Unbalanced droplets of one-dimensional mixtures of fermions

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By means of a diffusion Monte Carlo technique, we study one-dimensional unbalanced mixtures of fermionic Ytterbium atoms (173 Yb, 171 Yb). This means clusters in which the total number of 173 Yb particles is different from the sum of all the atoms belonging to the 171 Yb isotope. Our aim will be to check the possibility of having self-bound arrangements beyond the balanced compositions reported in previous literature rather than exploring all the situations in which that could be possible. In that vein, we focused mainly on mixtures in which the atoms belonging to one isotope are spin-polarized, while the spins of the particles in the other isotope are evenly distributed in two sets. What we found was that, even tough self-bound droplets are possible for different compositions, the most stable ones are clusters with a slight excess of attractively interacting 171 Yb particles with different spins with respect to the number of spin-polarized 173 Yb atoms. Clusters in which the number of repulsively interacting unequal-spin 173 Yb atoms are in excess with respect to the spin-polarized 171 Yb particles have a very narrow stability range.

I. INTRODUCTION

A droplet can be defined as a (relatively) small cluster of particles that stick together without collapse or evaporation during a reasonable long period of time. To be considered self-bound, a droplet has to be stable without the intervention of a external confining potential. When several species are present, the outcome of the mixing would depend on factors such as the bosonic or fermionic nature of the particles, their repulsive or attractive interactions and the dimensionality of the system [1–3]. The seminal work by Petrov [4], opened the field for ultracold Bose-Bose droplets [1, 2, 5–13], but other possibilities [14–21] are also viable.

Within this context, the consideration of onedimensional (1D) systems offers the advantage of the suppression of three-body losses with respect to their three-dimensional counterparts [3, 22]. In addition, if the interactions between species are the right ones, we can have self-bound Bose-Bose [11–13], Bose-Fermi [14, 17], and Fermi-Fermi 1D droplets [19, 20]. In this last case, when the number of spin-ups equals the number of spindowns, we end up with a set of composite bosons (or "molecules") with an effective repulsion between them [23, 24] that makes self-bound balanced 1D clusters of equal-mass fermions impossible [19, 25].

Fortunately, we can circumvent that limitation by considering at least three different types of fermionic species [19, 20]. This has been proved to work in small clusters of Ytterbium (173 Yb and 171 Yb) with attractive shortrange interactions between atoms of different isotopes. Since atoms belonging to the same isotope can have different spins, not all the 173 Yb- 171 Yb molecules are equal: we have as many types of composite bosons as possible spin pairings. Then, the relaxation of the Pauli avoidance between different kinds of molecules allows the attractive interaction between them to kick in, producing self-bound droplets.

What all previous cases have in common is that they consider only *balanced* clusters, i.e., ensembles in which the number of atoms of both species (or isotopes) is equal to each other. Very recently, that constraint has been removed in some studies of Bose-Bose clusters modeled by Gross-Pitaevskii equations [26–29] or within the framework of the discrete 1D Bose-Hubbard model [30]. All those works agreed in the existence of stable unbalanced clusters of particles, at least within certain values of the parameters defining the droplets. This opens the door to the study of differences in the behavior of those clusters with respect to the case of the balanced ones and to establish their stability ranges.

In this work, we will expand this new avenue by considering continuous 1D systems of self-bound unbalanced fermions. To do so, we will deal with ¹⁷³Yb-¹⁷¹Yb mixtures in which $N_{173} \neq N_{171}$ (N_{173} and N_{171} being their respective number of particles). We aim only to check whether those unequal particle clusters exist, rather than exhaustively testing all the situations in which we can find unbalanced self-bound setups. This is the reason why, to simplify things, we will consider mainly situations in which one of the components (either 173 Yb and 171 Yb) is spin-polarized while the atoms of the other are equally split into two unequal spin sets. In this, we are guided by the results of balanced clusters, in which all compositions including more than three types of spins or in which the numbers of atoms with the same spin are not the same, have qualitatively similar behaviors when the total number of particles is fixed [19, 20].

