Heavy-Light Few Fermion Clusters at Unitarity

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We examine the physics of two, three, and four heavy fermions interacting with a single light fermion via short-range interactions. Four-particle bosonic Efimov states have proven important experimentally and also been the subject of significant theoretical effort. Similar fermionic systems are just now being investigated. We find that with some simple interactions the four- and five-particle states collapse to the interaction range at smaller mass ratios than the three-body state, and also before larger clusters can collapse. These states and their excitations can be studied in cold atom experiments, providing unique insights into the role of few-body systems in many-body physics.

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The few- and many-body physics of heterogeneous mixtures of cold Fermi atoms is of great interest both experimentally[1,2] and theoretically[3–11]. For many-body systems, different mass ratios may allow for ‘exotic’ superfluid phases, or phases of mixtures of different condensates to be observed experimentally. Few-body mixtures of heavy and light fermions also allow us to study the role of new classes of fermionic few-body resonances, in particular searching for regimes in which four- and five-particle states can play a significant role.

The impact of few-body resonances in cold atomic gases has been confirmed recently for bosons, where Efimov states have been predicted theoretically and found experimentally[12–16]. These states can have significant effects on loss rates in cold-atom experiments, and are of course very intriguing in their own right. In the present work, we examine potential few-body fermion states and their impact. Such states are clearly very different from the bosonic Efimov states, but offer a potentially intriguing prospect for future studies.

In the many-body heterogeneous system, the simplest phase diagram at unitarity for a mass ratio relevant to mixtures of K and Li has been examined in Ref. [17]. A normal state is found at large polarization, particularly where the number of heavy fermions greatly exceed the number of light fermions. The resulting energy is very small, though, suggesting that intriguing states perhaps including multi-particle condensates may arise near this regime.

Theoretical investigations of the few-body problem with multiple heavy fermions and a one light fermion have already provoked a great deal of interest. Interestingly, calculations for two heavy and one light fermions find regions where collapse is possible at mass ratios significantly below the critical value of 13.6 where collapse and associated Efimov states are universal.[9] The few-body interactions must be fine-tuned to produce these states, and hence the few-body physics is non-universal. In this study, Nishida et al., discuss the potential effects of these states in many-body experiments, finding the potential to conduct examinations of strongly-interacting gases of dimers and trimers. Our results indicate that an even richer phase structure may be appropriate, as four- and five-body resonances can appear in addition to the resonances of two heavy and one light particle. In fact, these resonances can appear at lower mass ratios than the two-heavy one-light (2H1L) system.

Model Hamiltonian: We investigate this non-universal few-body regime by calculating ground states in a model system of three-, four- and many-fermions interacting with a single light particle via short-range interactions. The Hamiltonian considered for one light particle of mass \(m\) and \(N\) heavy fermions of mass \(M\) is:

\[
H = -\frac{\hbar^2}{2m} \nabla l^2 + \sum_{h=1}^{N} -\frac{\hbar^2}{2M} \nabla h^2 + \sum_{h} V_2(r_h) + \sum_{h_1<h_2} V_3(r_{h_1},r_{h_2}),
\]

where \(l\) labels the light particle, \(h\) the heavy particles, the two-body potential \(V_2\) acts only between light and heavy fermions, and the three-body potential is a function of the separations between the light and the two heavy particles. In all calculations the heavy-light effective mass \(\mu = Mm/(M+m)\) is used, along with the effective range of the two-body interaction \(r_{eff}\) to set the scales of energy and distance. The two-body interactions are tuned to unitarity or infinite scattering length. We use both Poschl-Teller and Gaussian two-body potentials:

\[
V_2 = -2\frac{\hbar^2}{2\mu} \lambda^2 \cosh^{-2}(\lambda r)
\]

\[
V'_2 = -2\nu_2^2 \frac{\hbar^2}{2\mu} \lambda^2 \exp[-(\lambda r)^2/2],
\]

where \(\nu_2^2 \approx 0.671\) is adjusted to unitarity. We also include a three-body interaction with the same range as
the two-body interaction for each pair:

\[ V_2(r, r') = \frac{\hbar^2}{2\mu} \lambda^2 \cos^{-2}(\lambda r) \cos^{-2}(\lambda r'). \]  

