Degeneracies in trapped two-component Fermi gases

K. M. Daily, D. Rakshit, and D. Blume

1Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

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We report on previously unobserved inter-system degeneracies in two-component equal-mass Fermi gases with interspecies zero-range interactions under isotropic harmonic confinement. Over the past 10 years, two-component Fermi gases consisting of $n_1$ spin-up and $n_2$ spin-down atoms with interspecies zero-range interactions have become a paradigm for modeling condensed matter systems, nuclear matter and neutron matter. We show that the eigen energies of the $(n_1+1, n_2-1)$ system are degenerate with the eigen energies of the $(n_1, n_2)$ system for any s-wave scattering length $a_s$, including infinitely large, positive and negative $a_s$. The existence of the inter-system degeneracies is demonstrated explicitly for few-body systems with $n_1 + n_2 = 4, 5$ and 6. The degeneracies and associated symmetries are explained within a group theoretical framework.

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Symmetry is one of the most fundamental concepts in physics, underlying our understanding of elementary particle physics, relativity and quantum mechanics, to name a few [1]. In quantum mechanics, symmetries manifest themselves in degeneracies of energy eigen values. If a Hamiltonian is invariant under rotations, for example, the eigen energies are $(2L + 1)$-fold degenerate, where $L$ denotes the orbital angular momentum quantum number [2]. Similarly, the fact that the energy spectrum of the non-relativistic hydrogen atom depends only on the principal quantum number is intimately related to conserved quantities associated with the orbital angular momentum and Runge-Lenz vectors [2].

Dilute atomic two-component Fermi gases with short-range interspecies s-wave interactions can nowadays be realized routinely in many cold atom laboratories [3]. In these experiments, the atoms occupy two different hyperfine states that are interpreted as spin-1/2 pseudo states. Ultracold atomic Fermi gases have emerged as model systems with which to study condensed matter phenomena such as the BCS-BEC crossover and nuclear physics phenomena such as the equation of state of superfluid neutron matter [4–6]. A multitude of results have been obtained for two-component equal-mass Fermi gases with s-wave zero-range (ZR) interactions. A notable milestone is the derivation of various universal relations by Tan [7–9], which are centered around the “contact” and now form the basis for novel spectroscopic techniques [10–11]. Another notable milestone is the identification of a hidden SO(2,1) symmetry of the two-component Fermi gas with ZR interactions at unitarity in an isotropic harmonic trap by Werner and Castin [12], which manifests itself in ladders of uniformly spaced excitation frequencies.

Our work identifies another symmetry that manifests itself in the existence of degenerate energy eigen values of two-component equal-mass Fermi gases with the same number of particles but different numbers of spin-up and spin-down atoms, i.e., of $(n_1, n_2)$ and $(n_1', n_2')$ systems with $n_1 + n_2 = n_1' + n_2'$. These “inter-system degeneracies” emerge in the ZR limit for any value of the interspecies s-wave scattering length and are broken for finite-range interactions or unequal-mass systems.

Our starting point is the non-relativistic Hamiltonian $H$ of the two-component Fermi gas with $n_1$ spin-up atoms and $n_2$ spin-down atoms $(n = n_1 + n_2)$,

$$H = H_0 + V_{\text{int}},$$

where

$$H_0 = \sum_{j=1}^{n} \left( -\frac{\hbar^2}{2m} \nabla_{\vec{r}_j}^2 + \frac{1}{2} m \omega^2 \vec{r}_j^2 \right)$$

and $V_{\text{int}}$ describes the interactions between the spin-up and spin-down atoms,

$$V_{\text{int}} = \sum_{j=1}^{n_1} \sum_{k=n_1+1}^{n} V_{\text{th}}(r_{jk}).$$

In Eq. (1), $m$ denotes the atom mass, $\omega$ the angular trapping frequency, and $\vec{r}_j$ the position vector of the $j$th atom measured with respect to the trap center. Following the literature [4], the spin-up and spin-down components by themselves are assumed to be non-interacting (NI). We model the intercomponent atom-atom interactions by a short-range Gaussian potential $V_g$ [13] with depth $V_0$ and range $r_0$, $V_g(r_{jk}) = -V_0 \exp[-r^2/(2r_0^2)]$, where $r_{jk} = |\vec{r}_j - \vec{r}_k|$. For a fixed $r_0$, we adjust the depth $V_0$ such that $V_g$ reproduces the desired free-space zero-energy atom-atom s-wave scattering length $a_s$. We restrict ourselves to two-body potentials that support no two-body s-wave bound state in free-space for negative $a_s$ and one two-body s-wave bound state in free-space for positive $a_s$. In the $r_0 \to 0$ limit, our interaction model provides a realization of the ZR $\delta$-function interaction. In practice, we determine the eigen energies of $H$ for a sequence of $r_0$ values and then extrapolate the eigen energies to the $r_0 \to 0$ limit. Throughout, we consider ranges $r_0$ that are much smaller than the harmonic oscillator length $a_{\text{ho}}$, where $a_{\text{ho}} = \sqrt{\hbar/(m\omega)}$. 

