Three and Four Harmonically Trapped Particles 
in an Effective Field Theory Framework

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Abstract

We study systems of few two-component fermions interacting via short-range interactions within a harmonic-oscillator trap. The dominant interactions, which are two-body, are organized according to the number of derivatives and defined in a two-body truncated model space made from a bound-state basis. Leading-order (LO) interactions are solved for exactly using the formalism of the No-Core Shell Model, whereas corrections are treated as many-body perturbations. We show explicitly that next-to-LO and next-to-next-to-LO interactions improve convergence as the model space increases. We present results at unitarity for three- and four-fermion systems, which show excellent agreement with the exact solution (for the three-body problem) and results obtained by others methods (in the four-body case). We also present results for finite scattering lengths and non-zero range of the interaction, including (at positive scattering length) observation of a change in the structure of the three-body ground state and extraction of the atom-dimer scattering length.

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The details of an interparticle potential of finite range $R$ are largely irrelevant in few-body systems when the two-body scattering length $a_2 \gg R$. This feature, which is referred to as universality, and its associated simplicity make such systems fertile testing ground for methods designed to tackle larger ones. While the measured two-nucleon scattering length happens to be large compared to the inverse of the pion mass, use of magnetic fields to create Feshbach resonances in cold, trapped atomic systems has opened up the possibility of dialing two-atom scattering lengths to values much larger than the typical range of the van der Waals potential. A recent ground-breaking achievement \cite{1} is the ability to further confine just a few atoms in nearly isolated sites of optical lattices formed by laser beams. At low temperatures, the lattice sites may be considered as harmonic oscillator (HO) traps. As long as the HO length $b$ is large, $b \gg R$, a trapped system still displays universal properties, although for $b \lesssim a_2$ these are rather different from those in a large trap or free space.

At sufficiently low energies, an effective field theory (EFT) has been formulated which uses the separation between the scales $a_2$ and $R$ to build an expansion in powers of $R/a_2$ \cite{2-4}. It replaces the underlying interparticle potential by a series of contact interactions with increasing numbers of derivatives of delta functions, akin to the multipole expansion in classical electrodynamics. Except for isospin, which does play a role in the relative relevance of few-body forces, the version of this EFT used in nuclear physics \cite{5} is formally indistinguishable from the one describing atomic systems \cite{6}. (Nevertheless, the underlying theories for the two cases are very different.)

As a consequence, atomic systems characterized by large scattering lengths can be studied with techniques developed in nuclear physics and, conversely, can provide tests for few- and many-body methods that can be further applied, with little or no change, to the description of nuclear systems at low energies. One such method is the No-Core Shell Model (NCSM), in which the solution to the non-relativistic Schrödinger equation for many-nucleon systems is obtained by numerical diagonalization using a discrete single-particle basis, typically a HO basis \cite{7}. This method is characterized by its flexibility, being able to reach medium-mass nuclei with no limitation to closed or nearly-closed shells and, at the same time, handle local and non-local interactions on the same footing. The cost of diagonalization is controlled by restriction to a “model space” with a maximum number $N_{\text{max}}$ of accessible shells above the minimum configuration. The NCSM is well suited to handle EFT interactions \cite{8}, which are in general non-local (in the sense of involving momenta) and always defined up to a maximum momentum $\Lambda$, the ultraviolet (UV) cutoff.

In Ref. \cite{9}, we formulated an EFT for two particles that support $S$-wave interactions with $a_2 \gg R$ in a HO trap of length $b \gg R$. The EFT interactions are defined within a model space with cutoff $\Lambda = \sqrt{2N_{\text{max}}} + 3/b$. We considered explicitly the first three orders in the expansion, up to which point only the $S$ wave is modified by the short-range potential. In leading order (LO), there exists only one, non-derivative contact interaction, which captures the physics of the scattering length and thus reproduces the results \cite{10} obtained with a pseudopotential \cite{11}. Subleading orders involve derivatives of contact interactions treated in perturbation theory. The next-to-leading-order (NLO) and next-to-next-to-leading-order (NNLO) corrections account for the physics of the effective range $r_2$ and lead to generalized pseudopotential results \cite{12-14}. Higher orders can be calculated similarly. We showed how convergence of the theory as function of $N_{\text{max}}$ can be improved systematically, and is in fact better than for an exact diagonalization of subleading orders.
In this paper we discuss systems of three and four two-state fermions in a trap. For these fermions, which we can think of as having spin \( s = 1/2 \), the approach of Ref. [9] applies and we again consider explicitly the EFT to NNLO. Thanks to the Pauli principle, three- and higher-body interactions appear only at higher orders [15], so the properties of few-body systems can be predicted. At LO, we solve the few-body problem using the NCSM formalism, as done before [16]. Beyond LO, we employ many-body perturbation theory.

A critical aspect is the use of different values of the model-space cutoff for systems with different number of particles, which leads to improved convergence. This is because the spectator particles in a many-body system can carry some of the excitation energy, leaving less available to an interacting pair. If the two-body and many-body spaces are cut off at the same number of quanta, some states of the two-body system will simply be omitted from the many-body space without their effects being taken into account by renormalization. One way to avoid this is to use a cutoff for the space where the many-body system is solved that is higher than that in the two-body subsystem where the two-body interaction was defined. A related approach, in which the two-body cutoff is taken to depend on the state of the spectators, was originally considered within the NCSM formalism in Ref. [17], but it was later abandoned in favor of the simpler approach with equal cutoffs.

