Universal Properties of a Trapped Two-Component Fermi Gas at Unitarity

D. Blume,[1,2] J. von Stecher,[1] and Chris H. Greene[1]

[1]*Department of Physics and JILA, University of Colorado, Boulder, Colorado 80309-0440, USA*

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

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We treat the trapped two-component Fermi system, in which unlike fermions interact through a two-body short-range potential having no bound state but an infinite scattering length. By accurately solving the Schrödinger equation for up to $N = 6$ fermions, we show that no many-body bound states exist other than those bound by the trapping potential, and we demonstrate unique universal properties of the system: Certain excitation frequencies are separated by $2\hbar\omega$, the wave functions agree with analytical predictions and a virial theorem is fulfilled. Further calculations up to $N = 30$ determine the excitation gap, an experimentally accessible universal quantity, and it agrees with recent predictions based on a density functional approach.

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Ultracold Fermi gases are pure and controllable systems where few- and many-body properties can be studied. Experiments now routinely convert a weakly interacting atomic Fermi gas into a molecular Bose-Einstein condensate (BEC) by tuning the scattering length near a Fano-Feshbach resonance. While the limiting behaviors of this BCS-BEC crossover are well understood, the strongly interacting regime remains fundamental and challenging. In particular, the unitary regime, characterized by a diverging two-body s-wave scattering length a_s, has been the subject of much experimental and theoretical research in the cold-atom community (see Ref. [1] for a review and an exhaustive list of references). Of course, two-component Fermi gases at unitarity also greatly interest the nuclear physics community. Cold atomic Fermi gases and neutron matter with large a_s are two physical realizations of the idealized system described in the "Bertsch problem" [2]. Despite its importance, few essentially exact calculations exist for its energy eigenstates, in part because the system is strongly correlated and has no small parameter for controlled perturbative treatments.

Here, we solve the many-body Schrödinger equation for the trapped unitary Fermi gas with an even or odd number of fermions by two different numerical techniques: a basis set expansion technique that uses correlated Gaussians (CG) and a fixed-node diffusion Monte Carlo (FN-DMC) method. Our energies provide much needed benchmarks for few-body systems with short-range interactions that are important for the atomic, nuclear, and condensed matter physics communities. A key result of our study is a demonstration that this system exhibits unique universal properties resembling those of the noninteracting system.

For the class of two-body potentials that support no s-wave bound state, we find that many-body bound states do not exist for systems with $N \leq 6$ fermions. Our calculated excited-state spectrum for $N \leq 6$ explicitly confirms, to within our numerical accuracy, the assertion by Werner and Castin [3] that the excitation spectrum consists of families of breathing-mode states separated by $2\hbar\omega$. These excitations are nontrivial in the sense that they are not associated with center-of-mass (c.m.) excitations. We interpret this spacing using hyperspherical coordinates and show that in addition to these families of breathing-mode excited states, other excitation frequencies exist that equal noninteger multiples of the trapping frequency. Moreover, the wave functions agree with analytically determined solutions [3], whose functional form was derived on the basis of a universality assumption. Finally, we show that a virial theorem is fulfilled [3,4]. This, together with our finding that negative energy states do not exist, shows explicitly that the entire spectrum of systems with $N \leq 6$ is universal; previously this had been shown explicitly only for the three-body system [5,6], but its likely validity had also been speculated for larger N (see, e.g., Ref. [3], and references therein). A final key point of the present study is a calculation of the excitation gap, for $N \leq 29$. Encouraging agreement is found with results obtained within a density functional theory (DFT) framework [7], and it also sheds light on the applicability of the local density approximation (LDA).

Our starting point is the Hamiltonian H for N mass-m fermions under spherical external confinement with angular trapping frequency ω, $H = T + V_{\rm tr} + V_{\rm int}$, where $T = -\hbar^2/(2m)\sum_{i=1}^{N}\nabla_i^2$, $V_{\rm tr} = \sum_{i=1}^{N} m\omega^2\vec{r}_i^{\,2}/2$, and $V_{\rm int} = \sum_{j=1}^{N_1}\sum_{k=1}^{N_2} V_0(r_{jk})$. Here N_1 and N_2 denote, respectively, the number of spin-up and spin-down fermions ($N = N_1 + N_2$), and $\vec{r}_i$ denotes the position vector of the ith atom. The purely attractive short-range potentials V_0 (identical to those of Ref. [8]) depend on the interparticle distance r_{jk} and are parametrized by two parameters, the depth d and the range R_0, where $R_0 \ll a_{ho}$ and $a_{ho} = \sqrt{\hbar/(m\omega)}$. For a given R_0, d is adjusted so that the first free-space two-body s-wave bound state is just about to exist (i.e., so that $|a_s| = \infty$). To study even-odd oscillations, we set $N_1 = N_2$ for even N, and $N_1 = N_2 + 1$ for odd N. Two numerical

methods are applied to solve the Schrödinger equation for H: the CG and the FN-DMC approach.