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We first consider the Hamiltonian $H_0$, which describes $n$ NI particles under isotropic harmonic confinement. As an example, Figs. 1(a) and 1(b) illustrate the ground state configurations of the $(n_1, n_2) = (3, 1)$ and $(2, 2)$ systems. The lowest single particle orbital with energy $3\hbar\omega/2$ can be occupied by a spin-up atom and a spin-down atom. To obey the Pauli exclusion principle, the other spin-up and spin-down atoms need to occupy one of the three excited state orbitals with energy $5\hbar\omega/2$. This simple picture yields a ground state energy of $8\hbar\omega$ for both the $(3, 1)$ and $(2, 2)$ systems. It can be readily shown that the ground state of the $(3, 1)$ system has $L^\Pi = 1^+$ symmetry, where $L$ denotes the orbital angular momentum quantum number and $\Pi$ the parity; this ground state is three-fold degenerate due to the rotational invariance of the Hamiltonian. The ground state of the $(2, 2)$ system is nine-fold degenerate. Just as the NI ground state manifolds of the $(3, 1)$ and $(2, 2)$ systems contain degenerate energies corresponding to the same $L^\Pi$ symmetry, so do the NI excited state manifolds. Moreover, analogous degeneracies are readily identified for NI systems with larger $n$.

In this paper, we are interested in the “inter-system degeneracies”, i.e., in the fact that the $(n_1 + 1, n_2 - 1)$ and $(n_1, n_2)$ systems support degenerate energies corresponding to the same $L^\Pi$ symmetry. Specifically, we analyze what happens to the inter-system degeneracies when the interactions are turned on. For example, since the $(3, 1)$ system contains three spin-up—spin-down pairs while the $(2, 2)$ system contains four [see Figs. 1(c) and 1(d)], it seems natural to expect that the interactions break the inter-system degeneracies discussed above for the NI $n = 4$ systems. As we will show, however, this is not the case if $r_0$ is taken to zero: For ZR interactions, the eigen energies of the $(3, 1)$ system form, within our numerical accuracy, a subset of the eigen energies of the $(2, 2)$ system. Analogous results are found for systems with $n = 5$ and 6.

To determine the eigen energies of the Hamiltonian $H$ for finite depth $V_0$ of the Gaussian model potential $V$, we resort to the stochastic variational approach [13]. We separate the center of mass motion and expand the relative eigen functions in terms of a basis set with good orbital angular momentum quantum number $L$ and parity $\Pi$ [13,17]. The proper permutation symmetry under the exchange of identical fermions is imposed by applying an appropriately chosen anti-symmetrization operator to the basis functions. Our implementation [18] allows for the treatment of states with all $L^\Pi$ symmetries. The stochastic variational approach results in variational upper bounds to the exact eigen energies [15].

As an example, Fig. 2 shows the extrapolated ZR energies for the $(3, 1)$ and $(2, 2)$ systems with $1^+$ symmetry as a function of the inverse $s$-wave scattering length $a_s^{-1}$. In this representation, the weakly-attractive BCS regime ($a_s < 0$ and $|a_s|/a_{ho} \ll 1$) is realized on the left of the graph and the repulsive BEC regime ($a_s > 0$) on the right of the graph. Lines show the relative eigen energies of the $(3, 1)$ system and symbols those of the $(2, 2)$ system for $r_0 = 0$. The extrapolated ZR energies are estimated to have a combined basis set and ZR extrapolation error smaller than 0.001 % for the energetically lowest-lying state and smaller than 0.01 % for the energetically second lowest-lying state. On the scale shown, the eigen energies of the $(3, 1)$ and $(2, 2)$ systems are, somewhat surprisingly, indistinguishable for both the lowest and second lowest states for all scattering lengths considered. The inset shows that the fractional difference is smaller than $2 \times 10^{-4}$ % for the energetically lowest lying $1^+$ state.
Symbols show the fractional difference $\Delta_s$ the crossover. As numerical accuracy, the energy curves agree throughout and the scattering lengths considered. Thus, within our $\Delta_s$, the (3^r \text{perturbative calculations [21].}

