Natural and unnatural parity states of small trapped equal-mass two-component
Fermi gases at unitarity and fourth-order virial coefficient

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Equal-mass two-component Fermi gases under spherically symmetric external harmonic confinement with large \( s \)-wave scattering length are considered. Using the stochastic variational approach, we determine the lowest 286 and 164 relative eigenenergies of the (2, 2) and (3, 1) systems at unitarity as a function of the range \( r_0 \) of the underlying two-body potential and extrapolate to the \( r_0 \rightarrow 0 \) limit. Our calculations include all states with vanishing and finite angular momentum \( L \) (and natural and unnatural parity \( \Pi \)) with relative energy up to 10.5\( \hbar \Omega \), where \( \Omega \) denotes the angular trapping frequency of the external confinement. Our extrapolated zero-range energies are estimated to have uncertainties of 0.1% or smaller. The (2, 2) and (3, 1) energies are used to determine the fourth-order virial coefficient of the trapped unitary two-component Fermi gas in the low-temperature regime. Our results are compared with recent predictions for the fourth-order virial coefficient of the homogeneous system. We also calculate small portions of the energy spectra of the (3, 2) and (4, 1) systems at unitarity.

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I. INTRODUCTION

Small trapped Fermi gases with contact or short-range interactions have attracted a great deal of attention recently \cite{1}. Using lithium or potassium, for example, equal-mass two-component systems can be realized experimentally by occupying two different hyperfine states. For typical experimental conditions, \( p \)-wave or higher partial wave interactions between two like atoms (say, two spin-up atoms) and between two unlike atoms (a spin-up and a spin-down atom) are negligibly small. Furthermore, by tuning an external magnetic field in the vicinity of a Fano-Feshbach resonance, the \( s \)-wave scattering length \( a_s \) can be adjusted to essentially any value \cite{2}. In this paper, we consider the regime where the \( s \)-wave scattering length is much larger than the range \( r_0 \) of the underlying two-body model potential. In the limit that \( r_0 \) goes to zero and \( a_s \) goes to infinity, the unitary regime is realized. In this regime, the only meaningful length scale of the system is given by the oscillator length \( a_{ho} \) that characterizes the external confining potential \cite{1,3}. Throughout, we assume a spherically symmetric harmonic potential with angular trapping frequency \( \Omega \) (i.e., \( a_{ho} = \sqrt{\hbar/m\Omega} \) with \( m \) denoting the atom mass).

From a theoretical point of view, small harmonically trapped Fermi gases with central short-range interactions are particularly appealing since they can be treated with comparatively high accuracy by a variety of methods, including techniques that have been developed in the context of atomic physics, nuclear physics and quantum chemistry problems \cite{4,10}. For the harmonically trapped equal-mass system, the center of mass degrees of freedom separate. Furthermore, the relative orbital angular momentum quantum number \( L \), the projection quantum number \( M \) and the parity \( \Pi \) are good quantum numbers. This implies that the Hilbert space can be divided into subspaces, which significantly reduces the complexity of the calculations compared to, for example, systems confined to move within a box with periodic boundary conditions \cite{17}. The harmonically trapped Fermi gas consisting of two spin-up and two spin-down atoms with vanishing angular momentum has been treated by a variety of techniques in the literature (see Refs. \cite{1,18} for reviews).

The ground state energy and ground state properties of the (2, 2) system in the zero-range limit, for example, are by now well characterized \cite{3,11}. Much less, however, is known about the excitation spectrum \cite{3,4,12,19}, which contains both natural and unnatural parity states, i.e., states with parity \( \Pi = (-1)^L \) and \( \Pi = (-1)^{L+1} \), respectively. While a good portion of the excitation spectrum of the (2, 2) system with natural parity has been determined throughout the crossover and at unitarity \cite{12}, little is known about the properties of states with unnatural parity. Moreover, the energy spectra of the (3, 1), (3, 2) and (4, 1) systems have not yet been characterized in detail.

