Quasi-one-dimensional Bose gases with large scattering length

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Bose gases confined in highly-elongated harmonic traps are investigated over a wide range of interaction strengths using quantum Monte Carlo techniques. We find that the properties of a Bose gas under tight transverse confinement are well reproduced by a 1d model Hamiltonian with contact interactions. We point out the existence of a unitary regime, where the properties of the quasi-1d Bose gas become independent of the actual value of the 3d scattering length $a_{3d}$. In this unitary regime, the energy of the system is well described by a hard rod equation of state. We investigate the stability of quasi-1d Bose gases with positive and negative $a_{3d}$.

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In recent years the study of quasi-1d quantum Bose gases has attracted a great deal of interest. Intriguing properties of quasi-1d gases, such as the exact mapping between interacting bosons and non-interacting fermions, have been predicted [1, 2, 3]. A bosonic gas that behaves as if it consisted of spinless fermions, a so-called Tonks-Girardeau (TG) gas, cannot be described within mean-field theory since it exhibits strong correlations; instead, a many-body framework is called for. While experimental evidence of quasi-1d behavior has been reported for bosonic atomic gases under highly-elongated harmonic confinement [4], TG gases have not been observed yet. It has been suggested, however, that TG gases can be realized experimentally for either low atomic densities or strong atom-atom interaction strengths. The 3d s-wave scattering length $a_{3d}$, and hence the strength of atom-atom interactions, can be tuned to essentially any value, including zero and $\pm \infty$, by utilizing a magnetic atom-atom Feshbach resonance [4, 5].

Utilizing a two-body Feshbach resonance, 3d degenerate gases with large scattering length $a_{3d}$ have been studied experimentally and theoretically. For $a_{3d} \to \pm \infty$, it is predicted that the behavior of the strongly-correlated gas is independent of $a_{3d}$ [4]. For homogeneous 3d Bose gases, this unitary regime can most likely not be reached experimentally since three-body recombination is expected to set in when $a_{3d}$ becomes comparable to the average interparticle distance. Three-body recombination leads to cluster formation, and hence “destroys” the gas-like state. The situation is different for Fermi gases, for which the unitary regime has already been achieved experimentally [6]. In this case, the Fermi pressure stabilizes the system even for large $|a_{3d}|$. It has been predicted that three-body recombination processes are suppressed for strongly interacting 1d Bose gases [3]. These studies raise the question whether a highly-elongated inhomogeneous Bose gas, that is, an inhomogeneous quasi-1d Bose gas, is stable as $a_{3d} \to \pm \infty$.

This Letter investigates the properties of a quasi-1d Bose gas at zero temperature over a wide range of interaction strengths within a microscopic, highly accurate many-body framework. We find that the system i) is well described by a 1d model Hamiltonian with contact interactions and renormalized coupling constant [2] for any value of the 3d scattering length $a_{3d}$; ii) behaves like a TG gas for a critical positive value of $a_{3d}$; iii) reaches a unitary regime for large values of $|a_{3d}|$, where the properties of the quasi-1d Bose gas become independent of the actual value of $a_{3d}$ and are similar to those of a hard-rod gas; and iv) becomes unstable against cluster formation for a critical negative value of $a_{3d}$.

Our study is based on the 3d Hamiltonian $H_{3d}$,

$$H_{3d} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{m}{2} \left( \omega_r^2 \rho_i^2 + \omega_z^2 z_i^2 \right) \right] + \sum_{i<j} V(r_{ij}),$$