To see if the (3, 1) and (2, 2) energies are also degenerate for other symmetries and for higher-lying excitations, we focus on the infinite scattering length regime. We analyze the extrapolated ZR energies of the (3, 1) and (2, 2) systems at unitarity for all states with relative energy $E^{\text{rel}}$ equal to or smaller than $21\hbar\omega/2$, which were determined in Ref. [18] with an accuracy of 0.1% or better. In this energy window, there exist 164 and 286 eigen energies for the (3, 1) and (2, 2) systems, respectively [19]. As pointed out by Werner and Castin [12], the existence of a hidden SO(2,1) symmetry leads to ladders of energies spaced by $2\hbar\omega$, i.e., the relative eigen energies at unitarity can be written as $E^{\text{rel}} = (s^{\nu,L,\Pi} + 2q + 1)\hbar\omega$, where $q = 0, 1, \cdots$. The separation constants $s^{\nu,L,\Pi}$ arise when solving the $(n_1,n_2)$-fermion problem within the hyperspherical framework. We find that the relative eigen energies with $E^{\text{rel}} \leq 21\hbar\omega/2$, corresponding to (3, 1) and (2, 2) states that are affected by the interactions, are characterized by 89 and 170 $s^{\nu,L,\Pi}$ values, respectively [20]. Quite surprisingly, every $s^{\nu,L,\Pi}$ value of the (3, 1) system, within the numerical accuracy [18], appears in the sequence of $s^{\nu,L,\Pi}$ values of the (2, 2) system. Figure 8 shows that the fractional difference between the $s^{\nu,L,\Pi}$ values of the (3, 1) and (2, 2) systems is of order of or smaller than the numerical accuracy of the extrapolated ZR energies. This suggests that the exact ZR energies of the (3, 1) system at unitarity form a subset of the exact ZR energies of the (2, 2) system at unitarity. These findings are corroborated by extensive perturbative calculations [21].

The calculations presented so far strongly suggest that the (3, 1) energies are degenerate with a subset of the (2, 2) energies in the $r_0 \to 0$ limit for all $a_\nu$. The supplemental material [21] shows, using the stochastic variational and perturbative approaches, that analogous intersystem degeneracies exist for systems with $n = 5$ and 6.

To interpret our observations, we construct a new Hamiltonian $H'$,

$$H' = H_0 + V^{\text{int}},$$

that reproduces the eigen energies of the $(n_1 + 1, n_2 - 1)$ and $(n_1, n_2)$ systems described by $H$ when $r_0 \to 0$. The interaction potential $V^{\text{int}}$ includes interactions between all atom pairs and not just between the spin-up and spin-down pairs,

$$V^{\text{int}} = \sum_{j<k} V_{1b}(r_{jk}).$$

The Hamiltonian $H'$ treats all atom pairs on equal footing. In particular, $V^{\text{int}}$ is the same for the $(n_1 + 1, n_2 - 1)$ and $(n_1, n_2)$ systems. Intuitively, it is clear that the antisymmetry of the eigen functions under the exchange of like atoms “turns off” the interactions between the like atoms when $r_0 \to 0$, thereby ensuring that the energy spectra of $H$ and $H'$ are identical when $r_0 \to 0$. This behavior is illustrated exemplarily in Fig. 4 for the energetically lowest-lying state of the $n = 4$ systems with 1$^+$ symmetry interacting through the Gaussian model potential. In the $r_0 \to 0$ limit, the eigen energies of $H$ and $H'$ agree for the (2, 2) and (3, 1) systems; moreover, as already pointed out above, the eigen energies of the (3, 1) and (2, 2) systems described by $H$ are characterized by different slopes while the eigen energies of the (3, 1) and (2, 2) systems described by $H'$ agree within our numerical accuracy for all $r_0$.

The key motivation for introducing the Hamiltonian $H'$ is that it describes all $n$-particle systems with ZR $s$-wave interactions, regardless of the particle statistics. The fact that the $(n_1 + 1, n_2 - 1)$ and $(n_1, n_2)$ systems are described by the same Hamiltonian allows us to tie.
the evidenced degeneracy of the eigen energies to the existence of a symmetry. In particular, according to quantum mechanics \cite{2}, the existence of degenerate eigen energies of a Hamiltonian is a manifestation of an underlying symmetry. Since the Hamiltonian $H'$ is invariant under the permutation of any pair of atoms, the inter-system degeneracies are intimately related to the structure of the permutation group $S_n$. Group theoretical tools are widely used in quantum chemistry and molecular physics to (anti-)symmetrize the wave functions associated with the electronic and nuclear degrees of freedom \cite{22}. Here, they are employed to analyze the properties of the Hamiltonian $H'$, which has been shown to reproduce the eigen spectrum of the original Hamiltonian $H$.

The Hilbert space of the $(n_1, n_2)$ system is spanned by the direct product of the Hilbert spaces of the two single components or, in terms of Young tableaux, $[1^{n_1}] \otimes [1^{n_2}] \ (22, 23)$. Here, $[1^n] = [1, 1, \ldots, 1]$ indicates the fully anti-symmetric tableau of the $n_1$ spin-up fermions. The direct product can be decomposed into a direct sum of Young tableaux that consist of at most two columns $(n_1 \geq n_2)$ \cite{24},

$$[1^{n_1}] \otimes [1^{n_2}] = [1^{n_1+n_2}] \oplus [2, 1^{n_1+n_2-2}] \oplus [2^2, 1^{n_1+n_2-4}] \oplus \cdots \oplus [2^{n_2}, 1^{n_1+n_2-2n_2}].$$