This paper presents extensive benchmark results for the (2, 2) and (3, 1) energies of natural and unnatural parity states at unitary. In addition, we present portions of the energy spectra of the (3, 2) and (4, 1) systems. We then use the energy spectra of the (2, 2) and (3, 1) systems at unitarity to determine the fourth-order virial coefficient \( b_4 \) of the trapped system in the low-temperature regime. The fourth-order virial coefficient enters into the virial equation of state, which allows for the determination of the universal thermodynamics of two-component Fermi gases in the temperature regime down to about half the Fermi temperature \( T_F \) \cite{21,27}. For the temperature regime in which we have convergence, i.e., for \( k_B T \lesssim 2\hbar \Omega/3 \), where \( T \) denotes the temperature and \( k_B \) Boltzmann’s constant, we find that the fourth-order virial coefficient \( b_4 \) of the trapped system is negative and decreases monotonically with increasing tempera-
ture. If we assume that $b_4$ continues to change monotonically with increasing temperature in the medium-and high-temperature regime, our results predict that the fourth-order virial coefficient of the trapped system and—through application of the local density approximation (LDA)—that of the homogeneous system approach a negative value in the high-temperature limit. This is in contrast to recent results [26, 28] based on the equation of state, determined both experimentally and calculated via a diagrammatic Monte Carlo technique. These studies predict that the fourth-order virial coefficient of the homogeneous system is positive. The discrepancy would be resolved if the fourth-order virial coefficient of the trapped system was changing non-monotonically with temperature, allowing for a sign change of $b_4$ in the medium- or high-temperature regime. Analogous non-monotonic behavior was found for one of the third-order virial coefficients of the trapped unequal-mass two-component Fermi gas at unitarity [29]. While we do not have access to sufficiently large portions of the energy spectra of the (2, 2) and (3, 1) systems to determine the fourth-order virial coefficient of the trapped system in the medium- and high-temperature regimes (thereby preventing us from drawing definite conclusions), our results illuminate a number of aspects related to the determination of the virial coefficients from few-body energy spectra.

Section II introduces the system under study, reviews the stochastic variational approach, and presents details regarding our implementation. Compact expressions for venting us from drawing definite conclusions), our results predict that the fourth-order virial coefficient of the trapped system in unitarity [29]. While we do not have access to sufficiently large portions of the energy spectra of the (2, 2) and (3, 1) systems to determine the fourth-order virial coefficient of the trapped system in the medium- and high-temperature regimes (thereby preventing us from drawing definite conclusions), our results illuminate a number of aspects related to the determination of the virial coefficients from few-body energy spectra.

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II. SYSTEM UNDER STUDY AND STOCHASTIC VARIATIONAL APPROACH

We consider a two-component Fermi gas with $n_1$ spin-up and $n_2$ spin-down atoms of mass $m$ with $n = n_1 + n_2$. We assume that the atoms are confined by a spherically symmetric trapping potential with angular frequency $\Omega$. Furthermore, we assume that the spin-up and spin-down atoms interact through a short-range interaction potential $V_{\text{int}}(r_{pq})$, where $r_{pq} (p = 1, \cdots, n)$ denotes the position vector of the $p^{\text{th}}$ atom measured relative to the center of the trap and $r_{pq} = |\vec{r}_p - \vec{r}_q|$, and that atoms with like spins do not interact. The model Hamiltonian $H$ then reads

$$H = \sum_{p=1}^{n} \left( \frac{-\hbar^2}{2m} \nabla_{\vec{r}_p}^2 + \frac{1}{2} m \Omega^2 \vec{r}_p^2 \right) + V_{\text{int}},$$