We calculate the lowest levels of the three- and four-fermion systems allowing for finite values of both \( a_2 \) and \( r_2 \). At unitarity, our three-fermion results converge to the semi-analytical values of Ref. [18]. Our improved convergence allows to better pinpoint the scattering length at which the ground-state parity changes, a phenomenon first identified in Ref. [16] and subsequently confirmed [19]. We also investigate atom-dimer scattering and compare with Ref. [20]. In the case of four fermions, we find a ground-state energy similar to values in the literature [21–23], and give an example of an excited level. Systems with larger numbers of fermions can be dealt with at the expense of more computer time.

Our approach has similarities to the one followed in Ref. [21], where an effective short-range interaction is fitted to several levels of the pseudopotential at unitarity, but diagonalized exactly. To the extent that they are model-independent, results from finite-range potentials [12] should be equivalent to ours.

The paper is organized as follows. In Sec. II we first briefly recall how interactions are generated using EFT and then outline their solution in the NCSM formalism. In the following section, Sec. III we show results for three and four fermions. We conclude and discuss future applications in Sec. IV.

### II. FORMALISM

We consider a non-relativistic system of \( A \) fermions of spin \( s = 1/2 \) and mass \( m \) in a HO trap of frequency \( \omega \). The HO potential can be decomposed into two pieces, one acting on the center of mass (CM) of the \( A \) particles and one on their relative coordinates. We denote by \( \vec{r}_i \) (\( \vec{p}_i \)) the position (momentum) of particle \( i \) with respect to the origin of the HO potential. The Hamiltonian describing the relative motion of the particles is given by

\[
H = H_0 + \sum_{i<j} V_{ij} + \ldots,
\]

with

\[
H_0 = \frac{1}{2mA} \sum_{i<j} (\vec{p}_i - \vec{p}_j)^2 + \frac{m\omega^2}{2A} \sum_{i<j} (\vec{r}_i - \vec{r}_j)^2, \tag{2}
\]
$V_{ij}$ being the two-fermion interaction, and “…” denoting three- and more-body interactions. In the following, the zero-point of the energy scale is such that the CM motion in the trap is omitted.

The HO introduces an energy scale $\omega$, or equivalently a length scale, the HO length

$$b = \sqrt{\frac{2}{m\omega}}. \hspace{1cm} (3)$$

We are interested in systems where $b \gg R$, the range of the force between the particles. We discuss in this section the construction and solution of $V_{ij}$ for few-particle systems.

A. Construction of the interaction using EFT

The interactions are constructed using EFT for the trapped few-fermion system. In free space the two-body interaction can be characterized by its scattering phase shifts. For small enough values of the on-shell momentum, $k \ll 1/R$, the phase shifts can be described by the Effective Range Expansion (ERE) [24]. Potentials that generate the same values for the ERE parameters cannot be distinguished at low energies: they all lead to the same wavefunction for distances beyond the range of the force, $r > R$. This universality can be made manifest by taking, instead of a specific finite-range potential, an interaction expanded as a Taylor series in momentum space.

For two-state fermions, we can use the results of Ref. [9], as long as we interpret the $\sum_{i \neq j} V_{ij}$ in Eq. (1) as a sum over pairs of particles in different states. In this case, an $S$-wave interaction is allowed and dominates. In the CM of the two fermions, and expressed in terms of relative coordinates, the interactions considered in this paper are

$$V(\mathbf{r}', \mathbf{r}) = C_0 \delta(\mathbf{r}') \delta(\mathbf{r}) - C_2 \left\{ \left[ \nabla^2 \delta(\mathbf{r}') \right] \delta(\mathbf{r}) + \delta(\mathbf{r}') \left[ \nabla^2 \delta(\mathbf{r}) \right] \right\} + C_4 \left\{ \left[ \nabla^4 \delta(\mathbf{r}') \right] \delta(\mathbf{r}) + \delta(\mathbf{r}') \left[ \nabla^4 \delta(\mathbf{r}) \right] + 2 \left[ \nabla^2 \delta(\mathbf{r}') \right] \left[ \nabla^2 \delta(\mathbf{r}) \right] \right\} + \ldots, \hspace{1cm} (4)$$

where $C_0$, $C_2$, and $C_4$ are parameters and “…” denote terms of higher orders. Since these interactions are singular, a regularization procedure is introduced in form of a UV cutoff $\Lambda$. This separates the short-distance physics, which is not included explicitly in the dynamics of this problem at low energy, and the long-distance physics, which is. In order for observables to be renormalization-group invariant, i.e. independent of the arbitrary cutoff, the parameters $C_i$ must depend on $\Lambda$.

