Three Fermions in a Box

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I calculate finite-volume effects for three identical spin-1/2 fermions in a box assuming short-ranged repulsive interactions of 'natural size'. This analysis employs standard perturbation theory in powers of 1/L, where L^3 is the volume of the box. I give results for the ground states in the A_1, T_1, and E cubic representations.

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1. Introduction

Recently much progress has been made in calculating two-body low-energy constants (LECs) directly from QCD in the mesonic sector (see [1] for a recent review). Lattice QCD (LQCD) calculations of two-meson interacting energies are performed and, using Lüscher's formalism[2], the scattering lengths are extracted. The exceptionally clean signals obtained in the mesonic sector have allowed for the extraction of pure three-body LECs [3, 4] using the multi-boson finite volume effects derived in [5, 6]. In the three-pion sector, the extracted three-body LEC is consistent with a repulsive three-body interaction[3].

Lüscher's formalism can be used to extract scattering phase shifts of two interacting baryons just as in the mesonic sector[7]. However, due to Pauli's exclusion principle, there is no general formula for relating LECs to interacting energy shifts for three (and more) fermions. In this proceeding I present finite volume effects for three identical spin-1/2 particles within a box, thereby generalizing Lüscher's formalism to three fermions. This analysis uses repulsive, short-ranged interactions of 'natural size', which is amenable to perturbation theory. Results are given for T_1 states that are accurate to order $1/L^5$, whereas results for A_1 and E states are accurate to order $1/L^4$. Here L is the length of a side of the box.

In the next section I give a heuristic explanation of how to construct three-fermion states of definite cubic symmetry. The anti-symmetry restrictions makes this construction non-trivial. Section 3 then enumerates the perturbative results in powers of 1/L using these basis states. I conclude in sect. 4.

2. Constructing anti-symmetrised three-fermion states of good cubic symmetry

2.1 Jacobi basis

The three-body single-particle eigenstates of the dimensionless kinetic energy operator $\hat{T}$ (in units of $\varepsilon_0 = 4\pi^2/mL^2$) in a box of volume L^3 are given by $|\vec{n}_1\,\vec{n}_2\,\vec{n}_3 >$, where

$$\hat{T}|\vec{n}_1\,\vec{n}_2\,\vec{n}_3 >= |\vec{n}_1\,\vec{n}_2\,\vec{n}_3 > \left(\frac{\vec{n}_1^2}{2} + \frac{\vec{n}_2^2}{2} + \frac{\vec{n}_3^2}{2}\right) . \tag{2.1}$$

Here $\vec{n}_i = (n_{ix}, n_{iy}, n_{iz})$ represents the wave number vector for the ith particle and I have assumed all particles have equal mass m. Other quantum numbers, such as spin (and isospin), have been suppressed.

For reasons which will become apparent below, the single-particle states are now transformed to a Jacobi basis using

$$\begin{aligned}
\vec{R}_{12} &= \vec{r}_1 - \vec{r}_2 \\
\vec{R}_3 &= \vec{r}_3 - \frac{1}{2}(\vec{r}_1 + \vec{r}_2) \\
\vec{R}_{cm} &= \frac{1}{3}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3) .
\end{aligned} \tag{2.2}$$

Here $\vec{R}_{12}$ represents the relative motion between particles 1 and 2, $\vec{R}_3$ represents the relative motion between particle 3 and the center-of-mass (CM) of particles 1 and 2, and $\vec{R}_{cm}$ is the total CM
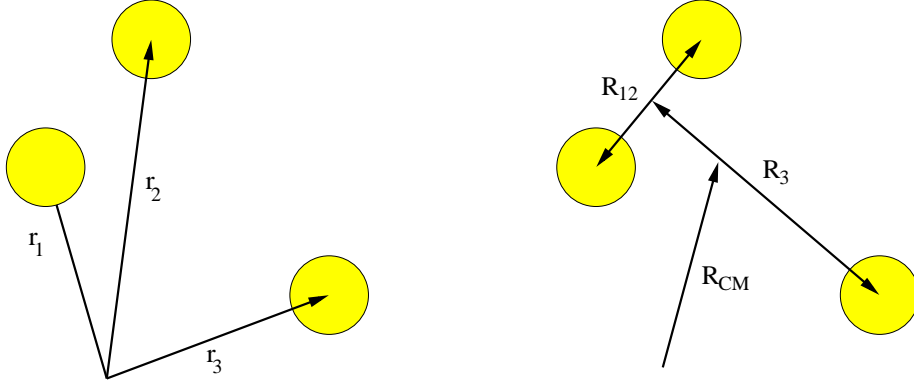
Figure 1: Depiction of transformation from independent degrees of freedom in the single-particle basis (left) to the independent degrees of freedom in the Jacobi basis (right).

