Metal and insulator states of SU(6) \times SU(2) clusters of fermions in one-dimensional optical lattices

M C Gordillo

Departamento de Sistemas Físicos, Químicos y Naturales, Universidad Pablo de Olavide, E-41013 Seville, Spain

* Author to whom any correspondence should be addressed.

E-mail: cgorbar@upo.es

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Abstract

We studied the behavior of mixtures of $^{173}$Yb (with symmetry up to SU(6)) and $^{171}$Yb (up to SU(2)) fermionic isotopes loaded in one-dimensional (1D) optical lattices. To do so, we solved the Schrödinger equation describing different systems using a diffusion Monte Carlo technique. We considered continuous Hamiltonians in which the interactions between atoms of different species (isotopes and/or spins) were modeled by contact potentials with parameters derived from their experimental scattering lengths. This implies that we can find both attractive and repulsive interactions between fermion pairs in the same cluster. The strength of those interactions can be changed by varying the transverse confinement, leading to different cluster behaviors. Only balanced clusters, i.e. with the same number of $^{173}$Yb and $^{171}$Yb atoms were considered. We found that the standard state for these clusters is a metallic-like one with different populations of $^{173}$Yb–$^{171}$Yb molecule-like pairs in each optical lattice potential well. However, for big enough clusters, insulator-like states are also possible.

1. Introduction

A lot of attention has been devoted recently to the study of fermionic mixtures made up of more than two different spins. Typically, this means alkali-earth metal atoms and their analogues [1, 2], specially $^{87}$Sr [3, 4] and $^{173}$Yb atoms [5–8]. The nuclear and electronic configuration of these isotopes implies that up to ten different spin flavors are possible, producing systems with SU(10) symmetry in the first case, and up to six in the second, i.e. SU(6) arrangements. However, since not all the spin levels need to be populated, we can have clusters with SU(N) symmetry with N < 10, 6, respectively. The interactions between pairs of particles with different spins were found to be repulsive in both cases, due to their positive three-dimensional (3D) scattering lengths.

Nevertheless, you can have attractive interactions if you consider pairs of different Sr or Yb isotopes. In the Sr case, the isotope family comprises three bosons and a fermion [2], while for Yb you have five bosons and two fermions [10]. Of all the possible Sr combinations, only the pair $^{86}$Sr (a boson)–$^{87}$Sr (a fermion) attract each other [9], while in the Yb case there are more possibilities to create molecule-like pairings. In this work we will be concerned only with a mix of two kinds of fermions, SU(6) $^{173}$Yb and SU(2) $^{171}$Yb, an arrangement that has been experimentally produced [11, 12], even though boson–fermion attractive mixtures are also possible [13, 14]. The $^{173}$Yb–$^{173}$Yb interaction is strongly attractive, while the $^{173}$Yb–$^{171}$Yb and $^{171}$Yb–$^{171}$Yb are strongly repulsive and weakly attractive, respectively. In this work, we will study one dimensional (1D) $^{173}$Yb–$^{171}$Yb fermi–fermi mixtures loaded in optical lattices. These combinations can be experimentally produced both in 3D [11, 12] or in 1D [15]. Only clusters, i.e., sets of few atoms were considered, since the creation of these structures is perfectly feasible from the experimental point of view [16].

The modelization of SU(N) systems in 1D optical lattices is usually done using the discrete Hubbard model [17–21], even tough some descriptions using continuous Hamiltonians can be found in the literature [22–28], most of them considering only repulsive interspecies interactions. The exception is reference [28],
were both attractive and repulsive fermi–fermi mixtures were contemplated. Following that previous literature, we described the set of atoms by the strictly 1D continuous Hamiltonian:

\[
H = \sum_{i=1}^{N_\alpha} \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega_\perp^2 x_i^2 + V_{\text{ext}}(x_i) \right] + + g_{1D}^{173-171} \sum_{i=1}^{N_{173}} \sum_{j=1}^{N_{171}} \delta(x_{i}^{173} - x_{j}^{171}) \\
+ g_{1D}^{173} \sum_{b,a} \sum_{i=1}^{n_{173, a}} \sum_{j=1}^{n_{173, b}} \delta(x_{i}^{173} - x_{j}^{173}) + g_{1D}^{171} \sum_{b,a} \sum_{i=1}^{n_{171, a}} \sum_{j=1}^{n_{171, b}} \delta(x_{i}^{171} - x_{j}^{171}).
\] (1)

