Binding between two-component bosons in one dimension

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Abstract. We investigate the ground state of one-dimensional few-atom Bose–Bose mixtures under harmonic confinement throughout the crossover from weak to strong inter-species \textit{attraction}. The calculations are based on the numerically exact multi-configurational time-dependent Hartree method. For repulsive components, we detail the condition for the formation of a molecular Tonks–Girardeau gas in the regime of intermediate inter-species interactions, and the formation of a molecular condensate for stronger coupling. Beyond a critical inter-species attraction, the system collapses to an overall bound state. Different pathways emerge for unequal particle numbers and intra-species interactions. In particular, for mixtures with one attractive component, this species can be viewed as an effective potential dimple in the trap center for the other, repulsive component.

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1. Introduction

Cold atoms have become an important tool to create and study strongly correlated quantum systems [1, 2]. One main reason is that it is possible to experimentally tune the effective low-energy interaction strength between the atoms using Feshbach resonances [3]. This has proven useful particularly for Fermi gases [4], whereas for bosons the creation of strong interactions is limited by three-body collisions. However, in lower (here: one) dimensions there are also other possibilities of achieving effectively strong correlations—as e.g. by lowering the atom-number density [5] and via confinement-induced resonances, which exploit the parametric dependence on the transverse trapping potential [6]. This allows one to practically adjust the coupling strength all the way from infinite attraction to hard-core repulsion.

For single-component bosons in one dimension (1D), the extreme case of infinitely repulsive interactions is known as the Tonks–Girardeau (TG) gas, which has been realized experimentally [7, 8]. Here, the system maps to an ideal gas of fermions, in the sense that the exclusion principle emulates the effect of hard-core repulsion [9]. The microscopic mechanism of the crossover from the weakly interacting Bose gas to the above fermionization limit has been investigated in detail [10]–[15]. By contrast, the ground state for strong attraction is an N-atom molecule [16]. However, exotic fermionized excitations exist for sufficiently attractive interactions [17]–[19].

In the case of two (or more) bosonic components, a plethora of configurations exists: on top of varying both intra- and inter-species interactions, also the trapping potentials may be made species dependent. Moreover, the experimental availability of different two-component mixtures (involving not only different hyperfine components [20, 21] or isotopes [22, 23] but also altogether different atomic species like K–Rb [24]) adds another degree of flexibility. For two 1D Bose gases with inter-species repulsion, a generalized, composite fermionization exists that may lead to demixing of the two components atom-by-atom [25]–[28]. In a lattice potential, even more complex patterns have been found, cf [29]–[32] and references therein.
In this work, we are interested in the binding between two bosonic species, i.e. the crossover from weak to strong inter-species attraction. Here little is known except for a general classification based on the harmonic-fluid approximation [33]. For fermions, pairing between the two components has been predicted, which then form a TG gas of molecules [34]. Similarly, pairing has been found in attractive Bose–Fermi mixtures in various settings [35]–[37]. While, in principle, a 1D fermionic component maps to a strictly fermionized bosonic one, the physics of realistic Bose–Bose mixtures differs in two ways: for one thing, the finite intra-species repulsion must compete with strong inter-species attraction. More generally, in contrast to fermions all possible intra-species interactions are possible and make for interesting phases. The key goal of this work is to demonstrate effects due to the interplay between intra-species and inter-species forces.

This paper is organized as follows. Section 2 introduces the model and briefly reviews the computational method. The pairing between repulsive components is elucidated in section 3, first for the case of a mixture of balanced components (sections 3.1 and 3.2), complemented by a discussion of atom-number imbalances and unequal intra-species interactions (section 3.3). Section 4 deals with the question of how the presence of attractive components alters the picture.

2. Model and computational method

2.1. Model

The object of investigation is a two-component Bose gas (denoted \( \alpha \in \{ A, B \} \)) subjected to a 1D confinement, where the external potentials acting on the different species are assumed to be the same, i.e. \( U_\alpha (x) = U (x) \). The two species can be considered as two internal states (pseudospin \(| \uparrow \rangle \) and \(| \downarrow \rangle \)) of the same kind of Bose atoms, or as different isotopes with the mass \( m_\alpha \approx m \). In the subsequent sections, we denote the atom number of each species with \( N_\alpha \) and the total number with \( N = N_A + N_B \). This kinematically 1D system of trapped bosons can be described in the low-energy limit by an effective 1D Hamiltonian with contact interactions. The second quantized Hamiltonian \( H \) then reads

\[
H = \int dx \sum_{\alpha = A, B} \left\{ \hat{\Psi}_\alpha^\dagger (x) \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + U (x) \right] \hat{\Psi}_\alpha (x) + \frac{g_\alpha}{2} \hat{\Psi}_\alpha^\dagger (x) \hat{\Psi}_\alpha^\dagger (x) \hat{\Psi}_\alpha (x) \hat{\Psi}_\alpha (x) \right\} \\
+ g_{AB} \int dx \hat{\Psi}_A^\dagger (x) \hat{\Psi}_B^\dagger (x) \hat{\Psi}_B (x) \hat{\Psi}_A (x),
\]