If we replace $n_1$ and $n_2$ in Eq. (6) by $n_1 + 1$ and $n_2 - 1$, respectively, and then compare with the decomposition for the $(n_1, n_2)$ state space, we find that the composition of the $(n_1, n_2)$ state space contains the decomposition of the $(n_1 + 1, n_2 - 1)$ state space,

$$[1^{n_1}] \otimes [1^{n_2}] = ([1^{n_1+1}] \otimes [1^{n_2-1}]) \oplus [2^{n_2}, 1^{n_1-n_2}].$$

This decomposition into irreducible representations shows explicitly that the decomposition of the $(n_1 + 1, n_2 - 1)$ system is contained in that of the $(n_1, n_2)$ system. Correspondingly, the eigen energies of the $(n_1 + 1, n_2 - 1)$ system with ZR interactions form a subset of those of the $(n_1, n_2)$ system with ZR interactions for all $a_s$. Equation (7) shows, in agreement with our earlier discussion, that the $(n_1, n_2)$ system contains additional eigen energies.

In summary, we have identified and interpreted inter-system degeneracies of two-component Fermi gases with ZR interactions under spherically symmetric confinement. The fact that the eigen energies of the $n = 4$ system with spin projection quantum number $M_S = 1$ form a subset of the eigen energies of the $n = 4$ system with $M_S = 0$ (and similarly for $n > 4$) has multiple implications. From a computational point of view, the degeneracies can be used to test the accuracy of various schemes employed to solve the $n$-fermion Schrödinger equation. Moreover, in certain cases it may be easier to treat the energetically lowest lying state of a system with larger $M_S$ than an excited state of a system with smaller $M_S$, allowing one to substitute an excited state calculation by a ground state calculation for a system of the same size but with different $M_S$. The inter-system degeneracies also have experimentally observable implications. Since the change of the energy with scattering length coincides for certain eigen states of the $(n_1 - 1, n_2 + 1)$ and $(n_1, n_2)$ systems, the corresponding eigen states, which characterize two distinctly different physical systems, have the same contact \cite{7,8}. Moreover, the two distinctly different systems share a common set of eigen frequencies. These frequencies can be measured via microwave spectroscopy \cite{26}.

The discussed inter-system degeneracies do not only exist for systems with ZR interactions but also for systems with finite-range interactions such as electronic systems, provided the Hamiltonian under study is invariant under permutation of all particle pairs. This also implies that the degeneracies are not limited to harmonically confined systems but also exist for systems in free space or under non-harmonic confinement, provided the Hamiltonian under study is invariant under permutation. We conclude by noting that our analysis is based on the assumption that the interaction potential is constructed from pairwise two-body interactions. The presence of three-body forces, which are needed to describe non-universal Efimov states or nuclear systems, introduces a new degree of freedom not considered here.

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K. M. Daily, D. Rakshit, and D. Blume

Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

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This material summarizes details of our calculations and results that support the conclusions drawn in the main part of the paper. Sections II and III show, within a perturbative framework, that the inter-system degeneracies exist in the weakly-interacting limits. Section III provides numerical examples for the inter-system degeneracies for two-component gases at unitarity with \( n = 4 \) and 5 atoms. Last, Sec. IV discusses the application of the group theoretical framework discussed in the main text to systems with up to \( n = 6 \) atoms.

I. WEAKLY-ATTRACTIVE FERMI GAS

When \( |a_s|/a_{ho} \ll 1 \) and \( a_s < 0 \), the two-component Fermi gas can be described perturbatively assuming \( \delta \)-function interactions between the spin-up and spin-down atoms. For the perturbative analysis of this regime, we assume that the two-body potential \( V_b(\vec{r}_{jk}) \) in Eq. (3) of the main text is written as \( (4\pi\hbar^2a_s/m)\delta(\vec{r}_{jk}) \). Within first-order degenerate perturbation theory, the relative energy \( E_{n_1,n_2}^{rel} \) of the \((n_1,n_2)\) system can be written in terms of the non-interacting energy \( E_{n_1,n_2}^{rel,ni} \) and an energy shift that is proportional to \( a_s/a_{ho} \):

\[
E_{n_1,n_2}^{rel} = E_{n_1,n_2}^{rel,ni} + (2\pi)^{-1/2} c_{n_1,n_2} a_s a_{ho} \omega.
\]  

The coefficients \( c_{n_1,n_2} \) are system and state dependent. The non-interacting wave functions can be constructed within the hyperspherical coordinate approach \cite{1} or by writing the non-interacting wave functions in terms of a product of determinants built using the single particle harmonic oscillator orbitals \cite{2}. We checked explicitly for \( n = 4 - 6 \) and all possible \((n_1,n_2)\) combinations that the energy shifts are the same for the interaction potentials \( V_{int} \) and \( V'_{int} \), supporting our finding that the Hamiltonians \( H \) and \( H' \), Eqs. (1) and (4) of the main text, are equivalent in the zero-range limit.