In this equation \( V_{\text{ext}}(x) \) is the 1D optical lattice potential:

\[
V_{\text{ext}}(x) = V_0 \sin^2 (2\pi/\lambda)x,
\] (2)

with \( \lambda \) the wavelength of the lasers creating the optical lattice \([29]\), and \( V_0 \) the depth of the potential minima. In those lattices, the distance between neighboring potential wells is \( \lambda/2 \). In equation (1), \( m_{173} \) is the number of \(^{173}\text{Yb} \) fermionic species, and \( m_{171} \) is the number of \(^{171}\text{Yb} \) types of spins. \( N_\alpha \) the total number of \(^{173}\text{Yb} \) and \(^{171}\text{Yb} \) atoms, respectively. \( n_{\alpha, a} \) and \( n_{\alpha, b} \) \((\alpha = 173, 171)\) represent the number of atoms of a particular isotope with a given value of the spin. So the first pair sum takes into account the interaction between atoms of different isotopes, irrespectively of their spins, and the second and third ones consider the interactions between different spins of the same isotope.

We considered the \(^{173}\text{Yb} \) and \(^{171}\text{Yb} \) masses to be similar enough to assign them the same value, spins, and the second and third ones consider the interactions between different spins of the same isotope. For example, we can have a six sets (corresponding to the six different spin types involved, \( (173, 171), \) not on their spin \([10]\).

This parameter can be calculated from its three-dimensional (3D) counterpart, \( a_{3D} \), using the prescription given in reference \([30]\):

\[
a_{1D} = \frac{\sigma_\perp^2}{2A_{3D}} \left( 1 - \frac{\sigma_{3D}}{\sigma_\perp} \right),
\] (4)

with \( A = 1.0326 \). \( \sigma_\perp \) is the oscillator length in the direction perpendicular to the x-axis. Equation (4) implies that we can vary \( g_{1D} \) by changing \( \sigma_\perp \), whose experimental value is in the range of kHz \([5, 14]\).

However, it is also possible to use an optical Feschbach resonance \([1, 31, 32]\) to change the strength of the interactions, something we did not consider here.

In this work, we used frequencies in the range \( \omega_\perp = 0 - 2\pi \times 50 \text{ kHz} \), since no significant changes in the cluster properties were found for tighter confinements. The experimental value in reference \([5]\) was \( \omega_\perp = 2\pi \times 25 \text{ kHz} \), what implies \( \sigma_\perp \sim \sim 48 \text{ nm} \). The \( a_{3D} \) values are \( 10.55 \text{ nm} \) \((^{172}\text{Yb} - ^{173}\text{Yb})\), \(-0.15 \text{ nm} \) \((^{171}\text{Yb} - ^{173}\text{Yb})\) and \(-30.6 \text{ nm} \) \((^{171}\text{Yb} - ^{171}\text{Yb})\) \([10]\). It is clear from equations (3) and (4) that confinement cannot vary the nature of the \(^{171}\text{Yb} - ^{171}\text{Yb} \) and \(^{171}\text{Yb} - ^{173}\text{Yb} \) interactions, since the corresponding 3D-scattering lengths are negative. On the other hand, since \( a_{3D}(173, 173) \) is positive, in principle one can change the sign of the term in parenthesis in equation (4) by varying \( \sigma_\perp \) and flip the interaction from repulsive to attractive. To do so, \( \sigma_\perp \) should be smaller than \( Aa_{3D}(173, 173) \). A quick calculation indicates that to fulfill that condition the transverse confinement should be \( \sim 2\pi \times 500 \text{ kHz} \), well out of the range of the standard experimental values. From equations (3) and (4), we can see that, for \( \omega_\perp = 2\pi \times 10 \text{ kHz} \), \( g_{1D}(173, 173) = 3.63\hbar \omega_\perp \), \( g_{1D}(173, 171) = -6.33\hbar \omega_\perp \) and \( g_{1D}(171, 171) = -0.04\hbar \omega_\perp \). On the other hand, for \( \omega_\perp = 2\pi \times 30 \text{ kHz} \), \( g_{1D}(173, 173) = 12.33\hbar \omega_\perp \), \( g_{1D}(173, 171) = -15.63\hbar \omega_\perp \) and \( g_{1D}(171, 171) = -0.13\hbar \omega_\perp \).
of a system with SU(6) symmetry) of two \(^{173}\)Yb atoms or two sets (spin up and down) of six \(^{171}\)Yb atoms, but not a set of seven spin-up \(^{171}\)Yb together with a five spin-down \(^{171}\)Yb atoms.