(1)

where the field operator \( \hat{\Psi}_\alpha (x) \) (\( \hat{\Psi}_\alpha^\dagger (x) \)) annihilates (creates) a boson of the \( \alpha \)-species at the position \( x \). The effective intra- and inter-species couplings \( g_\alpha \) and \( g_{AB} \) characterize the interaction between the atoms and can be controlled experimentally by the scattering lengths \( a_0^{(\alpha)} \) and \( a_0^{(AB)} \), respectively, in analogy to the single species case [6]. Furthermore, the standard rescaling procedure to harmonic oscillator units has been carried out (cf [26] for details). For technical reasons, we apply the Hamiltonian in the first quantized form. The eigenvalue problem reduces to solve the stationary Schrödinger equation \( H \Psi = E \Psi \), with \( H \equiv \sum_\alpha H_\alpha + H_{AB} \) composed of the single species Hamiltonian

\[
H_\alpha = \sum_{i=1}^{N_\alpha} \left[ \frac{1}{2} \tilde{p}_{\alpha_i}^2 + U (x_{\alpha_i}) \right] + \sum_{i<j} g_\alpha \delta_\alpha (x_{\alpha_i} - x_{\alpha_j})
\]

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and the inter-species coupling part

\[ H_{AB} = \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} g_{AB} \delta_\sigma (x_{A_i} - x_{B_j}). \]

Here the effective 1D contact interaction potential is mollified with a Gaussian \( \delta_\sigma (x) \equiv e^{-x^2/2\sigma^2} / \sqrt{2\pi \sigma} \) (of width \( \sigma = 0.05 \)) for numerical reasons. In the further examination, we focus on the case of a harmonic confinement, \( U(x) = \frac{1}{2}x^2 \), and on attractive inter-species forces \( g_{AB} \in (-\infty, 0] \). (The case of repulsive inter-species couplings has already been investigated in [26]. Note that, in the case of \( U = 0 \) and \( g_a = g_{AB}, \) this system is integrable via Bethe’s ansatz as in [5].)

### 2.2. Computational method

Our approach relies on the numerically exact multi-configuration time-dependent Hartree method [38]–[40], a quantum-dynamics approach that has been applied successfully to systems of few identical bosons [12, 13, 19], [41]–[43] as well as to Bose–Bose mixtures [26]. Its principal idea is to solve the time-dependent Schrödinger equation \( i\dot{\Psi}(t) = H\Psi(t) \) as an initial-value problem by expanding the solution in terms of direct (or Hartree) products \( \Phi_j \equiv \varphi_1^{(1)} \otimes \cdots \otimes \varphi_N^{(N)}. \)

\[ \Psi(t) = \sum_j A_j(t) \Phi_j(t). \quad (2) \]

The unknown single-particle functions \( \varphi_j^{(\kappa)} \) \( (j = 1, \ldots, n_\kappa) \) are in turn represented in a fixed basis of, in our case, harmonic-oscillator orbitals. The specific feature of the system at hand is the indistinguishability within each species. Therefore the single-particle functions are identical within each subset \( K_A = \{1, \ldots, N_A\} \) and \( K_B = \{N_A + 1, \ldots, N\} \) (i.e. \( \varphi_j^{(\kappa)} = \varphi_j^{(\alpha)}, \forall \kappa \in K_a \)). The permutation symmetry within each subset is ensured by the correct symmetrization of expansion coefficients \( A_j \). In analogy to the wave function, also non-separable terms of the Hamiltonian such as the two-body interaction are expanded in terms of direct products [44].

Note that, in the above expansion, not only the coefficients \( A_j \) but also the single-particle functions \( \varphi_j \) are time dependent. Using the Dirac-Frenkel variational principle, one can derive equations of motion for both \( A_j, \varphi_j \) [39]. Integrating this differential-equation system allows us to obtain the time evolution of the system via (2). This has the advantage that the basis set \( \{\Phi_j(t)\} \) is variationally optimal at each time \( t \); thus it can be kept relatively small. Still, its exponential growth with the number of particles limits our approach to only a few atoms \( N < 10 \), depending on how many single-particle functions need to be included to describe inter-particle correlations.

Although designed for time-dependent studies, it is also possible to apply this approach to stationary states. This is done via the so-called relaxation method. The key idea is to propagate some wave function \( \Psi(0) \) by the non-unitary \( e^{-H\tau} \) (propagation in imaginary time.) As \( \tau \to \infty \), this exponentially damps out any contribution but that originating from the true ground state like \( e^{-\left(E_{\text{true}} - E_0\right)\tau} \). In practice, one relies on a more sophisticated scheme termed improved relaxation, which is much more robust, especially for excitations. Here \( \langle \Psi | H | \Psi \rangle \) is minimized with respect to both the coefficients \( A_j \) and the orbitals \( \varphi_j \). The effective eigenvalue problems thus obtained are then solved iteratively by first solving for \( A_j \) with fixed orbitals and then ‘optimizing’ \( \varphi_j \) by propagating them in imaginary time over a short period. That cycle will then be repeated.

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3. Mixture of two repulsive components

In this section, we investigate two repulsive components ($g_\alpha > 0$) with increasing inter-species attraction $g_{AB} \in (-\infty, 0]$. We start with components of equal intra-species settings, such as equal intra-species interaction strengths, $g_A = g_B$, and particle numbers $N_A = N_B$ and discuss subsequently the changes in the system’s behavior when relaxing these conditions.

