Beyond the Tonks-Girardeau Gas: Strongly Correlated Regime in Quasi-One-Dimensional Bose Gases

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We consider a homogeneous 1D Bose gas with contact interactions and a large attractive coupling constant. This system can be realized in tight waveguides by exploiting a confinement induced resonance of the effective 1D scattering amplitude. By using the diffusion Monte Carlo method we show that, for small densities, the gaslike state is well described by a gas of hard rods. The critical density for cluster formation is estimated using the variational Monte Carlo method. The behavior of the correlation functions and of the frequency of the lowest breathing mode for harmonically trapped systems shows that the gas is more strongly correlated than in the Tonks-Girardeau regime.

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The study of quasi-1D Bose gases in the quantum-degenerate regime has become a very active area of research. The role of correlations and of quantum fluctuations is greatly enhanced by the reduced dimensionality, and 1D quantum gases constitute well-suited systems to study beyond mean-field effects [1]. Among these, particularly intriguing is the fermionization of a 1D Bose gas in the strongly repulsive Tonks-Girardeau (TG) regime, where the system behaves as if it consisted of noninteracting spinless fermions [2]. The Bose-Fermi mapping of the TG gas is a peculiar aspect of the universal low-energy properties which are exhibited by bosonic and fermionic gapless 1D quantum systems and are described by the Luttinger liquid model [3]. The concept of a Luttinger liquid plays a central role in condensed matter physics, and the prospect of a clean testing for its physical implications using ultracold gases confined in highly elongated traps is fascinating [4].

Bosonic gases in 1D configurations have been realized experimentally. Complete freezing of the transverse degrees of freedom and fully 1D kinematics has been reached for systems prepared in a deep 2D optical lattice [5,6]. The strongly interacting regime has been recently achieved using different techniques [7]. Alternatively, the strength of the interactions can be increased by using a Feshbach resonance[8]. With this method one can tune the effective 1D coupling constant g_{1D} to essentially any value, including $\pm\infty$, by exploiting a confinement induced resonance [9]. For large and positive values of g_{1D}, the system is a TG gas of pointlike impenetrable bosons. On the contrary, if g_{1D} is large and negative, we will show that a new gaslike regime is entered (super-Tonks gas regime) where the hard-core repulsion between particles becomes of finite range and correlations are stronger than in the TG regime. Some consequences of this new regime on the energetics of small systems in harmonic traps have already been pointed out in a preceding study [10]. In this Letter, we investigate the equation of state and the correlation functions of a homogeneous 1D Bose gas in the super-Tonks regime. We find that the particle-particle correlations decay faster than in the TG gas and that the static structure factor exhibits a peak. The momentum distribution and the structure factor of the gas are directly accessible in experiments by using, respectively, time-of-flight techniques and two-photon Bragg spectroscopy. The study of collective modes also provides a useful experimental technique to investigate the role of interactions and beyond mean-field effects [5]. Within a local density approximation (LDA) for systems in harmonic traps, we calculate the frequency of the lowest compressional mode as a function of the interaction strength. We find that in the super-Tonks regime the frequency is larger than for a TG gas.

We consider a 1D system of N spinless bosons described by the following contact-interaction Hamiltonian:

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

where m is the mass of the particles, $z_{ij} = z_i - z_j$ denotes the interparticle distance between particles i and j, and g_{1D} is the coupling constant which we take to be large and negative. The study of the scattering problem of two particles in tight waveguides yields the following result for the effective 1D coupling constant g_{1D} in terms of the 3D s-wave scattering length a_{3D} [9]:

$$g_{1D} = -\frac{2\hbar^2}{ma_{1D}} = \frac{2\hbar^2 a_{3D}}{ma_\perp^2}\frac{1}{1 - Aa_{3D}/a_\perp}, \quad (2)$$

where $a_\perp = \sqrt{\hbar/m\omega_\perp}$ is the characteristic length of the transverse harmonic confinement producing the waveguide and $A = |\zeta(1/2)|\sqrt{2} = 1.0326$, with $\zeta(\cdots)$ the Riemann zeta function. The confinement induced resonance is located at the critical value $a_{3D}^c = a_\perp/A$ and corresponds to the abrupt change of g_{1D} from large positive values ($a_{3D} \lesssim a_{3D}^c$) to large negative values ($a_{3D} \gtrsim a_{3D}^c$). The renormalization (2) of the effective 1D coupling constant has been recently confirmed in a many-body calculation of Bose gases in highly elongated harmonic traps using quantum Monte Carlo techniques [10].

