Density-functional theory of two-component Bose gases in one-dimensional harmonic traps

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We investigate the ground-state properties of two-component Bose gases confined in one-dimensional harmonic traps in the scheme of density-functional theory. The density-functional calculations employ a Bethe-ansatz-based local-density approximation for the correlation energy, which accounts for the correlation effect properly in the full physical regime. For the binary Bose mixture with spin-independent interaction, the homogeneous reference system is exactly solvable by the Bethe-ansatz method. Within the local-density approximation, we determine the density distribution of each component and study its evolution from Bose distributions to Fermi-like distribution with the increase in interaction. For the binary mixture of Tonks-Girardeau gases with a tunable inter-species repulsion, with a generalized Bose-Fermi transformation we show that the Bose mixture can be mapped into a two-component Fermi gas, which corresponds to exact soluble Yang-Gaudin model for the homogeneous system. Based on the ground-state energy function of the Yang-Gaudin model, the ground-state density distributions are calculated for various inter-species interactions. It is shown that with the increase in inter-species interaction, the system exhibits composite-fermionization crossover.

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I. INTRODUCTION

Experimental realization of the atomic mixtures and progress in manipulating cold atom systems have opened exciting new possibilities to study many-body physics of low-dimensional quantum gases beyond the mean-field theory. In comparison with the single-component systems, mixtures of quantum degenerate atoms may form novel quantum many-body systems with richer phase structures. Particularly, two-component Bose gases have been under intensive studies both experimentally [1, 2, 3, 4, 5] and theoretically [6, 7, 8, 9, 10]. Due to the competition among the inter-species and intra-species interactions, many interesting phenomena such as phase separation, new quantum states and phase transitions arise in two-component cold atomic gases [6, 7, 8, 9, 10]. With strong anisotropic magnetic trap or two-dimensional optical lattice the radial degrees of freedom of cold atoms are frozen and the quantum gas is described by an effective one-dimensional (1D) model [11, 12, 13]. As a textbook example the 1D Tonks-Girardeau (TG) gas [14] was observed firstly [12, 13]. Since then, not only the single-component bosonic gas but also 1D multi-component atomic mixtures have become the current research focus. In principle, both the intra-component and inter-component interactions can be tuned via the magnetic Feshbach resonance, which allows us to study the bosonic mixture in the whole interaction regime. Very recently, two-species Bose gases with tunable interaction have been successfully produced [4, 5].

In general, 1D quantum systems exhibit fascinating physics significantly different from its three-dimensional counterpart because of the enhanced quantum fluctuations in 1D [15, 16, 17, 18, 19, 20]. The mean-field theory generally works not well for the 1D systems except in very weakly interacting regime. When interaction is strong enough, non-perturbation methods, for instance, Bose-Fermi mapping (BFM), Bethe ansatz and Bosonization method, have to be exerted to properly characterize the features of the system [21, 22, 23, 24, 25, 26, 27, 28, 29]. For a single-component Bose gas, it has been shown that the density profiles continuously evolve from Gaussian-like distribution of bosons to shell-structured distribution of fermions [20, 21, 22, 23, 24, 25, 26, 27, 28, 29] with the increase in repulsion strength. Similar behavior of composite fermionization has been observed in the 1D Bose-Bose mixtures [27, 28, 29]. For two-component Bose mixture with spin-independent repulsions, the normalized density distribution of each component displays the same behavior up to a normalized constant which is proportional to respective atomic number of each component [27]. While the extended Bose-Fermi mappings [21, 22, 23] are restricted to the infinitely repulsive limit, some sophisticate methods, such as multi-configuration self-consistent Hartree method [28], numerical diagonalization method [29], and Bethe ansatz method [24, 25, 26, 27], have been applied to study the two-component Bose gases in the whole repulsive regime. Nevertheless, the above methods either suffer the small-size restriction [26, 27] or only limit to the integrable models [24, 25, 26, 27] which generally do not cover the realistic system confined in an external harmonic trap.
In this work, we use the basic idea of density functional theory (DFT) to investigate the ground-state properties of the two-component Bose gases trapped in harmonic potential in the full interacting regime. It is well known that the DFT can handle the system with large sizes and will not encounter the exponential wall that the above traditional multiparticle wave-function methods faced. The effects of the external potential will be accounted for by using the local-density approximation (LDA) \([19, 34, 35, 36, 57, 58, 69, 40, 41, 42]\). The combination of DFT and LDA had been applied to deal with the confined 1D single-component Bose gas \([19, 34, 35, 56]\) and Fermi gas \([37, 38, 39, 40, 41, 42]\) successfully. However, the two-component Bose gas has rarely been studied. The present work will study the ground-state properties of the confined Bose mixture and focus on two cases where the ground state energy function for the homogeneous system can be obtained exactly. In the first case, we consider the two-component Bose gas with spin-independent interaction. In the absence of external potential, this model is exactly solvable by the Bethe-ansatz method and thus the ground-state energy function can be extracted from the Bethe-ansatz solution \([24, 25, 26, 27]\). In the second case, we consider the two-component Bose gas with infinitely repulsive intra-component interactions and a tunable inter-component interaction. We will show that such a model can be mapped into the Yang-Gaudin model with generalized Bose-Fermi transformation and thus the ground-state energy function can be obtained from the Bethe-ansatz solution of the Yang-Gaudin model \([43]\). In the scheme of DFT, the ground-state density profiles are obtained by numerically solving the coupled nonlinear Schrödinger equations (NLEs) for both the equal-mixing Bose mixture and polarized Bose mixture.