3.1. Mixture of two fermionized components

The starting point is the highly repulsive limit of the components, i.e. two quasi-fermionized states within the two species with the inter-species interactions $g_A = g_B = 25.0$. For small inter-species attraction $g_{AB} = -0.001$ the system is well described by the uncorrelated product of two TG states $\Psi = \Psi_A \otimes \Psi_B$, where $\Psi_A = \Psi_B \approx |\Psi_0^F\rangle$. This means the state of each species $\alpha$ in the high-interaction limit ($g_\alpha \to +\infty$) can be mapped to a non-interacting state $\Psi_0^F$ of identical fermions [9], also commonly termed fermionization. By extension, a mixture of two fermionized Bose gases has similarities with a two-component Fermi gas.

The characteristic fermionic pattern of the TG-state is displayed in the one-body density (which is the same for both species $\alpha$ for symmetry reasons) $\rho(x) = \rho^{(\alpha)}(x)$ (with $\alpha \in \{A, B\}$), which measures the probability distribution of finding one $\alpha$ particle at the position $x$ pictured in figure 1. One recognizes the density concentrating more and more in the center of the trap with increasing inter-species attraction $g_{AB}$. Concurrently, in the intermediate interaction regime $|g_{AB}| = 5$ the initial two density peaks are at first getting increasingly pronounced, whereas the density in the center of the trap grows slowly. That intensification of the fermionic characteristic is due to molecule formation, as discussed in the following. By contrast, in the very high interaction regime ($|g_{AB}| = 20 \sim g_\alpha$) the two peaks merge into one single peak in the center of the trap.

Figure 1. One-body density $\rho(x) \equiv \rho^{(\alpha)}(x)$ ($\alpha \in \{A, B\}$) for a quasi-fermionized mixture ($g_\alpha = 25.0$) with the particle numbers $N_\alpha = 2$, plotted for different inter-species interactions $g_{AB}$ (see legend).
A more detailed insight into the system’s behavior is given by the two-body correlation functions. In the case of a binary mixture, these are defined as

$$
\rho_{aa}(x_1, x_2) = \frac{1}{N_a(N_a - 1)} \left\langle \hat{\Psi}_a^\dagger(x_1) \hat{\Psi}_a^\dagger(x_2) \hat{\Psi}_a(x_2) \hat{\Psi}_a(x_1) \right\rangle,
$$

$$
\rho_{AB}(x_A, x_B) = \frac{1}{N_A N_B} \left\langle \hat{\Psi}_A^\dagger(x_A) \hat{\Psi}_B^\dagger(x_B) \hat{\Psi}_B(x_B) \hat{\Psi}_A(x_A) \right\rangle.
$$

The two-body correlation functions $\rho_{aa}(x_1, x_2)$ and $\rho_{AB}(x_A, x_B)$ in figure 2 depict the conditional probability of measuring the one $\alpha$-particle at the position $x_1$ and the other at the position $x_2$, and likewise for the different species, $\rho_{AB}(x_A, x_B)$. The left column in figure 2 indicates that the two species keep their ‘fermionic’ character, i.e. the probability of finding particles of the same kind at the same position $\{x_1 = x_2\}$ stays very low up to high interspecies attractions ($|g_{AB}| \ll 20$). But according to $\rho_{AB}(x_A, x_B)$ (right column), the two species concentrate more and more at the same position, which means on the diagonal in two separate peaks either side of the center of the harmonic trap (see figure 2, $\rho_{AB}(x_A, x_B)$ for $g_{AB} = -5.0$).

This can be understood as formation of a molecular TG (MTG) state: as we shall argue below, two distinguishable particles form a bound state that is a molecule (in the following denoted as $AB$-molecule). These indistinguishable $AB$-molecules in turn form a (MTG) TG state. Whereas for two-component Fermi gases this MTG state remains stable even in the strongly attractive inter-species attraction regime [34], this is not the case in a pure bosonic mixture (see also figure 2).

### 3.1.1. Pairing description

For a better understanding of this behavior, we examine the Hamiltonian for the exemplary case $N_a = 2$. To this end, we transform $X \equiv (x_{A_1}, x_{A_2}, x_{B_1}, x_{B_2})^\top$ to the relative coordinates $Y = (R_{CM}, R_1, r_1, r_2)^\top$ specified by

$$
Y = \mathcal{O} X, \quad \mathcal{O} = \begin{pmatrix}
\frac{1}{\sqrt{4}} & \frac{1}{\sqrt{4}} & \frac{1}{\sqrt{4}} & \frac{1}{\sqrt{4}} \\
\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\
\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\
0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}}
\end{pmatrix}.
$$

(3)