For positive g_{1D}, the Hamiltonian (1) corresponds to the Lieb-Liniger (LL) model. The ground state and excited states of the LL Hamiltonian have been studied in detail [11], and, in particular, the TG regime corresponds to the limit $g_{1D} \to +\infty$. The ground state of the Hamiltonian (1) with $g_{1D} < 0$ has been investigated by McGuire [12], and one finds a solitonlike state with energy $E/N = -mg_{1D}^2(N^2-1)/24\hbar^2$. The lowest-lying gaslike state of the Hamiltonian (1) with $g_{1D} < 0$ corresponds to an excited state that is (meta)stable if the gas parameter $na_{1D} \ll 1$, where n is the density and a_{1D} is the 1D effective scattering length defined in Eq. (2). This state can be realized in tight waveguides by crossing adiabatically the confinement induced resonance. The stability of the gaslike state can be understood from a simple estimate of the energy per particle. For a contact potential the interaction energy $E_{\rm int}/N = g_{1D}ng_2(0)/2$ can be written in terms of the local two-body distribution function $g_2(0) = \langle\psi^\dagger(z)\psi^\dagger(z)\psi(z)\psi(z)\rangle/n^2$, where $\psi^\dagger$, ψ are the creation and annihilation particle operators. In the limit $g_{1D} \to -\infty$, one can use for the distribution function the result in the TG regime [13] $g_2(0) \simeq \pi^2n^2a_{1D}^2/3$, which does not depend on the sign of g_{1D}. In the same limit, the kinetic energy can be estimated by $E_{\rm kin}/N \simeq \pi^2\hbar^2n^2/(6m)$, corresponding to the energy per particle of a TG gas. For the total energy $E = E_{\rm kin} + E_{\rm int}$, one finds the result $E/N \simeq \pi^2\hbar^2n^2/(6m) - \pi^2\hbar^2n^3a_{1D}/(3m)$, holding for $na_{1D} \ll 1$. For $na_{1D} < 0.25$ this equation of state yields a positive inverse compressibility $mc^2 = n\partial\mu/\partial n$, where $\mu = dE/dN$ is the chemical potential and c is the speed of sound, corresponding to a gaslike phase. We will show that a more precise estimate yields that the gaslike state is stable against cluster formation for $na_{1D} \lesssim 0.35$.

The analysis of the gaslike equation of state is carried out using both the diffusion Monte Carlo (DMC) and variational Monte Carlo (VMC) methods. The trial wave function employed in the VMC calculation, as well as in the DMC one as importance sampling, is of the form $\psi_T(z_1,\ldots,z_N) = \prod_{i<j} f(z_{ij})$, where the two-body Jastrow term is chosen as

$$f(z) = \begin{cases} \cos[k(|z|-\bar{Z})] & \text{for } |z| \le \bar{Z}, \\ 1 & \text{for } |z| > \bar{Z}. \end{cases} \quad (3)$$

The cutoff length $\bar{Z}$ is a variational parameter. The wave vector k for a given $\bar{Z}$ is chosen such that the boundary condition at $z = 0$ imposed by the δ-function potential is satisfied: $-k\tan(k\bar{Z}) = 1/a_{1D}$. For distances smaller than the cutoff length, $|z| \le \bar{Z}$, the above wave function corresponds to the exact solution with positive energy of the two-body problem with the interaction potential $g_{1D}\delta(z)$. For $g_{1D} < 0$ ($a_{1D} > 0$) the wave function $f(z)$ changes sign at a nodal point which, for $\bar{Z} \gg a_{1D}$, is located at $|z| = a_{1D}$. In the calculations, we have used $N = 100$ particles with periodic boundary conditions. The variational energy slowly decreases by increasing the parameter $\bar{Z}$ and saturates for large values of $\bar{Z}$. We have chosen to use in all simulations the value $\bar{Z} = L/2$, where L is the size of the simulation box. Calculations carried out with larger values of N up to $N = 400$ have shown negligible finite size effects. The nonpositive character of $f(z)$ in Eq. (3) introduces a sign problem in the DMC calculation, which is overcome using the standard fixed-node (FN) approximation. This technique provides a rigorous upper bound to the energy determined by the nodal constraint of the trial wave function [14].