2. Method

To obtain the proper conclusions about the systems under consideration, we have to solve the Schrödinger equation derived from the Hamiltonian in equation (1). Since we are dealing with fermions, we used the fixed-node diffusion Monte Carlo (FN-DMC) method, that produces the exact ground state energy when the positions of the nodes of the real many-body wavefunction are known. To use that algorithm we should provide an initial approximation to the real many-body wavefunction of the system, the so-called trial function. That expression should contain as much information about the system as possible in order to be the basis for an importance sampling procedure [33]. In particular, it should include the exact position of the nodes of the real wavefunction (if known) and consider all the possible correlations between any pair of particles.

To describe all the clusters in this work we used as first guess the expression derived in reference [28]:

\[
\Phi(x_1, \ldots, x_{N_p}) = \mathcal{A} \left[ \phi(r_{11'}) \phi(r_{22'}) \ldots \phi(r_{N_{173}N_{171}}) \right] \prod_{i} \psi(x_i)
\]

\[
\times \prod_{a=1}^{m_{173}} \prod_{b=1}^{m_{171}} \prod_{i=1}^{n_{173}} \prod_{j=1}^{n_{171}} \frac{\psi\left(\sum_{a}^{173} x_{ai} - \sum_{b}^{171} x_{bj}\right)}{\prod_{a=1}^{m_{173}} \prod_{b=1}^{m_{171}} \prod_{i=1}^{n_{173}} \prod_{j=1}^{n_{171}} \psi\left(x_{ai} - x_{bj}\right)}
\]

(5)

where \(\mathcal{A}\) is an antisymmetric operator [34–36] and stands for the determinant of a matrix whose dimension is \(N_{173} \times N_{171}\) (a geminal). Each of the elements of that geminal, \(\phi(r_{ij})\) is a function that depends on the distance between a pair of particles of different isotopes, regardless of their spins \(r_{ij} = |x_i^{^{173}} - x_j^{^{171}}|\). In our case we chose:

\[
\phi\left(|x_i^{^{173}} - x_j^{^{171}}|\right) = \exp\left[-\frac{|g_{1D}(173, 171)|}{2}|x_i^{^{173}} - x_j^{^{171}}|\right]
\]

(6)

This is the exact solution of the Schrödinger equation corresponding to a pair of non-confined 1D-particles interacting with an attractive delta potential defined by \(g_{1D}\) [37]. This means that the solution depends exclusively on \(g_{1D}\) with no unknown parameters. The use of the geminal implies also that the trial function is antisymmetric with respect to the interchange of a couple of particles of the same isotope and spin, forcing the wavefunction to be zero when two of those particles are on top of each other. Those nodes are the only possible on 1D-systems [38].