which describes $N$ spin-polarized mass $m$ bosons under highly-elongated confinement with $\omega_z = \lambda \omega_r$, where $\lambda \ll 1$. The coordinates $\rho_i = \sqrt{x_i^2 + y_i^2}$ and $z_i$ denote, respectively, the radial and axial position of the $i$-th particle, $r_{ij} = |\vec{r}_i - \vec{r}_j|$ denotes the interparticle distance between atom $i$ and $j$, and $V(r)$ denotes the two-body interatomic potential. We consider two different potentials: i) a purely repulsive hard-sphere (HS) potential, $V^{HS}(r) = \infty$ for $r < a_{3d}$, and zero otherwise; and ii) a more realistic short-range (SR) potential, which can support two-body bound states, $V^{SR}(r) = -V_0/cosh^2(r/r_0)$, with well depth $V_0$. For $V^{HS}$, the s-wave scattering length $a_{3d}$ coincides with the range of the potential. For $V^{SR}$, in contrast, $r_0$ determines the range of the potential, while the scattering length $a_{3d}$ is a function of $r_0$ and $V_0$. In our calculations, $r_0$ is fixed at a value much smaller than the transverse oscillator length, $r_0 = 0.1a_\rho$, where $a_\rho = \sqrt{\hbar/m\omega_r}$. To simulate the behavior of $a_{3d}$ near a field-dependent Feshbach resonance, we vary the well depth $V_0$ and consequently the scattering length $a_{3d}$. 


Importantly, $a_{3d}$ diverges for particular values of $V_0$ (the inset of Fig. 1 shows one such divergence). At each divergence, a new two-body s-wave bound state is pulled in. Our numerical calculations (see below) are performed for the well depths $V_0$ shown in the inset of Fig. 1.

We consider situations where the bosonic gas described by Eq. (1) is in the 1d regime for any value of the 3d scattering length $a_{3d}$, which implies $N\lambda < 1$. If the range of $V(r)$ is much smaller than $a_{3d}$, it is predicted [2] that the properties of the 3d gas are well described by the 1d contact-interaction Hamiltonian $H_{1d}$,

$$
H_{1d} = \sum_{i=1}^{N} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z_i^2} + \frac{m}{2} \omega_z^2 z_i^2 \right) + g_{1d} \sum_{i<j} \delta(z_{ij}) + N\hbar\omega_{p},
$$

where $g_{1d}$ is an effective coupling constant. The limit $g_{1d} \to 0$ corresponds to the weakly-interacting mean-field regime, while $g_{1d} \to \infty$ corresponds to the strongly-interacting TG regime. For positive $g_{1d}$ and vanishing confinement ($\omega_p = \omega_z = 0$), Eq. (2) reduces to the Lieb-Liniger (LL) Hamiltonian [2], whose gas-like properties have been studied in detail. For negative $g_{1d}$ and $\omega_z = \omega_p = 0$, Eq. (2) supports cluster-like bound states [10]; little is known about gas-like states in this case.

Below, we solve the many-body Schrödinger equation for the 1d Hamiltonian with confinement, Eq. (2), for positive and negative $g_{1d}$, and relate our results to those for the 3d Hamiltonian, Eq. (1). Considering two bosons in a highly-elongated geometry that interact through a regularized zero-range pseudo-potential, Olshanii [2] shows that the effective 1d coupling constant $g_{1d}$ can be expressed in terms of the known 3d scattering length $a_{3d}$,

$$
g_{1d} = \frac{2\hbar^2 a_{3d}}{ma_p^2} \frac{1}{1 - Aa_{3d}/a_p},
$$

where $A = |(1/2)|/\sqrt{2} = 1.0326$. Alternatively, $g_{1d}$ can be expressed through the effective 1d scattering length $a_{1d}$, $g_{1d} = -2\hbar^2/(ma_{1d})$ [2], where

$$
a_{1d} = -a_p \left( \frac{a_p}{a_{3d}} - A \right).
$$

For $a_{3d} > 0$ (but $a_{3d} \lesssim a_p$), $g_{1d}$ approaches the unrenormalized coupling constant, $g_{1d}^0 = 2\hbar^2 a_{3d}/(ma_p^2)$, which is obtained by averaging the 3d coupling constant

$$
g_{3d} = 4\pi\hbar^2 a_{3d}/m 
$$

over the transverse oscillator ground state (see, e.g., Ref. [3]). For these values of $a_{3d}$, the 1d Hamiltonian given in Eq. (2) with $g_{1d}$ replaced by $g_{1d}^0$ describes a quasi-1d system accurately [11].

