One-dimensional SU($N$) clusters of fermions in optical lattices

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Abstract
The behaviour of fermion clusters with SU($N$) symmetry loaded in one-dimensional optical lattices and described by continuous Hamiltonians was studied using a diffusion Monte Carlo (DMC) technique. The state diagrams of SU(6) and SU(2) arrangements with the same number of particles were calculated and found virtually identical. The only difference was the absence of a band insulator in the SU($N$) case in the range of optical lattice depths considered ($V_0 = 0–12 E_R$; $E_R$, recoil energy of the lattice) in the non-interacting limit for $N > 2$. The appearance of that state was signalled by a noticeable change in the shape of the momentum distributions in going from a metal to a band insulator.

1. Introduction
The majority of the studies of ultracold bosons or fermions harmonically confined or loaded in optical lattices have been devoted to alkali metal atoms [1]. In the case of fermions, this means mainly systems with SU(2) symmetry, as $^4$Li or $^{40}$K. Nevertheless, other options are possible [2] for example, alkali-earth species, as $^{87}$Sr, or atoms that behave in a similar way, as $^{173}$Yb. Both are fermions with a maximum of ten or six spin states, respectively. This implies SU($N$) symmetries, with $N$ either 10 or 6, with characteristic behaviours depending on their lack of hyperfine structure. However, the total number of states can be reduced simply by not populating the highest spin levels. $^{173}$Yb atoms have been harmonically confined forming one-dimensional (1D) SU(6) clusters [3], and loaded in three-dimensional optical lattices, alone [4, 5], in mixtures with other SU(2) fermions [6, 7], or with bosons [8]. $^{87}$Sr SU(10)-symmetry sets of atoms can also be loaded in optical lattices [9].

In general, SU($N$) systems present enhanced atom correlations with respect to their SU(2) counterparts, a characteristic that is exacerbated in 1D-arrangements. That circumstance makes their descriptions by mean-field techniques not very accurate [3]. In this work, we will be concerned with 1D-clusters of SU($N$) atoms loaded in optical lattices. Those systems were traditionally described by the discrete Hubbard model, in which the atoms are confined to the absolute minima of the laser-induced potential wells. This approximation, even though computationally very efficient, is known to break down for shallow optical lattices, both for bosons [10] and fermions [11]. Another possibility is to use the Heisenberg model, also a discrete approximation. However, this is only valid in the limit of infinitely repulsive spin-spin interactions [2].

We will remove that approximation by considering continuous Hamiltonians, whose associate Schrödinger equations were solved using a diffusion Monte Carlo (DMC) technique, that takes correlations into account. The basic idea is to study the differences in the behaviour of SU(6) and SU(2) clusters all other things (such as interaction parameters and total number of atoms) being equal. In line with previous works on SU(2) clusters [12–16], we write the Hamiltonian as:

$$H = \sum_{i=1}^{N_s} \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} m \omega^2 x_i^2 + V_{ext}(x_i) \right] + g_{1D} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} \sum_{i=1}^{N_s} \sum_{j=1}^{N_s} \delta(x_i^\alpha - x_j^\beta).$$

(1)

Here, $N$ is the number of spin species. All atoms involved were considered to have the same mass, $m$, and the interaction strength between particles of spin $\alpha$ and $\beta$, with $\alpha \neq \beta$, was also fixed to $g_{1D} = -2\hbar^2/m a_{1D}$ for all possible pairs of atoms. $N_s$ stands for the total number of particles. We considered only balanced clusters, i.e. $N_\alpha = N N_{\alpha}$, with $N_{\alpha}$ the number of atoms with spin of type $\alpha$. $a_{1D}$ is the one-dimensional scattering length, that
can be derived from its three-dimensional s-wave counterpart [17] using the prescription in [18], and varied using a confined-induced resonance (CIR). The particularities of species with SU(N) symmetry make its modification by magnetic fields impossible and by optical techniques problematic due to three-body losses [2]. Thus, we kept to the repulsive-type interaction imposed by the positive sign of \(a_{1D} \) in the SU(6) \(^{173}\)Yb manifold [17] that we try to model.

