1D Bose gas at finite temperature and classify various physical regimes. We present the exact numerical solution by using the Yang-Yang equations and Hellmann-Feynman theorem and develop analytical approaches. Our results draw prospects for identifying the regimes of coherent output of an atom laser, and of finite-temperature "fermionization" through the measurement of the rates of two-body inelastic processes, such as photoassociation.

Recent observations of the one-dimensional (1D) regime in trapped Bose gases [1] offer unique opportunities for extending our understanding of the physics of these quantum many-body systems. The reason is that the 1D regime can be investigated theoretically by making use of the known exactly solvable 1D models [2], which have been the subject of extensive studies since the pioneering works of Girardeau [3], Lieb and Liniger [4], and Yang and Yang [5] (see [6–8] for reviews). With the development of experimentally viable Bose gases, these field theory models — once of theoretical relevance only — are now becoming testable in tabletop experiments.

The knowledge of the exact solutions to the 1D models allows us to go far beyond the mean-field Bogoliubov approximation. In the current stage of studies of experimentally feasible 1D Bose gases, one of the most important issues that requires such an approach is understanding the correlation properties in the various regimes at *finite temperatures*.

In this Letter, we give an exact calculation of the finite-temperature two-particle local correlation for an interacting uniform 1D Bose gas, $g^{(2)} = \langle \hat{\Psi}^\dagger(x)^2 \hat{\Psi}(x)^2 \rangle / n^2$, where $\hat{\Psi}(x)$ is the field operator and $n = \langle \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \rangle$ is the linear (1D) density. As a result, we identify and classify various finite-temperature regimes of the 1D Bose gas. Aside from this, the pair correlations are responsible for the rates of inelastic collisional processes [9], and are of particular importance for the studies of coherence properties of atom "lasers" produced in 1D waveguides.

At $T = 0$, the local two- and three-particle correlations of a uniform 1D Bose gas have recently been calculated in Ref. [10]. Here one has two well-known and physically distinct regimes of quantum degeneracy. For weak couplings or high densities, the gas is in a coherent or Gross-Pitaevskii (GP) regime with $g^{(2)} \to 1$. In this regime, long-range order is destroyed by long-wavelength phase fluctuations [11] and the equilibrium state is a quasicon-

densate characterized by suppressed density fluctuations. For strong couplings or low densities, the gas reaches the strongly interacting or Tonks-Girardeau (TG) regime and undergoes fermionization [3,4]: The wave function strongly decreases as particles approach each other, and $g^{(2)} \to 0$.

At the nonzero temperatures studied here, one has to further extend the classification of different regimes. For strong enough couplings or low densities, we obtain the TG regime with $g^{(2)} \to 0$ not only at low temperatures, but also at high temperatures. In addition, and in contrast to previous $T = 0$ results, we find a weak-coupling or high-density regime in which fluctuations are enhanced. Asymptotically, they reach the noninteracting Bose gas level of $g^{(2)} \to 2$ (rather than $g^{(2)} \to 1$), for any finite-temperature T.

The emergence of this behavior at low temperatures implies that one can identify *three* physically distinct regimes of quantum degeneracy: the strong-coupling TG regime of fermionization with $g^{(2)} \to 0$, a coherent GP regime with $g^{(2)} \simeq 1$ at intermediate coupling strength, and a fully decoherent quantum (DQ) regime with $g^{(2)} \simeq 2$ at very weak couplings. In the GP regime, where the density fluctuations are suppressed and one has a quasicondensate, the local correlation approaches the coherent level of $g^{(2)} \simeq 1$. However, a free (noninteracting) Bose gas at any finite T must have $g^{(2)} = 2$. So, below a critical density- and temperature-dependent level of interaction strength, one must have an increase in thermal fluctuations, until the ideal-gas level is reached in a continuous transition. At $T = 0$, the transition is discontinuous and occurs at zero interaction strength, so that it can be viewed as a zero-temperature phase transition. At high temperatures the GP regime vanishes and a decrease of coupling strength transforms the high-temperature TG regime directly into a classical ideal gas.