\(\psi(x_i^{\alpha} - x_j^{\beta})\) (\(\alpha = 173, 171\)) is a Jastrow function that introduces the correlations between pairs of particles of the same isotope with different spins. Particles of the same isotope with the same spin are assumed to interact via Pauli exclusion only. Since the \(^{172}\)Yb–\(^{173}\)Yb is repulsive, we took the Jastrow as the solution of the scattering equation describing the pair of particles in an homogeneous (not harmonically confined) setup [39]:

\[
\psi(x_i^{173} - x_j^{173}) = \begin{cases} \cos(k(|x_i^{173} - x_j^{173}| - R_m)) & |x_i^{173} - x_j^{173}| < R_m \\ 1 & |x_i^{173} - x_j^{173}| \geq R_m \end{cases}
\]

(7)

\(k\) was obtained by numerically solving the equation:

\[
ka_{1D}(173, 173) \tan(kR_m) = 1,
\]

(8)

for the value of \(a_{1D}\) corresponding to the \(^{173}\)Yb–\(^{172}\)Yb pair for a given transverse confinement [39]. In practice, we guess a value for \(R_m\), obtain the value of \(k\), and solve variationally the Schrödinger equation describing those pair of particles using as input equation (7). We kept the value of \(R_m\) that gave us the minimum energy.

On the other hand, if the pair of particles attract each other, as in the \(^{171}\)Yb–\(^{171}\)Yb case, the Jastrow has the same form given in equation (6) [39, 40], but with a different value of \(g_{1D}\). The term \((x_i^{\alpha} - x_j^{\alpha})\) in the denominator is included to avoid the spurious nodes in the geminal when two atoms of the same isotope with different spin are on top of each other. In introducing this term, we followed the prescription of reference [28]. Finally, \(\Psi(x_i)\) is the ground state of the Schrödinger equation corresponding to the Hamiltonian in equation (1) for a single particle in the external (harmonic + optical lattice) potential, obtained numerically.
We described the different states (phases are not possible since clusters are finite systems), using the density profiles, the atom populations of the optical lattice potential minima and the momentum distributions, \( n_\alpha (k) \). Pure estimators, obtained by the forward walking technique \([41]\) to calculate all observables other than the energy were used. The site occupations and the moment distributions can be experimentally obtained \([5]\). The particle population at each optical lattice potential well \( i \) can be calculated using the expression \([27, 42, 43]\):

\[
 n_i = \int_{x_i' - \lambda/4}^{x_i' + \lambda/4} \rho(x)dx.
\]  

(9)

Here, \( \rho(x) \) is the particle density around a potential minimum whose center is at coordinate \( x_i \). \( n_\alpha (k) \) is the Fourier transform of the one-body density matrix, \( \rho_\alpha (x, x') \), and can be defined for each spin species as:

\[
 n_\alpha (k) = \frac{1}{2\pi} \int dx dx' \rho_\alpha (x, x') \exp[-ik(x - x')],
\]  

(10)

with

\[
 \rho_\alpha (x, x') = N_\alpha \int dx_2 \ldots dx_N \Phi(x_i, \ldots, x_{N_\alpha}) \Phi(x'_i, \ldots, x'_{N_\alpha}),
\]  

(11)

that in the system under consideration depends on both \( x \) and \( x' \) and not only on the relative distance between them, as in an non-confined system. \( \Phi(x_i, \ldots, x_{N_\alpha}) \) represents the ground-state wavefunction of the cluster, as corrected by the forward walking technique in the DMC method.

3. Results

Our goal in this work is to establish the states of clusters of 24 atoms under different external conditions. This is small enough that it is not computationally too expensive and large enough to produce different states when varying the interaction between particles and/or the external parameters. In any case, those clusters are larger than the repulsively-interacting SU(6) clusters dealt with in the previous literature \([22–24, 26, 27]\). Moreover, there are indications that the behavior of clusters of this particular size could be close to that of a similarly composed infinity system \([26]\). We varied the potential depths of the optical lattices, \( \omega \)'s, and the perpendicular confinements, \( \omega_\perp \). As it can be deduced from equation (4), larger \( \omega_\perp \)'s imply larger \( ^{173}\text{Yb} - ^{171}\text{Yb} \) attractive interactions together with an increase in the \( ^{173}\text{Yb} - ^{173}\text{Yb} \) repulsion. The remaining \( ^{171}\text{Yb} - ^{171}\text{Yb} \) is so weak that can be considered to be constant and almost zero.