The present paper is organized as follows. Section II investigates two-component Bose gas with spin-independent interaction and introduce the method. Section III is devoted to the mixture of two TG gases with tunable inter-species repulsion. A summary is given in the last section.

II. BINARY BOSE MIXTURE WITH SPIN-INDEPENDENT INTERACTION

We consider a two-component Bose gas confined in the external potential \(V_{\text{ext}}(x)\) independent of the species of atoms, where the atomic mass of the \(i\)-component is \(m_i\). The atom numbers in each component are \(N_1\) and \(N_2\) and \(N = N_1 + N_2\) is the total atom number. The many-body Hamiltonian in second quantized form can be formulated as

\[
\mathcal{H} = \int dx \sum_{i=1,2} \left\{ \hat{\Psi}_i^+(x) \left[ -\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x^2} + V_{\text{ext}}(x) \right] \hat{\Psi}_i(x) + \frac{g_i}{2} \hat{\Psi}_i^+(x) \hat{\Psi}_i^+(x) \hat{\Psi}_i(x) \hat{\Psi}_i(x) \right\} + g_{12} \int dx \hat{\Psi}_1^+(x) \hat{\Psi}_2^+(x) \hat{\Psi}_2(x) \hat{\Psi}_1(x),
\]

(1)

in which \(g_i\) (\(i = 1, 2\)) and \(g_{12}\) denote the effective intra- and inter-species interaction that can be controlled experimentally by tuning the corresponding scattering lengths \(a_1, a_2\) and \(a_{12}\), respectively \([4, 5]\). \(\hat{\Psi}_i(x)\) (\(\hat{\Psi}_i(x)\)) is the field operator creating (annihilating) an \(i\)-component atom at position \(x\). Here we will consider the two-component Bose gas composed of two internal states of same species of atoms such that we have the same mass for all atoms \(m_1 = m_2 = m\). When the intra- and inter-component interactions are equal \((g_1 = g_2 = g_{12} = g)\), the system is governed by the spin-independent Hamiltonian with the first quantized form:

\[
H = \sum_{j=1}^{N} \left[ -\frac{\partial^2}{\partial x_j^2} + V_{\text{ext}}(x_j) \right] + 2c \sum_{j<l} \delta(x_j - x_l),
\]

(2)

where \(c = mg/\hbar^2\). The model in the absence of external trap is integrable and can be diagonalized via Bethe ansatz method \([24, 26]\).

We first focus on the homogeneous case by setting \(V_{\text{ext}}(x) = 0\). The effects of the external potential will be discussed latter in the scheme of the LDA and DFT. Before the application of DFT based on the Bethe-ansatz solution, we first give a brief summary of the Bethe-ansatz solution for the integrable two-component Bose gas. For the eigenstate with total spin \(S = N/2 - M\) (\(0 \leq M \leq N/2\)), the Bethe ansatz equations for the integrable two-component Bose gas take the following form \([24, 26]\):

\[
k_j L = 2\pi I_j - \sum_{i=1}^{N} \tan^{-1} \frac{k_j - k_i}{c} + \sum_{\alpha=1}^{M} \tan^{-1} \frac{k_j - \Lambda_{\alpha}}{c/2},
\]

\[
\sum_{j=1}^{N} \tan^{-1} \frac{\Lambda_{\alpha} - k_j}{c/2} = 2\pi J_{\alpha} + \sum_{\beta \neq \alpha}^{M} \tan^{-1} \frac{\Lambda_{\alpha} - \Lambda_{\beta}}{c}.
\]