where

$$V_{\text{int}} = \sum_{p=1}^{n_1} \sum_{q=n_1+1}^{n} V_{\text{int}}(r_{pq}).$$

Throughout, we are interested in the regime where the $s$-wave scattering length $a_s$ of the interspecies interaction potential $V_{\text{int}}$ becomes infinitely large. For the $(n_1, n_2) = (1, 1)$ and $(2, 1)$ systems, semi-analytical solutions are known if $V_{\text{int}}$ coincides with the zero-range $\delta$-function potential [4, 31]. For $(n_1, n_2)$ systems with $n_1 + n_2 \geq 4$, however, no such semi-analytical solutions are known. To determine the eigenenergies of $(n_1, n_2)$ systems with $n_1 + n_2 = 4$ and 5, we separate off the center of mass motion and resort to a numerical technique, the stochastic variational approach [32]. In this approach, it is convenient to model the interactions between the unlike atoms through a Gaussian potential $V_g(r)$ with depth $-V_0$ ($V_0 > 0$) and range $r_0$ [33],

$$V_g(r) = -V_0 \exp \left( - \frac{r}{\sqrt{2}r_0} \right).$$

To treat the unitary system, we adjust the depth $V_0$ of $V_g$ for a given $r_0$ such that the two-body system in free space supports one zero-energy $s$-wave bound state but no deep-lying bound states. To determine the zero-range energies, we consider a number of $r_0$, $r_0 \ll a_{\text{ho}}$, and extrapolate the finite-range energies to the $r_0 \rightarrow 0$ limit (see Sec. III for examples).

We take advantage of the fact that the Hamiltonian $H$ separates into the center of mass Hamiltonian $H_{\text{cm}}$ and the relative Hamiltonian $H_{\text{rel}}$, $H = H_{\text{rel}} + H_{\text{cm}}$. In the following, we consider the relative Hamiltonian $H_{\text{rel}}$ and use the stochastic variational approach to determine the eigenenergies and eigenstates of the Schrödinger equation $H_{\text{rel}} \Psi_{\text{rel}} = E_{\text{rel}} \Psi_{\text{rel}}$. Here, we explicitly indicate the dependence of the eigenenergies on $n_1$ and $n_2$ but, for notational simplicity, not that of the Hamiltonian and the wave function. To compact the notation, we write $H_{\text{rel}}$ as $H_{\text{rel}} = T_{\text{rel}} + V_{\text{rel}} + V_{\text{int}}$, where $T_{\text{rel}}$ denotes the kinetic energy operator associated with the relative motion, and $V_{\text{rel}}$ the contribution of the confining potential associated with the relative degrees of freedom.

The stochastic variational approach is a basis set expansion approach that writes the relative wave function $\Psi_{\text{rel}}$ of a given state in terms of a set of basis functions $\psi_k$ [32],

$$\Psi_{\text{rel}} = \sum_{k=1}^{N_k} c_k A \psi_k.$$

Here, the $c_k$ denote expansion coefficients and $A$ an antisymmetrization operator that ensures that the wave function is anti-symmetric under the exchange of any pair of like fermions. In Eq. (4), $N_k$ denotes the number of basis functions. As with other basis set expansion approaches,
the Ritz variational principle ensures that the lowest
energy as well as the higher-lying energies obtained by
the stochastic variational approach are rigorous upper
bounds to the exact eigenenergies of the system \[32\]. In
the following, we introduce the basis functions used in
this work, which have good orbital angular momentum
\(L\), projection quantum number \(M\) and parity \(\Pi\); here, \(L\),
\(M\) and \(\Pi\) are associated with the relative motion.

Following Refs. \[32-38\], we write the basis functions
\(\psi_k\) as a product of a correlated Gaussian [second line
of Eq. (5)] and a “prefactor” [first line of Eq. (5)] that
carries the angular momentum \(L\) of the system,
\[
\psi_k(\vec{x}) = |\vec{v}_1k|^l_1|\vec{v}_2k|^l_2|Y_{l_1}(\vec{v}_1k) \otimes Y_{l_2}(\vec{v}_2k)|_{LM}
\times \exp\left(-\frac{\vec{x}^T A_k \vec{x}}{2}\right).
\]
(5)