We start by considering a uniform gas of N bosons interacting via repulsive delta-function potential in a 1D

box of length L with periodic boundary condition. In the thermodynamic limit ($N, L \to \infty$, while the density $n = N/L$ is fixed), the system is exactly integrable by using the Bethe ansatz, both at $T = 0$ and finite temperature [4,5]. In second quantization, the Hamiltonian is

$$\hat{H} = \frac{\hbar^2}{2m} \int dx \, \partial_x \hat{\Psi}^\dagger \partial_x \hat{\Psi} + \frac{g}{2} \int dx \, \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \, \hat{\Psi}, \quad (1)$$

where $\hat{\Psi}(x)$ is the field operator, m is the mass, and $g > 0$ is the coupling constant. For Bose gases in highly elongated traps to be described by this 1D model, the coupling g is expressed through the 3D scattering length a. This is done assuming that a is much smaller than the amplitude of transverse zero point oscillations $l_0 = \sqrt{\hbar/m\omega_0}$, where ω_0 is the frequency of the transverse harmonic potential. For a positive $a \ll l_0$, one has

$$g = 2\hbar^2 a / m l_0^2, \quad (2)$$

and the 1D scattering length a_{1D} is $\hbar^2/mg \simeq l_0^2/a \gg l_0$ [12]. The 1D regime is reached if l_0 is much smaller than the thermal de Broglie wavelength of excitations $\Lambda_T = (2\pi\hbar^2/mT)^{1/2}$ and a characteristic length scale l_c [13] responsible for short-range correlations. On the same grounds as at $T = 0$ [10], one finds that for fulfilling this requirement it is sufficient to satisfy the inequalities $a \ll l_0 \ll \{1/n, \Lambda_T\}$.

The uniform 1D Bose gas with a short-range repulsive interaction can effectively be characterized by two parameters: the dimensionless coupling parameter

$$\gamma = mg / \hbar^2 n, \quad (3)$$

and the reduced temperature $\tau = T/T_d$, where the temperature of quantum degeneracy is given by $T_d = \hbar^2 n^2 / 2m$, in energy units ($k_B = 1$).

For calculating the local two-body correlation $g^{(2)}$ at any values of γ and τ, we use the Hellmann-Feynman theorem [14]. At $T = 0$, it has been used for calculating the mean interaction energy [4], and for expounding the issue of local pair correlations [10]. Consider the partition function $Z = \exp(-F/T) = \mathrm{Tr}\exp(-\hat{H}/T)$ which determines the free energy F. Here the trace is taken over the states of the system with a fixed number of particles in the canonical formalism. For the grand canonical description, one has to replace the condition of a constant particle number by the condition of a constant chemical potential μ and add a term $-\mu\hat{N}$ to the Hamiltonian. For the derivative of F with respect to the coupling constant, one has $\partial F/\partial g = -T\partial(\log Z)/\partial g$ and, hence,

$$\frac{\partial F}{\partial g} = \frac{1}{Z}\mathrm{Tr}[e^{-\hat{H}/T} \, \partial \hat{H}/\partial g] = (L/2)\langle \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \, \hat{\Psi}\rangle. \quad (4)$$

Introducing the free energy per particle $f(\gamma, \tau) = F/N$, the normalized two-particle correlation is

$$g^{(2)} = \frac{\langle \hat{\Psi}^\dagger \hat{\Psi}^\dagger \hat{\Psi} \, \hat{\Psi}\rangle}{n^2} = \frac{2m}{\hbar^2 n^2}\left(\frac{\partial f(\gamma, \tau)}{\partial \gamma}\right)_{n,\tau}. \quad (5)$$

We have calculated the free energy $f(\gamma, \tau)$ by numerically solving the Yang-Yang exact integral equations for the excitation spectrum and the distribution function of "quasimomenta" [5]. By implementing a postselective algorithm that ensures that the derivative of $f(\gamma, \tau)$ is taken for constant n, we then calculate $g^{(2)}$ from Eq. (5). The results of our calculations are presented in Fig. 1. We now give a physical description of different regimes determined by the values of the coupling constant γ and the reduced temperature τ.

