

# Trapped unitary two-component Fermi gases with up to ten particles

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The properties of two-component Fermi gases with zero-range interactions are universal. We use an explicitly correlated Gaussian basis set expansion approach to investigate small equal-mass two-component Fermi gases under spherically symmetric external harmonic confinement. At unitarity, we determine the ground-state energy for systems with up to 10 particles interacting through finite-range two-body potentials for both even and odd numbers of particles. We extrapolate the energies to the zero-range limit using a novel scheme that removes the linear and, in some cases, also the quadratic dependence of the ground-state energies on the two-body range. Our extrapolated zero-range energies are compared with results from the literature. We also calculate the two-body Tan contact and structural properties.

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## I. INTRODUCTION

The properties of two-component Fermi gases interacting through two-body zero-range potentials with  $s$ -wave scattering length  $a_s$  are universal [1,2]. At unitarity, i.e., for infinitely large  $a_s$ , the two-body interaction does not define a meaningful length scale and the strongly interacting Fermi gas is characterized by the same number of length scales as the noninteracting Fermi gas. Approximate realizations of the unitary Fermi gas include dilute neutron matter in the crusts of neutron stars [3] and ultracold atom gases such as  $^6\text{Li}$  [4] and  $^{40}\text{K}$  [5]. The properties of homogeneous and inhomogeneous unitary Fermi gases have attracted a great deal of experimental and theoretical attention. For spherically symmetric external confinement, the harmonic oscillator length  $a_{\text{ho}}$  defines the only length scale of the system. It is hence interesting to determine how the properties of trapped unitary Fermi gases vary with the number of particles.

Harmonically trapped Fermi gases at unitarity have been treated by quantum Monte Carlo methods [6–13], density functional theory (DFT) [11,14–17], and basis set expansion approaches. The accuracy of the fixed-node diffusion Monte Carlo (FN-DMC) energies [7,8,11,12] depends on the quality of the many-body nodal surface. The resulting energies provide upper bounds to the exact ground-state energies and the zero-range limit is reached through extrapolation [11,12]. Auxiliary-field quantum Monte Carlo (AFMC) methods, on the other hand, work on a finite lattice and extrapolation to the infinite lattice limit is required to obtain fully converged results [12]. The quality of DFT calculations depends critically on the underlying functional. Since the functional is typically obtained by matching to data for the homogeneous system, the analysis of results for the trapped system can provide insights into gradient corrections and other finite-size features [15–17]. Trapped unitary Fermi gases with up to six particles have been calculated by explicitly correlated Gaussian (ECG) basis set expansion approaches [7,8,18–22] with better than about 1% accuracy. Application of the ECG method to systems with more than six particles has been challenging due to the rapid increase of the number of permutations and the larger number of degrees of freedom. Recently, Ref. [23] treated the  $(N_1, N_2) = (4, 4)$  system at unitarity using a basis set that accounts for the most important but not all correlations.

Here we present results for small trapped unitary Fermi gases with  $N \leq 10$  particles, where  $N = N_1 + N_2$  and  $N_1 - N_2 = 0$  or 1. Our extrapolated zero-range energy of the (4,4) system is 0.9% lower than that reported in Ref. [23]. A new aspect of our work is that we developed an improved scheme for extrapolating the finite-range energies to the zero-range limit. This new scheme eliminates the linear and, in some cases, the quadratic dependence of the ground-state energies on the two-body range. The scheme provides a consistency check on the range dependence of our energies and reduces the errors that result from the extrapolation to the zero-range limit. Our results suggest that the developed range correction scheme allows one to obtain a reliable approximation to the zero-range energy from a single finite-range calculation. The scheme can be applied to other numerical calculations that work with finite-range interactions. We use our range correction scheme to determine the zero-range energies and the Tan contact for two-component Fermi gases with  $N \leq 10$  at unitarity. In addition, we present selected structural properties.

The remainder of this paper is organized as follows. Section II discusses the theoretical framework and our extrapolation scheme to the zero-range limit. Section III presents our results for systems with up to 10 particles and compares, where available, with results from the literature. Last, Sec. IV concludes.

## II. THEORETICAL FRAMEWORK

We consider equal-mass two-component Fermi gases with  $N_1$  spin-up and  $N_2$  spin-down atoms ( $N = N_1 + N_2$  and  $N_1 - N_2 = 0$  or 1) under external spherically symmetric harmonic confinement with angular trapping frequency  $\omega$ . The system Hamiltonian  $H(r_0)$  reads

$$H(r_0) = \sum_{i=1}^N -\frac{\hbar^2}{2m} \nabla_i^2 + V_{\text{tr}}(\vec{r}_1, \dots, \vec{r}_N) + \sum_{i=1}^{N_1} \sum_{j=N_1+1}^N V_{2b}(r_{ij}, r_0), \quad (1)$$

where  $m$  denotes the atom mass,  $\vec{r}_i$  denotes the position vector of the  $i$ th particle with respect to the trap center, and

$$V_{\text{tr}}(\vec{r}_1, \dots, \vec{r}_N) = \sum_{i=1}^N \frac{1}{2} m \omega^2 \vec{r}_i^2 \quad (2)$$

is the trapping potential.  $V_{2b}$  is the interspecies two-body interaction potential that depends on the interparticle distance  $r_{ij}$ ,  $r_{ij} = |\vec{r}_i - \vec{r}_j|$ . In our work, it is modeled by a finite-range Gaussian potential with range  $r_0$  and depth  $V_0$  ( $V_0 < 0$ ),

$$V_{2b}(r, r_0) = V_0 \exp\left(-\frac{r^2}{2r_0^2}\right). \quad (3)$$

For a fixed  $r_0$ ,  $V_0$  is adjusted such that  $V_{2b}(r, r_0)$  has an infinitely large  $s$ -wave scattering length  $a_s$  and supports one zero-energy two-body bound state in free space. The ranges  $r_0$  considered depend on the size of the system and vary from  $0.01a_{\text{ho}}$  to  $0.12a_{\text{ho}}$ , where  $a_{\text{ho}}$  denotes the harmonic oscillator length [ $a_{\text{ho}} = \sqrt{\hbar/(m\omega)}$ ]. For the Gaussian potential with one zero-energy bound state, the effective range  $r_{\text{eff}}$  is approximately equal to  $2.032r_0$ .

To numerically solve the Schrödinger equation for the Hamiltonian given in Eq. (1), we separate off the center-of-mass degrees of freedom and expand the eigenstates of the relative Hamiltonian in terms of ECG basis functions, which depend on a set of nonlinear variational parameters that are optimized through energy minimization (see below) [18,24]. The unsymmetrized basis functions for states with  $L^\pi = 0^+$  and  $1^-$  symmetry ( $L$  denotes the relative orbital angular momentum and  $\pi$  the relative parity) read  $\exp(-\frac{1}{2}\vec{x}^T A \vec{x})$  and  $\mathcal{Y}_{10}(\vec{u}^T \vec{x}) \exp(-\frac{1}{2}\vec{x}^T A \vec{x})$ , respectively, where  $A$  is a symmetric and positive definite  $(N-1) \times (N-1)$  parameter matrix,  $\vec{u} = (u_1, u_2, \dots, u_{N-1})^T$  is a  $N-1$  dimensional vector, and  $\mathcal{Y}_{10}$  is a solid spherical harmonic function [24].  $\vec{x} = (\vec{x}_1, \vec{x}_2, \dots, \vec{x}_{N-1})^T$  collectively denotes a set of  $N-1$  Jacobi vectors. The ground state of even- $N$  systems has  $0^+$  symmetry and that of odd- $N$  systems has  $1^-$  symmetry. A key advantage of these basis functions is that the corresponding overlap and Hamiltonian matrix elements can be calculated analytically [24].