Here, \(\vec{x}\) collectively denotes the \(n-1\) Jacobi vectors
\(\vec{v}_k\), where \(p = 1, \ldots, n-1\). The notation \(|Y_{l_1}(\vec{v}_1k) \otimes \nolimits
Y_{l_2}(\vec{v}_2k)|_{LM}\) indicates that the spherical harmonics
\(Y_{l_1,m_1}\) and \(Y_{l_2,m_2}\) are coupled to form a function with angular
momentum \(L\) and projection quantum number \(M\). For
states with natural parity, \(\Pi\), i.e., for states whose parity
is given by \(\Pi = (-1)^L\), we choose \(l_1 = L\) and \(l_2 = 0\) \[32–
33\]. For states with unnatural parity \((L > 0)\), i.e., for
states whose parity is given by \(\Pi = (-1)^{L+1}\), we choose
\(l_1 = L\) and \(l_2 = 1\) \[36\]. The basis functions that
describe unnatural parity states with \(L = 0\) have a slightly
different form since the construction of states with \(L = 0\)
and \(\Pi = -1\) requires the coupling of three spherical
harmonics with \(l_1, l_2\) and \(l_3 > 0\) \[32–38\]. The matrix \(A_k\)
is symmetric and positive-definite, and has dimensions
\((n-1) \times (n-1)\). The \((n(n-1)/2\) independent elements of
\(A_k\) are treated as variational parameters and optimi-
zed semi-stochastically. The three-dimensional vectors
\(\vec{v}_1k\) and \(\vec{v}_2k\), referred to as global vectors since they
depend on all \(n-1\) Jacobi vectors, are defined through
\(\vec{v}_1k = \sum_{p=1}^{n-1} u_{1k,p} \vec{x}_p = \vec{u}_{1k} \vec{x}\) and similarly
for \(\vec{v}_2k\). The vectors \(\vec{u}_{1k}\) and \(\vec{u}_{2k}\) are optimized semi-stochastically,
where \(\vec{u}_{1k} = (u_{1k,1}, \ldots, u_{1k,n-1})\) and similarly
for \(\vec{u}_{2k}\).

A key benefit of the basis functions given in Eq. (4) is
that the overlap matrix element \(O_{k'k} = \langle \psi_{k'} | \psi_k \rangle\), the
matrix element for the kinetic energy operator \(\langle T^{\text{rel}} \rangle_{k'k} = \langle \psi_{k'} | T^{\text{rel}} | \psi_k \rangle\),
and the matrix element for the confining potential \(\langle V_{\text{int}}^{\text{rel}} \rangle_{k'k} = \langle \psi_{k'} | V_{\text{int}}^{\text{rel}} | \psi_k \rangle\) reduce to compact expressions \[32, 37\]. Here, it is understood that
the integration is performed over all \(3n-3\) Jacobi coordinates
and that \(\psi_k\) is characterized by \(A_k\), \(\vec{u}_{1k}\) and \(\vec{u}_{2k}\) while \(\psi_{k'}\)
is characterized by \(A_{k'}\), \(\vec{u}_{1k'}\) and \(\vec{u}_{2k'}\). Moreover, a com-
 pact expression can also be found for the matrix elements
\(\langle V_{\text{int}}^{\text{rel}} \rangle_{k'k} = \langle \psi_{k'} | V_{\text{int}}^{\text{rel}} | \psi_k \rangle\) associated with the atom-atom
interaction if \(V_{\text{th}}\) is modeled by the Gaussian potential
\(V_g\). Appendix A summarizes explicit expressions of the
matrix elements with natural parity (any \(L\)) and unnatural
parity \((L > 0)\). The matrix elements for states with
\(0^-\) symmetry can be found in Refs. \[36, 38\].