For $a_{3d} \gtrsim a_p$ and for negative $a_{3d}$, in contrast, the confinement induced renormalization becomes important, and the effective 1d coupling constant $g_{1d}$ and scattering length $a_{1d}$, Eqs. (3) and (4), have to be used. Figure 1 shows $g_{1d}$ (dashed line) and $a_{1d}$ (solid line) as a function of $a_{3d}$. At the critical value $a_{3d}^c = 0.9684\rho a_p$, indicated by a vertical arrow in Fig. 1, $g_{1d}$ diverges while $a_{1d}$ goes through zero. At the 3d resonance, that is for $a_{3d} \to \pm\infty$, $g_{1d}$ and $a_{1d}$ each reach an asymptotic value $(g_{1d} = -1.9368\rho a_p \hbar \omega_p$ and $a_{1d} = 1.0326\rho a_p$, respectively, indicated by horizontal arrows in Fig. 1). Tuning $a_{3d}$ to large values hence allows a unitary quasi-1d regime, where $g_{1d}$ and $a_{1d}$ are independent of $a_{3d}$, to be entered.

We solve the Schrödinger equation for the many-body 3d Hamiltonian, Eq. (1), numerically using the diffusion quantum Monte Carlo (DMC) technique. Our interest is in the lowest gas-like many-body state. For $V^{HS}$, the lowest gas-like state of $H_{3d}$ coincides with the many-body ground state; to describe this state we hence use the “standard” DMC technique (see, e.g., [12]). For $V^{SR}$, in contrast, the many-body ground state is a cluster-like bound state. To describe the lowest-lying gas-like state, i.e., an excited state, we hence use the fixed-node DMC (FN-DMC) method [13]. For a given many-body nodal surface, the FN-DMC method allows the Schrödinger equation to be solved for approximate excited states. For $N = 2$, we obtain the exact nodal surface by direct diagonalization. Assuming that the scattering properties between each atom pair are unaltered by the presence of other atoms, we then use the $N = 2$ nodal surface to construct the many-body nodal surface. For dilute quasi-1d gases we expect that the FN-DMC approach as implemented here results in highly accurate many-body energies.

Figure 2 shows the resulting 3d energy per particle, $E/N - \hbar\omega_p$, as a function of $a_{3d}$ for $N = 5$ under quasi-1d confinement, $\lambda = 0.01$, for the hard-sphere and the short-range two-body potential, $V^{HS}$ (diamonds) and
The statistical uncertainty of the DMC energies is smaller than the symbol size. Dotted and solid lines show the 1d energy per particle calculated within the LDA for $g_{1d}^0$ (using the LL equation of state) and for $g_{1d}$, Eq. (3) (using the LL equation of state for $g_{1d} > 0$, and the HR equation of state for $g_{1d} < 0$), respectively. A dashed horizontal line indicates the TG energy, and a vertical arrow the position where $g_{1d}$, Eq. (3), diverges.

To compare our results obtained for the 3d Hamiltonian, $H_{3d}$, with those for the 1d Hamiltonian, $H_{1d}$, we also solve the Schrödinger equation for $H_{1d}$, Eq. (2). For positive values of the coupling constant $g_{1d}$ we calculate the many-body ground state energy by the exact DMC method. For $g_{1d} < 0$, however, the 1d Hamiltonian supports many-body bound states, and, as in the 3d case, we use the FN-DMC method to describe the lowest-lying gas-like state. For $N = 2$ and $g_{1d} < 0$, the first excited state of the Schrödinger equation for $H_{1d}$, Eq. (2), has a node at $\gamma_{1d} = a_{1d}$. To solve the many-body Schrödinger equation for $H_{1d}$ with negative $g_{1d}$ for the lowest gas-like state by the FN-DMC technique, we parameterize our many-body nodal surface in terms of $a_{1d}$. This many-body nodal surface is expected to be good if the density of the gas is low.