The HO provides a natural basis on which to expand wavefunctions: its eigenfunctions $\phi_{nl}$, which can be labeled by the quantum numbers $n$ (radial) and $l$ (orbital), have energies $(N_2 + 3/2)\omega$, with

$$N_2 = 2n + l. \hspace{1cm} (5)$$

The HO basis in turn offers a natural cutoff in the form of a maximum number of shells included in the basis: there exists a maximum relative momentum

$$\Lambda = \frac{\sqrt{2}}{b} \sqrt{N_{2,\text{max}}^2 + 3/2},$$

with $N_{2,\text{max}}$ the number of quanta of the highest energy state in the basis. The wavefunction of the interacting system is a superposition of HO eigenfunctions within the model space, determined by a solution of the Schrödinger equation with the potential [4].
In the case we are interested in, $a_2 \gg R$, $S$-wave interactions are enhanced by powers of $a_2$ over their natural size $R$. The LO interaction is the $C_0$ term in the potential, which represents the physics of the scattering length $a_2$. The other terms are corrections, in particular $C_2$ at NLO and $C_4$ at NNLO, both of which contain the effective range $r_2$. Higher $S$-wave ERE terms and interactions in higher partial waves appear only beyond NNLO. To NNLO, then, the energies of the interacting system in waves with $l \geq 1$ are not changed relative to the HO energies.

For $l = 0$, on the other hand, the two-body energies $E_{2,n}$ are determined from the solution of the Schrödinger equation with a superposition of HO wavefunctions up to a maximum $N_{2,\text{max}} = 2n_{\text{max}}$, where $n_{\text{max}}$ is the largest radial quantum number carried by states in the two-body basis. The solution at LO is obtained by an exact diagonalization considering only the $C_0$ term in the potential. The parameter $C_0(N_{2,\text{max}})$ is fixed by imposing that one known energy, which we take as the ground-state energy, be reproduced at any $N_{2,\text{max}}$. At NLO, the $C_2$ term is included in first-order perturbation theory and $C_2(N_{2,\text{max}})$ is fitted to a second known energy, which we take as the first-excited-state energy. At NNLO, $C_2$ is treated in second-order perturbation theory while the $C_4$ term is included in first-order perturbation theory, $C_4(N_{2,\text{max}})$ being fitted to a third level, which we take as the second-excited-state energy.

The energies used as input are the exact two-body energies in the limit $N_{2,\text{max}} \to \infty$. These energies can be found by solving a simple transcendental equation involving the ERE parameters:

$$\frac{\Gamma(3/4 - E_{2,n}/2\omega)}{\Gamma(1/4 - E_{2,n}/2\omega)} = \frac{b}{2a_2} - \frac{r_2 E_{2,n}}{2b^2 \omega} + \ldots$$

In LO, we include only the $a_2$ term; at NLO and NNLO, we include also $r_2$. The levels not used as input depend on $N_{2,\text{max}}$, and for $\Lambda \gtrsim 1/R$ they are predictions of the method. It can be shown that including more corrections to the potential improves the convergence to the exact solutions as the size of the model space increases. More details on the construction of the interactions can be found in Ref. [9].

In this way, the two-body interaction is determined at each $N_{2,\text{max}}$ from the ERE (i.e. scattering) parameters, and can be used as input into the calculation of $A \geq 3$ systems. In general, for the latter we also have to include few-body interactions. For two-state fermions, however, the Pauli principle requires three- and more-body contact interactions to involve derivatives, so that the extra fermions are placed in states with different orbital quantum numbers. The extra bodies and derivatives come with extra factors of $R$, and the corresponding interactions are suppressed [13]. To NNLO, no few-body interaction needs to be included here.

**B. Many-body basis and truncation**

With $V_{ij}$ so constructed, we can predict the energy levels of larger systems. We need to solve exactly for the LO potential, and then higher-order corrections are calculated in perturbation theory, just as in the two-particle case [9].

In a shell-model approach, energy eigenstates are obtained by direct diagonalization in a many-body basis constructed with HO wavefunctions. There are essentially two equivalent ways to construct the basis states. In one, the basis states are Slater determinants.
constructed from single-particle HO wavefunctions in the lab frame. This leads to the wave-function of the CM of the system factorizing exactly from the internal coordinates, as long as one performs an energy truncation of the basis states such that all states up to a given energy $N_{\text{max}}\omega$, $N_{\text{max}}$ being an integer, are included. While antisymmetry is easily built into this approach, the dimension of the basis space grows quickly. None-the-less, this method can be applied efficiently to systems of more than five particles. In the second approach, one considers states that depend only on internal (Jacobi) coordinates and the dependence of each of these is described by a HO wavefunction \cite{25}. For up to five particles, this is more effective than a Slater-determinant basis, but the antisymmetrization becomes increasingly difficult as the number of particles grows. As long as the same energy truncation is applied to both, the Slater-determinant and Jacobi bases give identical results for the intrinsic state of any system. Since in the current paper we investigate only systems with three and four particles, we describe in some detail the internal-coordinate approach. The novel truncation that we employ in the few-body system becomes more transparent in Jacobi coordinates.

We work with Jacobi coordinates defined in terms of differences between the CM positions of sub-clusters within the $A$-body system:

\begin{align*}
\vec{\xi}_1 &= \sqrt{\frac{1}{2}} (\vec{r}_1 - \vec{r}_2), \\
\vec{\xi}_2 &= \sqrt{\frac{2}{3}} \left[ \frac{1}{2} (\vec{r}_1 + \vec{r}_2) - \vec{r}_3 \right], \\
&\vdots \\
\vec{\xi}_{A-1} &= \sqrt{\frac{A-1}{A}} \left[ \frac{1}{A-1} (\vec{r}_1 + \vec{r}_2 + \cdots + \vec{r}_{A-1}) - \vec{r}_A \right].
\end{align*}

(8)

Using these, the HO Hamiltonian (2) can be expressed as

\begin{equation}
H_0 = \sum_{\rho=1}^{A-1} \left( \frac{p_{\vec{\xi}_\rho}^2}{2m} + \frac{m\omega^2}{2} \xi_\rho^2 \right),
\end{equation}

(9)

where $\vec{p}_{\vec{\xi}_\rho}$ is the momentum canonically conjugated to $\vec{\xi}_\rho$.