The CG approach has previously been used to determine the energy spectrum of the four-fermion system with short-range interactions [8,9]. Here we extend these studies up to $N = 6$ and additionally present structural properties. In our implementation, each basis function is written as a product of the c.m. ground state and a symmetrized product of Gaussian functions each of which depends on one of the $N(N-1)/2$ interparticle distances. The resulting states have vanishing relative orbital angular momentum L_{rel}. To describe the N-atom states with arbitrary L_{rel} in our CG approach, we add an extra noninteracting particle. The Hamiltonian matrix is evaluated analytically. A stochastic variational approach [10] optimizes the basis set and convergence.

Table I summarizes a few selected total energies $E_{\nu n}$ for $N = 3$–6 (throughout this work, c.m. excitations are not considered, i.e., $E_{\mathrm{c.m.}} = \frac{3}{2}\hbar\omega$). For $N = 3$ and 4, calculations for different R_0 indicate that the finite range effect of the reported energies is $\approx 0.02\hbar\omega$ [8,9]. For $N = 5$ and 6, finite range effects are expected to be $\approx 0.1\hbar\omega$. Assignment of the quantum numbers ν and n is discussed below. Our $N = 3$ energies agree with those reported in Ref. [5] and the corresponding s_ν coefficients (defined below) agree with those reported in Ref. [11]. For $N = 5$ and 6, our energies are the first *ab initio* results obtained for this Hamiltonian by a method that is at least, in principle, free of any assumptions. We find that the systems with $N = 5$ ($L_{\mathrm{rel}} = 0$ and 1) and $N = 6$ ($L_{\mathrm{rel}} = 0$) support no negative energy states.

To treat up to $N = 30$ fermions, the Schrödinger equation is solved by the FN-DMC method [12,13]. The proper fermionic antisymmetry is imposed through the use of a guiding function ψ_T. To within statistical uncertainties, the FN-DMC algorithm provides an upper bound to the exact energy, i.e., to the lowest-lying state with the same symmetry as ψ_T. Following Ref. [8], we consider two different functional forms for ψ_T: The nodal surface of ψ_{T1} is constructed by antisymmetrizing a product of pair functions [14], and that of ψ_{T2} coincides with the nodal surface of the noninteracting Fermi gas. Odd N systems are studied using generalizations of the ψ_T defined in Ref. [8] for even N: We find that ψ_{T2} gives the lowest energy up to $N \lesssim 9$ and ψ_{T1} for larger N. Unlike the energy, the unbiased calculation by the FN-DMC approach of observables associated with operators that do not commute with the Hamiltonian is more involved. Here, we use the mixed estimator $\langle A\rangle_{\mathrm{mixed}}$, $\langle A\rangle_{\mathrm{mixed}} = 2\langle A\rangle_{\mathrm{DMC}} - \langle A\rangle_{\mathrm{VMC}}$ [13]. To improve ψ_T, we introduce additional two-body correlations [15,16].

Table II summarizes the ground state energies E_{00} obtained by the FN-DMC approach for $N \leq 30$ (the energies for even N, $N \leq 20$, were already presented in Ref. [8]). For $N \leq 22$, our energies provide more stringent bounds with smaller error bars than those reported previously [17]. For $N = 23$–30, these are the first *ab initio* results available. Comparison with Table I shows that the FN-DMC energies for $N \leq 6$ agree with the CG energies to within 2%. This agreement validates our construction of the nodal surface of ψ_T for $N \leq 6$.

Dilute gases with short-range interactions exhibit unique universal properties at unitarity, such as the predicted behavior that the energy spectrum contains sequences of excited universal breathing-mode states separated by $2\hbar\omega$ [3,18]. This unique feature, specific to the unitary gas, can be intuitively understood by realizing that the only length scale of the problem is given in this limit by the size of the system, i.e., the hyperradius R. Here, R is defined by removing the c.m. vector $\vec{R}_{\mathrm{c.m.}}$ and dividing the remaining $3N-3$ coordinates into the hyperradius R and $3N-4$ hyperangles Ω: $mR^2 = \sum_i m r_i^2 - M R_{\mathrm{c.m.}}^2$, where $M = Nm$. A dimensionality argument then suggests that the functional form of the universal hyperradial potentials $V_{s_\nu}(R)$ should be the same as that of the noninteracting system, which immediately implies the $2\hbar\omega$ energy spacing for any excitation operator that depends on only R.