In addition to the 3d energy per particle, Fig. 2 shows the resulting 1d energy per particle obtained by solving the Schrödinger equation for $H_{1d}$, Eq. (2), for the renormalized coupling constant $g_{1d}^*$ [squares, Eq. (2)], and the unrenormalized coupling constant $g_{1d}$ (pluses), respectively. The 1d energies calculated using the two different coupling constants agree well for small $a_{3d}$, while clear discrepancies become apparent for larger $a_{3d}$. Importantly, the 1d energies calculated using the renormalized 1d coupling constant $g_{1d}^*$ agree well with the 3d energies calculated using the short-range potential $V^{SR}$ (asterisks) up to very large values of the 3d scattering length $a_{3d}$, and also for negative $a_{3d}$. In contrast, at large $a_{3d}$ the 1d energies deviate clearly from the 3d energies calculated using the hard-sphere potential $V^{HS}$ (diamonds). We conclude that the renormalization of the effective 1d coupling constant $g_{1d}^*$ and the 1d scattering length $a_{1d}$ are crucial to reproduce the results of the 3d Hamiltonian $H_{3d}$ when $a_{3d} \gtrsim a_0$ and when $a_{3d}$ negative. Small deviations between the 1d energies calculated using the renormalized 1d coupling constant $g_{1d}^*$ and the 3d energies calculated using the short-range potential $V^{SR}$ remain; we attribute these to the finite range of $V^{SR}$.

If the size of the cloud is much larger than the harmonic oscillator length $a_z$, where $a_z = \sqrt{\hbar/m\omega_z}$, it has been shown that the properties of the 1d LL Hamiltonian $H_{1d}$, $g_{1d} > 0$, are well described by a simple equation of state using the local density approximation (LDA) [1]. For $g_{1d} < 0$, we instead apply the equation of state for 1d hard-rod systems with size $a_{1d}$. For $\gamma_{1d} > a_{1d}$, the corresponding wave function coincides with that of $N$ 1d hard rods of size $a_{1d}$. For small values of the 1d gas parameter, $n_{1d}a_{1d} \ll 1$, where $n_{1d}$ denotes the linear density, we hence expect that the lowest-lying gas-like state of the 1d many-body Hamiltonian with $g_{1d} < 0$ is well described by a system of hard rods of size $a_{1d}$. The exact energy per particle of the uniform hard rod system is given by $E/N = (\pi^2\hbar^2n_{1d}^2/6m)/(1 - n_{1d}a_{1d})^2$ [1]. For trapped systems with $N\lambda \ll 1$ we obtain the expansion

$$E/N - \hbar\omega_p = \hbar\omega_p \frac{N\lambda}{2} \left(1 + \frac{128\sqrt{2}}{45\pi^2} \sqrt{N\lambda} \frac{a_{1d}}{a_p} + \ldots\right).$$

The first term corresponds to the energy per particle in the TG regime. Similarly, the linear density in the center of the cloud is to lowest order given by the TG result, $n_{1d} = \sqrt{2N\lambda/(\pi a_p)}$. In the unitary limit, that is for $a_{1d}/a_p = 1.0326$, expression (5) becomes independent of $a_{3d}$, and depends only on $N\lambda$.