The fermionic exchange symmetry is ensured by acting with the anti-symmetrization operator  $\mathcal{A}$  on the unsymmetrized basis functions. The number of permutations  $N_p$  increases factorially with the number of identical fermions. For the (5,5) system, e.g.,  $\mathcal{A}$  contains  $(5!)^2 = 14\,400$  two-particle exchange operations with alternating plus and minus signs. The evaluation of each overlap and Hamiltonian matrix element involves a sum over  $N_p$  terms that are highly oscillatory. In a standard 16-digit floating point implementation, numerical challenges arise from the near-cancellation of the positive and negative terms for systems with  $N > 8$ . The near-cancellation of these terms of alternating signs can be interpreted as a relative of the fermion sign problem known from Monte Carlo simulations [25,26]. To ensure that the matrix elements for the largest systems considered are accurate to at least 10 significant digits, we implemented our C codes using extended precision. The eigenenergies and expansion coefficients are obtained by solving a generalized eigenvalue problem that involves the Hamiltonian matrix and the overlap matrix. The numerical error of the resulting eigenenergies is several orders of magnitude smaller than the errors that arise from the use of a finite basis set and the extrapolation to the zero-range limit. In Sec. III, we report the total ground-state energy  $E(r_0)$  of the Hamiltonian  $H(r_0)$ , i.e., we add the center-of-mass energy of  $3E_{\text{ho}}/2$  to the relative energy obtained by use of the ECG

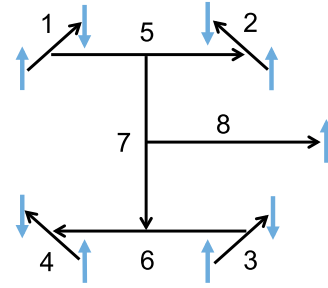


FIG. 1. (Color online) Illustration of the Jacobi coordinates employed in our work for the  $(N_1, N_2) = (5, 4)$  system. The dark vectors show the Jacobi vectors  $\vec{x}_1, \vec{x}_2, \dots, \vec{x}_8$ . The spin-up and spin-down fermions are represented by light vertical up and down arrows.

approach. Here  $E_{\text{ho}}$  denotes the harmonic oscillator energy ( $E_{\text{ho}} = \hbar\omega$ ).

We use a semistochastic variational approach to choose and optimize the variational parameters contained in  $A$  and  $\vec{u}$  [24]. Our Jacobi coordinates are chosen such that the first  $N_2$  Jacobi vectors correspond to distance vectors between unlike particle pairs. The next  $N_2/2$  Jacobi vectors correspond to the distance vectors between the center of mass of the first pair and the second pair, the distance vector between the center of mass of the third pair and the fourth pair, and so on. The remaining Jacobi vectors connect the larger subunits and, for odd  $N$ , the  $N$ th particle (see Fig. 1 for an illustration for  $N = 9$ ). For this choice of Jacobi coordinates, the first  $N_2$  diagonal elements of the  $A$  matrix represent correlations between unlike particles. We expect that these interspecies distances are, on average, smaller and more strongly correlated than those between like particles. This motivates us to choose the first  $N_2$  diagonal elements of the  $A$  matrix for each basis function from a preset nonlinear grid. Specifically, the minimum and maximum Gaussian widths for the unlike pairs are set to  $r_0/2$  and  $2a_{\text{ho}}$ , and a cubic grid, which places more points in the small-width region, is employed. The other diagonal elements are chosen stochastically from preset parameter windows. As in Ref. [23], we start with basis functions that are diagonal in  $A$ . These basis functions account for the most important correlations. Once a certain basis set size is reached (for the larger systems around  $N_b = 500$ ), we reoptimize the variational parameters contained in the diagonal of  $A$ , and for odd  $N$  in  $\vec{u}$ , and allow for off-diagonal  $A$  matrix elements. The off-diagonal matrix element at position  $(i, j)$  of the  $A$  matrix is chosen from 0 to the geometric mean of the  $i$ th and  $j$ th diagonal elements. We find that this choice results with high probability in positive-definite  $A$  matrices. The positive-definiteness of the  $A$  matrix is tested through diagonalization. We refer to the reoptimization of all variational parameters contained in  $A$  and, if applicable,  $\vec{u}$  of all  $N_b$  basis functions as a reoptimization cycle. The reoptimization cycle is repeated until the lowest energy changes by less than a preset value. After that, we extend the basis set by a hundred to several hundred basis functions and reoptimize the variational parameters of the enlarged basis set using a variable number of reoptimization cycles. This process is repeated a few times. At the end, the basis is enlarged to around 2000 basis functions without additional reoptimization of the nonlinear variational parameters.

TABLE I. Ground-state energy of the (3,2) system at unitarity. Column 2 shows the finite-range energy for the largest basis set considered. The estimated basis set error  $\Delta E(r_0)$  is reported in column 3. Columns 4 and 5 report the quantities  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$ ; error bars are given in parentheses. The energy derivatives are calculated for the largest basis set considered. Columns 6–8 report the energies  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ . These energies account for the estimated basis set extrapolation error, i.e.,  $E(r_0) - \Delta E(r_0)$  is being used to calculate  $E_{ZRA,j}(r_0)$  for  $j = 0, 1$ , and  $2$ . The error bars of  $E_{ZRA,1}(r_0)$  and  $E_{ZRA,2}(r_0)$  account for the uncertainties of  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$  but do not account for the uncertainty of  $\Delta E(r_0)$ . The last row reports the extrapolation of  $E_{ZRA,j}(r_0)$  to the zero-range limit.

$\frac{r_0}{a_{ho}}$	$\frac{E(r_0)}{E_{ho}}$	$\frac{\Delta E(r_0)}{E_{ho}}$	$E^{(1)}(r_0) \frac{a_{ho}}{E_{ho}}$	$E^{(2)}(r_0) \frac{a_{ho}^2}{E_{ho}}$	$\frac{E_{ZRA,0}(r_0)}{E_{ho}}$	$\frac{E_{ZRA,1}(r_0)}{E_{ho}}$	$\frac{E_{ZRA,2}(r_0)}{E_{ho}}$
0.07	7.5449	0.0001	1.148(7)	-5.13(12)	7.5448	7.4644(5)	7.4518(8)
0.06	7.5332	0.0001	1.201(8)	-4.61(25)	7.5331	7.4610(5)	7.4527(9)
0.05	7.5211	0.0004	1.240(12)	-4.11(28)	7.5207	7.4587(6)	7.4536(10)
0.04	7.5084	0.0004	1.284(15)	-2.85(33)	7.5080	7.4566(6)	7.4543(9)
0.03	7.4954	0.0006	1.297(26)	-0.32(46)	7.4948	7.4559(8)	7.4557(10)
0.02	7.4825	0.0009	1.290(120)	0.24(96)	7.4816	7.4558(24)	7.4559(26)
0					7.4557	7.4550	7.4563

The basis set errors reported in Tables I and II of Sec. III and Tables I–VI of the Supplemental Material [27] are estimated by analyzing the energy decrease that results from the basis set enlargements and the reoptimization cycles. Specifically, we find that the energy decrease decreases with each consecutive reoptimization cycle and enlargement of the basis set by the same number of basis functions, suggesting that the ground-state energy is converging. Based on extensive calculations for the smaller systems and selected tests for the larger systems, we estimate that the basis set error is roughly equal to 3 times the combined energy decrease of the last reoptimization cycle and the final basis set enlargement. It should be noted that our estimation of the basis set error depends on our implementation of the reoptimization cycle (e.g., how many “trials” are used to optimize each nonlinear variational parameter, etc.).