This argument has been formalized by Werner and Castin for the N particle unitary gas interacting through zero-range pseudopotentials under harmonic confinement [3]: It has been predicted that the adiabatic approximation

TABLE I. CG energies $E_{\nu n}$ for a Gaussian potential; $R_0 = 0.01a_{ho}$ for $N = 3$ and 4, and $0.05a_{ho}$ for $N = 5$ and 6.

N	L_{rel}	$E_{00}/(\hbar\omega)$	$E_{01}/(\hbar\omega)$	$E_{02}/(\hbar\omega)$	$E_{10}/(\hbar\omega)$	$E_{20}/(\hbar\omega)$
3	0	4.682	6.685	8.688	7.637	9.628
3	1	4.275	6.276	8.279	6.868	8.229
4	0	5.028	7.032	9.039	7.464	8.051
5	0	8.03	10.04	12.06	8.83	10.38
5	1	7.53			9.13	
6	0	8.48	10.50	12.52	10.44	11.00

TABLE II. FN-DMC energies E_{00} and expectation values $2\langle V_{\mathrm{tr}}\rangle$, both in units of $\hbar\omega$. The range R_0 of the square-well potential is $0.01a_{ho}$ for $N \leq 20$, and a bit smaller for larger N. Statistical uncertainties of E_{00} are reported in parentheses and of $2\langle V_{\mathrm{tr}}\rangle$ are a few times larger than those of E_{00}.

N	E_{00}	$2\langle V_{\mathrm{tr}}\rangle$	N	E_{00}	$2\langle V_{\mathrm{tr}}\rangle$	N	E_{00}
3	4.281(4)	4.255	13	24.79(9)	24.99	23	51.01(18)
4	5.051(9)	5.028	14	25.92(5)	26.21	24	52.62(20)
5	7.61(1)	7.48	15	29.59(10)	29.86	25	56.85(22)
6	8.64(3)	8.86	16	30.88(6)	31.11	26	58.55(18)
7	11.36(2)	11.20	17	34.64(12)	34.93	27	63.24(22)
8	12.58(3)	12.55	18	35.96(7)	36.39	28	64.39(31)
9	15.69(1)	15.55	19	39.83(15)	40.89	29	69.13(31)
10	16.80(4)	16.82	20	41.30(8)	41.84	30	70.93(30)
11	20.11(7)	19.81	21	45.47(15)			
12	21.28(5)	21.39	22	46.89(9)			

is exact for universal states. For these states, the wave function thus separates into a product of an, in general, unknown R-independent channel function $\Phi_\nu(\Omega)$ and a Ω-independent radial function $F_{\nu n}(R)$, $\Psi^{\rm rel}_{\nu n}(R,\Omega) = R^{(4-3N)/2}F_{\nu n}(R)\Phi_\nu(\Omega)$. For a given hyperangular quantum number ν ($\nu = 0, 1, \ldots$), the radial quantum number n takes the values $n = 0, 1, \ldots$. The description of the strongly interacting many-body system thus reduces to solving a one-dimensional Schrödinger equation for the hyperradial potential $V_{s_\nu}(R)$, which includes part of the kinetic energy and a contribution due to the two-body interactions,

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dR^2} + \frac{m\omega^2R^2}{2} + V_{s_\nu}(R)\right)F_{\nu n} = E^{\rm rel}_{\nu n}F_{\nu n}. \qquad (1)$$

Here, $V_{s_\nu}(R) = \hbar^2 s_\nu(s_\nu+1)/(2mR^2)$. The energies $E^{\rm rel}_{\nu n}$ are related to the total energies $E_{\nu n}$ through $E_{\nu n} = E^{\rm rel}_{\nu n} + E_{\rm c.m.}$. The coefficients s_ν are constants that arise from the integration over the hyperangular Schrödinger equation; their values are, in general, unknown. Owing to the simple functional dependence of Eq. (1) on R, the $E^{\rm rel}_{\nu n}$ and $F_{\nu n}$ can be written down readily [3], $E^{\rm rel}_{\nu n} = (s_\nu + 2n + 3/2)\hbar\omega$ and $F_{\nu n}(R) = R^{s_\nu+1}L_n^{(s_\nu+1/2)}(R^2/a_{ho}^2)\exp(-R^2/2a_{ho}^2)$ (not normalized), where n denotes a non-negative integer, and $L_n^{(s_\nu+1/2)}$ is the Laguerre polynomial. The expression for the $E^{\rm rel}_{\nu n}$ reveals immediately that the spacing between energy levels within a given hyperradial potential curve $V_{s_\nu}(R)$ is independent of s_ν and equals $2\hbar\omega$.