In the Hamiltonian of equation (1), \(V_{\text{ext}} \) represents the 1D optical lattice potential:

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

with \(\lambda\) the wavelength of the lasers creating the standing optical wave \([1]\), and \(V_0\) the depth of the lattice potential. This magnitude will be given in units of the so-called recoil energy, \(E_R = \hbar^2 / 2m\lambda^2\). In addition, the clusters were longitudinally confined by an harmonic oscillator potential, as in most experimental setups \([1]\). All distances will be given in units of that oscillator length, \(\sigma = \sqrt{\hbar / m\omega}\), while the unit for the total energy of the clusters will be \(\hbar\omega\), with \(\omega\) the oscillator frequency. In this work, we will consider only the case \(\lambda = \sigma\), for which \(E_R = 2\pi^2/\hbar\omega\).

In those lattices, the distance between potential minima is \(\lambda/2\). This values of \(\lambda\) and \(\sigma\) were chosen to conform to experimental data. For instance, from the experimental oscillator frequencies of in \([3]\), \(\sigma\) can be calculated to be in the range 760–1000 nm (see supplementary information of that work). Since the wavelength of the laser used to create the array of 1D tubes was \(\lambda = 759\) nm, we have \(\sigma = \lambda - 1.3\lambda\). In the three-dimensional lattice of \([5]\), \(\sigma \sim 1.2\lambda\).

In this work, we will try to study the differences in behaviour of clusters with the same number of fermions but for two different values of \(N\). Our main goal will be to characterize the stability ranges of all the possible states of the clusters, i.e. metals, band insulators and Mott insulators. To do so, we calculated different magnitudes using the diffusion Monte Carlo technique described in section 2. With all those data, we constructed the state diagram of \(N_p = 18\) clusters, characterizing the properties of the possible cluster states in section 3, with section 4 covering the main conclusions of this work.

\section*{2. Method}

As mentioned above, to solve the Schrödinger equation derived from the Hamiltonian in equation (1) we resorted to the diffusion Monte Carlo (DMC) method. This is an stochastic technique that allows us to obtain the exact energy for the ground state for a system of bosons or for a set of fermions for which the nodes of the exact many-body wavefunction describing them are known \([19]\). Fortunately, even though this is not generally the case, in strictly 1D systems we can have nodal points only when two particles of the same species are at the same position, i.e. when \(\langle x_i\alpha - x_j\beta \rangle = 0\) \([20]\), providing that the repulsive interactions between particles of different spins are finite. Thus, the inclusion of that prescription in the initial approximation to the real wavefunction (the so-called trial function) needed in the DMC algorithm produces the exact ground state energy for a 1D cluster of fermions. With that in mind, we chose:

\[
\Phi(x_0,\ldots,x_N) = \prod_{\alpha=1}^{N} D^{\alpha} \prod_{i}^{N_\sigma} \prod_{j}^{N_\sigma} \psi(x_i^\alpha - x_j^\beta),
\]

where the Slater determinant \(D^{\alpha}\) contains the lowest \(N_\sigma\) eigenvectors of the Hamiltonian in equation (1) including the harmonic and optical lattice potentials \([13–15]\) for the case in which \(N_p = 1\). That set of determinants assures us that this trial function has the nodes in the right positions, therefore the energy obtained will be the exact one within the statistical uncertainties associated to the method. The remaining part of equation (3) considers the correlation between unlike-spin particles via the Jastrow term: \([12–15,21]\),

\[
\psi(x_i^\alpha - x_j^\beta) = \begin{cases} \cos(k|\langle x_i^\alpha - x_j^\beta \rangle - R_m|) & |\langle x_i^\alpha - x_j^\beta \rangle > R_m \\ 1 & |\langle x_i^\alpha - x_j^\beta \rangle \leq R_m \end{cases}
\]

Here, \(R_m\) is a variationally optimized parameter, while \(k\) is obtained by solving:

\[
k a_{1D} \tan(k R_m) = 1,
\]

for each value of \(a_{1D}\) \([21]\). This form of the interspecies wavefunction assures that in the \(g_{1D} \to \infty\) limit there is a node for the case \(\langle x_i^\alpha - x_j^\beta \rangle = 0\), as it corresponds to a Tonks–Girardeau gas \([22]\).