The coordinates $R_{CM}(r_1, r_2)$ coincide—up to a factor—with the standard center-of-mass (interspecies relative) coordinates. The coordinate $R_1 = \frac{1}{2}[(x_{A_1} + x_{B_1}) - (x_{A_2} + x_{B_2})]$ specifies the distance between the centers of mass of two $(A, B)$-clusters. The orthogonal transformation leads to the Hamiltonian $H(Y) = h_{CM}(R_{CM}) + H_{rel}$, with

$$
H_{rel} = \left[\frac{1}{2} p_{R_1}^2 + \frac{1}{2} R_1^2 \right] + \sum_{i=1}^2 \left[\frac{1}{2} p_{R_i}^2 + \frac{1}{2} r_i^2 + \frac{g_{AB}}{2\sqrt{2}} \delta(r_i) \right] + g_A \delta \left(\frac{1}{\sqrt{2}} (r_1 - r_2) - R_1\right)
$$

$$
+ g_B \delta \left(\frac{1}{\sqrt{2}} (r_1 - r_2) + R_1\right) + g_{AB} \sum \delta \left(\frac{1}{\sqrt{2}} (r_1 + r_2) \pm R_1\right).
$$

(4)

If we assume the formation of, say, $A_i B_j$-bound states ($i, j \in \{1, 2\}$) (up to permutation symmetry), for high enough inter-species attraction $g_{AB}$ the extension of an $A_i B_j$-molecule is much smaller than the distances between two such molecules ($|r_i| \ll |R_i|$). One can check this in the two-body
Figure 2. Two-body correlation functions $\rho_{aa}(x_1, x_2)$ (left column) and $\rho_{AB}(x_A, x_B)$ (right column) of two quasi-fermionized components $g_A = g_B = 25.0$ for inter-species couplings $g_{AB} = -0.001, -5.0, -20.0$ and $-30.0$ (from top to bottom).

correlation functions (figure 2). In this limit, we can approximate (4) by the decoupled Hamiltonian

$$H_{rel} \approx \sum_{i=1}^{2} \left[ \frac{1}{2} p_i^2 + \frac{1}{2} r_i^2 + \frac{g_{AB}}{\sqrt{2}} \delta(r_i) \right] + \left[ \frac{1}{2} p_{R_i}^2 + \frac{1}{2} R_i^2 + \tilde{g} \delta(R_i) \right],$$

(5)
the last part describing the relative motion of the two $AB$-molecules with the effective interaction $\tilde{g} \equiv g_a + g_f + 2g_{AB}$. The analytic solution of the ground state is known [45] and the relative part (excluding the trivial CM factor) can be written as [19]

$$\psi_{\text{rel}}(X) \propto S_+ \left( \prod_{i=1,2} e^{-\left( g_{AB}/2 \right)|x_{A_i} - x_{B_i}|} \right) U \left( -\epsilon(\tilde{g}) ; \frac{1}{2} \left[ (x_{A_1} + x_{B_1}) - (x_{A_2} + x_{B_2}) \right] \right),$$

(6)

where $\epsilon(\tilde{g}) = \nu(\tilde{g}) + 1/2$ is determined by the transcendental equation $\nu(g) \in f^{-1}_g(0) : f_g(\nu) := 2^{3/2}[\Gamma(1-v)/\Gamma(\frac{1-v}{2})] + \tilde{g}$ and $U(a, b)$ denote the parabolic cylinder functions. The symmetry operator $S_+ := S^A_+ \otimes S^B_+$ serves to compensate the symmetry breaking introduced in the Hamiltonian (5).

This solution gives a good approximation of the density patterns in figure 2 for intermediate to strong attractions ($|g_{AB}| < g_a/2$). Also in the high coupling regime ($|g_{AB}| > g_a/2$) the model provides applicable predictions for the system’s behavior. Considering the molecule–molecule interaction term $\tilde{g}\delta(R_1) = (g_a + g_B + 2g_{AB})\delta(R_1)$, with large enough inter-species attraction $g_{AB}$ the effective molecule–molecule interaction $\tilde{g}$ vanishes and even becomes negative, i.e. attractive. That implies, more precisely, that for $g_{AB} \approx g_a/2$ a state forms where the $AB$-molecules are condensed similar to a Bose–Einstein condensate (BEC). For further increase of the interaction, the gas of $AB$-molecules collapses and forms a bound state. Even though the introduced approximation model gives reasonable predictions in that limit of very high inter-species attractions ($|g_{AB}| > g_a/2$), it should be handled with care, as the inter- and intra-species length scales become comparable and therefore the scale separation breaks down (see also figure 2).

These considerations can be supported by means of the quantities of the one-body density matrix $\rho^{(\alpha)}_1(x, x') = \frac{1}{N_\alpha} \langle \tilde{\Psi}^+_\alpha(x) \tilde{\Psi}_\alpha(x') \rangle$ and the pair density matrix

$$\tilde{\rho}(x, x') := \frac{1}{N_A N_B} \langle \Delta_{AB}^+(x) \Delta_{AB}(x') \rangle,$$

with the ‘pair’ operator $\Delta_{AB}(x) = \tilde{\Psi}_A(x) \tilde{\Psi}_B(x)$ that annihilates an $AB$-pair ‘particle’ at the position $x$. As $\Delta_{AB}(x)|\Psi\rangle$ is a ‘hole’-state, i.e. a state where an $AB$-pair has been removed at the position $x$, the pair density matrix embodies the overlap of two such ‘hole’-states. The pair density matrix reflects the correlation inherent in the state $\Psi$ between the positions $x$ and $x'$ on the level of $AB$-dimers, as opposed to correlations of single particles $\alpha$ described by $\rho^{(\alpha)}_1(x, x')$.