To illustrate the construction of the basis, let us consider three particles of spin $s$. In this case, two Jacobi coordinates $\vec{\xi}_1, \vec{\xi}_2$ are necessary to describe the internal motion. The basis states

\begin{equation}
A \left\{ \left[ \phi_{nl}(\vec{\xi}_1) \otimes \phi_{N\mathcal{L}}(\vec{\xi}_2) \right]_L | (ss)Ss; S \rangle \right\}
\end{equation}

(10)

have the spatial part constructed using HO wavefunctions with quantum numbers $n, l$ and $N, \mathcal{L}$ respectively, with the angular momentum coupled to $L$, while the spin part is constructed by coupling three spins $s$ to total spin $S$. In Eq. (10), $A$ stands for the operator that antisymmetrizes the three-particle wavefunction. If particles 1 and 2 are already described by an antisymmetric wavefunction, fulfilling the condition

\begin{equation}
(-1)^{s+l} = 1,
\end{equation}

(11)

then $A$ ensures the correct behavior of the three-body state under exchange of particles 1 or 2 and 3. The basis states thus constructed are eigenstates of the unperturbed Hamiltonian.
$H_0$ and the energy of each three-body state can be written as $(N_3 + 3)\omega$ where the quantum number $N_3$ is defined by

$$N_3 = 2n + l + 2N + \mathcal{L}.$$  

(12)

Details of the construction of a fully antisymmetrized basis from the states \([10]\), the calculation of two-body matrix elements of the interaction $V_{ij}$ in this basis, and the generalization to more particles and three-body forces can be found in Ref. \([25]\).

Because the NCSM is based on a direct numerical diagonalization, the basis must be truncated to a computationally tractable size. For a system of $A$ particles, the model space is truncated by introducing a cutoff $N_A^{\text{max}}$ defined as the largest number of quanta in the eigenstates of $H_0$ used to construct the $A$-body basis. Again using the three-body system as a concrete example, truncating the three-body basis at $N_3^{\text{max}}$ means keeping only states with HO energies such that $N_3 = 2n + l + 2N + \mathcal{L} \leq N_3^{\text{max}}$.

After the truncation of the many-body space, characterized by $N_A^{\text{max}}$, the natural question is what would be the consistent two-body interaction. Since the two-body interaction is defined in the two-body system, it is characterized by $N_2^{\text{max}}$. In the conventional NCSM approach, it is customary to choose the truncation in the two-body system so that the many-body space is the minimal required to include completely the two-body space. For example, if we consider just S-wave interactions, $N_2^{\text{max}} = N_3^{\text{max}}$ when one describes positive-parity states ($N_3^{\text{max}}$ has to be even), and $N_2^{\text{max}} = N_3^{\text{max}} - 1$ for negative-parity solutions ($N_3^{\text{max}}$ has to be odd). This was also the procedure used in Refs. \([8, 16]\).

However, one has to consider that the renormalization of the two-body system means that states lying above the cutoff $N_2^{\text{max}} = 2n_{\text{max}}$ have been “integrated out” rather than simply discarded. Their effects are thus included implicitly in the effective two-body interaction. When these two interacting particles are embedded in a system with a larger number of particles, the spectators will carry energies associated with the HO levels they occupy. For example, of the $(N_3 + 3)\omega$ total energy of one of the basis states \([10]\), $(2N + \mathcal{L} + 3/2)\omega$ is carried by the relative motion of the spectator. As a consequence, the maximum energy available to the two-body subsystem is smaller than that allowed by the $A$-body cutoff $N_A^{\text{max}}$ and some of the states removed by the truncation will not be accounted for by the renormalization. One way to correct for this is to use the interactions renormalized with a state-dependent two-body cutoff $N_2^{\text{max}} = N_3^{\text{max}} - (2N + \mathcal{L})$, as first suggested within an NCSM approach in Ref. \([17]\). However, the resulting state-dependent interaction is difficult to handle in Jacobi coordinates for systems with more than three particles, and cannot be incorporated in a Slater-determinant basis. In order to account for all the two-body physics beyond our cutoff without the use of such an interaction, we simply decouple the cutoff of the many-body problem from that of the subcluster defining any interaction. Such a prescription has some similarity to the truncation used in Ref. \([21]\).

Each of our calculations is characterized by two cutoff parameters: $N_2^{\text{max}}$ for the two-body subsystem, and $N_A^{\text{max}}$ for the few-body system. To the order we work, no three-body forces appear and so we do not need to consider a separate cutoff for renormalization of a three-body subsystem, when considering larger systems. Since to this order one has to include only S-wave interactions, $N_2^{\text{max}}$ is even, and $N_A^{\text{max}}$ is even (odd) for few-body states with even (odd) $\mathcal{L}$. Our final results are obtained by first increasing $N_A^{\text{max}}$ at fixed $N_2^{\text{max}}$ until they converge, and then increasing $N_2^{\text{max}}$. For two-body states with $N_2 > N_2^{\text{max}}$, we simply set the interaction matrix elements to zero. As we increase $N_A^{\text{max}}$ (at fixed $N_2^{\text{max}}$) from either $N_A^{\text{max}} = N_2^{\text{max}}$ or $N_A^{\text{max}} = N_2^{\text{max}} + 1$, we observe a rapid dependence on $N_A^{\text{max}}$. 

until it is somewhat larger than $N_{2}^\text{max}$, the difference reflecting the typical number of quanta carried by the spectators. For low-lying many-body states, further enlarging $N_{3}^\text{max}$ makes little difference because we are adding only two-body states where the two-body potential is switched off. Having achieved results for any observable of interest that are stable with respect to $N_{3}^\text{max}$ for each $N_{2}^\text{max}$, we can then take the limit of those values for large $N_{2}^\text{max}$. Examples are given next.