Using the expression for $E^{\rm rel}_{\nu n}$, the E_{00} reported in Tables I and II readily give s_0 for $N \le 30$. For $N \to \infty$, the ground state energy of the trapped and homogenous systems can be connected via the LDA (see, e.g., Ref. [19]), leading to $s_0 \approx \sqrt{\xi_{\rm hom}}E_{\rm NI}/\hbar\omega$. Here, $E_{\rm NI}$ denotes the energy of the noninteracting (NI) trapped system and $\xi_{\rm hom}$ denotes a universal parameter of the bulk system, $\xi_{\rm hom} = 0.42$ [14,16,20,21], which leads to $s_0 \approx 0.65E_{\rm NI}/\hbar\omega$. For the trapped system, we obtained $\xi_{\rm tr} = 0.465$ [8] and $s_0 \approx 0.68E_{\rm NI}/\hbar\omega$. The functional form of V_{s_ν} can also be obtained using a renormalization technique as $N \to \infty$ [22], which leads to $s_0 \approx 0.71E_{\rm NI}/\hbar\omega$ in fairly close agreement with the above values.

To date, the $2\hbar\omega$ spacing of the unitary gas has been verified explicitly only for $N = 3$ [5]. The spacing of the energies $E_{\nu n}$ reported in Table I for $N = 3$–6 for the first few states with $\nu = 0$ agrees with the predicted $2\hbar\omega$ spacing to better than 2%, i.e., within our numerical uncertainty. We additionally verified for $N \le 4$ that this spacing holds for the lowest states with $\nu = 1$ and 2.

Dash-dotted lines in Figs. 1(a) and 1(b) show the potential curves $V(R)$, $V(R) = V_{s_\nu}(R) + m\omega^2R^2/2$, for $N = 4$ for $\nu = 0$ and $\nu = 1$, respectively, calculated using the s_ν coefficients obtained from the CG energies. Dash-dotted lines in Fig. 1(c) show $V(R)$ for $\nu = 0$ for $N = 9$, 12, and 17 (from bottom to top) calculated using the s_0 coefficients

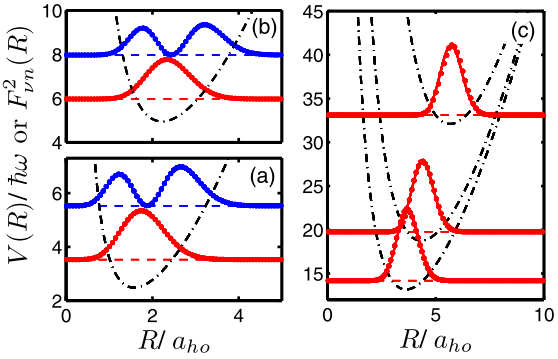

FIG. 1 (color online). Dash-dotted lines show $V(R)$ as a function of R/a_{ho} for (a) $N = 4$ with $\nu = 0$, (b) $N = 4$ with $\nu = 1$, and (c) $N = 9$, 12, and 17 (from bottom to top) with $\nu = 0$. Circles and solid lines show the corresponding $F^2_{\nu n}$ determined numerically and analytically, respectively. Dashed horizontal lines show the energies $E^{\rm rel}_{\nu n}$.

obtained from the FN-DMC energies. Circles and solid lines show the corresponding square of the radial functions $F^2_{\nu n}$ obtained numerically (by integrating $\Psi^2_{\nu n}$ over all coordinates but the hyperradius R) and analytically (using the s_ν coefficients calculated from the CG and FN-DMC energies), respectively. Clearly, our numerically determined $F^2_{\nu n}$ agree well with those determined analytically, providing the first quantitative numerical verification of the interpretation of the $2\hbar\omega$ spacing within the hyperspherical framework for $N > 3$.