Strong coupling regime $[\gamma \gtrsim \max(1, \sqrt{\tau})]$.—In the strong-coupling TG regime, the local correlation $g^{(2)}$ reduces dramatically due to the strong repulsion between particles, and becomes zero for $\gamma \to \infty$. In this regime the physics resembles that of free fermions, both below and above the quantum degeneracy temperature. Along the lines of Ref. [10], to leading order in $1/\gamma$ the finite temperature $g^{(2)}$ can be expressed through derivatives of Green's function of free fermions $G(x) = \int dk \, n_F(k) \times \exp(ikx)/(2\pi)$, where $n_F(k)$ are occupation numbers for free fermions. For the normalized local correlation, we obtain $g^{(2)} = 4[(G'(0))^2 - G''(0)G(0)]/\gamma^2 n^4$.

In the regime of quantum degeneracy, $\tau \ll 1$, the local correlation is dominated by the ground state distribution $n_F(k) = \theta(k_F^2 - k^2)$, where $k_F = \pi n$ is the Fermi momentum. Small finite-temperature corrections are obtained using the Sommerfeld expansion:

$$g^{(2)} = \frac{4}{3}\left(\frac{\pi}{\gamma}\right)^2\left[1 + \frac{\tau^2}{4\pi^2}\right], \qquad \tau \ll 1. \quad (6)$$

This low temperature result for $g^{(2)}$ has a simple physical meaning. A characteristic distance related to the interaction between particles is $a_{1D} = \hbar^2/mg \sim 1/\gamma n$, and fermionic correlations are present at interparticle distances $x \gtrsim a_{1D}$. For smaller x, the correlations practically do not change. Hence, the correlation $g^{(2)}$ for large γ is nothing else than the pair correlation for free fermions at a distance a_{1D}. The latter is $g^{(2)} \sim (k_F a_{1D})^2 \sim 1/\gamma^2$, which agrees with the result of Eq. (6) for $\tau \to 0$.

In the temperature interval $1 \ll \tau \ll \gamma^2$, the gas is nondegenerate, but the 1D scattering length a_{1D} is still

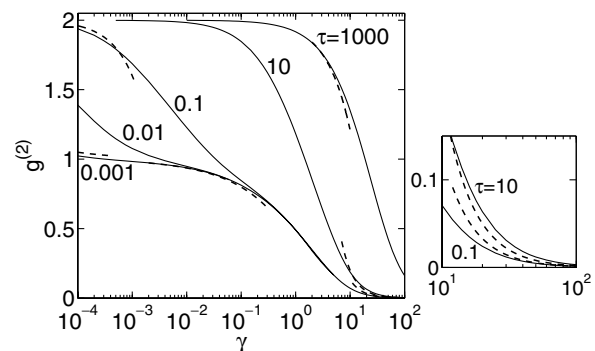FIG. 1. The local correlation $g^{(2)}$ versus γ at different τ. The solid curves are exact numerical results, while the dashed curves represent analytic results (see text).

much smaller than the thermal de Broglie wavelength Λ_T. As the characteristic momentum of particles is now the thermal momentum $k_T = \sqrt{2mT}/\hbar$, one estimates that $g^{(2)} \sim (k_T a_{1D})^2 \sim \tau/\gamma^2$. Calculating Green's function $G(x)$ for the classical distribution $n_F(k)$, we obtain

$$g^{(2)} = 2\tau/\gamma^2, \qquad 1 \ll \tau \ll \gamma^2, \qquad (7)$$

which agrees with the given qualitative estimate. The local correlation $g^{(2)}$ is still much smaller than 1, and we thus have a regime of high-temperature "fermionization."

The results of Eqs. (6) and (7) agree with the outcome of our numerical calculations. For $\tau = 0.1$ and $\tau = 10$, they are shown in Fig. 1 (in the region of large γ) by dashed curves next to the solid curves found numerically for the same values of τ.