III. FEW FERMIONS: RESULTS

In this section we present explicit results for energies of systems made of a few two-state fermions in a harmonic trap. Our goal is to show convergence as we increase the UV cutoff, $N_{2}^\text{max}$, and its systematic improvement as the order in the EFT increases.

Nothing in our method is specifically tied to unitarity ($b/a_2 = 0$ and $r_2/b = 0$) and we can carry out calculations for finite scattering length, as well as finite range, as long as $a_2 \gg r_2$. We can in fact obtain the $b/a_2$ and $r_2/b$ dependences of any state, improving on the $r_2/b = 0$ results of Ref. [16] because of both the accelerated convergence stemming from subleading orders and the inclusion of the finite range of the interaction (which in the absence of $r_2$ arises from the truncation of the two-body space). In this first study of subleading orders we limit ourselves to three and four fermions, where we can more extensively confront existing results. Systems of more particles can be attacked with larger computer resources.

A. $A = 3$ system

We consider first a system composed of three fermions, which allows us to illustrate the basic ideas of the method. Before considering the more realistic cases of finite scattering length and small effective range, we start with the unitary case, where semi-analytical results exist [18]. The three-fermion spectrum offers an excellent testing ground for numerical approaches, including the LO considered in our previous publication [16] and other methods to construct effective interactions [21]. We also use three-body energies to show how scattering information can be extracted for trapped few-body systems.

1. Unitary case

The ground state of the three-fermion system at $b/a_2 = 0$ and $r_2/b = 0$ has $L = 1$ and negative parity. Figure 1 shows the convergence of the energy of this state with the size of the three-body model space, $N_{3}^\text{max}$, for two values of the UV cutoff in the two-body system, (a) $N_{2}^\text{max} = 10$ and (b) $N_{2}^\text{max} = 18$. For fixed $N_{2}^\text{max}$, the Hamiltonian does not change, so that one expects a variational behavior of the ground-state energy with increasing the three-body model space. Indeed, as shown in Fig. 1, the energy decreases until convergence is reached for a large enough three-body model space. The value of $N_{3}^\text{max}$ for which the convergence is obtained depends on the particular value of $N_{2}^\text{max}$. Thus, for $N_{2}^\text{max} = 10$ the energy of the three-body ground state (in LO and corrections) does not change by more than $10^{-4}$ once $N_{3}^\text{max} \geq 19$, while for $N_{2}^\text{max} = 18$ convergence at this level is achieved for $N_{3}^\text{max} \geq 31$.

Even though for fixed $N_{2}^\text{max}$ the errors induced by the three-body cutoff are eliminated, the errors induced by the truncation in the two-body sector, where the interaction is defined,
FIG. 1: Energy in units of the HO frequency, $E/\omega$, of the ground state $L^\pi = 1^-$ of the $A = 3$ system at unitarity, as function of the three-body model-space size, $N_3^{\text{max}}$: (a) $N_2^{\text{max}} = 10$; (b) $N_2^{\text{max}} = 18$. (Black) Circles correspond to LO, (red) squares to NLO, and (green) diamonds to NNLO. The (black) dashed line marks the exact value [18].

can be eliminated either by taking $N_2^{\text{max}}$ to large values or by adding corrections that take into account physics left out by the truncation to a certain order, or by combination of the two. Figure 2 shows the convergence with respect to $N_2^{\text{max}}$ for the ground-state energy at unitarity. The LO calculation converges to the exact result [18], as has been shown before in the case $N_3^{\text{max}} = N_2^{\text{max}} + 1$ [16]. However, in Ref. [16] the ground-state energy had a faster running to the exact value: since convergence in $N_2^{\text{max}}$ is from below but in $N_3^{\text{max}}$ from above, increasing $N_3^{\text{max}}$ at fixed $N_2^{\text{max}}$ pushes the ground-state energy further away from the exact result. For example, when $N_2^{\text{max}} = 22$ the LO ground state is at $E/\omega = 2.7413$ in Ref. [16], while the present approach gives $E/\omega = 2.7386$. On the other hand, adding corrections to the potential speeds up the convergence: at NLO the agreement with the exact calculation is achieved faster than at LO, and improves still at NNLO. For the same $N_2^{\text{max}} = 22$, the energy at NNLO is $E/\omega = 2.7715$, very close to the exact solution $E/\omega = 2.7727$ found in Ref. [18]. Thus, subleading orders provide significant improvement over LO results.