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II. METHOD

Following the previous literature, the 1D clusters in this work will be described by the following Hamiltonian [19, 20, 31, 32]:

$$H = \sum_{i=1}^{N_p} \frac{-\hbar^2}{2m} \nabla_i^2 + g_{1D}^{173-171} \sum_{i=1}^{N_{173}} \sum_{j=1}^{N_{171}} \delta(x_i^{173} - x_j^{171}) + g_{1D}^{173-173} \sum_{b>a} \sum_{i=1}^{n_{173,a}} \sum_{j=1}^{n_{173,b}} \delta(x_{a,i}^{173} - x_{b,j}^{173}) + g_{1D}^{171-171} \sum_{b>a} \sum_{i=1}^{n_{171,a}} \sum_{j=1}^{n_{171,b}} \delta(x_{a,i}^{171} - x_{b,j}^{171}), \quad (1)$$

where N_p is the total number of fermions, with $N_p = N_{173} + N_{171}$, and will be in the range 24-36. As indicated above, $N_{173} \neq N_{171}$. Eq. 1 considers only interactions in which the atoms in the pair are different from each other, since Pauli's exclusion principle takes care of the avoidance between identical fermions. m is the mass of the atoms, described by a single parameter as in the previous literature [19, 20, 31, 32]. This is expected to be a reasonable approximation, since the mass difference between isotopes is around 1 %. $n_{173,ab}$ and $n_{171,ab}$ are the number of atoms with spins a and b. The g_{1D} parameters depend on the 1D-scattering lengths, a_{1D} , via $g_{1D}^{\alpha,\beta} = -2\hbar^2/ma_{1D}(\alpha,\beta)$. a_{1D} is defined by [33]:

$$a_{1D}(\alpha,\beta) = -\frac{\sigma_{\perp}^2}{a_{3D}(\alpha,\beta)} \left(1 - A\frac{a_{3D}(\alpha,\beta)}{\sigma_{\perp}}\right), \quad (2)$$

with A=1.0326 and $(\alpha, \beta) = (173, 171)$. $\sigma_{\perp} = \sqrt{\hbar/m\omega_{\perp}}$ is the oscillator length in the transverse direction, depending on the perpendicular confinement frequency, ω_{\perp} , taken to be in the range $2\pi \times 50-100$ kHz, tight enough to produce a quasi-one dimensional system. $a_{3D}(\alpha,\beta)$ are the three-dimensional experimental scattering lengths between isotopes, taken from Ref. 34 i.e., 10.55 nm $(^{173}\text{Yb}-^{173}\text{Yb})$, -0.15 nm $(^{171}\text{Yb}-^{171}\text{Yb})$ and -30.6 nm (¹⁷¹Yb-¹⁷³Yb), where the minus signs mean attractive interactions. Those scattering lengths cannot be changed via magnetic Feshbach resonances due to the closed-shell electronic structure of Yb atoms. The use of other kinds of Feshbach resonances is, at best, problematic [35], and to our knowledge, it has only been studied for setups containing a single Yb isotope [36–38]. However, the values of $g_{1D}^{\alpha,\beta}$ can be changed by modifying the external confinement, σ_{\perp} , via Eq. 2. That variation could also, in principle, change the nature of the interactions, determined by the sign of a_{1D} , through a confining-induced resonance. To do so, Aa_{3D}/σ_{\perp} should be greater than 1, something that does not happen for any of the a_{3D} values in the considered range of frequencies. This means that the nature of the interactions between isotopes is fixed by the sign of those a_{3D} 's: attractive for the ¹⁷³Yb-¹⁷¹Yb and 171 Yb 171 Yb pairs and repulsive in the 173 Yb 173 Yb case.