Columns 2 and 3 of Table I show the coefficients \( c_{2,2} \) and \( c_{3,1} \) for the \((2,2)\) and \((3,1)\) systems with \( L^\Pi = 1^+ \) symmetry and \( E^{rel,ni} \leq 21\hbar\omega/2 \). Table II shows that every energy shift of the \((3,1)\) system corresponds to an energy shift of the \((2,2)\) system. However, the \((2,2)\) system exhibits energy shifts that are not present in the \((3,1)\) system. We find similar results for the \( n = 4 \) systems with other \( L^\Pi \) symmetries and for the \( n = 5 \) and 6 systems. As an example, Table III summarizes the energy shifts for the \( n = 6 \) system for the first two non-interacting energy manifolds with \( E^{rel,ni} = 23\hbar\omega/2 \) and \( 25\hbar\omega/2 \). Columns 3, 4 and 5 of Table III list the \( c_{3,3}, c_{4,2} \) and \( c_{5,1} \) coefficients for all allowed \( L^\Pi \) symmetries. It can be seen that every energy shift of the \((5,1)\) system corresponds to an energy shift of the \((4,2)\) system. Moreover, every energy shift of the \((4,2)\) system corresponds to an energy shift of the \((3,3)\) system. However, the \((3,3)\) system exhibits energy shifts that are not present in the \((4,2)\) system, and the \((4,2)\) system exhibits energy shifts that are not present in the \((5,1)\) system.

| \( E^{rel,ni}/(\hbar\omega) \) | \( c_{2,2} \) | \( c_{3,1} \) |
|---|---|---|
| 17/2 | 4.50566 | 4.50566 |
| 3 | 1.73167 | 1.73167 |
| 0.512668 | 0.512668 |
| 0 | 0 | |
| 21/2 | 4.96842 | 4.96842 |
| 4.75108 | 4.75108 |
| 4.30231 | 4.30231 |
| 4.09201 | |
| 3 | 2.29699 | 2.29699 |
| 1.83736 | 1.83736 |
| 1.28299 | |
| 1.10983 | 1.10983 |
| 0.534486 | 0.534486 |
| 0 | 0 | |
| 0 | 0 | |
| 0 | 0 | |
| 0 | 0 | |
| 0 | 0 | |
TABLE II: Perturbative energy shifts for the (3, 3), (4, 2) and (5, 1) systems in the weakly-attractive \( a_s < 0 \) regime. The coefficients \( c_{3,3}, c_{4,2} \) and \( c_{5,1} \) are listed for the two energetically lowest lying non-interacting energy manifolds. Within each energy manifold, the coefficients are listed in decreasing order. The \( c_{4,2} \) and \( c_{5,1} \) column contain “blank rows” to highlight that only a subset of the (3, 3) shifts appears in the (4, 2) sequence and that only a subset of the (4, 2) shifts appears in the (5, 1) sequence.

| \( E_{\text{rel, eff}}/\hbar \omega \) | \( L^{\text{I}} \) | \( c_{3,3} \) | \( c_{4,2} \) | \( c_{5,1} \) |
|-----------------|-----------------|--------------|--------------|--------------|
| 23/2            | 0              | 11           | 8.5          | 8.5          |
|                 | 1              |              |              |              |
|                 | 2              |              |              |              |
| 25/2            | 0              | 7.75         | 7.75         |              |
|                 | 2              | 0            | 7            |              |
|                 | 1              |              | 6.25         | 6.25         |
|                 | 0              |              | 7.02013      |              |
|                 | 1              | 9.34613      | 9.34613      |              |
|                 | 1              | 8.58664      | 8.58664      |              |
|                 | 1              | 10.1049      |              |              |
|                 | 2              | 9.125        |              |              |
|                 | 2              | 9.04636      | 9.04636      |              |
|                 | 2              | 8.5          |              |              |
|                 | 2              | 8.11599      | 8.11599      |              |
|                 | 2              | 6.71264      | 6.71264      |              |
|                 | 2              | 5.5          | 5.5          | 5.5          |
|                 | 3              | 10.25        |              |              |
|                 | 3              | 8.59307      | 8.59307      |              |
|                 | 3              | 7.15693      | 7.15693      |              |
|                 | 4              | 8.25         |              |              |
|                 | 4              | 7.75         | 7.75         |              |