The calculation of $A = 3$ excited-state energies can be carried out similarly. We show in Fig. 3 the running with the three-body cutoff of the energy of the first excited state with $L^\pi = 1^-$, for the same two values of $N_2^{\text{max}}$ considered before, and in Fig. 4 the convergence with $N_2^{\text{max}}$. The same $10^{-4}$ precision for the same two-body UV cutoffs considered before is achieved at somewhat larger three-body cutoffs, $N_3^{\text{max}} \geq 23$ and $N_3^{\text{max}} \geq 35$ respectively. Like for the ground state, for a fixed $N_2^{\text{max}}$ the values of energies at all orders decrease until convergence is reached. Note the sharp decrease of the energy as $N_3^{\text{max}}$ goes from $N_2^{\text{max}} + 1$ to $N_2^{\text{max}} + 3$, followed by small change as the three-body cutoff is further increased. This suggests that a small number of quanta is carried out by the spectator, so that most of the two-body physics can be accommodated by a relatively small three-body space. The importance of having two different cutoffs in the two- and many-body systems clearly appears in this case. Indeed, if $N_3^{\text{max}}$ is fixed at $N_2^{\text{max}} + 1$ one can see from Fig. 3 that as corrections to the potential are added, results get worse: for both values of $N_2$ the energy at NLO and NNLO is farther away from the exact value than the value obtained at LO. As Fig. 4 shows, once $N_3^{\text{max}}$ is decoupled from $N_2^{\text{max}}$, the corrections to the potential again improve the energy systematically (except at very low two-body cutoff, i.e. $N_2^{\text{max}} \lesssim 10$). Agreement with the exact value [18] $E/\omega = 4.7727$ is very good: for $N_2^{\text{max}} = 22$, we find at LO $E/\omega = 4.7457$, ...
FIG. 2: Energy in units of the HO frequency, $E/\omega$, of the ground state $L^\pi = 1^-$ of the $A = 3$ system at unitarity, as function of the two-body cutoff, $N^{\text{max}}_2$. Notation as in Fig. 1.

FIG. 3: Same as Fig. 1 but for the first excited state with $L^\pi = 1^-$. Slightly below the value $E/\omega = 4.8554$ in Ref. 16; at NNLO, $E/\omega = 4.7721$.

The general features of convergence with $N^{\text{max}}_3$ and $N^{\text{max}}_2$ are also shown by states in other channels, although details vary. As an illustration, in Fig. 5 we show the energies for the first two states with $L^\pi = 0^+$. In this case, the convergence with $N^{\text{max}}_2$ is not always from below. For the lowest state, agreement with exact value [18] $E/\omega = 3.1662$ is very good already at NLO: for $N^{\text{max}}_2 = 26$, $E/\omega = 3.1652$, a difference of less than 0.05%. At NNLO, for the same $N^{\text{max}}_2$, the result is very close, but slightly worse, $E/\omega = 3.1641$. For the excited state, NLO is not as good, and at NNLO $E/\omega = 5.1614$, within 0.1% of the exact value [18], $E/\omega = 5.1662$.

Overall, there is systematic improvement as $N^{\text{max}}_2$ increases, which is accelerated by the inclusion of higher-order interactions.
2. Error analysis at unitarity

Truncation of the two-body space at $N_{2}^{\text{max}}$ corresponds to imposing a two-body UV cutoff at the momentum scale (6). The errors induced by this are expected to run as inverse powers of the cutoff scale, with a leading term of order $\Lambda^{-1}$ (see, for example, Ref. [26]). Since the terms in the effective potential represent short-range physics and thus must be analytic in $(p/\Lambda)^2$, only odd powers of $\Lambda^{-1}$ should appear. We therefore fit our cutoff-dependent energies with the form

$$\frac{E_3(N_{2}^{\text{max}})}{\omega} = \frac{E_3(\infty)}{\omega} + \frac{\alpha_1}{(N_{2}^{\text{max}} + 3/2)^{1/2}} + \frac{\alpha_3}{(N_{2}^{\text{max}} + 3/2)^{3/2}} + \frac{\alpha_5}{(N_{2}^{\text{max}} + 3/2)^{5/2}} + \ldots,$$

(13)

expressed, for convenience, in terms of dimensionless quantities. Here $E_3(\infty)$ is the semi-analytical result of Ref. [18] for the energy of the state. Some care is needed with this procedure since, with data for only a limited range of values of $N_{2}^{\text{max}}$, the fits can become unstable if too many terms are included.

The ground-state energy at LO in the range $N_{2}^{\text{max}} = 18$ to 30 can be well described by
fits with leading coefficients $\alpha_1 = -0.139$ and $\alpha_3 = -0.63$. At NNLO, fits to the ground state lead to values of $\alpha_1$ that are consistent with zero. Setting $\alpha_1$ to zero and refitting the NNLO energy over same range of $N_2^{\text{max}}$ yields $\alpha_3 = -0.30$ and $\alpha_5 = -5.8$. The greatly improved convergence at NNLO that is obvious from Figs. 2 and 4 is due to elimination of the leading ($\Lambda^{-1}$) term and reduction of the coefficient of the next one ($\Lambda^{-3}$).

The coefficients of the higher-order terms in these expansions are large, implying that the series in $\Lambda^{-1}$ is rather slowly converging for the values of the cutoff used here. This problem appears to be worse for the excited states, where we have not been able to find stable fits (i.e. fits where the values of the coefficients do not change appreciably as the number of terms is increased) to the energies for $N_2^{\text{max}} \leq 30$. However one should remember that the absolute errors on the NNLO energies are extremely small for $N_2^{\text{max}} \geq 20$ and so this has no practical consequences for our results.