To describe the different states (phases are not possible since clusters are finite systems), we will use the density profiles, the occupancies of each minimum of the optical lattice potential and the momentum distributions, \(n_i(k)\). Those correlation functions and the momentum distributions can be experimentally obtained \([3]\). \(n_i(k)\) is the Fourier transform of the one-body density matrix, \(\rho_i(x_i\alpha, x'_i\alpha)\), and can be defined for each spin species as:
that in a cluster depends on both $x_α$ and $x'_α$ and not only on the relative distance between them, as in an non-confined system. Here, $Ψ(x_1, ..., x_N)$ represents the ground state wavefunction of the cluster, as sampled in the DMC method.

3. Results

Our main goal in this work is to compute the state diagram of clusters with the same number of particles and different symmetries. To do so, we compared the cases $N = 2$ and $N = 6$ for $N_p = 18$, similar or larger than the one used in previous calculations that considered continuous Hamiltonians \[16, 23, 24\]. In a previous work in SU($2$) clusters with smaller number of particles \[14\], it was established that the only possible states for balanced clusters were metals, and Mott and band insulators. To distinguish one from the others, we have first to calculate the particle population, $n_i$, at each optical lattice potential well $i$. To do so, we used the expression \[25\]:

$$n_i(k) = \frac{1}{2\pi} \int dx dx' \rho_k(x_α, x'_α) \exp[-ik(x_α - x'_α)]$$

with

$$\rho_k(x_α, x'_α) = N_α \times \int dx_2 ... dx_N \; Ψ(x_1, ..., x_N) \; Ψ(x'_1, ..., x'_N),$$

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$$n_i = \int_{x_i-\lambda/4}^{x_i+\lambda/4} \rho(x) \, dx.$$

Here, $\rho(x)$ is the particle density around a potential minimum whose center is at coordinate $x_i$. We displayed several examples of those magnitudes in figure 1. We assigned the position and label ‘0’ to the central minimum of the cluster, and the values for all other wells were deduced accordingly. Both $\rho(x)$ and $n_i$ are calculated using all the particles in the cluster, without distinctions based on their spin type.

From those atom populations, we can calculate the local compressibility, $κ_i$, from \[25, 26\]:

$$κ_i = \frac{\partial n_i}{\partial n'_i}.$$
of those cases, corresponding to κi will allow us to distinguish between metals and insulators. We consider a cluster to be in an insulating state when there is a set of at least three consecutive sites for which \( \kappa_i = 0 \) [25]. According to equation (11), this means an array of sites for which the population is the same. That set of sites would constitute an insulating domain. The cases corresponding to \( N = 2 \), \( V_0 = 3E_R \) and \( g_{1D} = 30\hbar\omega\sigma \) and \( N = 6 \) for the same parameters shown in figure 1 are then insulators, since there are several sites at the center of the cluster for which \( n_i = 1 \). Note that this does not necessarily mean that the particle density in the maxima of the potential wells is zero, as it can be seen for the insulator example in the upper part of figure 1. In addition, due to the finite size of those arrangements, those insulating domains do not comprise the whole cluster; there are always sites for which \( \kappa_i \neq 0 \). In the examples shown, those sites conform a couple of metallic ‘wings’ at the outer part of the clusters.