(3)

where \(k_j\) and \(\Lambda_{\alpha}\) are the quasi-momentum and spin rapidity, respectively, the quantum numbers \(I_j\) and \(J_{\alpha}\) take integer or half-integer values, depending on whether \(N - M\) is odd or even. In term of the quasi-momentums, the energy eigenspectrum is given by \(E = \sum_{j=1}^{N} k_j^2\). In the thermodynamic limit, i.e., \(N, L \to \infty\) with \(N/L\) and \(M/L\) finite, if one introduces density of \(k\) roots \(\rho(k)\) and density of \(\Lambda\) roots \(\sigma(\lambda)\) as well as the corresponding hole root densities \(\rho^h(k)\) and \(\sigma^h(\lambda)\), the Bethe-ansatz equa-
tions thus is simplified to two coupled integral equations

\[ \rho(k) + \rho^h(k) = \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-Q}^{Q} \frac{2c\rho(k')}{c^2 + (k - k')^2} dk' \]

\[ -\frac{1}{2\pi} \int_{-B}^{B} \frac{c\sigma(\lambda)}{c^2/4 + (\lambda - k)^2} d\lambda \]  \hspace{1cm} (4)

\[ \sigma(\lambda) + \sigma^h(\lambda) = \frac{1}{2\pi} \int_{-Q}^{Q} \frac{c\rho(k)}{c^2/4 + (\lambda - k)^2} dk \]

\[ -\frac{1}{2\pi} \int_{-B}^{B} \frac{2c\sigma(\lambda)}{c^2 + (\lambda - k)^2} d\lambda'. \]  \hspace{1cm} (5)

The integration limits \( Q \) and \( B \) are determined by

\[ \rho = \int_{-Q}^{Q} \rho(k) dk \quad \text{and} \quad M/L = \int_{-B}^{B} \sigma(\lambda) d\lambda. \]

At zero temperature, the ground state corresponds to the case with

\[ Q/2 = J_0 = (N + 1)/2 - j \quad \text{and} \quad J_n \quad \text{an empty set.} \]

In other words, the ground state corresponds to the configuration \( \sigma(\lambda) = \rho^h(k) = 0 \), i.e., no holes in the charge degrees of freedom and no quasiparticles in the spin degrees of freedom. Consequently, the ground state reduces to

\[ \rho(k) = \rho = \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-Q}^{Q} \frac{2c\rho(k')}{c^2 + (k - k')^2} dk', \]

or

\[ g(x) = \frac{1}{2\pi} + \frac{1}{2\pi} \int_{-1}^{1} \frac{2\lambda g(x')}{\lambda^2 + (x - x')^2} dx', \]  \hspace{1cm} (6)

where we have made the replacement of variables \( k = Qx, c = Q\lambda \) and \( g(x) = \rho(Qx) \) according to \[13\]. The ground-state energy density can be expressed as

\[ \epsilon(\rho) = \frac{\hbar^2}{2m} \rho^2 e(\gamma) \]  \hspace{1cm} (7)

where \( \rho = \sum_i \rho_i \) is the total density and

\[ e(\gamma) = \frac{\gamma^3}{\lambda^3} \int_{-1}^{1} g(x)x^2 dx \]  \hspace{1cm} (8)

with the dimensionless parameter \( \gamma = \frac{\epsilon_x}{\rho} \). In terms of new variables, the equation \( \rho = \int_{-Q}^{Q} \rho(k) dk \) is rewritten as

\[ \lambda = \gamma \int_{-1}^{1} g(x) dx. \]  \hspace{1cm} (9)

The expression of ground state energy is identical to that of Lieb-Liniger Bose gas \[15\] except that now \( \rho \) should be replaced by the total density. Here \( e(\gamma) \) can be obtained by numerically solving the integral equations \[9\], \[8\] and \[9\] \[17\], \[19\] and we find that it can be fitted very accurately by the rational function

\[ e(\gamma) = \frac{\gamma(1 + p_1\gamma + p_2\gamma^2 + p_2\gamma^2)}{1 + q_0\gamma + q_1\gamma^2 + q_2\gamma^3}. \]  \hspace{1cm} (10)

FIG. 1: (color online) Fit function with four parameters and two parameters.

with \( p_1 = 2.05737, p_2 = 0.0688097, q_1 = 3.16861 \) and \( q_2 = 0.098297 \). In Fig. 1 we compare the fit function with the exact numerical result, where the exact match between them is displayed. In the weakly interacting TF regime \((\gamma \ll 1)\) \( e(\gamma) \) is approximated as \( e(\gamma) = \gamma \) and in the strongly interacting TG regime \((\gamma \gg 1)\) we have

\[ e(\gamma) = \frac{\pi^2/3}{\gamma} \]

Alternatively, \( e(\gamma) \) can also be formulated by the rational functional with only two parameters \( p = -5.0489470 \) and \( q = -20.8604983 \)

\[ e(\gamma) = \frac{\gamma(1 + p\gamma^2 + q\gamma^2)}{1 + q\gamma + p\gamma^2}. \]  \hspace{1cm} (11)

which also match well with the exact numerical result according to Fig. 1 although the accuracy is less perfect than Eq. \[10\].