Results for the energy as a function of the gas parameter na_{1D}, using both VMC and DMC methods, are shown in Fig. 1. For small values of the gas parameter $na_{1D} \le 0.1$, the DMC energies reproduce exactly the equation of state of a gas of hard rods (HRs) of size a_{1D} (thick dashed line). The HR energy per particle can be calculated exactly from the energy of a TG gas by accounting for the excluded volume [2]:

$$\frac{E_{\rm HR}}{N} = \frac{\pi^2\hbar^2n^2}{6m}\frac{1}{(1-na_{1D})^2}. \quad (4)$$

Up to $na_{1D} = 0.1$, the VMC energies are not distinguishable from the DMC ones, a feature that points out the high quality of the trial wave function in Eq. (3). Beyond this value of the gas parameter, the DMC energy begins to show instabilities which preclude to continue the calculation of the metastable gas. Therefore, for larger values of na_{1D} the energies are estimated only with the VMC energy. It is worth stressing that for the values of na_{1D} shown in Fig. 1 the VMC calculation is stable and does not show evidence of long-lived cluster states. This indicates that the overlap between the trial wave function and states with clusters

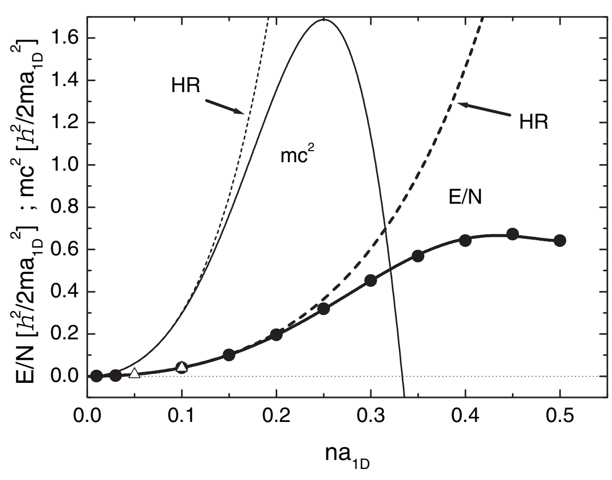

FIG. 1. Energy per particle and inverse compressibility as a function of the gas parameter na_{1D}. Open triangles, DMC results; solid symbols and thick solid line, VMC results and polynomial best fit; thick dashed line, HR equation of state [Eq. (4)]. Statistical error bars are smaller than the size of the symbols. Thin solid and dashed lines, mc^2 from the variational and HR equation of state, respectively.

formed is very small. By fitting a polynomial function to our variational results we obtain the best fit shown in Fig. 1 as a thick solid line. The inverse compressibility obtained from the best fit is shown in Fig. 1 as a thin solid line and is compared with mc^2 of a HR gas (thin dashed line). As a function of the gas parameter, mc^2 shows a maximum and then drops abruptly to zero. The vanishing of the speed of sound implies that the system is mechanically unstable against cluster formation. Our variational estimate yields the value $na_{1D} \simeq 0.35$ for the critical value of the density where the instability appears. This value coincides with the critical density for collapse calculated in the center of the trap for harmonically confined systems [10].

For small values of the gas parameter, the HR model also describes correctly the correlation functions of the super-Tonks gas. Where the DMC calculations are feasible, we will explicitly show the HR behavior by direct comparison with the DMC results based on the trial wave function Eq. (3). The correlation functions of a HR gas of size a_{1D} can be calculated from the exact wave function [15] $\psi_{HR} = \prod_{i<j}|\sin[\pi(z'_i - z'_j)/L]|$, where the set of coordinates $\{z'_j\}$ is obtained from the set $\{z_j\}$ with the ordering $z_1 < z_2 - a_{1D} < z_3 - 2a_{1D} < \cdots < z_N - (N-1)a_{1D}$ using the transformation $z'_j = z_j - ja_{1D}$, with $j = 1, 2, \ldots, N$. We focus our attention on the static structure factor $S(k)$, which in terms of the density fluctuation operator $\rho_k = \sum_{i=1}^{N} e^{ikz_i}$ is defined as

$$S(k) = \frac{1}{N}\frac{\langle\psi_{HR}|\rho_k\rho_{-k}|\psi_{HR}\rangle}{\langle\psi_{HR}|\psi_{HR}\rangle}, \tag{5}$$

and the one-body density matrix

$$g_1(z) = \frac{N}{n}\frac{\int\psi^*_{HR}(z_1+z,\ldots,z_N)\psi_{HR}(z_1,\ldots,z_N)dz_2\cdots dz_N}{\int|\psi_{HR}(z_1,\ldots,z_N)|^2dz_1\cdots dz_N}. \tag{6}$$

Contrary to the TG case, it is not possible to obtain analytical expressions for $g_1(z)$ and $S(k)$ in the HR problem. We have calculated them using configurations generated by a Monte Carlo simulation according to the exact probability distribution function $|\psi_{HR}|^2$. The results for the static structure factor are shown in Fig. 2. Compared to $S(k)$ in the TG regime, a clear peak is visible for values of k of the order of twice the Fermi wave vector $k_F = \pi n$ and the peak is more pronounced as na_{1D} increases. The change of slope for small values of k reflects the increase of the speed of sound c with na_{1D}. The DMC result for $S(k)$ at the density $na_{1D} = 0.1$ is also shown in Fig. 2; the agreement with the HR $S(k)$ at the same density is remarkable.