In figure 1 we can see a comparison between the pair densities of two systems with \( N_{^{173}} = N_{^{171}} = 12 \) in which all the atoms in both isotopes have the same spin. Since we are ignoring the mass differences, those clusters can be considered to have SU(2) symmetry. The full line represents an interacting cluster with \( \omega_\perp = 2\pi \times 30 \text{ kHz} \), while the dotted one corresponds to a non-interacting set of two types of fermions with an interspecies interaction \( g_{1D} = 0 \). In both cases the densities of the different isotopes were identical to each other, so instead of the single-particle density we represent the same magnitude for pairs of particles. This perfect pairing is due to the fact that the \( g_{1D} (173, 171) \) is much stronger than the other two interactions (when present), what makes it a very effective mechanism to decrease the energy of the entire system. This is also valid for the mixtures of fermions considered below.

The first conclusion is very apparent: the attractive systems are thinner in both cases, irrespective of the \( V_0 \) value. This is obvious since the interaction between pairs of particles makes them to be closer together, the only limit to collapse being Pauli’s exclusion principle. Moreover, for the deeper optical lattice, we can see that the density values at the central part of the cluster change from being similar to each other in the non interacting case to have a defined maximum at the center of the cluster for \( g_{1D} \neq 0 \). No significant change in the behavior of the density was observed for deeper lattices or larger \( \omega_\perp \)'s.

To establish the state of each cluster, we have to calculate the populations on each lattice site, using equation (9). Those states will be labeled in the same way as their thermodynamic limit counterparts, as in the previous literature (see for instance reference \([43]\) and references therein). A set of consecutive sites with an integer and constant value for those populations is the signature of an insulator \([42]\). When no set of equally populated lattice minima is present, we have a metal. The result of applying that procedure to the data of figure 1 is given in figure 2. From that figure, we can see that for low values of \( V_0 \), both systems are metals. On the other hand, the non-interacting system in the upper part of figure 2 is an insulator, in this case a band insulator, since the particle population in a set of sites around the center of the cluster is two (the number of pairs is one) \([27]\). Conversely, the attractive cluster is clearly a metal. In this kind of SU(2) clusters, no insulator of any kind was found up to values of \( V_0 = 14E_R \), and/or up to \( \omega_\perp = 2\pi \times 50 \text{ kHz} \). However, this does not preclude the formation of Mott or band insulators for larger values of \( V_0 \) and/or \( \omega_\perp \).
Figure 1. Pair density profiles for a cluster including 12 $^{173}\text{Yb}$ and 12 $^{171}\text{Yb}$ atoms confined in optical lattices of different depth, $V_0$. All the $^{173}\text{Yb}$ atoms have the same spin, and the same happens to the $^{171}\text{Yb}$ atoms. The profiles are normalized to the total number of pairs, in this case, 12. Full line, $\omega_\perp = 2\pi \times 30 \text{kHz}$; dotted one, non-interacting fermions with $g_{1D} = 0$. All densities are normalized to 12 atoms.

The composition of the cluster is also an important issue at determining its state. Figure 3 gives us an example of the pair density for systems with different spin configurations. Following reference [28], to characterize spin arrangements, we used labels of the type $n_{173} \times m_{173} + n_{171} \times m_{171}$ which meant $m_{173}$ sets of $n_{173}$ $^{173}\text{Yb}$ atoms with SU($m_{173}$) symmetry and $m_{173}$ sets of $n_{171}$ $^{171}\text{Yb}$ spins with SU($m_{171}$) symmetry. When $m_{173}$ or $m_{171}$ are 1, the index is not written down. In any case, since we are considering only balanced clusters, $n_{173} \times m_{173} = n_{171} \times m_{171}$. This means that $12 + 6 \times 2$ is a cluster with 12 $^{173}\text{Yb}$ atoms, 6 $^{171}\text{Yb}$ atoms with spin up and 6 $^{171}\text{Yb}$ atoms with spin down. Conversely, $2 \times 6 + 12$ means that we have an ensemble of $^{173}\text{Yb}$ atoms with six different spin types, each set including two atoms, together with 12 $^{171}\text{Yb}$ atoms, these last ones with the same spin.