In order to deduce the bulk properties of non-uniform systems, we have to combine the analytical solution of the homogeneous system with local density approximation. Within the local density approximation, one can assume that the system is in local equilibrium at each point \( x \) in the external trap, with local energy per particle provided by Eq. \[7\]. Therefore the energy functional of an inhomogeneous system can be formulated as

\[ \mathcal{E}(\rho) = \int dx \left[ \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \sqrt{\rho} \right]^2 + V_{ext}(x) \rho + \rho \epsilon(\rho) \]  \hspace{1cm} (12)

where \( \epsilon(\rho) \) takes the form of Eq. \[7\] which is the exact ground state energy density of the homogeneous system \[19\], \[38\], \[40\], \[41\]. The first gradient term represents additional kinetic energy associated with the inhomogeneity
of the gas that is not accounted for by the “local” kinetic energy included in the homogenous energy \([35,47]\). Next we shall consider the case with external potential being a weak harmonic trap \(V_{\text{ext}}(x) = \frac{1}{2}m\omega^2x^2\). For the convenience of latter calculation, we introduce \(\Phi_i = 1\) and thus we have \(\rho = |\Phi_1|^2 + |\Phi_2|^2\). In terms of \(\Phi_i\), the energy functional can be represented as

\[
E = \int dx \left[ \sum_{i=1,2} \Phi_i^* \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{\text{ext}} \right) \Phi_i + \rho \epsilon (\rho) \right].
\]

(13)

The ground state corresponds to the minimization of the energy functional Eq. (13). For the two-component bosonic system, the particle number of each component is conserved. In order to obtain the ground state from a global minimization of \(E\) with the constraints on both \(N_i\), we introduce Lagrange multiplier chemical potential \(\mu_i\) to conserve \(N_1\) and \(\mu_2\) to conserve \(N_2\). The ground state is then determined by a minimization of the free-energy functional \(\mathcal{F} = E - \mu_1 N_1 - \mu_2 N_2\). As shown in Ref. \([48]\), the minimization of energy functional corresponds to a more extensive area and the density profiles decrease to zero rapidly at the boundary. In order to compare the results obtained from the density-functional calculations to the exact results obtained by Bose-Fermi mapping method, in Fig. 3 we show the density profiles of each component and the total density profile in the strongly interacting limit for \(U = 500\). Here each components are normalized to their particle numbers and clearly they satisfy the relation of eq.(15). The total density profile obtained by BFM method is given by \(\rho_{\text{tot}}(x) = \rho_1(x) + \rho_2(x)\). Similar to the case of single species of Bose gas, all of them exhibit the evolution from Bose distribution to Fermi-like one with the increase in interaction constant. In the weakly interacting regime the density profiles display the Gauss-like Bose distribution, while in the strongly interacting regime Bose atoms behave like fermions, which distribute uniformly in a more extensive area and the density profiles decrease to zero rapidly at the boundary. In order to compare the results obtained from the density-functional calculations to the exact results obtained by Bose-Fermi mapping method, in Fig. 3 we show the density profiles of each component and the total density profile in the strongly interacting limit for \(U = 500\). Here each components are normalized to their particle numbers and clearly they satisfy the relation of eq.(15). The total density profile obtained by BFM method is given by \(\rho_{\text{tot}}(x) = \sum_{n=0}^{N-1} |\phi_n(x)|^2\) which is also shown in Fig. 3. Here \(\phi_n(x)\) denotes the eigenstate of the single particle Hamiltonian of harmonic oscillator. It turns out that the results obtained from both methods agree well with each other in the full space except that the density profile obtained by BFM displays oscillations. In the limit of large particle number, the differences become imperceptible.

III. MIXTURE OF TG GASES WITH TUNABLE INTER-COMPONENT INTERACTION

In this section, we focus on the mixture of two TG gases with infinitely strong intra-species interaction, i.e., \(g_i = \infty\) (\(i = 1,2\)) and a tunable inter-species interaction \(g_{12} = g\). In this limit, the original Hamiltonian Eq. (11)
is simplified to

\[ \mathcal{H}^{FG} = \int dx \sum_{i=1,2} \left\{ \hat{\Psi}_1^i(x) \left[ -\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x^2} + V_{ext}(x) \right] \hat{\Psi}_1^i(x) + g\hat{\Psi}_1^i(x)\hat{\Psi}_2^i(x)\hat{\Psi}_2^i(x) \hat{\Psi}_1^i(x) \right\}, \]