As shown in figure 3, the off-diagonal range of the pair density matrix $\tilde{\rho}(x, x')$ persists and even slightly increases for the inter-species attractions up to $|g_{AB}| \approx 5$, where its appearance agrees well with the corresponding one-body density matrix $\rho^{(M)}_1(x, x')$ of identical, fermionized bosons with mass $M = 2$ (in units of $m$). This proves the existence of a paired state (MTG), as discussed above. By contrast, the single-particle density matrix $\rho^{(\alpha)}_1(x, x')$ (see figure 3 left column) shows two peaks on the diagonal, while the off-diagonal density steadily diminishes with increasing $|g_{AB}|$. In this light a single $\alpha$-atom will be in an incoherent superposition of left- (right-) localized states, without any phase correlations. This has to be contrasted with the phase correlations present for the pair density matrix (see figure 3 right column for $g_{AB} = -5.0$). Interestingly this may be compared to a demixed state in the presence of repulsive inter-species interactions [26].

When further increasing the inter-species interaction to $|g_{AB}| \approx 20$ the size of the system decreases; however, a seemingly perfect off-diagonal long-range order [46] in the pair density

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Figure 3. One-body density matrix $\rho_1(x, x')$ (left column) and pair density matrix $\tilde{\rho}(x, x')$ (right column) for inter-species couplings $g_{AB} = -0.001, -5.0, -20.0$ and $-30.0$ (from top to bottom).

matrix is attained, which can be interpreted as (few-body analog of) a condensed state on the level of $AB$-molecules, $\tilde{\rho}(x, x') = \varphi^*_A(x) \cdot \varphi_B(x')$ (see figure 3 right column for $g_{AB} = -20.0$). By contrast, on the single-particle level, displayed in the one-body density matrix $\rho_1^{(\alpha)}(x, x')$, no condensed state exists, but the two correlation peaks merge into one centered peak concentrated on the diagonal $\{x = x'\}$. 

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For inter-species interaction strength larger than the order of magnitude of the intra-species interactions $|g_{AB}| \gg |g_\alpha|/2$, the system becomes highly bound beyond the $AB$-molecule level, as is reflected in the decrease of the off-diagonal elements in the pair density matrix $\tilde{\rho}(x,x')$. This can be seen as a collapse from a molecular gas to a strongly interacting cluster of $AB$-molecules. In contrast to a Bose–Fermi and Fermi–Fermi mixture the collapse in a pure bosonic mixture is qualitatively different: in a Bose–Fermi mixture only the bosons form a small region with high density, whereas the fermions will be attracted up to a ‘Pauli-allowed’ density, and Fermi–Fermi mixtures with $s$-wave interactions remain mechanically stable even in the strongly attractive inter-species regime.

Although, for definiteness, we restricted our discussion to a mixture with particle numbers $N_\alpha = 2$, the mechanism described by equation (5) extends to the case of more molecules, $N_\alpha > 2$. For much larger systems $N \gg 1$, of course, few-body effects as the density oscillations seen in figure 1 will be smeared out and the corresponding density profiles broadened due to repulsion, as in the single-component Bose gas [47]. Likewise, the collapse witnessed for $g_{AB} \to -\infty$ will be much more pronounced, as the center-of-mass width $\Delta R_{CM}$ shrinks with increasing atom number.

### 3.1.2. Fermionized attractive components

It is known for identical bosons that fermionization can also be obtained in the attractive interaction regime [17, 19], where it is called the super-Tonks-Girardeau state (STG). We show that the above pairing mechanism can also be observed in a mixture with two attractively interacting, fermionized components ($g_\alpha < 0, \alpha \in \{A, B\}$). In this case it is no longer the ground state but an excited state of the system. We performed the numerical investigation for the exemplary case of a mixture with $N_\alpha = 2$ being situated in the energetically lowest STG-state ($g_\alpha = -15.0$). Direct comparison with a system of repulsive, fermionized components shows the corresponding process analogous to the formation of the molecular TG-gas, but with smaller off-diagonal correlations (figure 4). Clearly the density profile of the STG-state is more localized in fragmented regions than that of the TG-state (figure 4). The reason is the finite intra-species interaction-strength (here $g_\alpha = -15.0$), where the state is not completely fermionized. Since this quasi-STG-state still has a non-vanishing, positive $1D$-scattering length $a_\alpha = -(2/g_\alpha) > 0$, it is closer to a gas of spatially extended, hard-core particles (so-called hard rods) than to a completely fermionized, point-like TG-gas [17], and localization effects are more pronounced, which can be observed in the more profiled density.