II. WEAKLY-REPULSIVE \( a_s > 0 \) REGIME

In the weakly-repulsive regime, the two-component Fermi gas can be thought of as consisting of up to \( n_2 \) composite bosonic molecules and unpaired spin-up and spin-down atoms. If no molecules are formed, the perturbative treatment is the same as for the \( a_s < 0 \) case discussed in the previous section. When molecules form, unpaired spin-up and spin-down fermions interact, as in the \( a_s < 0 \) case, through the \( \delta \)-function potential with s-wave atom-atom scattering length \( a_s \), while spin-up atoms and molecules (and spin-down atoms and molecules) interact through a \( \delta \)-function potential with s-wave atom-dimer scattering length \( a_{ad} \); in addition, the atom mass \( m \) is replaced by \( 4m/3 \) to account for the change of the mass of one of the collision partners. If two or more molecules form, the molecule-molecule interaction is modeled through the \( \delta \)-function potential with s-wave dimer-dimer scattering length \( a_{dd} \) and reduced mass \( m_1 \). Using this effective interaction model, we have calculated the energy shifts for the \( n = 4, 5 \) and 6 systems within first-order degenerate perturbation theory for good portions of the energy spectra. We find that the energy shifts of the \( (n_1 + 1, n_2 - 1) \) system form a subset of the energy shifts of the \( (n_1, n_2) \) system for \( n = 4, 5 \) and 6. Moreover, the energy shifts of the \( (n_1 + 2, n_2 - 2) \) system form a subset of the energy shifts of the \( (n_1 + 1, n_2 - 1) \) system for \( n = 6 \). In the following we provide a qualitative analysis of the \( a_s > 0 \) regime assuming at least one molecule forms.

Figure 1 schematically illustrates the effective systems encountered for \( n = 4, 5 \) and 6 when molecules are formed. The (3, 1) system can form one molecule, denoted by “D” (dimer) while the (2, 2) system can form one or two molecules. However, as we argue now, only a portion of the energy spectrum of the “F+D” system (see Fig. 1) is degenerate with the energy spectrum of the “2F+D” system. While the wave function of the effective (3, 1) system (the “2F+D” system) must be anti-symmetric under the exchange of the two spin-up fermions, no such constraint exists for the effective (2, 2) system (the “F+F+D” system). This implies that the energy spectrum of the effective (3, 1) system containing one molecule forms a subset of the energy spectrum of the effective (2, 2) system containing one molecule. The anal-
ysis of the (4, 1) and (3, 2) systems proceeds similarly. In particular, the “3F+F” system contains more symmetry constraints than the “2F+F′+D” system. The number of atom-dimer interactions are, however, the same. This implies that the energy spectrum of the effective (4, 1) system containing one molecule forms a subset of the energy spectrum of the effective (3, 2) system containing one molecule.

For the $n = 6$ system, the situations where respectively one and two bosonic molecules form need to be considered separately. We first consider the situation where one molecule forms. The degeneracy of a part of the energy spectrum of the “3F+F′+D” system with the energy spectrum of the “4F+D” system can be understood along the same lines as above. For the effective “3F+F′+D” and “2F+2F′+D” systems, in contrast, the situation is a bit more complicated. Intuitively, one may argue that it was shown in Sec. I that the energy shifts of the “3F+F′” system form a subset of the energy shifts of the “2F+2F′” system and that the distinguishable “D” particle cannot “destroy” the degeneracy. For the (4, 2) and (3, 3) systems, two molecules can form. Following the logic above, the effective “2F+2D” system contains more constraints than the “F+F′+D” system. This implies that the energy spectrum of the effective (4, 2) system containing two molecules forms a subset of the energy spectrum of the effective (3, 3) system containing two molecules.

We reiterate that the qualitative pictures discussed here have been confirmed by calculating the energy shifts for good portions of the energy spectra of the $n = 4$, 5 and 6 systems.

III. UNITARITY

Our numerical stochastic variational approach for determining the eigen energies of small trapped few-body systems under external spherical symmetric confinement, interacting through finite-range Gaussian model potentials, is discussed in detail in Ref. [2]. For the discussion here it is important that this approach yields the ground state and excited state energies of trapped few-body systems for any s-wave scattering length $a_s$ and that the accuracy of the eigen energies can be controlled systematically.

Reference [2] tabulates the extrapolated zero-range energies of the (3, 1) and (2, 2) systems described by the Hamiltonian $H$, see Eq. (1) of the main text, at unitarity. These energies and the associated $s_{ν,1/2}^{\nu}$ values were used to make Fig. 3 of the main text. To exemplarily illustrate the degeneracy of a subset of the (2, 2) energies and the (3, 1) energies, Table III summarizes the (2, 2) and (3, 1) energies with $E_{ν,1/2}^{\text{rel}} \leq 2\hbar\omega/2$ and $L^\Pi = 1^+$ symmetry. The second and fourth columns show the corresponding $s_{ν,1/2}^{\nu}$ values, derived from the energies with hyper-radial quantum number $q = 0$. It is easily checked that the relative energies of the (3, 1) system agree with the relative energies of the (2, 2) system to within the numerical uncertainty of 0.1 % of the extrapolated zero-range energies. Similarly good agreement is found for the $n = 4$ systems with other $L^\Pi$ symmetries.