motion. In momentum space, this corresponds to the following transformations,

$$
\begin{aligned}
\vec{P}_{12} &= \frac{1}{2}\left(\vec{p}_1 - \vec{p}_2\right) \\
\vec{P}_3 &= \frac{2}{3}\left(\vec{p}_3 - \frac{1}{2}\left(\vec{p}_1 + \vec{p}_2\right)\right) \\
\vec{P}_{cm} &= \vec{p}_1 + \vec{p}_2 + \vec{p}_3 \, .
\end{aligned}
\tag{2.3}
$$

Eigenstates in this Jacobi basis are defined as $|\vec{N}_{12}\,\vec{N}_3\,\vec{N}_{cm}>$, where now

$$
\hat{T}|\vec{N}_{12}\,\vec{N}_3\,\vec{N}_{cm}> = |\vec{N}_{12}\,\vec{N}_3\,\vec{N}_{cm}>\left(\vec{N}_{12}^2 + \frac{3}{4}\vec{N}_3^2 + \frac{1}{6}\vec{N}_{cm}^2\right) \, .
\tag{2.4}
$$

Figure 1 shows this transformation schematically.

Since interactions occur only between particles (I assume no external potential acting on the fermions) and typically only the lowest energy eigenstates are of interest, the utility of switching to the Jacobi basis is now manifest: one can simply set $\vec{N}_{cm} = 0$. Thus a three-body problem effectively becomes a 'two-body' problem. All results in the following section use $\vec{N}_{cm} = 0$, though it is straightforward (but tedious) to generalize to nonzero CM motion.

A subtle point comes about from the transformation to Jacobi basis since the box boundary conditions are originally defined in the single-particle basis. In the case when $\vec{N}_{cm} = 0$, for any component of $\vec{N}_3$ which is odd, the corresponding component of $\vec{N}_{12}$ must satisfy anti-periodic boundary conditions. Conversely, any component of $\vec{N}_3$ which is even has the corresponding component of $\vec{N}_{12}$ satisfying periodic boundary conditions. These restrictions can be derived by comparing the completeness relations within the single-particle basis and the Jacobi basis.

2.2 Three-body antisymmetrised states

The states $|\vec{N}_{12}\,\vec{N}_3>$ (the index $\vec{N}_{CM}$ is dropped since only zero CM motion is considered) are not anti-symmetric under exchange of any two particles. Anti-symmetric states are constructed by projecting onto the three-body anti-symmetriser,

$$
P_{\mathscr{A}}^{123} = \frac{1}{3}P_{\mathscr{A}}^{12}\left(1 - P_{13} - P_{23}\right) \, ,
\tag{2.5}
$$

where P_{ij} is the permutation operator that permutes particles i and j and

$$P_{\mathscr{A}}^{12} = \frac{1}{2}\left(1 - P_{12}\right) \tag{2.6}$$

is the two-body anti-symmetriser of particles 1 and 2. Note that Eq. 2.5 commutes with the parity operator. Thus the states of interest are ones that satisfy

$$P_{\mathscr{A}}^{123}|n\,i\,\pi> = |n\,i\,\pi>\,,$$

where $|n\,i\,\pi>$ represents the ith state of cubic shell n with definite parity π. It is made up of linear combinations of $|\vec{N}_{12}\,\vec{N}_3>$ such that $\vec{N}_{12}^2 + \vec{N}_3^2 = n$. For each cubic shell there is a finite number of anti-symmetric states D_n.