GP regime ($\tau^2 \lesssim \gamma \lesssim 1$).—In the intermediate coupling or GP regime, for sufficiently low temperatures the equilibrium state is a quasicondensate: The density fluctuations are suppressed, but the phase fluctuates [15]. As the phase-coherence length l_ϕ greatly exceeds the short-range characteristic length $l_c = \hbar/\sqrt{mng}$, for finding the local correlations the field operator can be represented as a sum of the macroscopic component Ψ_0 and a small component $\hat{\Psi}'$ describing finite-momentum excitations. Actually, the component Ψ_0 contains the contribution of excitations with momenta $k \lesssim k_0 \ll l_c^{-1}$, whereas $\hat{\Psi}'$ includes the contribution of larger k. At the same time, the momentum k_0 is chosen such that most of the particles are contained in Ψ_0. This picture is along the lines of Ref. [6], and the momentum k_0 drops out of the answer as the main contribution of $\hat{\Psi}'$ to $g^{(2)}$ is provided by excitations with $k \sim l_c^{-1}$ [16]. The two-particle local correlation is then reduced to $g^{(2)} = 1 + 2(\langle\hat{\Psi}'^\dagger\hat{\Psi}'\rangle + \langle\hat{\Psi}'\hat{\Psi}'\rangle)/n$. The normal and anomalous averages, $\langle\hat{\Psi}'^\dagger\hat{\Psi}'\rangle$ and $\langle\hat{\Psi}'\hat{\Psi}'\rangle$, can be calculated by using the same Bogoliubov transformation for $\hat{\Psi}'$ as in 3D. This gives the result that

$$g^{(2)} = 1 + \int_{-\infty}^{\infty} \frac{dk}{2\pi n}\left[\frac{E_k}{\varepsilon_k}(1 + n_k) - 1\right], \qquad (8)$$

where $E_k = \hbar^2 k^2/2m$, $\varepsilon_k = \sqrt{E_k^2 + 2ngE_k}$ is the Bogoliubov excitation energy, and n_k are occupation numbers for the excitations.

The integral term in Eq. (8) contains the contribution of both vacuum and thermal fluctuations. The former is determined by excitations with $k \sim l_c^{-1}$, and at $\tau = 0$ we immediately recover the zero-temperature result of Ref. [10]. For very low temperatures $\tau \ll \gamma$, thermal fluctuations give an additional correction, so that

$$g^{(2)} = 1 - 2\sqrt{\gamma}/\pi + \pi\tau^2/(24\gamma^{3/2}), \qquad \tau \ll \gamma \ll 1. \quad (9)$$

The phase-coherence length is determined by vacuum fluctuations of the phase and is $l_\phi \sim l_c \exp(\pi/\sqrt{\gamma})$ [11]. For $\tau = 0.001$, the above approximate result, shown in Fig. 1 at intermediate values of γ, practically coincides with the corresponding exact numerical result.

For temperatures $\tau \gg \gamma$, thermal fluctuations are more important than vacuum fluctuations. The main contribution to the local correlation is again provided by excitations with $k \sim l_c^{-1}$, and we obtain from Eq. (8)

$$g^{(2)} = 1 + \tau/(2\sqrt{\gamma}), \qquad \gamma \ll \tau \ll \sqrt{\gamma}. \quad (10)$$

The phase-coherence length is determined by long-wavelength phase fluctuations. The calculation similar to that for a trapped gas [17] gives $l_\phi \approx \hbar^2 n/mT$. The condition $l_\phi \gg l_c$, which is necessary for the existence of a quasicondensate and for the applicability of the Bogoliubov approach, immediately yields the inequality $\tau \ll \sqrt{\gamma}$. Thus, Eq. (10) is valid under the condition $\gamma \ll \tau \ll \sqrt{\gamma}$, and the second term on the right-hand side of this equation is a small correction. One can easily see that this correction is just the relative mean square density fluctuations. In the region of its validity, the result of Eq. (10) agrees well with our numerical data, and is shown in Fig. 1 for $\tau = 0.001$, in the region of small γ values. The exact results graphed in Fig. 1 for different values of τ show that the coherent or GP regime is not present for $\tau \gtrsim 0.1$, in the sense that $g^{(2)}$ as a function of γ does not develop a plateau around the value $g^{(2)} = 1$.