To reach the universal regime where  $a_{ho}$  defines the only length scale in the system, we need to extrapolate the numerically calculated finite-range energies to the zero-range limit. In previous ECG works [18,19,21–23], this was done by fitting the finite-range energies by a linear or quadratic function. We refer to this traditional extrapolation scheme as the zeroth-order extrapolation scheme. The difference between the finite-range energies and the extrapolated zero-range energies is, typically, at the order of a few percentages and can introduce a non-negligible extrapolation error. Moreover, for larger systems, it is computationally expensive, maybe even prohibitively expensive, to obtain energies at very small ranges. It should also be noted that the extrapolated zero-range energies do not provide variational upper bounds even though

the finite-range ECG energies do. It is thus desirable to remove the linear and, ideally, quadratic range dependence. Motivated by the generalized virial theorem

$$E(0) = 2V_{tr}(0) \quad (4)$$

[ $V_{tr}(0)$  denotes the expectation value of  $V_{tr}(\vec{r}_1, \dots, \vec{r}_N)$  for  $r_0 \rightarrow 0$ ] at unitarity, Werner [28] proposed to remove the linear range dependence of the ground-state energy by combining it with the expectation value  $V_{tr}(r_0)$  of the trapping potential  $V_{tr}(\vec{r}_1, \dots, \vec{r}_N)$  calculated for the same  $r_0$ ,

$$E(0) = 3E(r_0) - 4V_{tr}(r_0) + O(r_0^2). \quad (5)$$

While Eq. (5) removes the leading-order range dependence, it is associated with error bars that come from the basis set errors of  $E(r_0)$  and  $V_{tr}(r_0)$ . In our ECG method, the basis set is optimized by minimizing the ground-state energy. Not surprisingly, we find that the convergence of the expectation value of the trapping potential is not as good as that of the energy. This motivates us to propose an alternative scheme that can be carried out to higher orders.

The ground-state energy  $E(r_0)$  of the  $N$ -particle system is a smooth function of the two-body interaction range  $r_0$ . The  $n_{max}$ th order Taylor series of  $E(\bar{r}_0)$  around  $r_0$  is

$$E(\bar{r}_0) = \sum_{n=0}^{n_{max}} E^{(n)}(r_0) \frac{1}{n!} (\bar{r}_0 - r_0)^n + O[(\bar{r}_0 - r_0)^{n_{max}+1}], \quad (6)$$

where

$$E^{(n)}(r_0) = \left. \frac{\partial^n E(\bar{r}_0)}{\partial \bar{r}_0^n} \right|_{\bar{r}_0=r_0} \quad (7)$$

TABLE II. Same as Table I but for the (4,4) system at unitarity.

$\frac{r_0}{a_{ho}}$	$\frac{E(r_0)}{E_{ho}}$	$\frac{\Delta E(r_0)}{E_{ho}}$	$E^{(1)}(r_0) \frac{a_{ho}}{E_{ho}}$	$E^{(2)}(r_0) \frac{a_{ho}^2}{E_{ho}}$	$\frac{E_{ZRA,0}(r_0)}{E_{ho}}$	$\frac{E_{ZRA,1}(r_0)}{E_{ho}}$	$\frac{E_{ZRA,2}(r_0)}{E_{ho}}$
0.1	12.329	0.010	2.07(10)	-18(3)	12.319	12.113(10)	12.011(25)
0.08	12.287	0.018	2.44(16)	-16(4)	12.269	12.073(13)	12.015(26)
0.06	12.230	0.022	2.72(25)		12.208	12.045(15)	
0.05	12.204	0.025	2.71(32)		12.179	12.043(16)	
0.04	12.184	0.035	2.56(55)		12.149	12.047(22)	
0					12.015	12.019	

is the  $n$ th-order derivative of the ground-state energy with respect to the range evaluated at  $r_0$ .  $E^{(0)}(r_0)$  is simply the ground-state energy  $E(r_0)$  of  $H(r_0)$ .  $E^{(1)}(r_0)$  can be obtained through the Hellmann-Feynman theorem [29],

$$E^{(1)}(r_0) = \left\langle \frac{\partial H(\bar{r}_0)}{\partial \bar{r}_0} \bigg|_{\bar{r}_0=r_0} \right\rangle, \quad (8)$$

which is exact in the limit that the basis set is complete. The matrix elements needed to evaluate  $E^{(1)}(r_0)$  reduce to compact analytical expressions.  $E^{(2)}(r_0)$  can be obtained by the finite-difference method, i.e., by evaluating  $E^{(1)}(r_0)$  at two nearby  $r_0$ .

Our goal is to obtain the zero-range energy  $E(0)$ . Setting  $\bar{r}_0$  in Eq. (6) to 0, we obtain

$$E(0) = E_{\text{ZRA},n_{\text{max}}}(r_0) + O(r_0^{n_{\text{max}}+1}), \quad (9)$$

where

$$E_{\text{ZRA},n_{\text{max}}}(r_0) = \sum_{n=0}^{n_{\text{max}}} E^{(n)}(r_0) \frac{1}{n!} (-r_0)^n \quad (10)$$

is the  $n_{\text{max}}$ th-order approximation to the zero-range energy. Equations (9) and (10) establish a relation between the zero-range energy  $E(0)$  and the finite-range energy  $E(r_0)$  and its derivatives with respect to the two-body range.  $E_{\text{ZRA},0}(r_0)$  is simply the finite-range energy  $E(r_0)$  with linear leading-order range dependence. The leading-order range dependence of  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  is quadratic and cubic, respectively. Crucial is that  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  are obtained at finite  $r_0$  without extrapolation. They provide better approximations to the zero-range energy  $E(0)$  than  $E_{\text{ZRA},0}(r_0)$ . We refer to the extrapolations of  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  to the zero-range limit as the first- and second-order extrapolation schemes. For a complete basis,  $E_{\text{ZRA},1}(r_0)$  coincides with the quantity  $3E(r_0) - 4V_{\text{tr}}(r_0)$ , i.e., formally Eq. (9) with  $n_{\text{max}} = 1$  is equivalent to Eq. (5). It turns out, however, that our ECG implementation provides a more accurate estimate for  $E^{(1)}(r_0)$  than for  $V_{\text{tr}}(r_0)$ . In Sec. III, we independently fit  $E_{\text{ZRA},0}(r_0)$ ,  $E_{\text{ZRA},1}(r_0)$ , and  $E_{\text{ZRA},2}(r_0)$  and compare the resulting zero-range energies. The Appendix shows that the functional forms of  $E_{\text{ZRA},0}(r_0)$ ,  $E_{\text{ZRA},1}(r_0)$ , and  $E_{\text{ZRA},2}(r_0)$  are correlated and presents the results of a single combined fit of  $E_{\text{ZRA},0}(r_0)$ ,  $E_{\text{ZRA},1}(r_0)$ , and  $E_{\text{ZRA},2}(r_0)$ . The resulting zero-range energy is found to be consistent with the zero-range energies obtained from the independent fits.

The ECG calculations become numerically more challenging with decreasing two-body interaction range  $r_0$ . The challenges arise from the need to resolve length scales of different orders of magnitude. In previous ECG calculations [21,22], much effort was put on solving the Schrödinger equation for systems with small  $r_0$ . In this work, we show that a reliable approximation to the zero-range energy can be obtained by calculating  $E_{\text{ZRA},2}(r_0)$  at a range  $r_0 \approx 0.1a_{\text{ho}}$ . We demonstrate in Sec. III that  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  play important roles in obtaining the zero-range energy  $E(0)$  and its error bar.