where \( \hat{\Psi}_1^i(x) \) and \( \hat{\Psi}_2^i(x) \) are the creation and annihilation operators at location \( x \) for \( i \)-component fermions and \( n_i^F(x) = \hat{\Psi}_1^i(x)\hat{\Psi}_2^i(x) \). With the above transformations, the Hamiltonian (16) is mapped into the two-component fermionic gas with the Hamiltonian given by

\[ \mathcal{H}^F = \int dx \sum_{i=1,2} \left\{ \hat{\Psi}_1^F(x) \left[ -\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial x^2} + V_{ext}(x) \right] \hat{\Psi}_1^F(x) + g\hat{\Psi}_1^F(x)\hat{\Psi}_2^F(x)\hat{\Psi}_2^F(x)\hat{\Psi}_1^F(x) \right\}. \]

The first term on the right side of eq. (19) is introduced to enforce the fermionic annihilation operators \( \hat{\Psi}_1^F(x) \) and \( \hat{\Psi}_2^F(x) \) fulfilling the anti-commutation relations \( \{ \hat{\Psi}_1^F(x), \hat{\Psi}_2^F(x) \} = 0 \).

Since the bosonic model of (16) is related to the fermionic model of (19) by an unitary transformation, they have the same energy spectrum. Furthermore the ground-state properties which are independent of the statistical properties of bosonic system, for example, the ground-state density distribution, can be obtained by consulting for the corresponding fermionic model. Obviously the homogeneous system of (19) with \( V_{ext}(x) = 0 \) is the Yang-Gaudin model which can be solved exactly by means of the Bethe ansatz method [49]. The Bethe-ansatz equations take the form of

\[ k_j L = 2\pi I_j - 2 \sum_{a=1}^{M} \tan^{-1} \frac{k_j - \Lambda_a}{c/2} \]

\[ \sum_{j=1}^{N} \tan^{-1} \frac{\Lambda_a - k_j}{c/2} = \pi J_a + \sum_{\beta=1}^{M} \tan^{-1} \frac{\Lambda_a - \Lambda_{\beta}}{c} \]

for the quasi-momentum \( \{ k_j \} \) and rapidity \( \{ \Lambda_a \} \) with the quantum number \( I_j \) and \( J_a \). While in the thermodynamic limit the equations (20) reduce to two coupled integral equations

\[ \rho(k) = \frac{1}{\pi} \int_{-B}^{B} \frac{\sigma(\Lambda')}{c^2 + (k - \Lambda')^2} + \frac{1}{2\pi}, \]

\[ \sigma(\Lambda) = \frac{1}{\pi} \int_{-B}^{B} \frac{\alpha(\Lambda')}{c^2 + (\Lambda - \Lambda')^2} + \frac{1}{\pi} \int_{-Q}^{Q} \frac{\rho(k)}{c^2 + (\Lambda - k)^2} \]

with \( c' = c/2 \), where \( Q/B \) are determined by \( N/L = \int_{-Q}^{Q} \rho(k)dk \) and \( M/L = \int_{-B}^{B} \sigma(\lambda)d\lambda \). If we make the replacement of variables \( x = x/Q, y = \Lambda/B, g_c(x) = \rho(xQ) = \rho(k) \) and \( g_s(y) = \sigma(yB) = \sigma(\Lambda) \), the above integral equations (21) can be formulated as

\[ g_c(x) = \frac{1}{2\pi} + \frac{1}{2\pi \lambda_s} \int_{-1}^{1} dy \frac{\rho_s(y)}{1/4 + (x/\lambda_c - y/\lambda_s)^2} \]

\[ g_s(y) = \frac{1}{2\pi \lambda_c} \int_{-1}^{1} dx \frac{g_c(x)}{1/4 + (y/\lambda_c - x/\lambda_s)^2} - \frac{1}{\pi \lambda_s} \int 1 dy' \frac{\rho_s(y')}{1 + (y - y')^2/\lambda_s^2} \]

with \( \lambda_c = \gamma \int_{-1}^{1} dx g_c(x) \) and \( \lambda_s = \frac{2\pi}{1/\zeta} \int_{-1}^{1} dy g_s(y) \). After solving the integral equations the energy density of ground state can be evaluated by

\[ \varepsilon_{GS} = \frac{\hbar^2 N^2 \gamma^3}{2mL^2 \lambda_c} \int_{-1}^{1} x^2 g_c(x) dx \]

For the system with total density \( \rho = \rho_1 + \rho_2 \) and polarization \( \zeta = (\rho_1 - \rho_2)/\rho \), the energy density of ground state can be parameterized as

\[ \varepsilon_{GS}(\rho, \zeta) = \frac{\pi^2 \hbar^2 \rho^2}{8m} \left[ (1/3 + \zeta^2) + f(\chi, \zeta) \right] \]
with

\[ f(\chi, \zeta) = \left[ e(\chi) - 1/3 \right] \left\{ 1 + \alpha(\chi) \zeta^2 + \beta(\chi) \zeta^4 \right\} - \left[ 1 + \alpha(\chi) + \beta(\chi) \right] \zeta^6, \]