The long-range behavior of $g_1(z)$ can be obtained from the hydrodynamic theory of low-energy excitations [16]. For $|z| \gg \xi$, where $\xi = \hbar/(\sqrt{2}mc)$ is the healing length of the system, one finds the power-law decay $g_1(z) \propto 1/|z|^\alpha$, where the exponent α is given by $\alpha = mc/(2\pi\hbar n)$. For a TG gas, $mc = \pi\hbar n$ and thus $\alpha_{TG} = 1/2$. For a HR gas,

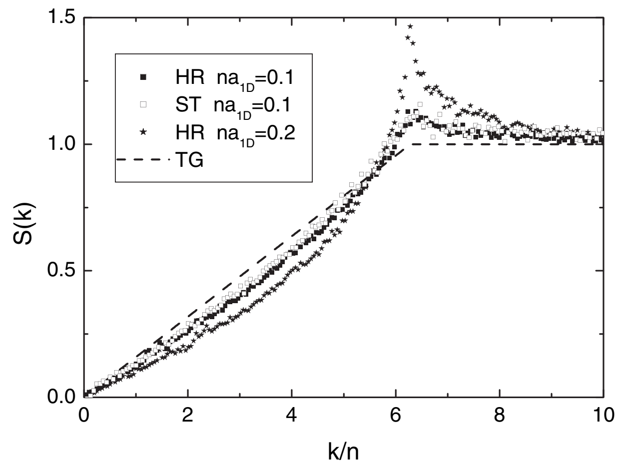

FIG. 2. Static structure factor $S(k)$ for a gas of HRs at different values of the gas parameter na_{1D} and for a TG gas (dashed line). Open symbols stand for the DMC result of the super-Tonks (ST) regime at $na_{1D} = 0.1$.

one finds $\alpha = \alpha_{TG}/(1 - na_{1D})^2$ and thus $\alpha > \alpha_{TG}$. This behavior is clearly shown in Fig. 3, where we compare $g_1(z)$ of a HR gas with $na_{1D} = 0.1$ and 0.2 to the result of a TG gas [17]. The DMC result for $g_1(z)$ at $na_{1D} = 0.1$ is also shown in the figure; its long-range behavior matches the expected behavior of the HR model at this density, $g_1(z) \propto 1/|z|^{0.617}$. The long-range power-law decay of $g_1(z)$ is reflected in the infrared divergence of the momentum distribution $n(k) \propto 1/|k|^{1-\alpha}$ holding for $|k| \ll 1/\xi$. The power-law decay of $g_1(z)$ and the linear slope of $S(k)$ at low momenta show that the super-Tonks gas belongs to the Luttinger liquid universality class [3]. The larger value of α and the peak in $S(k)$ show that correlations are stronger and more short ranged than in the TG gas.

Another possible experimental signature of the super-Tonks regime can be provided by the study of collective

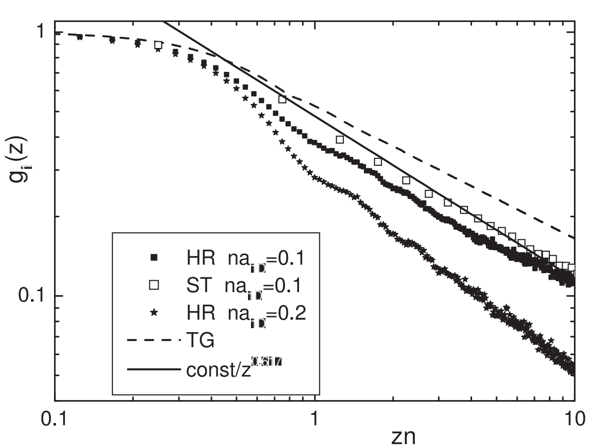

FIG. 3. One-body density matrix $g_1(z)$ for a gas of HR at different values of the gas parameter na_{1D} and for a TG gas (dashed line). Open symbols stand for the DMC result of the super-Tonks (ST) regime at $na_{1D} = 0.1$. The solid line corresponds to the power-law fit $g_1(z) = \text{const}/z^{0.617}$ to the DMC data.