When the populations in the insulator domain are equal to one, we have a Mott insulator; if there are equal to two (or to \( N \) in SU(N) clusters) we have band insulators. If there is no set of adjacent sites with equal integer populations, we label the entire cluster as a metal. For instance, the cases with \( N = 2 \), \( V_0 = E_R \) and \( g_{1D} = 30\hbar\omega\sigma \) and \( N = 6 \), \( V_0 = 3E_R \) and \( g_{1D} = 5\hbar\omega\sigma \) displayed in figure 1 correspond to metals. In this figure, we can see also that the population profiles of an SU(2) cluster are wider than the corresponding to a SU(N) arrangement with the same parameters, in accordance with experimental data for three-dimensional optical lattices [4, 5]. This is a direct consequence of Pauli’s exclusion principle. For finite values of the \( g_{1D} \) parameter, the number of spin pairs that cannot share the same \( x \) coordinate decreases with \( N \): 72 for a SU(2) cluster with \( N_p = 18 \) (9 \( \times \) 8/2 spin-up spin-up pairs plus the same number of spin-down spin-down couplings) to 18 for a SU(6) set of particles (3 same-spin pairs multiplied by the number of spin types). This means that the average distance between any pair of atoms is larger in the SU(2) case, widening both the particle density and population profiles.

Using the density and population profiles, we can establish the state diagram for a cluster of \( N_p = 18 \) particles. The results are displayed in figure 2. We can see that in the limits between the metal and the band insulator in the \( N = 2 \) case. No such limit exists for SU(6) clusters.

Here, \( \mu_i \) is the local chemical potential, defined as [26]:

\[
\mu_i = \mu - \frac{1}{2} m \omega^2 x_i^2,
\]

where \( \mu \) is the total chemical potential of the cluster. The combination of those two equations gives us:

\[
\kappa_i = - \frac{1}{m \omega^2 x_i} \frac{\partial n_i}{\partial \kappa_i}.
\]

The values of \( \kappa_i \) will allow us to distinguish between metals and insulators. We consider a cluster to be in an insulating state when there is a set of at least three consecutive sites for which \( \kappa_i = 0 \) [25]. According to equation (11), this means an array of sites for which the population is the same. That set of sites would constitute an insulating domain. The cases corresponding to \( N = 2 \), \( V_0 = 3E_R \) and \( g_{1D} = 30\hbar\omega\sigma \) and \( N = 6 \) for the same parameters shown in figure 1 are then insulators, since there are several sites at the center of the cluster for which \( n_i = 1 \). Note that this does not necessarily mean that the particle density in the maxima of the potential wells is zero, as it can be seen for the insulator example in the upper part of figure 1. In addition, due to the finite size of those arrangements, those insulating domains do not comprise the whole cluster; there are always sites for which \( \kappa_i \neq 0 \). In the examples shown, those sites conform a couple of metallic ‘wings’ at the outer part of the clusters.

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Using the density and population profiles, we can establish the state diagram for a cluster of \( N_p = 18 \) particles. The results are displayed in figure 2. We can see that in the limits between the metal and the Mott insulator are virtually equal to each other when we take into account the error bars, similar in both cases, and only shown in the SU(2) cluster. The only difference between those state diagrams is the existence of a band insulator limit for \( V_0 = 8E_R \) only present in the SU(2) arrangement. That band insulator appear only for low values of the \( g_{1D} \) interaction parameter, as seen in smaller balanced clusters [14].

As indicated above, clusters are band insulators when there is a domain of consecutive optical lattice sites for which \( n_i \) is an integer different from one. In the lower panel of figure 3 we can see the population profiles for two of those cases, corresponding to \( V_0 = 10E_R \) and \( V_0 = 12E_R \) for SU(2) arrangements, with \( g_{1D} = 0 \). The remaining population profiles correspond to metals. Apart from the number of atoms in each lattice site, there is
an additional difference between Mott insulators and band insulators, at least for the systems under study: in the last case, the particle density (an example of which is given in figure 4) at the maxima of the local lattice potential is very close to zero, something that does not happen for a Mott insulator.