3. Finite scattering length

Away from unitarity, universality can take on a different character. Results for the ground and first excited state at NNLO as a function of $b/a_2$, but keeping $r_2/b = 0$, are shown in Fig. 6. For each value of $b/a_2$, calculations were carried out with $N_2^{\text{max}} = 22$ and the value $N_3^{\text{max}}$ was increased to reach convergence (at the same level of $10^{-4}$ as before) of the energy. The values at $b/a_2 = 0$ are the same as in the previous section. As pointed out in Ref. [16] and reproduced in Ref. [19], at positive $b/a_2$ there is an inversion of parity for the ground state from $L^\pi = 1^-$, as expected from the HO levels with a weak interaction, to $L^\pi = 0^+$, as expected from one particle moving in an $S$-wave around a bound state of the other two. Here our use of higher orders in perturbation theory allows us to pinpoint this inversion to $b/a_2 \simeq 1.34$, very close to our original estimate of 1.5 [16]. This ground-state inversion is universal in the sense that it holds for all potentials with negligible $r_2$. It is one example of how a trap with $b \lesssim a_2$ can have different universal properties than a large, $b \gg a_2$, trap.

Positive scattering length means that the two-body ground state is bound as the trap
is removed, \( b \to \infty \). In this limit one is often interested in scattering on the bound state. Scattering observables are notoriously difficult to calculate in many-body systems, despite significant progress in this direction \[27\]. The presence of the trap, however, can simplify the calculation of low-energy scattering observables. In the two-body case, given energy levels \( E_{2,n} \) we can use Eq. (7) to extract \( S \)-wave scattering parameters. In Ref. \[9\] we examined the size of such parameters induced by our two-body truncation, and as the present manuscript was being written a study of the extent to which such an extraction is possible in the two-nucleon system within the NCSM scheme appeared \[28\]. Because similar connections between scattering properties and the spectrum of the trapped system exist for few-body systems, we can use our three-body energies to extract parameters for scattering of a particle on the two-body ground state. A similar procedure to determine the scattering length from the full three-body solution was presented in Ref. \[29\].

As noted in Ref. \[16\], in the limit \( b \gg a_2^2 \), the lowest three-body energy approaches the LO dimer energy, \(-1/2\mu a^2_2\), which corresponds to the threshold for the scattering of one particle on the bound state of the other two. Indeed, if one allows the dimer to form inside a wide-enough trap, \( b \gtrsim a_2^2 \), the low-lying three-body spectrum can be associated with the spectrum of two particles (one composite) in a trap. This spectrum is connected to the atom-dimer low-energy parameters (scattering length \( a_{ad} \), effective range \( r_{ad} \), etc.) \[9, 10, 12–14\]:

\[
\frac{\Gamma(3/4 - (E_{3,n} - E_{2,0})/2\omega)}{\Gamma(1/4 - (E_{3,n} - E_{2,0})/2\omega)} = \frac{b'}{2a_{ad}} - \frac{r_{ad}}{2b'} \frac{E_{3,n} - E_{2,0}}{\omega} + \ldots
\]  

Here, \( E_{3,n} - E_{2,0} \) is the energy of the three-body system above the dimer ground state, while \( b' = 1/\sqrt{\mu_{ad}\omega} \) is the HO parameter length calculated with the atom-dimer reduced mass, \( \mu_{ad} = 2m/3 \). Note that Eq. (14) is valid only for atom-dimer relative momenta smaller than \( 1/a_2 \), since \( a_2 \) is of the order of the size of the atom-dimer system, thus limiting the number of three-body states that can be used reliably for the extraction of atom-dimer properties.

In Fig. 7 we plot the atom-dimer scattering length \( a_{ad} \) obtained at fixed \( b/a_2^2 = 3 \) (circles) and \( b/a_2^2 = 4 \) (squares). For each two-body cutoff, we assume that the shape and higher-order parameters can be neglected and, using the lowest two \( L = 0 \) states obtained in NNLO, eliminate the atom-dimer effective range to obtain the scattering length. As shown in Fig. 7 the running is slower for \( b/a_2^2 = 4 \) than for \( b/a_2^2 = 3 \) because the interaction is stronger with respect to the HO strength. One thus would like smaller \( b/a_2^2 \) ratios so that better precision is reached for smaller cutoffs; however, for too small \( b/a_2^2 \) ratios the dimer might not be able to form inside the trap. In the limit of large \( N_{2}^{\text{max}} \) our results approach the continuum value of Ref. \[20\].

4. Finite effective range

As one moves away from a Feshbach resonance, effects of the interaction range should become more pronounced and universality reduced to some degree. Assuming a finite effective range, we can predict the changes in the properties of the three-body system. In particular, we can investigate the effect on the position of the crossing between the lowest \( L = 1 \) and \( L = 0 \) states.

In Fig. 8 we plot the corresponding energies as a function of \( b/a_2 \), for \( r_2/b = 0.1 \). As one can see, such an \( r_2 \) changes each of the energies by less than \( \omega \) in the interval displayed. One consequence is a change in the position where the \( L = 0 \) becomes lower in energy than
FIG. 7: Atom-dimer scattering length in units of the two-body scattering length, $a_{ad}/a_2$, as a function of the two-body cutoff, $N_2^{\text{max}}$. NNLO results for $b/a_2 = 3$ (black circles) and $b/a_2 = 4$ (red squares) are compared with the value (blue line) of Ref. [20].