We note that the overlap matrix element \(O_{k'k}\) between
two different basis functions does not vanish, i.e., the
basis set employed is not orthogonal. This implies that the
determination of the eigenenergies amounts to the diag-
onalization of a generalized eigenvalue problem defined
by the Hamiltonian and overlap matrices \[32\]. While one
might think, at first sight, that the non-orthogonality of
the basis functions could introduce numerical instabil-
ities, it has been shown in previous work \[5, 6, 8, 12-13\]
that numerical instabilities due to linear dependence is-
ses can be avoided completely for the systems of interest
in this work if the basis sets are chosen carefully.

Our strategy to optimize the large number of non-
linear variational parameters is quite simple \[32\]. We
start with a reference basis set, which could consist of
just one basis function or as many as several 100 or
1000 basis functions. We then enlarge this reference basis set
by one basis function, which is chosen from a large num-
ber of trial basis functions, typically between several
100 and several 1000. Each trial function is characterized by
a different set of variational parameters. To decide which
basis function to keep, we calculate the energy for each
of the enlarged trial basis sets, which consist of the refer-
ence basis set plus one of the trial basis functions, and
choose the one that results in the largest reduction of
the energy of the state of interest. The state of interest
could be the ground state or an excited state. The pro-
cedure is repeated until the basis set is sufficiently
complete to describe the state of interest with the desired accuracy.

When optimizing a state whose energy is nearly de-
generate with that of another state or when optimizing
highly excited states, some care needs to be exercised.
In the former case, we find it advantageous to optimize
two or more states simultaneously. In the latter case, we
find it beneficial to start with a basis set that provides
a reasonably accurate description of the lower lying part
of the energy spectrum. The advantage of our optimiza-
tion procedure is that the basis set is optimized for a
particular state or a particular subset of states. Corre-
spondingly, we work with comparatively small basis sets.
The energies of the \((2,2)\) and \((3,1)\) systems at unitari-
ity (see Table I and supplemental material) are obtained
using basis sets that consist of 700-3400 basis functions,
while the energies of the \((3,2)\) and \((4,1)\) systems (see
supplemental material) are obtained using basis sets that
consist of 1500-3800 basis functions.

III. ENERGIES OF SMALL TRAPPED FERMI
GASES

One key purpose of this paper is to elucidate how we
determine a large portion of the energy spectrum of
trapped two-component Fermi systems with \(n = 4\) and
5, and to tabulate the extrapolated zero-range energies.
We believe that the tabulation of the energies is useful
as these energies provide much needed highly accurate
benchmark results that can be used to assess the accu-
racry and validity regime of alternative approaches. We
anticipate that the tabulated energies will also prove use-
ful in other applications.
FIG. 1: (Color online) Illustration of convergence for the (3,1) system at unitarity with $1^+$ symmetry and $r_0 = 0.04a_{\text{ho}}$. Solid and dashed lines show the quantity $\Delta_{E_{3,1}}$, where $\Delta_{E_{3,1}} = [E_{3,1}^{\text{rel}}(N_b) - E_{3,1}^{\text{rel}}(N_b \to \infty)]/E_{3,1}^{\text{rel}}(N_b \to \infty)$, for states 1 and 12 as a function of $1/N_b$. The dotted lines show the extrapolation to the $N_b \to \infty$ limit. The inset shows a blow-up of the small $1/N_b$ region.

Figure 1 shows an example of our basis set optimization for the (3,1) system with $1^+$ symmetry and $r_0 = 0.04a_{\text{ho}}$ at unitarity. Solid and dashed lines show the fractional difference $\Delta_{E_{3,1}}$ for the ground state (state 1) and state 12, respectively, between the relative energy $E_{3,1}^{\text{rel}}$ for a basis set of size $N_b$ and the energy for an infinite basis set. The dotted lines in Fig. 1 show the extrapolation to the $N_b \to \infty$ limit. It can be seen that the ground state energy converges notably faster than the excited state energy. The energies for $N_b = 800$ and $N_b = 900$ are $E_{3,1}^{\text{rel}}(r_0 = 0.04a_{\text{ho}}) = 5.08294\hbar\Omega$ for state 1 and $E_{3,1}^{\text{rel}}(r_0 = 0.04a_{\text{ho}}) = 10.1788\hbar\Omega$ for state 12, respectively. The basis set errors for these basis sizes are 0.0002% and 0.003%, respectively, i.e., the energies of states 1 and 12 lie relatively $0.00001\hbar\Omega$ and 0.0003\hbar\Omega above the extrapolated energies for the infinite basis set. The low-lying states of the (3,1) system with $1^+$ symmetry at unitarity converge relatively quickly with increasing $N_b$. This can be observed, in general, we choose the size of our basis sets for the (2,2) and (3,1) systems such that the basis set extrapolation error is smaller than 0.1%.