Reference [2] also reports the extrapolated zero-range energies of the (3, 2) and (4, 1) systems at unitarity; these energies have an estimated accuracy of 1 %. For example, the extrapolated zero-range ground state energies of the (4, 1) system with $L^\Pi = 1^+$, $2^+$ and $3^+$ symmetry described by the Hamiltonian $H$ are $7.155\hbar\omega$, $7.494\hbar\omega$, and $7.502\hbar\omega$. For comparison, the extrapolated zero-range energy of the second excited state of the (3, 2) system with $L^\Pi = 1^+$ symmetry is $7.158\hbar\omega$, that of the fourth excited state of the (3, 2) system with $L^\Pi = 2^+$ symmetry is $7.497\hbar\omega$, and that of the second excited state of the (3, 2) system with $L^\Pi = 1^+$ symmetry is $7.504\hbar\omega$. These examples show that the extrapolated zero-range energies of the (4, 1) system described by $H$ form, within the numerical accuracy of Ref. [2], a subset of the extrapolated zero-range energies of the (3, 2) system described by $H$.

IV. APPLICATION OF GROUP THEORETICAL FRAMEWORK

As discussed in the main text, the Hamiltonian $H'$ is invariant under the exchange of any pair of particles and thus described by the symmetric group $S_n$ of degree $n$. In the following, we apply Eqs. (6) and (7) of the main text to weakly-interacting atomic Fermi gases (small $|a_s|$) with $n = 4, 5$ and 6 described by $H'$.

| $E_{ν,1/2}^{\text{rel}}/(\hbar\omega)$ | $s_{ν,2}^{\nu,L_{\Pi}}$ | $E_{ν,1/2}^{\text{rel}}/(\hbar\omega)$ | $s_{ν,1/2}^{ν,L_{\Pi}}$ |
|-------------------------------------|-----------------|-------------------------------------|-----------------|
| 5.0820                             | 4.0820          | 5.0819                              | 4.0819          |
| 7.0822                             |                 | 7.0820                              |                 |
| 7.185                              | 6.1895          | 7.6060                              | 6.6056          |
| 8.1459                             | 7.1459          | 8.1456                              | 7.1456          |
| 8.5000                             | 7.5000          | 8.5000                              | 7.5000          |
| 9.0827                             | 8.9848          | 8.9846                              | 7.9846          |
| 9.1341                             | 8.1341          | 9.1324                              | 8.1324          |
| 9.1908                             |                 | 9.3750                              | 8.3750          |
| 9.4561                             | 8.4561          | 9.4544                              | 8.4544          |
| 9.6070                             |                 | 9.6853                              | 8.6847          |
| 9.7798                             | 8.7798          |                                    |                 |
| 10.148                             | 10.147          |                                    |                 |
We first treat the \( n = 4 \) system. The \( S_4 \) group contains five conjugacy classes or irreducible representations that are characterized by the Young tableaux [4], [3, 1], [2, 2] = [2, 2], [2, 1, 1] = [2, 2, 1, 1] and [1, 1, 1] with degrees \( d_1 = 1, d_{11} = 3, d_{12} = 2, d_{111} = 3 \) and \( d_{1111} = 1 \). According to Eq. (6) of the main text, the properly anti-symmetrized states of the (2, 2) and (3, 1) systems can be decomposed as

\[
[1, 1] \otimes [1, 1] = [1, 1, 1, 1] \oplus [2, 1, 1] \oplus [2, 2]
\]  

and

\[
[1, 1, 1] \otimes [1, 1, 1] = [1, 1, 1, 1, 1] \oplus [2, 1, 1],
\]

respectively. By inspection, this yields Eq. (7) with \( n_1 = n_2 = 2 \) of the main text,

\[
[1, 1] \otimes [1, 1] = ([1, 1, 1] \otimes [1]) \oplus [2, 2].
\]

To see how these decompositions relate to the energy spectra of the (2, 2) and (3, 1) systems, we determine the eigen energies of \( H' \) for small \( |a_s|/\hbar \omega \) perturbatively. We start our discussion by considering the system consisting of four distinguishable particles with equal masses, referred to as the XYZA system. All six two-body interactions are assumed to be characterized by the same s-wave scattering length. Table IV lists the coefficients \( c \) [see Eq. (1)], which determine the perturbative energy shifts, for each \( L^\Pi \) symmetry. Column 4 lists the number of linearly independent eigen states with zero projection quantum number, i.e., the number of eigen states of the XYZA system with a given \( L, \Pi \) and energy shift (and \( M_L = 0 \)).

To construct eigen functions of four-particle systems with a given permutation symmetry, we perform a “post-symmetrization” of the linearly independent eigen functions of the XYZA system. There exist nine physical four-body systems with distinct exchange symmetry: BBBB, BBX, BBBB’, BBXY, BBFF, FFXY, FFFF’ [referred to earlier as the (2,2) system], FFFX [referred to earlier as the (3,1) system], and FFFF. Here, “B” stands for “boson” and “F”, as before, for “fermion”; the particle order does not matter (e.g., the XBBB is equivalent to the BBX) system). The number of properly symmetrized/anti-symmetrized eigen states for these physical systems are listed in columns 5-13 of Table IV for each \( L, \Pi \) and energy shift (\( M_L = 0 \)). The number of linearly independent eigen functions with a given \( L, \Pi \) and energy shift (and \( M_L = 0 \)) (see column four of Table IV) corresponds to the degree of the corresponding irreducible representation of the \( S_4 \) group.