The two-heavy one-light problem has been investigated by Nishida, et al.[9], who found a regime for $8.6 < \frac{M}{m} < 13.6$ where the interaction can be fine-tuned to produce three-body resonances. In a many-body system these states would yield an interacting gas of dimers and trimers. In this study they explicitly assume that collapse of four- and five-body states are not favored. However, for specific sets of geometrically symmetric heavy-particle coordinates (equilateral triangles and regular tetrahedrons, respectively), Nishida[18] used the Born-Oppenheimer approximation to study the static potential between the heavy fermions. Significant additional attraction was found for these multi-particle states, suggesting it is at possible that the larger clusters may be bound at lower mass ratios than the two-heavy one-light system.

Methods: We examine this possibility using Quantum Monte Carlo techniques. The calculations employ variational states to give a variational upper bound to the ground-state energy. We assume a trial wave function $\Psi_T = \phi_L \Phi_H$, where $\phi_L$ is a positive definite function of the light particle coordinates, and $\Phi_H$ is an antisymmetric state of the heavy particle coordinates. All coordinates are measured from the system center-of-mass to avoid spurious CM motion.

The calculations are variational and hence produce an upper bound to the ground state of the model Hamiltonian. We believe that these results are likely to be accurate in most regimes, as the nodal surfaces ($\Psi_T = 0$) are quite simple for these systems. For two, three, or four particles it is possible to put all the fermions in relative $p$-waves; larger systems require higher partial waves or radial excitations. The simplest possible nodal surfaces are, as in the Born-Oppenheimer approximation, independent of the position of the light particle. They are simply the projected length, projected area, and volume of the line, triangle, and tetrahedron connecting the two, three, and four heavy fermions, respectively:

\[
\begin{align*}
\Phi_H^2 &= (r_1 - r_2) \cdot \hat{z}, \\
\Phi_H^3 &= r_{3,12} \times (r_1 - r_2) \cdot \hat{z}, \\
\Phi_H^4 &= r_{4,123} \cdot (r_{3,12} \times (r_1 - r_2)),
\end{align*}
\]

where $\mathbf{r}_{i,j,k}$ is used to indicate the relative coordinate of particle $i$ from the center of mass of the pair or triplet $j,k$. These ground states have angular momentum $L = 1, 0, 0$, respectively, for $N = 2, 3, 4$. Slightly lower energies are obtained in the calculations reported here by putting the heavy particles in $s$- and $p$-wave orbitals measured from the system CM, yielding additional variational freedom.

Results: The results for the ground-state energies of the two-, three-, and four-heavy, one light systems are shown in Figure I for these specific two-body interactions. All energies are plotted in units of $E_0 \equiv \frac{\hbar^2}{2 \mu r_{\text{eff}}^2}$, where $r_{\text{eff}}$ is the effective range of the interaction. For these two-body interactions the regimes where $E \lesssim 0$ are shown, nevertheless they would collapse to large negative energies and zero radius as the two-body effective range is reduced. The few-particle system will collapse at this point independent of whether the particles are confined in a trap or not.

For these interactions we find that the four heavy one light system collapses at a much smaller mass ratio than the three heavy one light which, in turn, collapses before the two heavy one light. The additional attraction obtained from the light particle orbiting multiple heavy fermions is sufficient to bind them quite deeply. The increase in binding with mass ratio is very rapid for the 3H1L and particularly for the 4H1L system. For these simple interactions, the binding of the 3H1L and 4H1L clusters are very large at the mass ratio where the 2H1L system is near threshold. Results for the Poschl-Teller potential are given in Table I.