To calculate the two-body Tan contact  $C(r_0)$  at unitarity, we use the adiabatic energy relation [30],

$$C(r_0) = \frac{4\pi m}{\hbar^2} \frac{\partial E(r_0)}{\partial (-a_s^{-1})} \bigg|_{a_s^{-1}=0}. \quad (11)$$

To obtain the two-body contact for  $r_0 = 0$ , we use the zeroth- and first-order zero-range extrapolation schemes, i.e., we extrapolate  $C_{\text{ZRA},0}(r_0)$  and

$$C_{\text{ZRA},1}(r_0) = C(r_0) - \frac{\partial C(\bar{r}_0)}{\partial \bar{r}_0} \bigg|_{\bar{r}_0 \rightarrow r_0} r_0 \quad (12)$$

to the zero-range limit.

The contact alternatively can be calculated through the pair relation

$$C(r_0) = N_1 \times N_2 \times \lim_{r \rightarrow 0, r \gg r_0} (4\pi)^2 P_{12}(r) r^2, \quad (13)$$

where  $P_{12}(r)$  denotes the pair distribution function. The quantity  $r^2 P_{12}(r)$  with normalization  $4\pi \int_0^\infty P_{12}(r) r^2 dr = 1$  tells one the likelihood of finding two unlike particles at distance  $r$  from each other. The behavior of  $4\pi P_{12}(r) r^2$  around  $r \approx r_0$  depends on the details of the two-body interaction potential. Specifically, for finite-range potentials the quantity  $4\pi P_{12}(r) r^2$  goes to zero as  $r \rightarrow 0$ . For the zero-range potential, in contrast,  $4\pi P_{12}(r) r^2$  remains finite as  $r \rightarrow 0$ . Thus, to extract the finite-range contact via the pair relation, we consider the region where  $r \gg r_0$  but  $r \ll a_{\text{ho}}$ . In practice, the condition  $r \gg r_0$  translates to  $r \gtrsim 2r_0$ .

We also consider the spherically symmetric radial density  $P_j(r)$  of species  $j$ ,  $j = 1$ , and 2. For even  $N$ , we have  $P_1(r) = P_2(r)$ . The quantity  $P_j(r)$  tells one the likelihood of finding a particle at distance  $r$  from the trap center. The normalization is chosen such that  $4\pi \int_0^\infty P_j(r) r^2 dr = 1$ .

### III. RESULTS

This section discusses the energies and other observables of the systems with  $N \leq 10$  obtained by the ECG method. We use the (3,2) system to explain our new range correction scheme. Column 2 of Table I shows the finite-range energies  $E(r_0)$  obtained by use of the ECG approach for various two-body interaction ranges  $r_0$ . The reported energies are obtained for the largest basis set considered. They provide variational upper bounds for the finite-range Hamiltonian with Gaussian interaction. Column 3 reports the estimated basis set error  $\Delta E(r_0)$ . For all  $r_0$  considered, the basis set error is less than 0.02%. Columns 4 and 5 show the quantities  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$ , respectively. While  $E^{(1)}(r_0)$  increases slightly with decreasing range  $r_0$ , this increase is smaller than the decrease of  $r_0$ , implying that the range correction  $E^{(1)}(r_0)r_0$  decreases with decreasing  $r_0$ . The magnitude of  $E^{(2)}(r_0)$  decreases with decreasing  $r_0$ . Note that we are not able to estimate  $E^{(2)}(r_0)$  reliably for small  $r_0$  (the error bars are larger than the quantity itself). Yet, the error bars of  $E^{(2)}(r_0)$  allow us to estimate the maximal correction proportional to  $r_0^2$  for each  $r_0$ , thereby providing us with another means to estimate error bars. Columns 6–8 of Table I show  $E_{\text{ZRA},j}(r_0)$  with  $j = 0, 1$ , and 2. These values are obtained by subtracting the basis set error  $\Delta E(r_0)$ . The leading-order range dependence of  $E_{\text{ZRA},0}(r_0)$  is linear and we perform a fit of the form  $c_0 + c_1 r_0 + c_2 r_0^2 + c_3 r_0^3$ . The extrapolated zero-range energy is reported in the last row of column 6. The leading-order range dependence of  $E_{\text{ZRA},1}(r_0)$  is quadratic and we perform a fit of the form  $c_0 + c_2 r_0^2 + c_3 r_0^3 + c_4 r_0^4$ , weighted by the inverse square of the uncertainty. The extrapolated zero-range energy

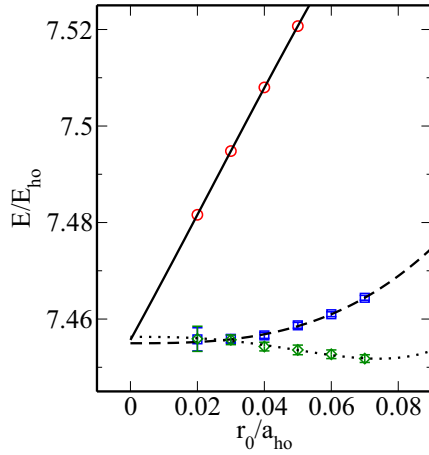


FIG. 2. (Color online) Ground-state energy of the (3,2) system at unitarity as a function of  $r_0$ . Circles, squares, and diamonds show the energies  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ , respectively, reported in the last three columns of Table I. The uncertainty of  $\Delta E(r_0)$  is not accounted for by the error bars. Solid, dashed, and dotted lines show polynomial fits to  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ .

is reported in the last row of column 7. The leading-order range dependence of  $E_{ZRA,2}(r_0)$  is cubic and we perform a fit of the form  $c_0 + c_3 r_0^3 + c_4 r_0^4$ , weighted by the inverse square of the uncertainty. The extrapolated zero-range energy is reported in the last row of column 8. Table I shows that the zeroth-, first-, and second-order extrapolation schemes yield zero-range energies that differ by at most  $0.0013 E_{ho}$ . This confirms that the range dependence of the (3,2) ground-state energy for the  $r_0$  considered is well described by a Taylor series. Moreover, we note that  $E_{ZRA,2}(r_0)$  for  $r_0 = 0.07 a_{ho}$  differs by only  $0.0045 E_{ho}$  from the extrapolated zero-range energy. This suggests that  $E_{ZRA,2}(r_0)$  obtained at a single (relatively large) range provides a very good estimate for the zero-range energy. Circles, squares, and diamonds in Fig. 2 show the energies  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ , respectively. The fits (see the discussion above) are shown by lines.

For systems with up to six particles (see the Supplemental Material [27] for a summary), we believe that our basis sets for all  $r_0$  are very close to complete. Specifically, (i) the energy changes very little upon further enlargement of the basis set; (ii) the first- and second-order derivatives  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$  are stable and their error bars can be estimated reliably; (iii) the extrapolations of  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$  are in very good agreement; and (iv) the quantities  $3E(r_0) - 4V_{tr}(r_0)$  and  $E_{ZRA,1}(r_0)$  agree quite well [see the discussion after Eq. (10)]. For systems with more than six particles, the construction of a nearly complete basis set is more challenging, especially for small  $r_0$ . As an example, we discuss the (4,4) system; for the (4,3), (5,4), and (5,5) systems, the reader is referred to the Supplemental Material [27].