In figure 3, we consider the case of $12 + 6 \times 2$ and $6 \times 2 + 12$ clusters loaded in an optical lattice with $V_0 = 10E_R$ and $\omega_\perp = 2\pi \times 30 \text{kHz}$. We display the aggregate total density for both $^{173}\text{Yb}$ spins in the first case, and for $^{171}\text{Yb}$ species in the second. If we want to get the density of any of the two $^{173}\text{Yb}$ species of the first cluster we would have to divide the values given in figure 3 by two. The same should be done for the $^{171}\text{Yb}$ species of the second arrangement, the reason being that the ground state of a mixture of species has the most symmetric possible wavefunction [23, 24], producing density distributions that are identical for spins belonging to the same isotope. This can be easily understood by taking into account that the Hamiltonian of equation (1) is invariant with respect to the interchanging of the positions of a whole set of atoms of a particular spin with those of another spin set if both belong to the same isotope. If this condition is not fulfilled, the densities of both species will be different [44].

Taking in mind all of the above, we can readily see that the cluster with both spin up and spin down $^{173}\text{Yb}$ atoms is appreciably more compact than the one in which we have two different $^{173}\text{Yb}$ spin types. This is due to the fact that the interactions between like spins are attractive in the first case and repulsive in the other. The more compact cluster have also different populations of atoms in each of the three lattice sites that it spans. It is, therefore, a metal, as the $12 + 12$ arrangement displayed in the upper panel of figure 1. An increase in $\omega_\perp$ and/or $V_0$ does not change that metallic character. Moreover, considering (for instance) a $3 \times 4 + 6 \times 2$ cluster instead of a $12 + 6 \times 2$ one would not change the metallic character of the arrangement. This is due to the fact that the relaxing of the Pauli’s exclusion in going from a single set of identical $^{173}\text{Yb}$ to four sets of three atoms of the same isotope would make the arrangement even thinner, increasing the density at the central well without the leveling off of the densities necessary to create an insulator. On the other hand, the $6 \times 2 + 12$ ensemble has a set of three consecutive sites at the center at which the densities are equal to each other, what implies that this cluster is an insulator.
Figure 2. Pair populations for the same systems in the previous figure. Open squares, $\omega_\perp = 2\pi \times 30$ kHz; full squares, non-interacting system. The corresponding error bars are of the size of the symbols and not shown for simplicity.

Figure 3. Pair density profile of two clusters of different spin compositions for $\omega_\perp = 2\pi \times 30$ kHz and $V_0 = 10E_R$. See further explanation on the text.

However, to fully characterize the clusters, we would have to calculate the populations at each potential minima using equation (9), as done for the 12 + 12 cluster. The results are represented in figure 4 for several representative cases. In both upper and lower panels, full squares correspond to $\omega_\perp = 2\pi \times 15$ kHz, $V_0 = 12E_R$. According to the previous definitions, both clusters are insulators, since they have three consecutive sites at the center with the same populations. The curious thing is that the number of atoms at each lattice site is four, i.e., we have two pairs of particles. This implies that the insulator cannot be classified either as a Mott insulator or a band insulator, in which the number of particles at each site is one or two, respectively [27]. In the upper panel of the same figure we can also see the change of the state of that insulator to a metal when we decrease the lattice depth (open squares, $\omega_\perp = 2\pi \times 15$ kHz, $V_0 = 10E_R$) or the interaction between particles ($\omega_\perp = 2\pi \times 10$ kHz, $V_0 = 12E_R$). From the lower panel results we can see also that the 6 $\times$ 2 + 12 cluster with $\omega_\perp = 2\pi \times 10$ kHz, $V_0 = 14E_R$ is also a metal.
Figure 4. Pair populations for different cluster compositions, confinements and lattice depths. Upper panel: $2 \times 6 + 12$ cluster; open squares, $\omega_\perp = 2 \pi \times 15$ kHz, $V_0 = 10E_R$; full squares, $\omega_\perp = 2 \pi \times 15$ kHz, $V_0 = 12E_R$; full circles, $\omega_\perp = 2 \pi \times 10$ kHz, $V_0 = 12E_R$. Lower panel: $6 \times 2 + 12$ cluster; open circles, $\omega_\perp = 2 \pi \times 10$ kHz, $V_0 = 14E_R$; full squares, $\omega_\perp = 2 \pi \times 15$ kHz, $V_0 = 12E_R$. Error bars are of the size of the symbols.