For the \( 9\hbar \omega/2 \) energy manifold, e.g., one eigen state exists. The “highest symmetry” of this eigen state corresponds to the BBBB system, which is associated with the fully symmetric Young tableau [4]. The BBBB state “automatically” also has the proper symmetry of the BBBX, BBBB’ and BBXY systems. The three linearly independent states in the \( 11\hbar \omega/2 \) energy manifold are associated with the Young tableau [3, 1]. Appropriate linear combinations of these linearly independent functions give the properly symmetrized/anti-symmetrized eigen functions of the BBBX, BBBB’, BBXY, BBFF and FFXY systems. The two linearly independent eigen states in the \( 13\hbar \omega/2 \) energy manifold with \( L^\Pi = 0^+ \) and \( c = 13/2 \) are associated with the Young tableau [2, 2]. Appropriate linear combinations of these linearly independent functions give the properly symmetrized/anti-symmetrized eigen functions of the BBBB’, BBXY, FFFX and FFFF’ systems. Lastly, the three linearly independent states in the \( 13\hbar \omega/2 \) energy manifold with \( L^\Pi = 1^+ \) are associated with the Young tableau [2, 1, 1]. Appropriate linear combinations of these linearly independent functions give the properly symmetrized/anti-symmetrized eigen functions of the BBBX, BBFF, FFXY and FFFF’ systems.

The perturbative calculations summarized above show that the eigen states of the FFFF system are, as predicted by Eq. (4), associated with either the [1, 1, 1, 1] or the [2, 1, 1] Young tableaux. In both cases, there exists a corresponding eigen state of the FFFF system [see also Eq. (2)]. It follows that the eigen energies of the FFFF system are degenerate. However, the perturbative calculations show—in agreement with Eqs. (2) and (4)—that there also exist eigen states of the FFFF system that are associated with the [2, 2] Young tableau. No corresponding eigen states with FFFF symmetry exist in this case, explaining the fact that the FFFF system supports a set of eigen energies that are absent in the FFFF spectrum. In selected cases, we have checked that the post-symmetrization approach, applied to the unsymmetrized eigenstates of the XYZA system at unitarity, reproduces the energies of the (2,2) and (3,1) systems reported in Ref. [7]. Similarly, we tied the energy spectra of the (4,1), (3,2), (5,1), (4,2) and (3,3) systems obtained perturbatively and by the stochastic variational approach to the irreducible representations of the symmetric groups \( S_5 \) and \( S_6 \).

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TABLE IV: Perturbative analysis of the trapped \( n = 4 \) system with various symmetries described by the Hamiltonian \( H' \). The first column lists the relative energy of the non-interacting energy manifold considered. The perturbative energy shifts for a given angular momentum \( L \) and parity \( \Pi \) are reported in column three. The energy shifts are calculated without imposing a specific symmetry on the wave functions; the corresponding degeneracies are listed in column four (only states with projection quantum number \( M_L = 0 \) are considered). Columns five through 13 list the number of linearly independent eigen states with a particular particle symmetry that can be constructed from the unsymmetrized states that describe the XYZA system.

| \( E_{\text{rel}}/\hbar \omega \) | \( L^x \) | \( c \) | XYZA | BBBB | BBBBB | BBXY | BBFF | FFXY | FFF'F' | FFFF |
|---|---|---|---|---|---|---|---|---|---|---|
| 9/2 | 0^+ | 12 | 1 | 1 | 1 | 1 | 1 |
| 11/2 | 1^- | 8 | 3 | 1 | 1 | 2 | 1 | 1 |
| 13/2 | 0^+ | 6.5 | 2 | 1 | 1 | 1 | 1 |
| | | 9 | 3 | 1 | 1 | 2 | 1 | 1 |
| | | 14 | 1 | 1 | 1 | 1 | 1 |
| 1^+ | 4 | 3 | 1 | 1 | 2 | 1 | 1 |
| 2^+ | 5 | 2 | 1 | 1 | 1 | 1 |
| | 6 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 8 | 1 | 1 | 1 | 1 | 1 |
| 15/2 | 0^- | 0 | 1 | 1 | 1 | 1 | 1 |
| 1^- | 2.82461 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 4.42539 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 5 | 2 | 1 | 1 | 1 | 1 |
| | 5.12271 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 7.42288 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 9.20442 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 11 | 1 | 1 | 1 | 1 | 1 |
| 2^- | 2 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 3 | 2 | 1 | 1 | 1 | 1 |
| | 4 | 3 | 1 | 1 | 2 | 1 | 1 |
| 3^- | 3.5 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 4 | 3 | 1 | 1 | 2 | 1 | 1 |
| | 6 | 1 | 1 | 1 | 1 | 1 |
| | 6.5 | 3 | 1 | 1 | 2 | 1 | 1 |

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