Table II summarizes our ECG results for the (4,4) system; the format is the same as that in Table I for the (3,2) system. The smallest range considered and the error bars for the  $N = 8$  system are larger than those for the  $N = 5$  system. For a fixed  $r_0$ , the quantities  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$  for the  $N = 8$  system are about twice as large as for the  $N = 5$  system and their error bars are notably larger. The overall trends,

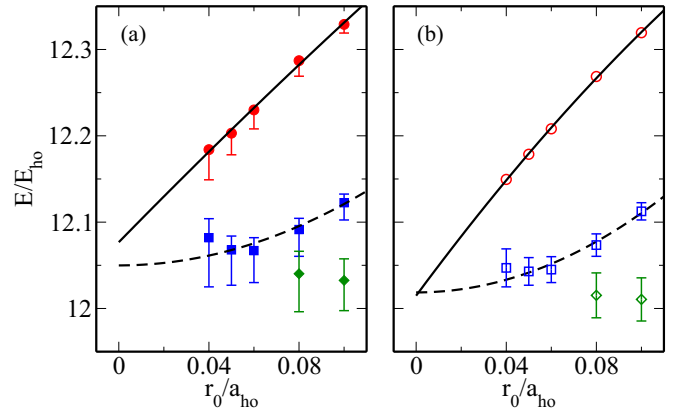


FIG. 3. (Color online) Ground-state energy of the (4,4) system at unitarity. (a) Circles, squares, and diamonds show  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ , respectively, for the largest basis set considered. The error bars of  $E_{ZRA,0}(r_0)$  show the estimated basis set error  $\Delta E(r_0)$  (see column 3 of Table II); they extend below the data points but not above. The error bars of  $E_{ZRA,1}(r_0)$  combine the estimated basis set error and the error of  $E^{(1)}(r_0)$  (see column 4 of Table II). Last, the error bars of  $E_{ZRA,2}(r_0)$  combine the estimated basis set error and the errors of  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$  (see column 5 of Table II). Solid and dashed lines show the extrapolations of  $E_{ZRA,0}(r_0)$  and  $E_{ZRA,1}(r_0)$  to the zero-range limit. (b) Same quantities as in (a) but corrected for the estimated basis set error. The open symbols show the energies  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$  reported in the last three columns of Table II. The uncertainty of  $\Delta E(r_0)$  is not accounted for by the error bars. It can be seen that the basis set error lowers the zero-range energy by about  $0.05 E_{ho}$  or, equivalently, 0.4%.

however, are similar: (i) the energy  $E(r_0)$  decreases with decreasing range, (ii)  $E^{(1)}(r_0)$  increases with decreasing range for  $r_0 \geq 0.06 a_{ho}$  (for smaller  $r_0$ , the trend reverses; we believe that this is a consequence of the numerics and not a real trend), and (iii)  $E^{(2)}(r_0)$  becomes less negative with decreasing range. Our numerics are not good enough to determine  $E^{(2)}(r_0)$  for  $r_0 \leq 0.06 a_{ho}$ . It can be seen, however, that the  $E_{ZRA,2}(r_0)$  for  $r_0 = 0.1 a_{ho}$  and  $0.08 a_{ho}$  agree quite well with the energies obtained by extrapolating  $E_{ZRA,0}(r_0)$  and  $E_{ZRA,1}(r_0)$  to the zero-range limit (see the last row of Table II). Since the basis set error is non-negligible for  $N = 8$ , Fig. 3 shows the energies  $E_{ZRA,0}(r_0)$  (circles),  $E_{ZRA,1}(r_0)$  (squares), and  $E_{ZRA,2}(r_0)$  (diamonds) before correcting for the basis set error [Fig. 3(a)] and after correcting for the basis set error [Fig. 3(b)]. We extrapolate  $E_{ZRA,0}(r_0)$  and  $E_{ZRA,1}(r_0)$  for both the largest basis set considered [Fig. 3(a)] and the infinite basis set [Fig. 3(b)] to the zero-range limit by performing fits of the form  $c_0 + c_1 r_0 + c_2 r_0^2$  and  $c_0 + c_2 r_0^2$ , respectively (see the solid and dashed lines in Fig. 3). To fit a function to  $E_{ZRA,1}(r_0)$ , the data points are weighted by the inverse square of the uncertainty. For the (4,4) and larger systems, we do not fit to higher-order polynomials because (i) the number of data points is five or less and (ii) the error bars are too large to determine the  $r_0^3$  dependence reliably. An alternative fit approach that includes the  $r_0^3$  term is discussed in the Appendix.

Table III summarizes our zero-range ground-state energies  $E(0)$  (column 2) obtained by extrapolating the energies  $E_{ZRA,1}(r_0)$ , which have been shifted down by the estimated basis set error, to the zero-range limit. The error bars given

TABLE III. Summary of our zero-range ground-state energies at unitarity and comparison with literature results for systems with  $N \leq 10$  and  $N_1 - N_2 \leq 1$ . Column 2 reports the zero-range ground-state energies  $E(0)$  calculated in this work. Columns 3 to 16 report ground-state energies from the literature calculated by use of different methods and their percentage differences from  $E(0)$ . All energies are reported in units of  $E_{\text{ho}}$ . The ground-state energy of the (2,1) system, obtained semianalytically [31], is  $4.272724E_{\text{ho}}$ . See text for more details.

$(N_1, N_2)$	$E(0)$	$E_{\text{ECG}}$	%	$E_{\text{DMC1}}^{\text{a}}$	%	$E_{\text{DMC2}}^{\text{b}}$	%	$E_{\text{AFMC2}}^{\text{c}}$	%	$E_{\text{AFMC4}}^{\text{c}}$	%	$E_{\text{CI}}^{\text{d}}$	%	$E_{\text{lattice}}^{\text{e}}$	%
(2,1)	4.2727(1)			4.281(4)	0.2							4.279	0.1		
(2,2)	5.0091(4)	5.0092(4) <sup>f</sup>		5.051(9)	0.8	5.028(2)	0.4					5.138	2.6	5.071(+32/−75)	1.2
(3,2)	7.455(1)	7.457(3) <sup>g</sup>		7.61(1)	2.1										
(3,3)	8.337(4)	8.34(9) <sup>g</sup>		8.64(3)	3.6	8.377(3)	0.5	8.26(1)	−0.9	8.21(1)	−1.6	8.601	3.2	8.347(+80/−66)	0.1
(4,3)	11.01(2)			11.36(2)	3.2							11.021	0.1		
(4,4)	12.02(3)	12.13(1) <sup>h</sup>	0.9	12.58(3)	4.7	12.04(1)	0.2	11.82(2)	−1.7	11.76(3)	−2.2	12.179	1.3	11.64(+11/−12)	−3.2
(5,4)	15.24(9)			15.69(1)	3.0										
(5,5)	16.12(6)			16.80(4)	4.2	16.10(1)	−0.1							16.05(+3/−7)	−0.4

<sup>a</sup>From Table II of Ref. [7]; the energies have been calculated for the square-well potential with range  $r_0 = 0.01a_{\text{ho}}$ , which—at unitarity—corresponds to  $r_{\text{eff}} = 0.01a_{\text{ho}}$ .

<sup>b</sup>Read off from Fig. 4 of Ref. [12]; the FN-DMC energies have been extrapolated to the zero-range limit.

<sup>c</sup>Read off from Fig. 4 of Ref. [12]; the error bars only account for the statistical uncertainty. A leading-order correction scheme has been applied to convert the finite lattice results to the infinite lattice limit [12,32].

<sup>d</sup>From Table I of Ref. [13]; the CI energies have been obtained for a finite shell-model space and the two-body coupling constant has been renormalized by matching the two-particle ground-state energy to the exact energy.