It could be possible that adding additional fermions would bind the system at even smaller mass ratios. To test this assertion we have performed calculations of the 9H1L and 10H1L systems using the same Quantum Monte Carlo techniques. These particle numbers are sug-

![Figure I: Binding Energies versus mass ratio](image-url)
suggested by filling single-particle states in the d (L=2) wave and a radial excitation into the 2s state. Adding additional fermions does not seem to reduce the minimum mass ratio further, presumably the additional energy cost of putting heavy fermions in higher angular-momentum or higher-energy radial states is too large to bind the overall system. There exists a mass ratio where a single light particle could bind an infinite number of heavy particles, however in our calculations to date this ratio appears significantly larger than the ratio where smaller systems can collapse.

We have calculated the root-mean-square radius for the heavy and light particles for the clusters near threshold. The results for a few cases are summarized in Table I. For the 2H1L system we find that the light-particle rms radius at very weak binding is about 3-4 times the heavy particle radius, consistent with simple expectations. The difference in radii decreases as we go to the larger systems and larger binding, though. In the table we report VMC results for the trial wave function $\Psi_T$ and the QMC results. The large extrapolations make very accurate results difficult to extract, but the trend is clear.

We’ve also examined the single-particle densities of the clusters. Because of the nodal structures defined above, the heavy particles have very small density near the cluster’s center-of-mass. In the case of the simple trial functions above, the density is exactly zero at the origin. The light particle, in contrast, has a maximum density at the origin, preferring to occupy a space in the middle of the heavy fermions.

It is clear from our results that different two-body potentials with the same effective range give different binding energies. In fact the mass ratio where the curves intercept $E = 0$ changes with different two-body interactions. To further quantify these results, we’ve also studied these systems including a repulsive three-body interaction $V_3$. The three-body interaction also shifts the zero binding energy intercept. These results underscore the non-universal nature of this regime. As an example, in Figure 2 we compare results with- and without a three-body interaction near threshold for the 3H1L and 4H1L systems. Even relatively small amplitudes of the three-body interaction shift the curves significantly, as is to be expected for a non-universal system. The 2H1L systems behaves similarly, with a significant impact of the three-body force. All systems can become unbound for a repulsive three-body interaction with a strength $V_3$ of order unity.

**Future Possibilities:** It would be interesting to know if a single three-body interaction parameter can simultaneously describe the binding of the 2H1L, 3H1L, and 4H1L systems. This has been found to be the case in few-body bosonic systems, or in fermionic systems where the number of spin degrees of freedom is larger than the number of particles. In particular this relation has been used to explain the relative binding of the deuteron, 3H, and 4He nuclei. Of course the interaction here cannot be a pure contact interaction but would require momentum-dependent terms for the two heavy fermions, which must be in an odd relative partial wave, coupled to one boson.

We are presently investigating the possibility of bound excited states in these systems in certain ratios of mass regimes, perhaps related by simple scaling laws. The large binding of the heavier systems relative to the smaller gives some reason to believe this may be possible. One can imagine states similar to those found for bosons where one heavy particle is in an excited loosely bound state. It would have to be in an s-wave or other low partial wave to have a significant attraction to the remaining N-1 particle cluster. Finally, it could be extremely interesting to study the systems described here in the many-body context. Optical lattices can be used to set the effective mass ratio as described in [8]. One could in principle set the mass ratio and the relative population of the heavy and light species to obtain strongly-interacting gases of 4H1L and 3H1L clusters. Many other possibilities can also be imagined.

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**TABLE II:** RMS radii for the heavy and light particles for the clusters. VMC and extrapolated QMC result are given, results are for the Poschl-Teller potential and all radii are given in units of $r_{eff}$.

| M/m | VMC L | VMC H | QMC L | QMC H |
|-----|-------|-------|-------|-------|
| 2H1L | 14.5  | 0.78  | 0.18  | 1.14  | 0.30  |
| 3H1L | 11.75 | 0.30  | 0.18  | 0.42  | 0.24  |
| 4H1L | 10.25 | 0.30  | 0.24  | 0.30  | 0.24  |

**FIG. 2:** (color online) The effect of three-body interactions on the binding energies of 3H1L. The three-body interaction can shift the mass threshold for collapse significantly.

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