2.3 Cubic group symmetry

The states $|n\,i\,\pi>$ are now anti-symmetrised but are not states of good cubic symmetry. Standard group-theoretical techniques can be used to obtain the appropriate linear combinations of $|n\,i\,\pi>$ such that the overall anti-symmetric state falls into one of the five irreducible representations (irreps) of the cubic group: A_1, A_2, E, T_1, and T_2[8]. A cursory description of this procedure is only given below.

Given the set of anti-symmetrised states $|n\,i\,\pi>$, matrix elements of the cubic rotation operators R_α are constructed using this basis, *i.e.* $<n\,j\,\pi|R_\alpha|n\,i\,\pi>$, forming a regular representation of the group. This regular representation consists of 24 matrices, all of dimension $D_n \times D_n$. Traces of these matrices give five distinct characters $\chi_R(r)$, and using the five characters of the irreps of the cubic group, $\chi_{IR}(r)$, and the number of rotation elements in each irrep, $n_{IR}(r)$, the multiplicity of each irrep in this regular representation,

$$m_{IR} = \frac{1}{24}\sum_{r=1}^{5} n_{IR}(r)\chi_R(r)\chi_{IR}(r),$$

for a given cubic shell n is found. Given the dimension of each irrep, $d_{IR}(r)$, projection operators for each irrep are then constructed,

$$P_{IR} = \frac{1}{24}\sum_r d_{IR}(r)\chi_{IR}(r)\sum_{\alpha\in r} R_\alpha\,,$$

from which the anti-symmetrised states of definite cubic symmetry are constructed. Table 1 enumerates the anti-symmetric states for the first three cubic shells. Note that Pauli's exclusion principle prevents any three spin-1/2 fermion states residing in the $n = 0$ cubic shell.

3. Perturbative results

At up to order $1/L^5$, only s-wave and p-wave interactions contribute. I parametrize these momentum space interactions in the following manner:

$$V_0(\vec{p}',\vec{p}) = \frac{4\pi a_0}{m}\left[1 + \frac{a_0 r_0}{2}\left(\frac{p'^2 + p^2}{2}\right) + \dots\right] \qquad \text{(s-wave)} \tag{3.1}$$

$$V_1(\vec{p}',\vec{p}) = \frac{12\pi a_1}{m}\vec{p}'\cdot\vec{p}\left[1 + \frac{a_1 r_1}{2}\left(\frac{p'^2 + p^2}{2}\right) + \dots\right] \quad \text{(p-wave)}\,. \tag{3.2}$$

n	Spin	Parity	A_1	A_2	E	T_1	T_2	D_n
1	$\frac{1}{2}$	+	1	0	1	0	0	3
1	$\frac{1}{2}$	-	0	0	0	1	0	3
1	$\frac{3}{2}$	-	0	0	0	1	0	3
2	$\frac{1}{2}$	+	2	1	3	1	2	18
2	$\frac{1}{2}$	-	0	0	0	3	3	18
2	$\frac{3}{2}$	+	0	1	1	1	0	6
2	$\frac{3}{2}$	-	0	0	0	2	2	12
3	$\frac{1}{2}$	+	4	0	4	3	6	39
3	$\frac{1}{2}$	-	0	3	3	7	3	39
3	$\frac{3}{2}$	+	1	1	1	2	2	16
3	$\frac{3}{2}$	-	0	3	1	4	1	20

Table 1: Dimension and multiplicity of anti-symmetric states of various cubic irreps for zero CM motion. n refers to value of cubic shell. The cubic irreps are A_1, A_2, E, T_1, and T_2 and refer to the spatial part of the wavefunctions. Numbers below these irreps correspond to the mulitplicity of the irrep within cubic shell n. Last column gives the total dimension of anti-symmetric states D_n in cubic shell n.

The parameters a_0 and r_0 are the scattering length and effective range, respectively. They both have units of length. The parameters a_1 and r_1 are the scattering volume and effective momentum, having units of length^3 and length^{-1}, respectively. The perturbative analysis assumes that $a_0/L \ll 1$ and $r_0/L \ll 1$, as well as $a_1/L^3 \ll 1$ and $r_1 L \ll 1$.