(23)

where \( \chi = 2\gamma/\pi \), and \( e(\chi) \), \( \alpha(\chi) \) and \( \beta(\chi) \) are given in Ref. [39, 40].

\[ e(\chi) = \frac{4\chi^2/3 + a_p \chi + b_p}{\chi^2 + c_p \chi + d_p}, \]

\[ \alpha(\chi) = \frac{-\chi^2 + a_\alpha \chi + b_\alpha}{\chi^2 + c_\alpha \chi - b_\alpha}, \]

\[ \beta(\chi) = \frac{a_\beta \chi}{\chi^2 + b_\beta \chi + c_\beta} \]

(24)

with \( a_p = 5.780126 \), \( b_p = -(8/9)ln2 + \pi a_p/4 \), \( c_p = (8/\pi)ln2 + 3a_p/4 \), \( d_p = 3b_p \), \( a_\alpha = -1.68894 \), \( b_\alpha = -8.0155 \), \( c_\alpha = 2.74347 \), \( a_\beta = -1.51457 \), \( b_\beta = 2.59864 \) and \( c_\beta = 6.58046 \).

Thus for the mixture of two-component TG gas, the energy density \( e(\rho) \) in energy functional [13] should be replaced by \( e_{CS}(\rho, \alpha, \zeta) = \chi(\rho) + \zeta(\rho) \) [38, 39]. With the same procedure as the former section, the coupled Schrödinger equations take the same formula as Eq. (14) and \( \tilde{F}(\rho) \) in the equation about \( \Phi_i \) (\( i = 1, 2 \)) should be replaced with

\[ \tilde{F}_i(\rho, \zeta) = \frac{\pi^2 \hbar^2}{8m} \frac{\partial}{\partial \rho_i} \rho^3 \left[ (1/3 + \zeta^2) + f(\chi, \zeta) \right]. \]

(25)

For the unpolarized case, it is reduced to

\[ \tilde{F}(\rho) = \frac{\pi^2 \hbar^2}{8m} \left[ 3\rho^2 e(\chi) + \rho^3 \frac{\partial e}{\partial \rho} \right]. \]

(26)

By numerically solving the coupled NLEs, we obtain the ground-state density distributions for different interacting constants \( U \) (\( U = g/\hbar \omega \)).

We first consider the unpolarized Bose mixture with \( N_1 = N_2 \), for which we always have \( \rho_1(x) = \rho_2(x) \). In Fig. 4, we show the density profiles \( \rho_1(x) \) for various inter-species interactions, which are normalized to the atom number \( N_1 \). When the inter-species interaction is zero, no correlation exists between two TG gases and \( \rho_1(x) \) is given by the density distribution of the single-component TG gas, which is identical to the density distribution of a polarized Fermi gas with \( N_1 \) fermions [14]. When the inter-species interaction is weak, the density distribution of each component does not deviate far from the distribution of the single-component TG gas. With the increase in inter-species interaction, the density profiles become broader and broader, and continuously evolve to the limit of strong inter-species interaction. As shown in Fig. 4, the density profile for \( U = 500 \) already agrees very well with the exact profile in the limit of \( U = \infty \) except the oscillation peaks. In this limit, the density profile for each component fulfills the relation [15] and displays \( N \) peaks, which can be exactly calculated by using the Bose-Fermi mapping method [21].

For the imbalance trapped mixture of TG gases, the distributions of each component will display different behaviors in the full interacting regime except in the limit of strong interspecies interaction, where the distributions display same behaviors only with different normalization condition, i.e., \( n_1(x) = n_2(x) \) with \( n_i(x) = \rho_i(x)/N_i \). The density profiles of each components and the total density profiles for the polarized mixture of TG gases are exhibited in Fig. 5a, Fig. 5b and Fig. 5c, respectively. The profiles for the case of vanished inter-species interaction and of infinitely strong inter-species interaction are also plotted (oscillating lines) in the figure, which are obtained by means of BFM method. It is shown that in the
regime close to these two limits the distributions agree well with the results of BFM method. It is feasible even in the situation of finite weak or strong inter-species interaction. With the increase in inter-species interaction both components distribute in more extensive regime and the density profiles of $i$-component evolve from the behavior of single-component TG gas with $\rho_i(x) = \rho_{TG}(x)|_{N=N_i}$ to the behavior of the fermionized Bose mixture with $\rho_i(x) = \sum_{n=N_i}^{N-1} |\phi_n(x)|^2$. In Fig. 5d, we show the spin density distribution defined as the density difference between two components. For $U = 0$, we have $\rho_1(x) - \rho_2(x) = \sum_{n=N_1}^{N-1} |\phi_n(x)|^2$. In the weakly and intermediately interacting regimes, the spin density distributions display two explicit peaks at the location far away from the center of trap and at the locations near the middle of trap spin density profiles are almost flat. That is to say, two weakly interacting TG gases form the shell structure of the coexisted regime of two components surrounded by the fully polarized majority component. With the increase in interspecies interaction, the peaks become smaller and smaller and disappear finally. In the limit of strong inter-species interaction, two components coexist in the full spaces and the spin density profile exhibits similar behavior to the total density profile. This could be understood because in the infinite-$U$ limit one has $\rho_1(x) - \rho_2(x) = \sum_{n=N_1}^{N-1} |\phi_n(x)|^2$ according to [12].