The upper part of the figure 3 allow us to characterize the crossover between those regimes using the momentum distributions. Those \( n(k) \)'s are the averages of all the \( n_{\alpha}(k) \) functions corresponding to the \( N \) spin types of the cluster. As we can see, there is a noticeable change for \( k \)-vectors around \( 6\sigma^{-1} \). This corresponds to a distance between particles of \( 2\pi/k \sim \sigma \), i.e. twice as much the separation between potential minima in the 1D

**Figure 3.** Upper panel: Momentum distributions for non-interacting \((g_{1D} = 0)\) SU(2) systems for different values of the optical potential depths. Lower panel: Population distributions for the same systems displayed above. The error bars are of the size of the symbols and not shown. Full squares: \( V_0 = 0 \); open circles, \( V_0 = 2\) \( \hbar \omega \); full circles, \( V_0 = 4\) \( \hbar \omega \); open triangles, \( V_0 = 10\) \( \hbar \omega \); full triangles, \( V_0 = 12\) \( \hbar \omega \). Those last two cases are band insulators. The momentum distributions are normalized to one.

**Figure 4.** Particle density, \( \rho(x) \), for the same Mott insulator SU(2) cluster already displayed in figure 1 (dashed line; \( N_p = 18 \), \( V_0 = 3\) \( \hbar \omega \), \( g_{1D} = 30\) \( \hbar \omega \) \( \sigma \) ), and for an band insulator SU(2) arrangement (full line; \( N_p = 18 \), \( V_0 = 10\) \( \hbar \omega \), \( g_{1D} = 0 \) ).
optical lattice. For $V_0$ values smaller than $8E_R$, $n(6\sigma^{-1}) \sim 0$, while for deeper potential wells, $n(6\sigma^{-1}) > 0$. This implies a correlation between atoms located at next-to-nearest neighbour minima. On the other hand, the maxima in the $n(k)$’s for $k > 8\sigma^{-1}$ are related to the distances between consecutive lattice sites ($0.5\lambda$), being absent in the $V_0 = 0$ case. That separation between the closest minima of the optical lattice potential corresponds to $k = 4\pi \sigma^{-1} \sim 12.57\sigma^{-1}$. The reason there is not a single peak but a broad band is because the atoms are not located exactly at the center of the lattice potential, as can be seen in the upper panel of figure 1. So, for small values of $g_{1D}$, a band insulator appears when there are correlations in the position of fermions located at the nearest and next-to-nearest lattice sites. If the last one is absent, we have a metal.

In addition, the momentum distributions for small values of $k (k < 6\sigma^{-1})$ are also different from metals and band insulators: while the first present as many peaks as the number of atoms of the species (nine in this case, considering $k$ and $-k$ values, those last ones not shown), the band insulator $n(k)$’s are smeared out. This is due to the introduction of effective correlations between atoms located in lattice sites further away from next-to-nearest neighbours. For instance, there is a local maximum in the $n(k)$ function for $V_0 = 10E_R$ at a $k$ vector around $\pi \sigma^{-1}$, corresponding to a distance $\sim 2\sigma$. However, the differences between the Mott insulator and band insulator momentum distributions functions displayed in figures 3 and 6, suggest that the optical lattice induced correlation only shows up when it completely overcomes the corresponding to the intrinsic atom-atom interaction characteristic of an harmonically confined cluster, i.e. when the particle density at the maxima of the optical lattice is approximately zero. To see that this is actually what happens, we display the particle densities for a Mott SU(2) insulator and a band SU(6) insulator in figure 4.

To prove that the differences in the momentum distributions are due to a metal-insulator crossover, we show in figure 5 exactly the same data as in figure 3 but for SU(6) clusters. The population distributions shown in the lower panel are those of metals, since we cannot see any consecutive set of sites with the exactly the same $n_i$. As before, the normalized momentum distributions are displayed in the upper part of the figure. In those, for all values of $V_0 = 0$, we observe the same band related to nearest neighbour correlations. The structure with three perfectly defined maxima (including the negative values not shown) for small values of $k$ is also seen. However, contrarily to what happens for the SU(2) clusters, no smeared out of the $n(k)$’s with increasing $V_0$ is found. In addition, $n(k) \sim 0$ for $k \sim 6\sigma^{-1}$. This means that in SU(6) clusters there is no crossover from a metal to a band insulator, at least in the range of optical potential wells considered.