### 3.2. Weakly interacting components

Following the pathway to weak intra-species repulsion, the mechanism of pair formation is getting constantly weaker until it vanishes in the weak-interaction regime ($g_\alpha \sim 1$). In this weakly interacting regime, we turn to the limit case of two hardly interacting, BEC-like components ($g_\alpha \approx 0$). Compared to the case of two strongly repulsive components, there is no formation of a condensed state of $AB$-molecules, but the system collapses with the increase of the inter-species attraction. In other words, between the $AB$-molecules there is always an effective attractive interaction and thus for strong interaction a bright-soliton-like state evolves. Figure 5 displays a comparison of the one-body densities of (i) two identical point-molecules each of mass $M = 2$, which mirrors the case of very tightly bound, point-like $AB$-molecules.
Figure 4. Pair density matrix $\tilde{\rho}(x, x')$ for $g_\alpha = 25.0$ (left column) and the super-TG (STG) state $g_\alpha = -15.0$ (right column) ($\alpha \in \{A, B\}$). The inter-species interaction parameters are $g_{AB} = -0.01, -5.0$ (from top to bottom).

Figure 5. One-body density $\rho(x)$ of $N = 2$ point-like molecules of mass $M = 2$ with interaction strength $\tilde{g} = 0$ (dashed), two non-interacting components with $g_{AB} = -10.0$ (solid thin), and two molecular components with $g_{AB} = -10.0$ (solid thick).

with no molecular interaction $\tilde{g} = 0$, (ii) an $N$-body bound state of the form

$$\Psi(X) \propto \Phi_0(R) \left\{ \exp \left[ -\frac{|g_{AB}|}{2} \left( \sum_{i,j \leq 2} |x_{A_i} - x_{B_j}| \right) \right] \prod_{\alpha \in \{A, B\}} \exp \left( -\frac{|g_\alpha|}{2} |x_{\alpha_1} - x_{\alpha_2}| \right) \right\}$$

and (iii) the case $g_\alpha = 0$, which is a solitonic state in between the two extremes.

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One-body density matrix $\rho_1^{(A)}(x, x')$ of two quasi-fermionized components ($g_\alpha = 25.0$) for the inter-species interaction strength $g_{AB} = -0.01$, $-10.0$, $-20.0$ (from left to right) of a mixture with particle numbers $N_A = 3$ and $N_B = 2$ (upper row), $N_A = N_B = 3$ (lower row).

We note that the coherence between the ‘$AB$-molecules’ (as evidenced in the pair density matrix) is slightly stronger compared to the one-body level $\rho_1^{(\alpha)}(x, x')$, as there is just explicit interaction between the species ($g_{AB}$). However, as there is no longer a scale separation, one cannot consider this system simply as a gas of point-like molecules.

### 3.3. Imbalanced components

After having studied the mechanism for equal component settings, we now want to highlight the effects of relaxing the equality of the particle numbers and the intra-species interaction strengths.

#### 3.3.1. Unequal particle numbers.

We first consider the case of unequal particle numbers $N_A \neq N_B$, but still the same intra-species interaction strengths ($g_A = g_B$). We exemplify this on the case of two quasi-fermionized species ($g_\alpha = 25.0$) with particle numbers $N_A = 3$ and $N_B = 2$. On the way from weak to very strong inter-species attractions $g_{AB}$, an analogous pathway occurs as for fermionized binary mixtures with equal particle numbers, as can be checked on the basis of the pair density matrix. That is, an MTG state forms in the intermediate inter-species interaction regime, followed by condensation and collapse for even higher inter-species attractions. The effect of the difference in the particle numbers (or particle densities) can be seen as a formation of two phases: one consists of tightly bound $AB$-molecules, as in the case of equal species numbers, and the other consists of $N_d \equiv |N_A - N_B|$ (here: $N_d = 1$) ‘loosely bound’ spare particles, i.e. particles that are hardly affected by the inter-species interaction (of course, taking into account the proper particle exchange symmetries.) This picture of loosely bound particles provides a good understanding of the two-body density patterns in the intermediate to strong inter-species interaction regime ($|g_{AB}| \lesssim 10$). Furthermore this formation of, in this case, two $AB$-molecules and one loosely bound particle manifests in the one-body density matrix $\rho_1^{(A)}(x, x')$ (figure 6) in the formation of two density peaks on the diagonal $\{x' = x\}$ and the
Figure 7. Pair density matrix $\tilde{\rho}(x, x')$ for the particle numbers $N_A = N_B = 2$ plotted along the diagonal \{x' = x\} for $x \in [-2.2, 0.0]$ and along the off-diagonal \{x' = -x\} for $x \in [0.0, 2.2]$, of one fermionized component $g_B = 25.0$ and intra-species interactions of the other component: (a) $g_A = 0.01$, (b) $g_A = 5.0$, (c) $g_A = 10.0$ and (d) $g_A = 25.0$. The highest inter-species interaction (solid line) shows the best possible symmetry between on- and off-diagonal. (The densities have been rescaled to the same maximal value at the position $x = 0$.)

larger off-diagonal density compared to the balanced counterpart ($N_A = N_B = 3$), respectively. This two-phase picture breaks down as the system starts to collapse for larger attraction (see figure 6, $g_{AB} = -20$).

3.3.2. Unequal inter-species repulsions. Now we consider unequal intra-species repulsions $g_A \neq g_B$. For the sake of clarity, we keep the particle numbers equal $N_A = N_B$. We start with the case of all intra-species interactions corresponding to the fermionization regime, here $g_A = 10.0$ and $g_B = 25.0$. In the chosen example the species $A$ is weakly fermionized, but still the system evolves similarly to the case of two strongly fermionized species discussed above, that is, we observe the formation of a pronounced TG pattern in the pair density matrix $\tilde{\rho}(x, x')$, indicating the MTG state. This is in line with figure 7, which pictures the $\tilde{\rho}(x, x')$-profile along the diagonal \{x' = x\} and along the off-diagonal \{x' = -x\}.