Figure 5. State diagrams of $2 \times 6 + 12$ (open squares) and $6 \times 2 + 12$ clusters (full squares). When only full squares are seen, the limit is common to both arrangements.

We summarized all the information gathered about the insulator or metallic state of the $2 \times 6 + 12$ and $6 \times 2 + 12$ clusters for different values of the defining parameters in the state diagram displayed in figure 5. Both systems present similar behavior except in the triangle-like region limited by the dotted lines in the figure. $6 \times 2 + 12$ clusters within that parameter range are metals, while $2 \times 6 + 12$ ones are insulators. From the shape of the density profile in figure 4 we can see that in the entire range of parameters studied, $12 + 6 \times 2$ clusters are metals. This suggests that, all other things being equal, insulator clusters are only possible when atoms of the same isotope with different spins do not attract each other, not even for weak interspecies interactions.

We also calculated the Fourier transform of the density matrix, $n(k)$, an observable that can be obtained experimentally [5], and that decays as $k^{-4}$ for $k \to \infty$. We start that by tackling in figure 6 the same systems...
Figure 6. Momentum distributions for the same $^{12}_+^{12}_+$ systems displayed in figure 1. Full line, non-interacting metallic system, dashed line, $^{12}_+^{12}_+$ non-interacting band insulator arrangement. Squares, $^{12}_+^{12}_+$ clusters with attractive interactions corresponding to a transverse confinement of $\omega_\perp = 2\pi \times 30$ kHz. The momentum distributions normalized to the number of particles per species, in this case, 12.

already considered in figure 1. The non-interacting systems have behaviors similar to those already found in smaller clusters [27]; for relatively small values of $V_0$, there is a pronounced minimum for $k$-vectors around $6\sigma^{-1}$, the tell-tale signature of a metal for these systems. On the other hand, an increasing depth of the potential lattice makes that minimum disappear when we change to a band insulator. $k \sim 6\sigma^{-1}$ corresponds roughly to the distance between next-nearest neighbors (located at distances $\sim \sigma$) in the optical lattice, so $n(6\sigma^{-1}) \neq 0$ implies a correlation between atoms beyond first neighbors (located at distances $\sim 0.5\sigma$, $k \sim 4\pi\sigma^{-1}$). That correlation is a necessary ingredient to have an insulator. This is exactly what we can see in figure 6. In addition, a deeper $V_0$ also implies a fatter tail of the momentum distribution. On the other hand, no relative minimum can be seen for the $^{12}_+^{12}_+$ attractive clusters, even though an increasing value of the interspecies interactions makes the tails of the $n(k)$ distributions fatter. The turning-on of the interactions also implies a washing-out of the maxima and minima found at low values of $k$, and the disappearance of the minimum around $6\sigma^{-1}$.