To solve the Schrödinger equation derived from the continuous Hamiltonian in Eq. 1, we used the fixed-node diffusion Monte Carlo (FN-DMC) algorithm, that gives us the exact ground state of a 1D system of fermions [39, 40], without resorting to any mean field treatment. We start from an initial approximation to the exact wavefunction, the so-called trial function. We used:

$$\Phi(x_1, \cdots, x_{N_p}) = \Phi(x_1, \cdots, x_{N_p}) = \mathcal{A}(x_1^{173}, x_2^{173}, \cdots, x_{N_{173}}^{N_{173}}, x_1^{171}, x_2^{171}, \cdots, x_{N_{171}}^{N_{171}})$$

$$\prod_{b>a} \prod_{i=1}^{n_{173,a}} \prod_{j=1}^{n_{173,b}} \frac{\psi(x_{a,i}^{173} - x_{b,j}^{173})}{(x_{a,i}^{173} - x_{b,j}^{173})}$$

$$\prod_{b>a} \prod_{i=1}^{n_{171,a}} \prod_{j=1}^{n_{171,b}} \frac{\psi(x_{a,i}^{171} - x_{b,j}^{171})}{(x_{a,i}^{171} - x_{b,j}^{171})}, \quad (3)$$

where $\mathcal{A}(x_1^{173}, x_2^{173}, \cdots, x_{N_{173}}^{N_{173}}, x_1^{171}, x_2^{171}, \cdots, x_{N_{171}}^{N_{171}})$ is the determinant of a square matrix that depends on the coordinates of all the particles in the system. The dimension of that square matrix will be $N_{max} \times N_{max}$, N_{max} being the maximum value between N_{173} and N_{171} . To build that matrix, we followed the prescription used in Ref. 41 for unbalanced sets of three-dimensional fermions. If, for the sake of the argument, we consider $N_{max} = N_{171} > N_{173}$, we will have a $N_{171} \times N_{171}$ matrix. Bearing in mind that the solutions of the Schödinger equation for a pair of 1D-particles interacting via an attractive delta potential can be written as [42]:

$$\phi(|x_i^{173} - x_{j'}^{171}|) = \exp\left[-\frac{|g_{1D}^{173,171}|}{2}|x_i^{173} - x_{j'}^{171}|\right], \quad (4)$$

then, we have that the first N_{173} rows of that $N_{171} \times N_{171}$ matrix are of the form:

$$\phi(|x_i^{173} - x_{1'}^{171}|), \phi(|x_i^{173} - x_{2'}^{171}|), \cdots, \phi(|x_i^{173} - x_{N_{171'}}^{171}|),$$
(5)

with *i* in the range $i=1, \dots, N_{173}$. The remaining $N_{171} - N_{173}$ rows have to include functions that depend exclusively on the coordinates of all the atoms of the ¹⁷¹Yb isotope. Following Ref. 43, we considered single-particle orbitals similar to the ones we would have in a Vandermonde matrix [44]. This means that the complete $N_{171} \times N_{171}$ determinant can be written as:

$$\begin{vmatrix} x_{1'}^{N_{171}-N_{173}-1} & x_{2'}^{N_{171}-N_{173}-1} & \cdots & x_{N_{171}}^{N_{171}-N_{173}-1} \\ & \ddots & \ddots & \ddots & & \ddots \\ & x_{1'}^2 & x_{2'}^2 & \cdots & x_{N_{171}}^2 \\ & x_{1'} & x_{2'} & \cdots & x_{N_{171}}^2 \\ & 1 & 1 & \cdots & 1 \\ \phi(r_{N_{173},1'}) & \phi(r_{N_{173},2'}) & \cdots & \phi(r_{N_{173},N_{171}}) \\ & \ddots & \ddots & \cdots & \cdots \\ & \phi(r_{2,1'}) & \phi(r_{2,2'}) & \cdots & \phi(r_{2,N_{171}}) \\ & \phi(r_{1,1'}) & \phi(r_{1,2'}) & \cdots & \phi(r_{1,N_{171}}) \end{vmatrix}$$

with $r_{i,j'} = |x_i^{173} - x_{j'}^{171}|$. This form does not include any confining wavefunction, as it is typically the case when

an harmonic potential is included in the Hamiltonian, [44] and generalizes the used in previous literature for balanced fermion clusters.