Lines in Fig. 2 show the resulting 1d energies per par-
ticle for the LL equation of state \((g_{1d} > 0)\) as well as the HR equation of state \((g_{1d} < 0)\) calculated within the LDA. Remarkably, the LDA energies nearly coincide with the 1d many-body DMC energies (pluses and squares, respectively); finite-size effects play a role only for \(a_{3d} \ll a_p\). Our calculations establish for the first time that a simple treatment, i.e., a HR equation of state treated within the LDA, describes trapped quasi-1d gases with negative coupling constant \(g_{1d}\) well over a wide range of the 3d scattering length \(a_{3d}\). For \(a_{3d} \to 0\), that is, for large \(a_{1d}\), the HR equation of state using the LDA, cannot properly describe trapped quasi-1d gases, which are expected to become unstable against formation of cluster-like many-body bound states for \(a_{1d} \approx 1/n_{1d}\). We hence investigate the regime with negative \(a_{3d}\) in more detail within a many-body framework.

By comparing with results for the 3d Hamiltonian, Eq. (1), we have shown above that the 1d Hamiltonian \(H_{1d}\), Eq. (2), provides an excellent description of quasi-1d gases. We hence base our stability analysis of quasi-1d gases with large effective 1d scattering length \(a_{1d}\) on \(H_{1d}\). We solve the many-body Schrödinger equation for \(H_{1d}\) using the variational quantum Monte Carlo (VMC) method. Our variational \(N\)-particle Bijl-Jastrow-type wave function consists of one- and two-body terms. The one-body terms are written as a function of a single variational parameter \(\alpha\), which determines the size of the atomic gas. The two-body term is parameterized by \(a_{1d}\), and explicitly accounts for correlations.

Figure 3 shows the resulting VMC energy per particle for \(N = 5\) and \(\lambda = 0.01\) as a function of the variational parameter \(\alpha\) (Gaussian width) for four different \(a_{1d}\). For \(a_{1d}/a_p = 1\) and 2, Fig. 3 shows a local minimum at \(\alpha_{\text{min}} \approx a_2\). The minimum VMC energy nearly coincides with the essentially exact DMC energy, which suggests that our variational wave function provides a highly accurate description of the quasi-1d many-body system. The energy barrier at \(\alpha \approx 0.2a_2\) decreases with increasing \(a_{1d}\) and disappears for \(a_{1d}/a_p \approx 3\). We interpret this vanishing of the energy barrier as an indication of instability \(\square\). For small \(a_{1d}\), the energy barrier separates the gas-like state from cluster-like bound states. For larger \(a_{1d}\), this energy barrier disappears and the gas-like state becomes unstable against cluster formation.

We additionally performed variational calculations for larger \(N\) and different \(\lambda\). We find that the onset of instability of quasi-1d Bose gases can be described by the product of the 1d scattering length \(a_{1d}\) and the linear density at the trap center \(n_{1d}\). To be specific, our many-body calculations suggest that a quasi-1d gas is stable for \(a_{1d}n_{1d} \lesssim 0.35\), and becomes unstable for \(a_{1d}n_{1d} \gtrsim 0.35\). Our analysis suggests that the quasi-1d unitary regime can be reached experimentally. By tuning the 3d scattering length, it is further possible to investigate the onset of instability. By reducing \(\lambda\) one should be able to stabilize relatively large quasi-1d systems.

In conclusion, we investigated the energetics of a Bose gas under highly elongated harmonic confinement over a wide range of the 3d scattering length. We find that the quasi-1d gas can be described by a many-body 1d model Hamiltonian with zero-range interactions and renormalized coupling constant. For \(a_{3d} \to \pm \infty\), the quasi-1d gas enters a unitary regime, where all properties of the system are independent of \(a_{3d}\). In the vicinity of the unitary regime, the quasi-1d system behaves like a gas of HRs. For negative \(a_{3d}\), quasi-1d gases become unstable against cluster formation for a critical value of \(a_{1d}n_{1d}\).

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![FIG. 3: VMC energy per particle as a function of the variational parameter \(\alpha\) for \(N = 5\), \(\lambda = 0.01\), and \(a_{1d}/a_p = 1.0326\) (pluses), 2 (asterisks), 3 (diamonds) and 4 (triangles).](image)
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