According to figure 5, for those values of $\omega_\perp$, clusters with $V_0 = 6E_R$ are metallic, while arrangements with $V_0 = 12E_R$ are insulators. Obviously, and contrarily to what happens in $^{12}_+^{12}_+$ clusters, the momentum distributions of the $^{173}$Yb atoms are different from those of the $^{171}$Yb ones, the reason being that atoms in both sets are not interchangeable. If we observe closely those last $n(k)$’s we can see that are basically featureless functions in all cases, with fatter tails for deeper optical potentials. On the other hand, the ones corresponding to the 6 sets of $^{173}$Yb atoms are appreciably different. Basically, we observe a maximum or a shoulder-like feature around a range of $k$-vectors between 10–15 $\sigma^{-1}$. That corresponds to distances of $\sim 0.5\sigma$, i.e. to next-neighbor minima in the optical lattice. This shoulder is made less prominent with the increasing of the interspecies interactions brought about by larger $\omega_\perp$, up to the point of practically disappear for $\omega_\perp = 2\pi \times 30$ kHz and $V_0 = 6E_R$, but it is readily observable in all the other cases.

Last, we display three $^{173}$Yb momentum distributions for clusters of different compositions, $\omega_\perp = 2\pi \times 20$ kHz and $V_0 = 6E_R$. According to what was said before, all those clusters are metals. What we see is that the smaller the number of species, the smoother the $n(k)$’s. For the arrangement with the larger number of spins, there is a maximum corresponding to occupations of distances around the distance corresponding to the closest minima in the optical lattices. This larger correlation in $2 \times 6 + 12$ clusters is probably due to the fact that atoms of different species are not limited by Pauli’s exclusion principle, and can come closer to each other that a set of with the same number of fermions but with the same spin, that cannot be at the same position due to the antisymmetry of the wavefunction. The comparison of the $n(k)$’s for these three kinds of metallic clusters also implies that the existence of a shoulder around 10–15 $\sigma^{-1}$ is not, by itself, a signature of an insulator state (figure 8).
4. Conclusions

In this work we have studied the states of clusters made up of 24 atoms containing different spins and/or isotopes of ytterbium, the main difference with previous studies being the consideration of attractive interactions between particles. We introduced the possibility of pairing between sets of atoms with different spins with a single ensemble of fermions of another isotope to form pairs of molecule-like arrangements. We found that the character of the cluster was mainly set by the type of interactions between the different spins sets of the same isotope.

When we have a single set of spins for each isotope, the system can be considered to have SU(2) symmetry. This is not completely true since we are ignoring the tiny mass difference between $^{173}$Yb and $^{171}$Yb atoms. In that case, figures 1 and 2 tell us that the attraction between different atoms destroys the band insulator we have in the non interacting systems. According to the standard nomenclature [27, 42, 43],...
the inequality of the populations in consecutive lattice sites, make those clusters metals, even tough the associations between pairs make them a non-typical kind of metal. That attraction produces, obviously, more compact clusters than in the non-interacting case. This metallic character is preserved for all the values of \( \omega \) and \( V_0 \) dealt with in this work.

The consideration of different spins per isotope produces richer behaviors. If the interaction between those spins is attractive, the atoms will try to occupy the smallest possible space, with only the Pauli’s exclusion principle applied to atoms of the single-spin isotope preventing the collapse of the ensemble. We can see an example of this in figure 3, where 24 atoms are confined in only three lattice sites. On the other hand, if we have a set of repulsive spins interacting attractively with the atoms of the other isotope, other states are possible. In particular, for some values of the parameters defining the nature of the cluster, we can have two sets of particles within a single lattice well for several consecutive sites (see figure 4). That number of atoms is larger than the one for a 12 + 12 cluster defined by the same parameters (see figure 2). This difference is due to the relaxing of the constraints due to Pauli’s exclusion principle. Two undistinguishable fermions cannot be on top of each other, but two distinguishable fermions can, even though the probability of that happening depends on the value of the \( g_{1D} \) repulsive parameter [45]. That effect is added to the tendency to form more compact clusters already displayed in SU(2)-like arrangements. All of this makes possible the existence of a crossover between metallic and insulator clusters.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

M C Gordillo © https://orcid.org/0000-0003-1521-483X

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