IV. SUMMARY

In summary, the ground-state properties of two-component Bose gases trapped in 1D harmonic traps have been studied in the scheme of DFT. On the basis of Bethe-ansatz solution, we calculate the ground-state density distributions of the confined systems for each component by combining the local density approximation with the exact solution of homogeneous system. For the case with spin-independent interaction, the distribution of each component is $N_i/N$ of the total density distribution in the full repulsive regime. With the increase in the interaction the density distributions show evolution from Gauss-like Bose distributions to Fermi-like distributions. For the mixture of two TG gases with tunable inter-species interaction, we show that it can be mapped into a two-component Fermi gas by a generalized Bose-Fermi transformation. Taking advantage of the exact ground-state energy of Yang-Gaudin model for the homogeneous system, we calculate the density profiles of the confined systems. For both balanced Bose mixture and polarized Bose mixture, the density profiles of each component display the continuum crossover from the distribution of single-component TG gas with $N_i$ atoms to that of composite-fermionization mixture as inter-species interaction increases. In the limit of strong repulsion, the results obtained from density-functional calculation are compared with the results from the Bose-Fermi mapping method and it turns out that they match very well in the full coordinate space.

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[1] C. J. Myatt, E. A. Burt, R. W. Ghrist, E. A. Cornell, and C. E. Wieman, Phys. Rev. Lett. 78, 586 (1997).
[2] G. Modugno, G. Ferrari, G. Roati, R. J. Brecha, A. Simoni, and M. Inguscio, Science 294, 1320 (2001).
[3] M. Erhard, H. Schmaljohann, J. Kronjager, K. Bongs, and K. Sengstock, Phys. Rev. A 69, 032705 (2004); C. Ospelkaus et al., Phys. Rev. Lett. 97, 120402 (2006).
[4] G. Thalhammer, G. Barontini, L. De Sarlo, J. Catani, F. Minardi, and M. Inguscio, Phys. Rev. Lett. 100, 210402 (2008); S. B. Papp, J. M. Pino, and C. E. Wieman, Phys. Rev. Lett. 101, 040402 (2008).
[5] K. Pich, A. D. Lange, A. Prantner, G. Kerner, F. Ferlaino, H.-C. Nägerl, R. Grimm, cond-mat/0812.3287.
[6] T.-L. Ho and V. B. Shenoy, Phys. Rev. Lett. 77, 3276 (1996).
[7] P. Ao and S. T. Chui, Phys. Rev. A 58, 4836 (1998).
[8] H. Pu and N. P. Bigelow, Phys. Rev. Lett. 80, 1130 (1998).
[9] M. A. Cazalilla and A. F. Ho, Phys. Rev. Lett. 91, 150403 (2003).
[10] L. Zhou, J. Qian, H. Pu, W. Zhang, and H. Y. Ling, Phys. Rev. A 78, 053612 (2008).
[11] T. Stöferle, H. Moritz, C. Schori, M. Köhl, and T. Esslinger Phys. Rev. Lett. 92, 130403 (2004).
[12] B. Paredes, A. Widera, V. Murg, O. Mandel, S. Fölling, I. Cirac, G. V. Shlyapnikov, T. W. Hänsch, and I. Bloch, Nature 429, 277 (2004).
[13] T. Kinoshita, T. Wenger and D. S. Weiss, Science 305, 1125 (2004).
[14] M. D. Girardeau, J. Math. Phys. (N.Y.) 1, 516 (1960); Phys. Rev. 139, B500 (1965).
[15] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).