FIG. 8: Same as Fig. 7 but for $r_2/b = 0.1$. In this case, the crossing point between the $L = 1^-$ and $L = 0^+$ lowest states moves to $b/a_2 \simeq 1.75$, a larger value than in the absence of effective range.

the $L = 1$ state, which is now at $b/a_2 \simeq 1.75$. Indeed, the effect of the finite positive range is a shift of the crossing point to larger values of $b/a_2$.

B. $A = 4$ system

We now consider the system made of four two-component fermions in a trap. As before, we fix the value of the two-body cutoff $N_2^{\text{max}}$ and increase the size of the many-body model.
space, defined here as $N_{4}^{\text{max}}$. We show only results at unitarity, although finite scattering length and effective range can be entertained as well. Of course, because of the larger number of particles we limit ourselves to smaller spaces.

For states with zero total angular momentum, the smallest value for the four-body cutoff is $N_{4}^{\text{max}} = N_{2}^{\text{max}}$. Results for the convergence of the ground-state energy at unitarity with respect to $N_{4}^{\text{max}}$ are plotted in Fig. 9 for two values of the two-body cutoff, (a) $N_{2}^{\text{max}} = 4$ and (b) $N_{2}^{\text{max}} = 8$. As for the $A = 3$ ground state, at each order convergence is from above. For the two values of $N_{2}^{\text{max}}$ displayed, we notice the same rather sharp decrease of the energy as for the $A = 3$, $L = 1^{-}$ first-excited state shown in Fig. 3. As in the latter case, improvement with order is visible only after this sharp decrease. Here near convergence is achieved when $N_{4}^{\text{max}}$ reaches $N_{2}^{\text{max}} + 4$ for $N_{2}^{\text{max}} = 4$ and $N_{2}^{\text{max}} + 8$ for $N_{2}^{\text{max}} = 8$, suggesting that more energy is taken away from the two-body subsystems than in the three-body case.

Figure 10 shows the convergence in $N_{2}^{\text{max}}$ for the ground and first-excited states at unitarity. For each cutoff $N_{2}^{\text{max}}$, the four-body model space was increased until convergence. In LO, the ground-state energy for $N_{2}^{\text{max}} = 10$ is $E/\omega = 3.64$, to be compared with $E/\omega = 4.01$ in Ref. [16]. With corrections up to NNLO $E/\omega = 3.52$, which is in good agreement with previous calculations where the ground-state energy was found to be $3.6 \pm 0.1$ [22], $3.551 \pm 0.009$ [23], and $3.545 \pm 0.003$ [21]. Like in the case of three particles, improvement is significant and systematic.

IV. CONCLUSIONS AND OUTLOOK

We have considered systems made out of a few two-component fermions in a HO trap of length $b$ using interactions generated by the application of effective field theory up to NNLO. To this order, the interactions are purely two-body and determined by the two-body scattering length $a_{2}$ and effective range $r_{2}$.

Calculations at LO were performed by solving the many-body Schrödinger equation via

FIG. 9: Energy in units of the HO frequency, $E/\omega$, of the ground state $L^{F} = 0^{+}$ of the $A = 4$ system at unitarity, as function of the four-body model space size, $N_{4}^{\text{max}}$: (a) $N_{2}^{\text{max}} = 4$; (b) $N_{2}^{\text{max}} = 8$. Notation as in Fig. 1.
a direct diagonalization, similar to the NCSM approach, whereas higher-order corrections were treated as perturbations. We have seen that, as in the two-body case, convergence is sped up by adding corrections to the potential. We have shown the necessity of using different values for the two- and many-body UV cutoffs in order to allow for enough two-body states in the many-body environment to match the two-body physics included in the construction of the interaction.

By doing so, results at unitarity for the three- and four-fermion systems agree very well with other solutions, either semi-analytical or using other numerical methods. We also have presented results for finite values of $a_2$ and $r_2$. We were able to more precisely determine the ratio $b/a_2$ where, with vanishing effective range, there is a parity inversion in the ground state of the three-body system. If the range is known, its effect on the location of this point can be calculated. On either side of this transition the ground state is universal in the sense of being the same regardless of the details of the potential, as long as its range $R \ll a_2$. However, the existence of the transition shows that the trap can lead to qualitatively different behavior compared to the free system.

Above the transition point, the ground state is the one expected from one atom moving in a $S$-wave around a dimer. We were able to use our calculated three-body energy levels to obtain an estimate for the atom-dimer scattering length comparable to the value found in Ref. [20].

This work can be extended in various directions. First, as more data on trapped few-fermion systems appear, one could determine $r_2$ for specific atoms and predict its effects on the few-body dynamics. Second, one can apply the same method to other systems, such as bosons or fermions with more components. In these cases a three-body force appears already at LO, whose parameter needs to be determined from the three-body system itself. The corresponding UV limit-cycle behavior is expected to survive the presence of the trap. A system of particular interest is the atomic nucleus, where $r_2$ is known and the LO three-nucleon force can be determined either from the triton binding energy or from the neutron-deuteron scattering length (through the lowest energy levels of the trapped system of two neutrons and one proton). We can now calculate such systems systematically.
to high orders.

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