The terms $(x_{a,i}^{\alpha} - x_{b,j}^{\alpha})$ in the denominator of Eq. 3 correct the spurious nodes between atoms of the same isotope with different spins (see Refs. 19 and 31 for further details). In Eq. 3, $\psi(x_{a,i}^{\alpha} - x_{b,j}^{\alpha})$'s are Jastrow functions that introduce the correlations between pairs of particles of the same isotope belonging to different spin species a, b. For the repulsively interacting ¹⁷³Yb-¹⁷³Yb pair, we have [45]:

$$\psi(x_{a,i}^{173} - x_{b,j}^{173}) = \cos(k[|x_{a,i}^{173} - x_{b,j}^{173}| - R_m])$$
(6)

when the distance between atoms, $|x_{a,i}^{173} - x_{b,j}^{173}|$, was smaller than a variationally obtained parameter, R_m , and 1 otherwise. k was obtained by solving the transcendental equation $ka_{1D}(173, 173) \tan(kR_m) = 1$. When the pair of particles of the same isotope attract each other, as in the ¹⁷¹Yb-¹⁷¹Yb case, the Jastrow has the form of Eq. 4 [31, 45], but with a different value of the defining constant, $g_{1D}^{171,171}$.

III. RESULTS

As shown in previous literature [19, 25], when $N_{173} = N_{171}$ and the atoms belonging to both isotopes are spin-polarized, we have a set of composite bosons with an effective repulsion between them due to a double Pauli avoidance that precludes the formation of selfbound clusters. One of the tell-tale signals of this behavior is that the energy per particle is exactly $E_b/2 =$ $-(g_{1D}^{173,171})^2/(8\hbar\omega_{\perp}\sigma_{\perp})$, with E_b the binding energy of a pair of particles interacting attractively via a 1D delta potential [42]. On the other hand, when $N_{171} > N_{173}$ (again for the sake of the argument) what we have is that the total energy of the system is $N_{173}E_b$ and the system is again unbound. As stated above, we have neglected the mass difference between isotopes ($\sim 1\%$) even tough that difference, if large enough, could induce the existence of self-bould boson [46] and fermion [46, 47] arrangements.

In Figs. 1-3 and Fig. 5, we display the dependence of the energy per particle on the cluster composition to check whether is smaller than $(N_{173}/N_p)E_b$ (or $(N_{171}/N_p)E_b$, depending on the case) and self-bound droplets are possible. The $|g_{1D}^{173,171}|$ range displayed is the result of taking ω_{\perp} 's in the interval $2\pi \times 50\text{-}100$ Hz, deducing the corresponding σ_{\perp} 's, and introducing those values in Eq. 2 to produce the magnitude of the interaction. The first of those figures show the case for clusters with total number of particles in the range 24-36, assembled by joining together a variable number of spin-polarized ¹⁷³Yb atoms and a evenly distributed set of spin-up and spin-down ¹⁷¹Yb particles. Since ¹⁷¹Yb atoms have SU(2) symmetry, we cannot consider more than two spin sets. To consider larger clusters in order to extrapolate our DMC results to the thermodynamic



FIG. 1. Energies per Yb atom for clusters of different compositions (see text for definitions) as a function of the interaction parameter between atoms of different isotopes. Error bars in all cases are similar to the ones displayed and not shown for simplicity. Dotted line is a least-squares third orden polynomial fit to the 36-18/(9+9) case and it is intended as a guide-to-the eye.