[16] M. Olshanii, Phys. Rev. Lett. 81, 938 (1998).
[17] T. Bergeman, M. G. Moore, and M. Olshanii, Phys. Rev. Lett. 91, 163201 (2003).
[18] D. S. Petrov, G. V. Shlyapnikov, and J. T. M. Walraven, Phys. Rev. Lett. 85, 3475 (2000).
[19] V. Dunjko, V. Lorent and M. Olshanii, Phys. Rev. Lett. 86, 5413 (2001).
[20] S. Chen and R. Egger, Phys. Rev. A. 68, 063605 (2003).
[21] M. D. Girardeau and A. Minguzzi, Phys. Rev. Lett. 99, 230402 (2007).
[22] F. Deuretzbacher, K. Fredenhagen, D. Becker, K. Bongs, K. Sengstock, and D. Pfannkuche, Phys. Rev. Lett. 100, 160405 (2008).
[23] L. Guan, S. Chen, Y. Wang and Z. Q. Ma, Phys. Rev. Lett. 102, 160402 (2009).
[24] Y. Q. Li, S. J. Gu, Z. J. Ying and U. Eckern, Europhys.
[25] J. N. Fuchs, D. M. Gangardt, T. Keilmann, and G. V. Shlyapnikov, Phys. Rev. Lett. 95, 150402 (2005); M. T. Batchelor, M. Bortz, X. W. Guan, and N. Oelkers, J. Stat. Mech. P03016 (2006).
[26] X.-W. Guan, M. T. Batchelor, and M. Takahashi, Phys. Rev. A 76, 043617 (2007); N. Oelkers, M. T. Batchelor, M. Bortz and X.-W. Guan, J. Phs. A 39, 1073 (2006).
[27] Y. Hao, Y. Zhang, X. W. Guan, and S. Chen, Phys. Rev. A 79, 033607 (2009).
[28] S. Zöllner, H.-D. Meyer, and P. Schmelcher, Phys. Rev. A 78, 013629 (2008).
[29] Y. Hao, and S. Chen, Eur. Phys. J. D 51, 261 (2009).
[30] Y. Hao, Y. Zhang, J. Q. Liang and S. Chen, Phys. Rev. A 73, 063617 (2006).
[31] F. Deuretzbacher, K. Bongs, K. Sengstock, and D. Pfannkuche, Phys. Rev. A 75, 013614 (2007); X. Yin, Y. Hao, S. Chen and Y. Zhang, Phys. Rev. A 78, 013604 (2008).
[32] S. Zöllner, H.-D. Meyer, and P. Schmelcher, Phys. Rev. A 74, 063611 (2006).
[33] O. E. Alon, and L. S. Cederbaum, Phys. Rev. Lett. 95, 140402 (2005).
[34] E. B. Kolomeisky, T. J. Newman, J. P. Straley, and X. Qi, Phys. Rev. Lett. 85, 1146 (2000).
[35] P. Öhberg and L. Santos, Phys. Rev. Lett. 89, 240402 (2002).
[36] Y. E. Kim and A. L. Zubarev, Phys. Rev. A 67, 015602 (2003); J. Brand, J. Phys. B, 37 S287 (2004).
[37] G. E. Astrakharchik, D. Blume, S. Giorgini, and L. P. Pitaevskii, Phys. Rev. Lett. 93, 050402 (2004).
[38] Y. E. Kim and A. L. Zubarev, Phys. Rev. A 70, 033612 (2004); R. J. Magyar and K. Burke, Phys. Rev. A 70, 032508 (2004).
[39] G. Xianlong, M. Polini, R. Asgari, and M. P. Tosi, Phys. Rev. A 73, 033609 (2006).
[40] S. H. Abedinpour, M. Polini, G. Xianlong and M. P. Tosi, Phys. Rev. A 75, 015602 (2007).
[41] G. Xianlong, and R. Asgari, Phys. Rev. A 77, 033604 (2008).
[42] H. Hu, X.-J. Liu, and P. D. Drummond, Phys. Rev. Lett. 98, 070403 (2007).
[43] C. N. Yang, Phys. Rev. Lett. 19, 1312 (1967); M. Gaudin, Phys. Lett. A 24, 55 (1967).
[44] E. Eisenberg and E. H. Lieb, Phys. Rev. Lett. 89, 220403 (2002).
[45] K. Yang and Y. Q. Li, Int. J. Mod. Phys. B 17, 1027 (2003).
[46] A. Minguzzi, S. Succi, F. Toschi, M.P. Tosi, P. Vignolo, Phys. Rep. 395, 223 (2004).
[47] E. H. Lieb, R. Seiringer, and J. Yngvason, Phys. Rev. Lett. 91, 150401 (2003).
[48] F. Dalfovo and S. Stringari, Phys. Rev. A 53, 2477 (1996).
[49] S. Chen, J. Cao, and S. J. Gu, Europhys. Lett. 85, 60004 (2009).