The results, when expressed with dimensional units, are accurate to order $1/L^5$ for the T_1 states. For E and A_1 states, the results are accurate to order $1/L^4$. However, since results are presented in units of $\varepsilon_0 = \frac{4\pi^2}{mL^2}$ (*i.e.* results are dimensionless), at most terms of order $1/L^3$ are shown explicitly. Only states perturbatively connected to the first cubic shell $n = 1$ are shown. To facilitate the presentation, a list of the various lattice sums and their numerical values that are inherent to these calculations is given in tab. 2.

3.1 T_1^- Spin=$\frac{3}{2}$

This channel is only sensitive to the effective range,

$$\frac{\varepsilon}{\varepsilon_0} = 1 + 36\pi \frac{a_1}{L^3} + \mathcal{O}(L^{-5}) \,. \tag{3.3}$$

Furthermore, there are no terms that come in at $1/L^4$ on the right-hand side of eq. 3.3.

3.2 T_1^- Spin=$\frac{1}{2}$

$$\frac{\varepsilon}{\varepsilon_0} = 1 + 3\frac{a_0}{\pi L} + \left(\frac{3}{2} - 3\mathscr{L}_2\right)\frac{a_0^2}{\pi^2 L^2} + 27\pi\frac{a_1}{L^3} + \frac{3}{2}\pi\frac{a_0^2 r_0}{L^3}$$
$$+ \left(\frac{9}{4} - 3\mathscr{L}_2 + 3\mathscr{L}_2^2 - 6\mathscr{M}_2\right)\frac{a_0^3}{\pi^3 L^3} + \mathcal{O}(L^{-4}) \,. \tag{3.4}$$

Label	Expression	Numerical value
$\mathscr{L}_1$	$\sum^{|\vec{n}|\leq\Lambda}\frac{1}{\vec{n}^2-1}-4\pi\Lambda$	-1.21134
$\mathscr{L}_2$	$\sum^{|\vec{n}|\leq\Lambda}\frac{1}{n_x^2+n_y^2+n_z(n_z+1)}-4\pi\Lambda$	-6.37481
$\mathscr{M}_1$	$\sum\frac{1}{(\vec{n}^2-1)^2}$	23.24322
$\mathscr{M}_2$	$\sum\frac{1}{(n_x^2+n_y^2+n_z(n_z+1))^2}$	18.3

Table 2: Lattice sums and their numerical values. Sums are over all triplet of integers $\vec{n}=(n_x,n_y,n_z)$ such that the denominator does not vanish. The limit $\Lambda\to\infty$ is implicit.

3.3 E^+ Spin=$\frac{1}{2}$

$$\frac{\varepsilon}{\varepsilon_0}=1+\frac{a_0}{\pi L}-\left(\frac{3}{2}+\mathscr{L}_2\right)\frac{a_0^2}{\pi^2 L^2}+\mathscr{O}(L^{-3}) .$$

(3.5)

3.4 A_1^+ Spin=$\frac{1}{2}$

$$\frac{\varepsilon}{\varepsilon_0}=1+7\frac{a_0}{\pi L}-\left(\frac{3}{2}+\mathscr{L}_2+6\mathscr{L}_1\right)\frac{a_0^2}{\pi^2 L^2}+\mathscr{O}(L^{-3}) .$$

(3.6)

4. Conclusion

I have presented finite volume effects for three identical spin-1/2 fermions in a box interacting via short-ranged, repulsive interactions of 'natural' size. Results are given for states in the first cubic shell $n=1$ and are valid up to order $1/L^5$ for the T_1 states and $1/L^4$ for the A_1 and E states. These results generalize Lüscher's formalism to three spin-1/2 fermions in a box.

A similar analysis can be performed on nucleons by the introduction of isospin degrees of freedom[9]. Here the spectra of states is extremely rich and the structure of the interactions is complex due to the presence of tensor forces and pure s-wave three-body interactions. Furthermore, at the physical pion mass the interactions are no longer of 'natural' size and non-perturbative formalisms must be employed[9].

Ultimately, LQCD will answer current outstanding nuclear physics questions, such as the nature and origin of the tensor force and three-nucleon interaction. This work represents a necessary step towards obtaining these answers.

Acknowledgments

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