The band insulator states appear only when the unlike-spin interaction parameters is small or even zero. When $g_{1D} > 0$, an increase in $V_0$ makes the metal clusters turn into a Mott insulator [14, 15]. Figure 6 addresses the change in the $n(k)$’s when that happens. It is well established that the momentum distribution tails of harmonically confined clusters for $g_{1D} > 0$ are fatter than for non-interacting clusters [16, 23, 24], something...
that has been experimentally proven [3]. The harmonically trapped cases would correspond to the limit \( V_0 = 0 \) in figure 2, being therefore metals. According to that same figure, all the clusters considered in this work for which \( V_0 < 3E_R \) are also metals, irrespectively of their \( g_{1D} \) and \( N \) values. On the other hand, their momentum distributions, shown in figure 6 for \( g_{1D} = 30\hbar\omega \sigma \), are similar to those of harmonically confined clusters, i.e. they decrease monotonically with \( k \), for \( k > 4\sigma^{-1} \). They have also the \( N_{\alpha} \) maxima in the region low \( k \)-vectors that can also be seen in the previous figures for the \( g_{1D} = 0 \) case. The only difference between the metal and Mott insulator \( n(k) \)'s is displayed in the inset of figure 6: there is a small maxima in the region \( k > 10-12\sigma^{-1} \), corresponding approximately to the distance between consecutive minima of the optical lattice potential. That feature shows up above the fat tail due to unlike-spin repulsion. No specific trace of the next-to-nearest neighbour correlation characteristic of the band insulator in shown.

4. Discussion

In this work we have established that the state diagram of a set of atoms loaded in a one-dimensional optical lattice depends basically on the total number of atoms, \( N_p \), and not on the number of spin species, \( N \). The only feature for which there is an appreciable difference for SU(2) and SU(6) clusters is the appearance of a band insulator in the first case and not in the second. This can be easily understood using an extension of the findings of [14]: for a SU(\( N \)) cluster of \( N_p \) particles to be a band insulator, an associated SU(1) arrangement with \( N_p/N \) particles has to be an insulator. The state diagram for SU(1) arrangements with different number of particles and \( V_0 < 14E_R \) is given in [14]. An inspection of that diagram indicates that for \( V_0 = 12E_R \) (the maximum well depth considered in this work), the minimum number of particles for a cluster of identical fermions to be an insulator is 6. Smaller arrangements are metals. In our clusters, the \( N_p/N \) ratios are 9 and 3, for SU(2) and SU(6) symmetries. This means that a SU(6) cluster with 18 particles cannot be a band insulator. On the other hand, to have a Mott insulator in the limit \( g_{1D} \rightarrow \infty \), a SU(1) cluster of \( N_p \) particles has again to be an insulator. For \( N_p = 18 \), this means \( V_0 \geq 3E_R \) [14]. This condition depends on the total number of particles, and not on \( N \). This is exactly what we can see in the state diagram of figure 2.

Figures 3 and 6 display how the introduction of correlations due to the presence of an optical lattice or to the crossover to an insulator state change the momentum distributions. Those variations are interesting since they can be measured experimentally by time-of-flight absorption imaging [3]. As indicated above, the correlation between nearest neighbours shows up as a band around a \( k \) vector corresponding to the inverse of the distance between potential minima (0.5\( \sigma \)). However, for metallic clusters, this band is washed out when the repulsive interaction is large enough, only to reappear when a Mott insulator is formed, as it can be seen in figure 6. Mott insulators can also be identified from density profiles obtained by different spectroscopic techniques [4, 5].

On the other hand, in the limit of non-interacting fermions, the appearance of a band insulator is related to correlations between spins on next-to-nearest neighbour optical lattice sites. This means that the \( n(k) \)'s changes from \( \sim 0 \) to \( > 0 \) for \( k \sim 6\sigma^{-1} \). However, the increasing in the \( g_{1D} \) interaction parameter also makes this feature disappear.

**Figure 6.** Momentum distributions for SU(2) and SU(6) clusters for two values of the optical potential well and a common interaction parameter of \( g_{1D} = 30\hbar\omega \sigma \). Inset: Same as in the main figure but for a restricted range of \( k \) vectors.
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