Degeneracies in Trapped Two-Component Fermi Gases

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

Phys. Rev. Lett. **109**, 030401 — Published 17 July 2012

DOI: 10.1103/PhysRevLett.109.030401

Degeneracies in trapped two-component Fermi gases

K. M. Daily,[1] D. Rakshit,[1] and D. Blume[1]

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

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.

PACS numbers:

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 unitary 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 eigen energies 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 ($n = n_1+n_2$),

$$H = H_0 + V_{\rm int}, \tag{1}$$

where

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

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

$$V_{\rm int} = \sum_{j=1}^{n_1}\sum_{k=n_1+1}^{n} V_{\rm tb}(r_{jk}). \tag{3}$$

In Eq. (1), m denotes the atom mass, ω the angular trapping frequency, and $\vec{r}_j$ the position vector of the jth 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 $V_{\rm g}$ [13] with depth V_0 and range r_0, $V_{\rm g}(r_{jk}) = -V_0\exp[-r^2/(2r_0^2)]$, where $r_{jk} = |\vec{r}_j - \vec{r}_k|$. For a fixed r_0, we adjust the depth V_0 such that $V_{\rm g}$ 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 δ-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 $a_{\rm ho}$, where $a_{\rm ho} = \sqrt{\hbar/(m\omega)}$.

We first consider the Hamiltonian H_0, which describes n NI particles under isotropic harmonic confinement. As

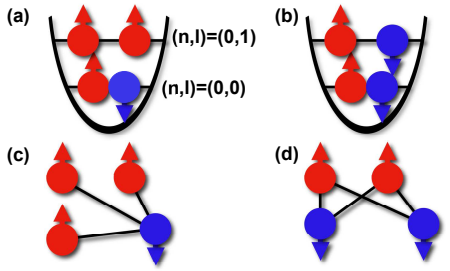

FIG. 1: (Color online) Illustration of the $n = 4$ systems. Panels (a) and (b) show the ground state configurations of the NI trapped $(3, 1)$ and $(2, 2)$ systems. The horizontal solid lines indicate the single particle harmonic oscillator orbitals with energy $(2n + l + 3/2)\hbar\omega$; the $(n, l) = (0, 0)$ and $(0, 1)$ orbitals are respectively one-fold and three-fold degenerate. Solid lines in panels (c) and (d) illustrate the spin-up—spin-down interactions of the $(3, 1)$ and $(2, 2)$ systems.

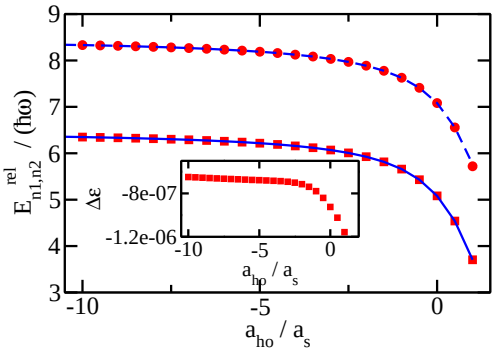

FIG. 2: (Color online) Relative extrapolated ZR energies for the $n = 4$ systems described by H as a function of $a_{\rm ho}/a_s$. Solid and dashed lines show the extrapolated ZR energies of the energetically lowest-lying and second lowest-lying states of the $(3, 1)$ system with 1^+ symmetry while squares and circles show those of the $(2, 2)$ system. The energies of the $(3, 1)$ and $(2, 2)$ systems are indistinguishable on the scale shown. The inset shows the fractional difference $\Delta\epsilon$, $\Delta\epsilon = (E^{\rm rel}_{2,2} - E^{\rm rel}_{3,1})/E^{\rm rel}_{3,1}$, for the energetically lowest-lying state.