Decoherent regime.—At very weak couplings, $\gamma \lesssim \min(\tau^2, \sqrt{\tau})$, the gas enters a decoherent regime. Both phase and density fluctuations are large. At small enough γ the local correlation is always close to the result for free bosons, $g^{(2)} = 2$. In this regime, the only consequence of quantum degeneracy is the quantum Bose distribution for occupation numbers of particles, so we can further divide it into a decoherent quantum (DQ) regime for $\tau < 1$ and a decoherent classical (DC) regime for $\tau > 1$.

The result of Eq. (10) cannot be used for $\gamma = 0$. In this case one has a gas of free bosons, and Wick's theorem leads to $g^{(2)} = 2$ at any τ. For small τ, our data in Fig. 1 show a sharp increase of $g^{(2)}$ from almost 1 to almost 2 when $\gamma \lesssim \tau^2$. This is a continuous transition from the quasicondensate to the DQ regime [18]. Lowering the temperature lowers the value of γ at which this transition occurs. For $\tau = 0$, the transition takes place at $\gamma = 0$. In this case it is discontinuous and can be regarded as a zero-temperature phase transition.

The DQ regime can be treated asymptotically by employing a standard perturbation theory with regard to the coupling constant g. Omitting the details of calculations, which will be published elsewhere, for the local correlation we obtain

$$g^{(2)} = 2 - 4\gamma/\tau^2, \qquad \sqrt{\gamma} \ll \tau \ll 1. \quad (11)$$

At higher temperatures $\tau \gtrsim 1$, the decoherent *quantum* regime ($\sqrt{\gamma} \lesssim \tau \lesssim 1$) transforms to the decoherent *classical* regime ($\tau \gtrsim \max\{1, \gamma^2\}$) and $g^{(2)}$ remains close to 2 (see Fig. 1). The local correlation is found in the same way as in the DQ regime and takes the asymptotic form

$$g^{(2)} = 2 - \gamma\sqrt{2\pi/\tau}, \qquad \tau \gg \max\{1, \gamma^2\}. \quad (12)$$

The result of Eq. (12) remains valid for large values of γ, provided that $\gamma^2 \ll \tau$. Here the de Broglie wavelength Λ_T becomes smaller than a_{1D} and the regime of high-temperature fermionization continuously transforms into the decoherent regime of a classical gas. The corrections to $g^{(2)} = 2$, given by Eqs. (11) and (12), are in agreement with the exact numerical calculations. In Fig. 1, the approximate analytical results are shown by the dashed lines next to the corresponding solid lines found numerically, for $\tau = 0.1$ and $\tau = 1000$.

In conclusion, we have calculated the two-particle local correlation $g^{(2)}$ for a uniform 1D Bose gas at finite temperatures [19]. Within their range of validity, the analytical results agree with exact numerical calculations based on the Hellmann-Feynman theorem and the Yang-Yang equations. The knowledge of $g^{(2)}$ allows one to deduce when the approximate GP equation often used for first-order phase-coherence calculations is valid. The value of $g^{(2)} \simeq 1$ indicates that the correlation function factorizes, which is a necessary condition for using the GP approach. The prediction of coherent behavior only for certain temperatures and interaction strengths, $\tau^2 \lesssim \gamma \lesssim 1$, may be an important criterion for atom lasers where spatial coherence is a necessary ingredient in obtaining interference and high-resolution interferometry. Our results are also promising for identifying the regime of fermionization in finite-temperature 1D Bose gases through the measurement of inelastic processes in pair interatomic collisions such as photoassociation. Here the transitions occur at interatomic distances which are much smaller than the short-range correlation length l_c and, therefore, the rate will be proportional to the local correlation $g^{(2)}$.

We also find a fully decoherent quantum regime in the case of very weak interactions or high densities. There is a *continuous* transition from the GP regime to the ideal-gas limit ($\gamma \to 0$), where the gas displays large thermal (Gaussian) density fluctuations with $g^{(2)} = 2$ at any finite temperature [20]. As γ is decreased towards the ideal gas, the GP result holds only above a certain ratio of interaction strength to density. Below this, the GP approach becomes invalid and there is a dramatic increase in fluctuations, with $g^{(2)} \to 2$ as $\gamma \to 0$.

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