<sup>e</sup>From Table VI of Ref. [10]; the upper and lower limits of the error bars differ and are separated by a slash. The error bars account for statistical, fitting, finite-volume, and spatial-discretization errors, but do not account for systematic errors due to the contributions from excited states. We note that odd- $N$  systems were considered in Ref. [9]. The results in Ref. [9] were described as “preliminary” and are not included here.

<sup>f</sup>From Ref. [20]; the energy has been obtained by solving the hyperangular Schrödinger equation.

<sup>g</sup>From Table XXI of Ref. [18]; the energies have been extrapolated to the zero-range limit using the zeroth-order extrapolation scheme.

<sup>h</sup>From Table II of Ref. [23]; the energy has been extrapolated to the zero-range limit using the zeroth-order extrapolation scheme.

in parentheses are estimated by combining the zero-range extrapolation error, the uncertainty of the basis set error, and the uncertainty of  $E^{(1)}(r_0)$ .

Our ground-state energy for the (2,1) system agrees excellently with the semianalytic energy obtained using the zero-range framework of Ref. [31]. For comparison, Table III includes the ground-state energies from the literature obtained by various methods. Column 3 of Table III reports the zero-range ground-state energies  $E_{\text{ECG}}$  calculated by the ECG method in previous works [18,20,23]. Our results for the (2,2), (3,2), and (3,3) systems agree within error bars with the literature results. For the (3,3) system, we provide a notably tighter error bar. The ECG energy for the (4,4) system by Bradley *et al.* [23] is about 0.9% higher than our (4,4) energy. Bradley *et al.* estimate that the error due to the use of a restricted basis set is about 0.6% for the relative energy, translating to 0.53% for the total energy. This estimate is in reasonable agreement with the difference between their energy and our energy. Column 5 reports the FN-DMC energies  $E_{\text{DMC1}}$  calculated for the square-well potential with range  $0.01a_{\text{ho}}$  [7]. The deviations between the FN-DMC and our ECG energies are due to the positive effective range correction and the approximate nature of the nodal surface of the trial wave function (the latter dominates). Column 7 reports highly improved FN-DMC energies  $E_{\text{DMC2}}$  [12]. These energies have been extrapolated to the zero-range limit. The FN-DMC energies from Ref. [12] agree very well with our ECG energies (the agreement is better than 0.6% and, for  $N = 8$  and 10, the error bars overlap). Unfortunately, Ref. [12] considered only spin-balanced systems. Columns 9 and 11 report the energies  $E_{\text{AFMC2}}$  and  $E_{\text{AFMC4}}$  calculated using the AFMC approach with  $q^2$  and  $q^2 + q^4$  dispersion relations, respectively [12].

These energies have been obtained by applying a leading-order correction scheme to convert the finite lattice results to the infinite lattice limit but have not been extrapolated to the infinite lattice size limit [12,32]. Note that the AFMC energies for fixed  $N$  but different dispersion relations do not agree within error bars. The reason may be that the corrections due to the finite lattice spacing behave differently for the different dispersion relations and that the error bars are purely statistical. Column 13 reports the configuration interaction (CI) energies  $E_{\text{CI}}$  obtained using a limited CI shell-model space [13]. The authors of Ref. [13] noted that the two-body interaction strength was renormalized using an approach that could be improved upon. Improvement to both these aspects (enlarged CI model space and refined renormalization approach) could change the CI energies. Interestingly, the odd- $N$  CI energies agree quite well with our ECG energies while the even- $N$  CI energies are higher by between 1.3% and 3.2%. It is not clear to us what the origin of the different even- and odd- $N$  behaviors is. Column 15 reports the lattice MC energies  $E_{\text{lattice}}$  [10]. The lattice MC energies exhibit shell effects that are absent in the FN-DMC, AFMC, and—for small  $N$ —ECG energies (our energies for  $N \leq 10$  do not exhibit shell effects). The lattice MC energy for  $N = 8$  is 3.2% lower than our ECG, reflecting the shell effects exhibited by the lattice MC energies in the small- $N$  regime. For systems with  $N > 10$ , the lattice MC energies are higher than or equal to (within error bars) the FN-DMC energies  $E_{\text{DMC2}}$  from Ref. [12]. The difference between the lattice MC energies and FN-DMC energies for  $N > 10$  is smallest for closed-shell systems. Besides the results summarized in Table III, we also compared our ground-state energies with DFT energies [14] for both even- and odd- $N$  systems. The DFT energies are 5% to 10% higher than our ECG energies.

TABLE IV. Zero-range contact  $C(0)$  at unitarity for  $N = 3 - 10$ . Column 2 reports the zero-range contact  $C(0)$  determined using the adiabatic energy relation.  $C(0)$  for the (1,1) system, obtained analytically from the implicit eigenequation derived in Ref. [33], is  $4\sqrt{2\pi}a_{\text{ho}}^{-1} = 10.026513a_{\text{ho}}^{-1}$ .  $C(0)$  for the (2,1) system, obtained semianalytically using the hyperspherical coordinate framework [31,34,35], is  $10.468967a_{\text{ho}}^{-1}$ .

$(N_1, N_2)$	$C(0)a_{\text{ho}}$
(2,1)	10.469(1)
(2,2)	25.74(1)
(3,2)	25.20(1)
(3,3)	40.39(8)
(3,4)	38.2(2)
(4,4)	55.4(5)
(5,4)	56.9(9)
(5,5)	72.3(8)

In addition to the energies, we calculate the contact at unitarity. To remove the leading-order range dependence, we analyze the quantities  $C_{\text{ZRA},0}(r_0)$  and  $C_{\text{ZRA},1}(r_0)$ . While the energies  $E_{\text{ZRA},0}(r_0)$  and  $E_{\text{ZRA},1}(r_0)$  approach the  $r_0 = 0$  limit from above and below, respectively, for all  $N$  considered, the contacts  $C_{\text{ZRA},0}(r_0)$  and  $C_{\text{ZRA},1}(r_0)$  approach the  $r_0 = 0$  limit from either above or below. Specifically, fitting  $C_{\text{ZRA},0}(r_0)$  to a function of the form  $c_0 + c_1 r_0 + c_2 r_0^2$ , we find that  $c_1$  is positive for  $N = 4$ , very close to zero for  $N = 6$ , negative for  $N = 8$ , and again positive for  $N = 10$ . For the odd- $N$  systems,  $c_1$  is always positive. The pair distribution functions exhibit an analogous range dependence in the  $r_0 \ll r \ll a_{\text{ho}}$  region (see Figs. 9 and 10 of the Supplemental Material for the  $N = 5$  and 8 systems), suggesting that the intricate  $N$  and  $r_0$  dependence of the contact is a real effect and not an artifact of our numerics. Our convergence studies support this interpretation. Table IV reports the zero-range contact  $C(0)$  for  $N = 3 - 10$  at unitarity obtained by extrapolating  $C_{\text{ZRA},1}(r_0)$  to the zero-range limit. The error bars in parentheses account for the zero-range extrapolation error and the basis set error. The  $r_0 = 0$  extrapolations of  $C_{\text{ZRA},0}(r_0)$  and of the contact extracted from the pair distribution functions agree with the values reported in Table IV but have larger error bars. The contact exhibits an interesting even-odd pattern. Specifically, for the  $N = 4$  and 5 systems (and the 6 and 7 systems and the 8 and 9 systems), the contacts are roughly equal, reflecting the fact that these neighboring even-odd systems contain the same number of pairs. To zeroth order, the contact scales as  $N_2$  times the contact of the two-body system, i.e., linearly with the number of pairs. Since  $C(0)$  scales with  $N_2$ , the  $r_0 \ll r \ll a_{\text{ho}}$  region of the scaled pair distribution functions  $4\pi P_{12}(r)r^2$  approximately collapse to a single curve if multiplied by  $N_1$ . This approximate collapse is illustrated in Figs. 4(c) and 4(d).