limit $N_p \to \infty$ is computationally very expensive and beyond the scope of this work. In this example, we fixed $N_{171}/2 = 9$, but the results are similar for clusters with different compositions. To name those clusters, we used the convention $N_p - N_{173} / (N_{171}/2 + N_{171}/2)$. Since their energies per particle are smaller than E_b , we may say that, in principle, the droplets are self-bound, this being due to the attractive interactions between atoms in different (with unequal spins for the atoms in the ¹⁷¹Yb isotope) molecules. We can see also that, for the same total number of ¹⁷¹Yb atoms, the stability of the cluster increases with the number of 173 Yb particles. In Fig. 1 we display also the case of two unequal sets of spin-up and spin-down 171 Yb atoms (30-12/(10+8)). The energy per particle is virtually identical that that of the more balanced 30-12/(9+9) one. This implies that our results are robust with respect to a slight change in spin composition. Larger differences in the number of spin up and spin down ¹⁷¹Yb numbers produce unstable clusters (see below). On the other hand, when we keep N_{173} constant, the energy per particle also decreases with N_{171} , as can be seen in Fig. 2. Last, we display in Fig. 3, a couple of representative examples that indicate that, when N_p is constant, the most stable arrangements are those with a small imbalance in the N_{173}/N_{171} ratio.

However, to make sure that we have a stable self-bound droplet we have to check that the cluster will not eventually break during the course of the simulation. To do that, we calculated the density profiles for different arrangements and checked that they remained invariant



FIG. 2. Same as in Fig. 1 but for clusters in which the number of atoms in the spin-polarized 173 Yb subcluster is fixed. As in the previous figure, the error bars are comparable in all cases and only shown for the 28-12/(8+8) droplet for clarity. The dotted line is also intended as a guide-to-the-eye.



FIG. 3. Energies per particle for different cluster compositions. In all cases the error bars are of the size of the ones displayed and the dotted lines are again guides-to-the eye.

and finite in width throughout each simulation. As a example of such circumstance, we display in Fig. 4 one of those profiles for a 28-12/(8+8) droplet, representative of clusters in which the spin-polarized component is 173 Yb, for two different values of transverse confinement. The profiles are normalized to the total number of particles for the 173 Yb isotope (12) and to the number of particles per spin for the 171 Yb one (8). Those are equilibrium



FIG. 4. Density profiles for a 28-12/(8+8) cluster for two different values of transverse confinement. Open symbols and dashed line correspond to ¹⁷³Yb densities, while solid symbols and full line display the behavior of each spin component of the ¹⁷¹Yb isotope. Error bars are of the size of the symbols and not displayed by simplicity.

profiles, unchanged along a DMC simulation comprising 3×10^5 Monte Carlo steps after thermalization and averaged over 3 independent Monte Carlo histories. To avoid spurious correlations, we considered only configurations separated 100 steps apart, i.e., we kept 3000 sets of data. To be sure about stability of the clusters, we compared those total averages with the ones obtained considering the first 1000 DMC steps, the 1000 in the middle, and the 1000 final configurations of each history. In all cases, the results were identical to those shown in Fig. 4. As to the properties of the droplet itself, we can see that the tighter the confinement, the larger the width of the atoms of the cluster in the longitudinal direction, in accordance with what happens in balanced clusters [19]. We can see also that the ¹⁷¹Yb densities spread outside the locations of the spin-polarized ¹⁷³Yb isotope, but not too far. This allows the excess ¹⁷¹Yb atoms in the wings to bind with the $^{173}\mathrm{Yb's}$ closer to them.