During the formation of the MTG state, one can observe an assimilation of, for instance, the one-body density matrices $\rho_1^{(A)}(x, x')$ and $\rho_1^{(B)}(x, x')$. The best overlap is achieved about
Figure 8. Distance Dist between the one-body density maxima $\text{Max}[\rho_1^{(\alpha)}(x, x')]$ of the components $\alpha \in \{A, B\}$ for different inter-species interaction strength $g_{AB}$ and the intra-species interactions $g_A = 10.0$ and $g_B = 25.0$.

the value $|g_{AB}| \approx 5.0$. To characterize this increasing similarity, let us define the distance between the peak positions $x_{\text{max}, \alpha}$ of each component’s (diagonal) density profile, i.e. where $\rho_1^{(\alpha)}(x_{\text{max}, \alpha}, x_{\text{max}, \alpha})$ is maximal. For a given inter-species coupling $g_{AB}$, this is denoted by $\text{Dist} := ||x_{\text{max}, A}| - |x_{\text{max}, B}||$ (see figure 8).

With a further increase of the inter-species interaction ($|g_{AB}| > 5$), the system collapses in a way characteristic for Bose–Fermi mixtures [37]. That is, the less repulsive component $A$ forms a high density region in the center of the trap, whereas the strongly fermionized component keeps its fermionic character up to higher inter-species interactions ($|g_{AB}| \approx 8.0$). That decrease of the density overlap is visualized in the light increase of the distance Dist of the extrema of the one-body density for $5 < |g_{AB}| \lesssim 8$ (figure 8). This characteristic does not hold for very high inter-species interactions ($|g_{AB}| \gtrsim 10$), where the system collapses similarly to that of two equally fermionized Bose components, discussed above. The comparison of the case at hand (see figure 7(c)) with that of two fermionized components (see figure 7(d)) shows that the length scale of the off-diagonal profile is always smaller than that of the diagonal profile. Thus no $g_{AB}$ exists for which a perfect off-diagonal long range order is achieved in the pair density matrix $\tilde{\rho}(x, x')$. In this sense, the system starts to collapse, without forming a condensed state on the $AB$-molecule level. It is noteworthy that if both components are equally weakly fermionized ($g_A = g_B = 10.0$), no partial collapse occurs as in the above case, and a condensed state can be observed.

Going towards components with intermediate and weak intra-species repulsions (like $g_A \lesssim 5$ shown in figures 7(a) and (b)) the pair-formation is not visible anymore, and the system immediately starts to collapse without forming a condensed state as in the case before. In the extreme case of one ‘condensed’ component ($g_A \to 0^+$), the approximation (5) above is not valid as the length scales cannot be separated anymore. For unequal particle numbers, the system can again be thought of as a two-phase system; hence if the particle number of the fermionized state (say $B$) exceeds the number of condensed particles, the coherence in the one-body density $\rho_1^{(B)}(x, x')$ has larger off-diagonal elements due to spare (unbound) $B$-particles.
4. Mixture with attractive components

In this section, we complete our investigation by exploring mixtures with one or more attractively interacting components \( g_{\alpha} < 0 \).

4.1. Repulsive and attractive components

We start in the spirit of the above section with one component in the fermionized interaction limit, i.e. \( g_B = 25.0 \), and the other in a bound state \( g_A = -10.0 \). The bound species are strongly localized in the center of the trap and the feedback on that component is negligible for any inter-species attraction. To explore this situation it is natural to consider a simplified Hamiltonian, where the effect of the localized species \( A \) is replaced by an additional external potential for the \( B \) atoms \( \delta U_B(x) = g_{AB} N_A \rho^A(x) \).

Furthermore for \( g_B \gg 1 \), one can map the fermionized component on a non-interacting fermionic system \([9]\). Consequently one obtains for the exemplary case of \( N_B = 2 \) particles the simple solution \( \Psi_0^F = |\Psi_0^{\text{fermion}}| = \frac{1}{\sqrt{2}} \left[ \Phi_0(x_1) \Phi_1(x_2) - \Phi_0(x_2) \Phi_1(x_1) \right] \), where \( \Phi_i \) denotes the \( i \)th single-particle eigenstate of a split-trap.

The validity of the approximation becomes rapidly better with increasing numbers of particles \( N_A \) in the bound state, as the width of one-body density \( \rho^A(x) \) scales as \( \frac{1}{\sqrt{N_A}} \), and hence converges towards a \( \delta \)-type potential in the limit of large particle numbers \( N_A \to \infty \). The agreement is astonishingly good already with relatively few particles \( N_A \geq 4 \). In figure 9, the exact two-body correlation function \( \rho_{BB}(x_1, x_2) \) for \( N_B = 2 \) particles is shown. As it turns out, the picture of a non-interacting fermionic system applies very well up to intermediate inter-species interactions \( |g_{AB}| < 2 \) (in the case of \( N_A = 4 \)). This predicts that if for intermediate inter-species interaction \( g_{AB} \approx -1 \) one detects a \( B \)-particle aside the trap center \( (x_{B_1} \approx \pm 1) \), the other \( B \)-particle is located at the center of the trap \( (x_{B_2} \approx 0) \). (For \( N_B > 2 \) an additional density contribution emerges on the off-diagonal.)