Figure 5 shows the radial density  $P_1(r)$  of the ground state at unitarity for even  $N$  and  $r_0 = 0.06a_{\text{ho}}$ . We note that the convergence of the radial density in the small- $r$  regime is not as good as that of the pair distribution function, especially for large  $N$  and small  $r_0$ .  $P_1(r)$  peaks at  $r = 0$  for the (2,2) system, is relatively flat in the small- $r$  region for the (3,3) and (5,5) systems, and peaks around  $0.6a_{\text{ho}}$  for the (4,4) system. To estimate the range dependence, we calculate  $P_1(r)$

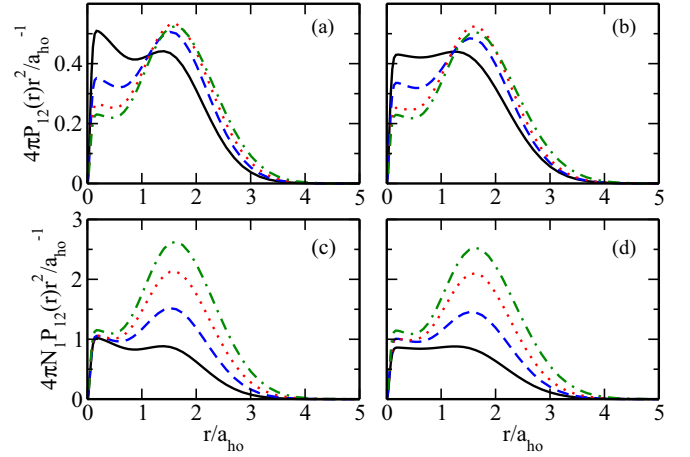


FIG. 4. (Color online) Panels (a) and (c) show the scaled pair distribution functions  $4\pi P_{12}(r)r^2$  and  $4\pi N_1 P_{12}(r)r^2$ , respectively, of the ground state at unitarity for the (2,2) system (solid line), (3,3) system (dashed line), (4,4) system (dotted line), and (5,5) system (dash-dotted line). Panels (b) and (d) show the scaled pair distribution functions  $4\pi P_{12}(r)r^2$  and  $4\pi N_1 P_{12}(r)r^2$ , respectively, of the ground state at unitarity for the (2,1) system (solid line), (3,2) system (dashed line), (4,3) system (dotted line), and (5,4) system (dash-dotted line). The calculations are performed for  $r_0 = 0.06a_{\text{ho}}$ .

for different  $r_0$  for the (2,2), (3,3), and (4,4) systems. For a given system, the  $r \lesssim 0.5a_{\text{ho}}$  region of  $P_1(r)$  increases with decreasing two-body range  $r_0$  (see Fig. 8 of the Supplemental Material [27]). The changes with  $r_0$  are relatively small and the densities displayed in Fig. 5 show the generic behavior of trapped Fermi gases with short-range interactions. Figure 6 shows  $P_j(r)$ ,  $j = 1$  and 2, for the odd- $N$  systems at unitarity for  $r_0 = 0.06a_{\text{ho}}$ .  $P_1(r)$  and  $P_2(r)$  peak at  $r = 0$  for the (2,1) system, are relatively flat in the small- $r$  region for the (3,2) and (5,4) systems, and peak around  $0.5a_{\text{ho}}$  for the (4,3) system. We find that the range dependence of the radial density for the odd- $N$  systems is similar to that for the even- $N$  systems (see Fig. 7 of the Supplemental Material [27]).

To gain insights into the pairing of the particles, Fig. 7 shows the integrated quantities  $\bar{N}_j(r)$ ,

$$\bar{N}_j(r) = 4\pi N_j \int_0^r P_j(r')r'^2 dr', \quad (14)$$

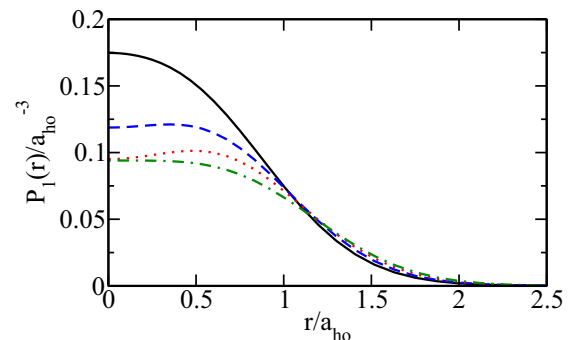


FIG. 5. (Color online) Radial density  $P_1(r)$  of the ground state at unitarity for the (2,2) system (solid line), (3,3) system (dashed line), (4,4) system (dotted line), and (5,5) system (dash-dotted line). The calculations are performed for  $r_0 = 0.06a_{\text{ho}}$ .

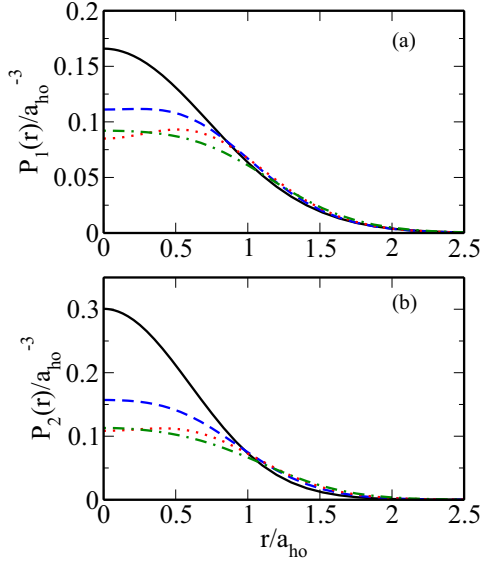


FIG. 6. (Color online) Panels (a) and (b) show the radial density of the majority species  $P_1(r)$  and the minority species  $P_2(r)$ , respectively, for the ground state of the (2,1) system (solid line), (3,2) system (dashed line), (4,3) system (dotted line), and (5,4) system (dash-dotted line). The calculations are performed for  $r_0 = 0.06a_{ho}$ .

for the odd- $N$  systems. Solid and dashed lines show  $\bar{N}_j(r)$  for the majority ( $j = 1$ ) and minority ( $j = 2$ ) species, respectively.  $\bar{N}_j(r)$  monitors the number of particles of species  $j$  located between zero and  $r$  and approaches  $N_j$  in the large- $r$  limit. We find that  $\bar{N}_1(r)$  and  $\bar{N}_2(r)$  take, for  $N$  fixed, different values for all  $r$ , suggesting that there exists no core region where the systems are fully paired. This is in contrast to an earlier FN-DMC study [8] which suggested that the  $N = 9$  system has a fully paired core. It should be noted that a fully paired core is expected in the large- $N$  limit [36]; however, how many particles are needed to be in the large- $N$  limit is not clear.