Fig. 5 gives us the same information as Fig. 1, but for arrangements in which the spin-polarized component belongs to the ¹⁷¹Yb isotope. This implies that the interactions between the two (or three) sets of ¹⁷³Yb atoms are repulsive, as corresponds to the positive threedimensional scattering length [34] between them. In that figure, we only display energies per particle for four clusters. The reason is that they are the only ones for which the density profiles are stable according to the criterion described in the previous paragraph. When the number of ¹⁷¹Yb decreases (or, equivalently, the number of ¹⁷³Yb increases), the clusters end up either splitting into smaller units or regularly spreading along the simulation runs



FIG. 5. Energies per particle for stable clusters in which the spin-polarized component is 171 Yb. Error bars are similar in both cases, but they are only shown for the 35-(9+9)/17 and 35-(6+6+6)/17 clusters.

with no equilibrium final position. This last circumstance would be akin to "evaporation". This happens also when we considered clusters in which the spin-polarized part corresponds to ¹⁷³Yb and the two-spin ¹⁷¹Yb sets are too unequal, for instance for a 30-12/(12+6) arrangement or for the case in which the number of unequal sets of spins is three (out of the 6 possible for the 173 Yb SU(6) atoms), as in the 35-(6+6+6)/17 atoms. The density profile for the stable 35-(9+9)/17 cluster is displayed in Fig. 6. There, we can see that this droplet is wider than its counterpart of the same size. Obviously, this is due to the repulsive interactions between atoms in the (9+9) subcluster. In any case, the nine atom subunits are contained within the limits of their spin-polarized counterparts and the whole cluster is stable due to the attractive ¹⁷¹Yb-¹⁷³Yb interactions.

IV. CONCLUSIONS

In this work we have dealt with the possibility of having 1D self-bound unbalanced clusters of fermions. By that, we meant mixtures of Ytterbium isotopes in which the total number of ¹⁷³Yb atoms is different than the total number of ¹⁷¹Yb particles. As in the case of balanced droplets ($N_{173}=N_{171}$), when both components are spin-polarized, it is impossible to have a self-bound system. On the other hand, when the atoms of one of the isotopes have different spin values, those droplets are stable. In this work we have considered mainly examples of evenly split spin populations, but the results are similar for other distributions.

We saw also that the relative stability of the droplets

FIG. 6. Same as in Fig. 4 for two different droplets with the same size and different compositions for a transverse confinement of $\omega_{\perp} = 2\pi \times 90$ Hz. Dashed lines and open symbols correspond to the spin-polarized component, while solid lines and symbols show the results for one of the spin components corresponding to atoms in the other isotope.

depends on their composition. Unbalanced droplets in which the interactions between particles of the same isotope and unequal spins are repulsive have a very narrow stability range. What we have found is that when N_{173} (two or three different spins) > $(N_{171}+1)$ the clusters either break into smaller units or evaporate. Conversely, when the unequal-spin atoms attract each other (spinup and spin-down ¹⁷¹Yb), the variability in the cluster compositions is larger. In particular, for the majority of the cases considered in this work, i.e., for N_p - $N_{173}/(N_{171}/2+N_{171}/2)$ arrangements with fixed N_p , we found that the most stable droplets were those of the type N_{p} - $(N_{p}/2-2)/(N_{p}/4+1,N_{p}/4+1)$, as can be seen in Fig. 3. That can be understood as the result of having a balanced cluster with two additional ¹⁷¹Yb atoms located in both wings, as can be seen in the density profiles of the 28-12/(8+8) arrangement displayed in Fig. 4. The relative reduction in the number of spin-polarized ¹⁷³Yb atoms decreases the effective repulsive interaction between identical fermions, lowering the total energy per particle. However, if we further deplete the ¹⁷³Yb part of the cluster, the reduction in the ¹⁷¹Yb-¹⁷³Yb interactions de-stabilize the entire structure. This is because the ¹⁷¹Yb atoms in the outer part of the wings are progressively further away from the ¹⁷³Yb's at the center, and unable to form molecules. In addition, those $^{171}\mathrm{Yb}$ atoms should bind to other ¹⁷¹Yb's to stay in the cluster, the ¹⁷¹Yb-¹⁷¹Yb interactions being too weak to stabilize the wings if they are made up of more than two ¹⁷¹Yb atoms.



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