Figure 9. Two-body correlation function \( \rho_{BB}(x_1, x_2) \) of a mixture with one molecular species \( g_A = -10.0 \) \( (N_A = 4) \) and one species of \( N_B = 2 \) repulsive bosons, \( g_B = 25.0 \), for the inter-species interaction parameter \( g_{AB} = -0.01 \), \(-1.0\), \(-5.0\) (from left to right).
Figure 10. One-body density $\rho^{(B)}(x)$ of $N_B = 2$ non-interacting $B$-particles ($g_B = 0.0$), with different $A$-particle numbers $N_A$ in a bound state ($g_A = -10.0$) and the inter-species interaction strength $g_{AB} = -10.0$.

Whereas for the model $\delta$-type potential the two-body density $\rho_{BB}(x_1, x_2)$ would remain in the (increasingly sharp) cross-shaped pattern even for $g_{AB} \to -\infty$, this is not the case for the system at hand (see figure 9 for $g_{AB} = -5.0$). Due to the nonzero width of the additional potential caused by the $A$-particles, for high enough inter-species attraction all of the $B$ particles can be accommodated in the ‘$A$-potential’ as a whole (unlike for a $\delta$-type potential). That is illustrated in figure 9 for $g_{AB} = -5.0$, where again the familiar TG-density pattern can be observed, but with the spatial extension of the $A$-particle density (compare with figure 10). This behavior in the high interaction regime can also be observed for higher $B$-particle numbers.

4.2. Two attractive components

Extending the results of the last section, we start with the case of one weakly interacting, i.e. ‘condensed’ component ($g_B \approx 0$), and the other component again in a bound state ($g_A = -10.0$). We can again apply the previous split-trap approximation on a system with $N_B = 2$, i.e. the condensed $B$-particle feel an effective short-range potential at the center of the harmonic trap. Again with increasing particle-number $N_A$ in the molecular state, the approximation is getting better. However, for the length scales of the two components to differ as distinctly as in the case of a fermionized component, the agreement with the split-trap model above requires more $B$-particles in the bound state. If we assume as a model a condensed state in component $B$ ($g_B = 0$) and a tightly bound, $\delta$-type state in component $A$, the model Hamiltonian 7 reduces to

$$\tilde{H}_B = \sum_{i=1}^{N_B} \left( \frac{1}{2} p_{B_i}^2 + \frac{1}{2} x_{B_i}^2 + N_A g_{AB} \delta(x_{B_i}) \right),$$

with the solution [49]

$$\Psi_0(X_B) \propto \exp \left( -\frac{(x_{B_1}^2 + x_{B_2}^2)}{2} \right) \prod_{i=1}^{N_B} U \left( \frac{1}{2} - \frac{E_0}{2}, \frac{1}{2}, x_{B_i}^2 \right),$$
which evolves with increasing inter-species attraction towards a state analogous to the bound state of the $\delta$-potential.

For higher attractive interactions also in component $B$, the model is not applicable anymore. In the limit of highly attractive components, with increasing inter-species interaction strength the system forms an entire bound state. For the special case of equal interaction strength $g_A = g_{AB} \equiv g$, one can map the system to a bound state of $N_A + N_B$ identical particles

$$\Psi_0(X \equiv (X_A, X_B)) \propto \Phi_0(R) \exp \left( -\frac{|g|}{2} \sum_{i<j} |x_i - x_j| \right).$$

5. Summary

In conclusion, we have investigated the ground state of a two-component Bose gas in a 1D harmonic trap throughout the crossover from weak to strong inter-component attraction. We have highlighted different pathways depending on the choices of the different intra-component couplings, and indicated how they can be understood in terms of simplified models. For two quasi-fermionized components (i.e. TG states), the system forms an MTG gas in the intermediate inter-component interaction regime, which consists of bound pairs containing one particle of each component. In the strongly attractive regime, we demonstrated the condensation of the bound pairs, followed by the collapse of the system beyond a critical attraction. We showed the analogous mechanism for attractively fermionized components, that is, components in the STG regime. Relaxation of the condition of two equally fermionized components leads to a modified pathway: in the case of just one fermionized component, the formation of an MTG gas can still be observed for high enough repulsion within the second component, but the collapse occurs in analogy to Bose–Fermi mixtures without condensation of the bound pairs, in contrast to the case of comparable repulsions. In the regime of intermediate (inter-species) attraction, unequal (number-) densities in the components have been found. These can be understood as two phases, one consisting of molecular pairs of each component, and the other phase consisting of loosely bound particles. For mixtures with one strongly attractive component, we showed that this component can be interpreted as an additional external $\delta$-function potential for the other component, in the case that both length scales can be well separated. The investigation of these intriguing pairing scenarios paves the way toward studying their quantum dynamics, such as the tunneling of molecular pairs in multi-well traps.

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