Another property of the unitary Fermi gas is that all of its universal states follow a virial theorem, i.e., $E_{\nu n} = 2\langle V_{\rm tr}\rangle_{\Psi^2_{\nu n}}$ [3,4]. Table II shows that the energy expectation value (columns 2 and 5) and the energy obtained using the virial theorem (columns 3 and 6) for $N \le 20$ agree well, providing further evidence for the separability of universal states of the unitary gas and, on the other hand, suggesting that our parametrization of the nodal surface used in the FN-DMC calculations is adequate. The virial theorem has previously been tested at various levels of approximation [7,17,23].

We now use the ground state energies reported in Table II to determine the experimentally measurable exci-

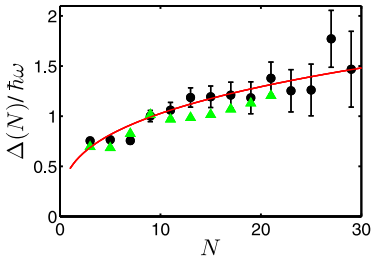

FIG. 2 (color online). Circles show the excitation gap $\Delta(N)$ determined from our FN-DMC energies. A solid line shows $\Delta_{\rm LDA}(N)$ using $\xi_{\rm tr}$ and $\alpha_{\rm tr}$. For comparison, triangles show $\Delta(N)$ determined from the DFT energies [7].

tation gap $\Delta(N)$ for the trapped unitary Fermi gas as a function of N. The definition of the excitation gap for the homogeneous system [20], which equals half the energy it takes to break a pair, can be readily extended to the trapped system [7,17], $\Delta(N) = E_{00}(N) - [E_{00}(N-1) + E_{00}(N+1)]/2$. Circles in Fig. 2 show the excitation gap $\Delta(N)$ obtained from our FN-DMC energies. $\Delta(N)$ increases from $\approx 0.75\hbar\omega$ for $N = 3$ to $\approx 1.5\hbar\omega$ for $N = 29$. For comparison, triangles show $\Delta(N)$ calculated using the DFT energies obtained recently by Bulgac [7]. The agreement between ours and Bulgac's $\Delta(N)$ is quite good.

To gain further insight, we calculate the gap in the LDA, $\Delta_{\mathrm{LDA}}(N) = 3\alpha_{\mathrm{hom}}(3N)^{1/3}\hbar\omega/(8\sqrt{\xi_{\mathrm{hom}}})$. The universal parameter α describes the even-odd oscillations: α_{hom} equals 0.85 for the bulk system [21], and we find $\alpha_{\mathrm{tr}} = 0.60$ for the trapped system. $\Delta_{\mathrm{LDA}}(N)$, shown in Fig. 2 by a solid line using ξ_{tr} and α_{tr}, provides a good description of our FN-DMC results. The fact that α_{tr} is noticeably smaller than α_{hom} suggests that the extra particle is not distributed uniformly throughout the cloud. Indeed, our density profiles for $N \gtrsim 11$ (not shown) indicate that the extra particle sits near the surface of the cloud. In the LDA, the center should be described well but not the surface, so LDA might fail here. Recently, Son proposed that the gap increases with $N^{1/9}$ as $N \to \infty$ [24]. A fit of our results for $\Delta(N)$ for $N \geq 9$ shows consistency with the $N^{1/9}$ dependence but does not conclusively confirm it.

In summary, we have shown that trapped two-component unitary Fermi gases with $N \leq 6$ support no negative energy states. While our FN-DMC calculations do not exclude the presence of negative energy states for larger N, we find no evidence for their existence. A variational analysis predicts an upper bound for the system size N_{cr} at which nonuniversal states exist of ≈ 40. To obtain N_{cr} we consider the Gaussian two-body potential and take the variational many-body wave function of the untrapped system to coincide with that of a trapped noninteracting two-component Fermi gas. The confinement width is treated as a variational parameter, and N is increased till a negative energy state is found. The absence of negative energy states for $N \leq 6$ fermions explains the stability of equal-mass two-component Fermi gases. Furthermore, we explicitly verify a number of unique properties of the universal states of the unitary Fermi gas. The particular form of the energy spectrum has consequences: It should be possible to verify experimentally that for each excitation frequency ω_{ex} there exists a ladder of non c.m. excitations $\omega_{\mathrm{ex}} + 2n\omega$ (n integer). Furthermore, the s_ν coefficients calculated here for the trapped system remain valid for the free-space system [3]. Finally, we calculate the excitation gap $\Delta(N)$ for $N \leq 29$ and find good agreement with recent DFT results. $\Delta(N)$ increases with N and the excess atom leads for $N \gtrsim 11$ to an increase of the density in the surface region.

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