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 Π 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 [14]. Just as the NI ground state manifolds of the $(3, 1)$ and $(2, 2)$ systems contain degenerate energies corresponding to the same L^Π 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^Π 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 $V_{\rm g}$, we resort to the stochastic variational approach [13, 15]. 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 Π [15–17]. 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^Π 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 $|a_s|/a_{\rm ho} \ll 1$) 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 2×10^{-4} % for the energetically lowest lying 1^+ state and the scattering lengths considered. Thus, within our numerical accuracy, the energy curves agree throughout

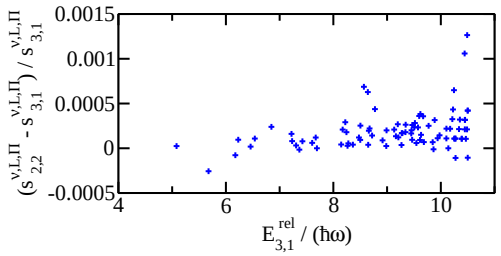

FIG. 3: (Color online) Analysis of the extrapolated ZR energies of the $n = 4$ systems described by H at unitarity. Symbols show the fractional difference Δs, $\Delta s = (s^{\nu,L,\Pi}_{2,2} - s^{\nu,L,\Pi}_{3,1})/s^{\nu,L,\Pi}_{3,1}$, between $s^{\nu,L,\Pi}_{2,2}$ and $s^{\nu,L,\Pi}_{3,1}$ as a function of $E^{\rm rel}_{3,1}$. Δs is of the order of or smaller than the fractional numerical uncertainty of the extrapolated ZR energies.

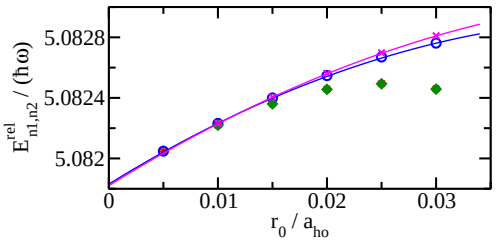

FIG. 4: (Color online) Comparison of the eigen energies of the Hamiltonian H and H' with Gaussian model interactions as a function of $r_0/a_{\rm ho}$ at unitarity. Crosses and circles show the relative eigen energies $E^{\rm rel}_{n_1,n_2}$ of the energetically lowest-lying state with 1^+ symmetry described by H while diamonds and stars show the relative eigen energies of the energetically lowest-lying state with 1^+ symmetry described by H' (on the scale shown, the diamonds and stars are indistinguishable). Solid lines show fits to the relative eigen energies of H.

the crossover.

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 $E^{\rm rel}$ 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 $E^{\rm rel} = (s^{\nu,L,\Pi} + 2q + 1)\hbar\omega$, 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 $E^{\rm rel} \leq 21\hbar\omega/2$, 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 3 shows that the fractional difference between the $s^{\nu,L,\Pi}$ values of the $(3,1)$ and $(2,2)$ systems is of the 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 corrobated 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_s. The supplemental material [21] shows, using the stochastic variational and perturbative approaches, that analogous inter-system degeneracies exist for systems with $n = 5$ and 6. To interpret our observations, we construct a new Hamiltonian H',

$$H' = H_0 + V'_{\rm int}, \tag{4}$$

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 $V'_{\rm int}$ includes interactions between all atom pairs and not just between the spin-up and spin-down pairs,

$$V'_{\rm int} = \sum_{j<k}^{n} V_{\rm tb}(r_{jk}). \tag{5}$$

The Hamiltonian H' treats all atom pairs on equal footing. In particular, $V'_{\rm int}$ is the same for the (n_1+1, n_2-1) and (n_1, n_2) systems. Intuitively, it is clear that the anti-symmetry 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 agree. For finite r_0, 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 quan-

tum mechanics [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 [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, $[1^{n_1}] = [1, 1, \cdots, 1]$ 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 $(n_1 \geq n_2)$ [24],

$$[1^{n_1}] \otimes [1^{n_2}] = [1^{n_1+n_2}] \oplus [2, 1^{n_1+n_2-2}] \oplus \left[2^2, 1^{n_1+n_2-4}\right] \oplus \cdots \oplus [2^{n_2}, 1^{n_1+n_2-2n_2}]. \quad (6)$$

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 decomposition of the (n_1, n_2) state space contains the decomposition of the $(n_1 + 1, n_2 - 1)$ state space,

$$[1^{n_1}] \otimes [1^{n_2}] = \left([1^{n_1+1}] \otimes [1^{n_2-1}]\right) \oplus \left[2^{n_2}, 1^{n_1-n_2}\right]. \quad (7)$$

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 [7–9]. Moreover, the two distinctly different systems share a common set of eigen frequencies. These frequencies can be measured via microwave spectroscopy [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.

Support by the NSF through grant PHY-0855332 and by the ARO is gratefully acknowledged.

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