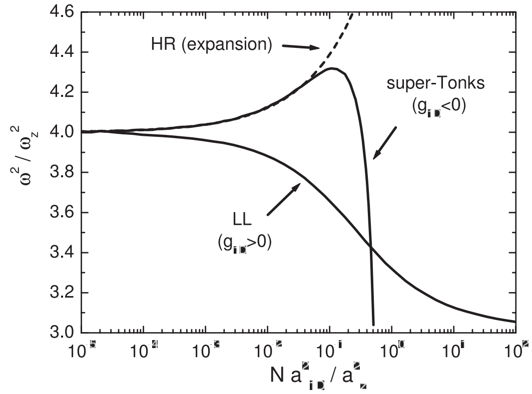

FIG. 4. Square of the lowest breathing mode frequency, ω^2, as a function of the coupling strength Na_{1D}^2/a_z^2 for the LL Hamiltonian ($g_{1D} > 0$) and in the super-Tonks regime ($g_{1D} < 0$). The dashed line refers to the HR expansion (see text).

modes. We calculate the frequency of the lowest compressional mode of a system of N particles in a harmonic potential $V_{ext} = \sum_{i=1}^{N} m\omega_z^2 z_i^2/2$. We make use of LDA, which allows us to calculate the chemical potential of the inhomogeneous system $\tilde{\mu}$ and the density profile $n(z)$ from the local equilibrium equation $\tilde{\mu} = \mu[n(z)] + m\omega_z^2 z^2/2$, and the normalization condition $N = \int_{-R}^{R} n(z)dz$, where $R = \sqrt{2\tilde{\mu}/(m\omega_z^2)}$ is the size of the cloud. For densities n smaller than the critical density for cluster formation, $\mu[n]$ is the equation of state of the homogeneous system derived from the fit to the VMC energies (Fig. 1). From the knowledge of the density profile $n(z)$, one can obtain the mean square radius of the cloud $\langle z^2 \rangle = \int_{-R}^{R} n(z) z^2 dz/N$, and thus, making use of the result [18] $\omega^2 = -2\langle z^2\rangle/(d\langle z^2\rangle/d\omega_z^2)$, one can calculate the frequency ω of the lowest breathing mode. Within LDA, the result will depend only on the dimensionless parameter Na_{1D}^2/a_z^2, where $a_z = \sqrt{\hbar/m\omega_z}$ is the harmonic oscillator length. For $g_{1D} > 0$, i.e., in the case of the LL Hamiltonian, the frequency of the lowest compressional mode increases from $\omega = \sqrt{3}\omega_z$ in the weak-coupling mean-field regime ($Na_{1D}^2/a_z^2 \gg 1$) to $\omega = 2\omega_z$ in the strong-coupling TG regime ($Na_{1D}^2/a_z^2 \ll 1$). The results for ω in the super-Tonks regime are shown in Fig. 4 as a function of the coupling strength. In the regime $Na_{1D}^2/a_z^2 \ll 1$, where the HR model is appropriate, we can calculate analytically the first correction to the frequency of a TG gas. One finds the result $\omega = 2\omega_z[1 + (16\sqrt{2}/15\pi^2)(Na_{1D}^2/a_z^2)^{1/2} + \cdots]$. Figure 4 shows that this expansion accurately describes the frequency of the breathing mode when $Na_{1D}^2/a_z^2 \ll 1$, for larger values of the coupling strength the frequency reaches a maximum and drops to zero at $Na_{1D}^2/a_z^2 \simeq 0.6$. The observation of a breathing mode with a frequency larger than $2\omega_z$ would be a clear signature of the super-Tonks regime.

In conclusion, we have pointed out the existence of a strongly correlated regime in quasi-1D Bose gases beyond the Tonks-Girardeau regime. This regime can be entered by exploiting a confinement induced resonance of the effective 1D scattering amplitude. A FN-DMC simulation of the super-Tonks metastable gas up to a value of the gas parameter $na_{1D} = 0.1$ has been carried out. In this regime, the results obtained for the energy, the structure factor, and the one-body density matrix are reproduced by the exactly solvable HR model. An upper bound of the critical density for the onset of instability against cluster formation is estimated using the VMC method. For harmonically trapped systems, we calculate the frequency of the lowest compressional mode.

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