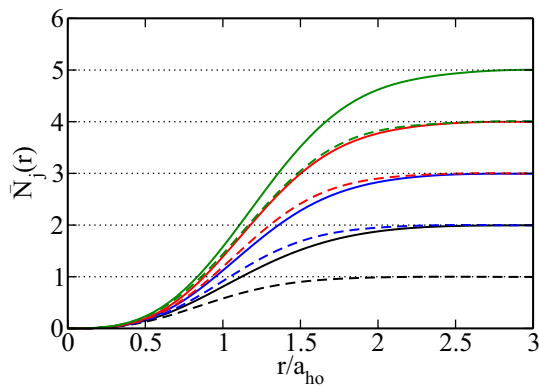


FIG. 7. (Color online) Solid and dashed lines show the integrated quantities  $\bar{N}_1(r)$  and  $\bar{N}_2(r)$ , respectively, for odd- $N$  systems as a function of  $r$ . From bottom to top, the curves correspond to systems with  $N = 3, 5, 7,$  and  $9$ . The horizontal dotted lines at 1 to 5 serve as a guide to the eye. The calculations are performed for  $r_0 = 0.06a_{ho}$ .

#### IV. CONCLUSIONS

This paper considered the ground-state properties of trapped two-component Fermi gases at unitarity with up to 10 particles. The calculations were performed for interspecies finite-range Gaussian interaction potentials using the ECG approach. Previous ECG calculations were limited to  $N = 3-6$  and 8. The present work additionally considered the spin-imbalanced  $N = 7$  and 9 systems with  $L^x = 1^-$  symmetry and the spin-balanced  $N = 10$  system with  $L^x = 0^+$  symmetry. A new range-correction scheme, which allows for the leading and—in some cases—the subleading range dependence to be removed, was introduced. The accuracy of the range correction scheme was tested extensively for small- $N$  systems ( $N \leq 6$ ) and then applied to larger systems ( $N = 7-10$ ). Our final results for the ground-state energy, reported in column 2 of Table III, are obtained by extrapolating  $E_{ZRA,1}(r_0)$ —corrected for by the basis set error—to the zero-range limit. The resulting extrapolated zero-range energies have error bars that range from 0.002% for  $N = 3$  to 0.6% and 0.4% for  $N = 9$  and 10. The energies agree well with the FN-DMC energies from Ref. [12], suggesting that the zero-range energies of harmonically trapped two-component Fermi gases with  $N \leq 10$  ( $N_1 - N_2 = 0$  or 1) are now known with an accuracy better than 1%. The finite-range energies were reported for finite  $r_0$  and all  $N$ . These finite-range energies provide variational upper bounds and are expected to help assess the accuracy of future finite-range calculations (the range  $r_0$  can be easily converted to the effective range). In addition to the energy, the pair distribution functions and radial densities were analyzed. The Tan contacts obtained through the adiabatic and pair relations were found to agree within error bars.

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#### APPENDIX: ADDITIONAL COMMENTS ON THE RANGE-CORRECTION SCHEME

In the main text, we independently fit the quantities  $E_{ZRA,0}(r_0)$ ,  $E_{ZRA,1}(r_0)$ , and  $E_{ZRA,2}(r_0)$ . The resulting zero-range energies were found to be in good agreement. This appendix discusses that a single correlated fit yields results that are consistent with those obtained from the independent fits.

We assume that the ground-state energy  $E(r_0) = E_{ZRA,0}(r_0)$  is a polynomial in the two-body interaction range  $r_0$ ,

$$E(r_0) = c_0 + c_1 r_0 + c_2 r_0^2 + c_3 r_0^3 + O(r_0^4). \quad (\text{A1})$$

Using Eq. (A1) to calculate  $E^{(1)}(r_0)$  and  $E^{(2)}(r_0)$  and inserting the results into Eq. (10), we find

$$E_{ZRA,1}(r_0) = c_0 - c_2 r_0^2 - 2c_3 r_0^3 + O(r_0^4) \quad (\text{A2})$$



and

$$E_{\text{ZRA},2}(r_0) = c_0 + c_3 r_0^3 + O(r_0^4). \quad (\text{A3})$$

As expected, the leading-order range dependencies of  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  are quadratic and cubic, respectively, and the functional forms of  $E_{\text{ZRA},j}(r_0)$  are not independent. Specifically, the quadratic coefficient of  $E_{\text{ZRA},1}(r_0)$  has the opposite sign but the same magnitude as that of  $E_{\text{ZRA},0}(r_0)$ , the cubic coefficient of  $E_{\text{ZRA},1}(r_0)$  has the opposite sign but twice the magnitude as that of  $E_{\text{ZRA},0}(r_0)$ , and the cubic coefficient of  $E_{\text{ZRA},2}(r_0)$  is the same as that of  $E_{\text{ZRA},0}(r_0)$ . Interestingly, our independent fits shown in Figs. 2 and 3 of the main text and Figs. 1–6 of the Supplemental Material are largely consistent with Eqs. (A1)–(A3). For example, our fits of  $E_{\text{ZRA},0}(r_0)$  yield a negative  $r_0^2$  coefficient and those of  $E_{\text{ZRA},1}(r_0)$  yield a positive  $r_0^2$  coefficient. The magnitudes of these coefficients, however, depend fairly sensitively on the number of terms included in the independent fits.

As an alternative, we perform a simultaneous four-parameter fit of  $E_{\text{ZRA},0}(r_0)$ ,  $E_{\text{ZRA},1}(r_0)$ , and  $E_{\text{ZRA},2}(r_0)$  using Eqs. (A1)–(A3). Each data point is weighted by the inverse square of the uncertainty [for  $E_{\text{ZRA},0}(r_0)$  we assume an uncertainty of  $0.3\Delta E(r_0)$  and the uncertainties of  $E_{\text{ZRA},1}(r_0)$  and  $E_{\text{ZRA},2}(r_0)$  are given in Tables I and II of the main text and Tables I–VI of the Supplemental Material]. The resulting zero-range energies for  $N = 3$ –10 are  $4.2726E_{\text{ho}}$ ,  $5.0088E_{\text{ho}}$ ,

$7.454E_{\text{ho}}$ ,  $8.335E_{\text{ho}}$ ,  $11.01E_{\text{ho}}$ ,  $12.02E_{\text{ho}}$ ,  $15.25E_{\text{ho}}$ , and  $16.12E_{\text{ho}}$ , respectively. These energies lie within the error bars of the zero-range energies reported in Table III. The simultaneous fit yields a positive  $c_1$  coefficient and negative  $c_2$  and  $c_3$  coefficients for all  $N$ . The  $c_1$  coefficient obtained from the independent fit of  $E_{\text{ZRA},0}(r_0)$  differs from that obtained from the simultaneous fit by less than 10% for all  $N$ .

We also apply the simultaneous fit approach to the contact. We fit our numerically obtained  $C_{\text{ZRA},0}(r_0)$  and  $C_{\text{ZRA},1}(r_0)$  to functions of the form  $c_0 + c_1 r_0 + c_2 r_0^2 + c_3 r_0^3$  and  $c_0 - c_2 r_0^2 - 2c_3 r_0^3$ , respectively, for  $N < 6$ , and to functions of the form  $c_0 + c_1 r_0 + c_2 r_0^2$  and  $c_0 - c_2 r_0^2$ , respectively, for  $N = 7$ –10. The resulting zero-range contacts  $C(0)$  for  $N = 3$ –10 lie within the error bars of the zero-range contacts reported in Table IV.

The observed leading and subleading corrections to the ground-state energy for systems at unitarity with  $N_1 - N_2 = 0$  or 1 (positive  $c_1$  and negative  $c_2$ ) have the same sign as those reported for the homogeneous system (see, e.g., Ref. [11]). For the two-particle system, this can be seen directly from the analytically known solutions given in Refs. [33,37–39]. It is interesting that this behavior does not change with increasing number of particles. Importantly, though, the sign of the leading-order range correction of the trapped system does depend on the  $s$ -wave scattering length (see, e.g., Ref. [19]).

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