Figure 2 exemplarily illustrates the range dependence for the relative energy of the (3,1) system with $1^+$ symmetry. Figure 2(a) shows the range dependence of the ground state energy, Fig. 2(b) shows the range dependence of the energy associated with state 12, and Fig. 2(c) shows the range dependence of the energy for a state that depends comparatively weakly on $r_0$ (state 5). In Figs. 2(a) and 2(b), the energies vary to a very good approximation linearly with $r_0$ for sufficiently small $r_0/a_{\text{ho}}$. This finding is in agreement with earlier work [9, 11, 12, 13]. For the ground state [see Fig. 2(a)], the range dependence is quite weak and linear behavior is only observed for $r_0 \lesssim 0.03a_{\text{ho}}$.

In Fig. 2(c), the zero-range energy agrees to within 0.00002$\hbar\Omega$ with the energy of the non-interacting system. This, combined with the very weak dependence of the energy on $r_0$ and the fact that the energy approaches the zero-range limit from below, suggests that this state is not affected by $s$-wave scattering but only by higher-partial wave scattering. In the zero-range limit, energy shifts associated with higher-partial wave scattering processes vanish. Our interpretation is corroborated by a perturbative calculation along the lines of that performed in Refs. 9, 12, which utilizes zero-range contact interactions. For the (3,1) system with $L^\Omega = 1^+$ symmetry, we find, in agreement with our results based on the stochastic variational approach, that there exists one state with relative energy $17\hbar\Omega/2$ and six states with relative energy...
2\hbar\Omega/2 that are independent of \(a_s\).

We refer to states that are unaffected by \(s\)-wave interactions as unshifted states. We find that a relatively large number of states fall into this category. Their existence and likelihood of occurrence has already been discussed for the (2, 1) and (2, 2) systems in the literature \([4, 12]\). For the (2, 1) system, e.g., all unnatural parity states are unaffected by \(s\)-wave interactions in the zero-range limit. For the (2, 2) and (3, 1) systems, unnatural parity states can be affected by \(s\)-wave interactions in the zero-range limit. The only exception are states with \(0^-\) symmetry, which are unshifted. This behavior can be intuitively understood within a picture that utilizes angular momentum coupling. To construct a state with \(0^-\) symmetry, the coupling of three finite angular momenta is needed. These angular momenta can be envisioned as being each associated with one of the three Jacobi vectors that characterize the \(n = 4\) system. As a consequence, the \(s\)-wave interactions are effectively turned off by the nodal structure of the wave function. For \(n = 5\), this argument predicts that states with \(0^-\) symmetry can be affected by \(s\)-wave interactions since the system is characterized by one more Jacobi vector than angular momenta needed to ensure the \(0^-\) symmetry. Indeed, this prediction is in agreement with our results from the perturbative and stochastic variational calculations.

Table I summarizes our extrapolated zero-range energies \(E_{\text{rel}}^{(3)1}(r_0 = 0)\), \(E_{\text{rel}}^{(5)2}(r_0 = 0)\), \(E_{\text{rel}}^{(3)1}(r_0 = 0) = 10.56\hbar\Omega\), for states with \(1^+\) symmetry at unitarity that are affected by \(s\)-wave interactions. The zero-range energies are obtained by calculating the energies of a given state for several ranges \(r_0\) between 0.0025 \(\leq r_0/a_{ho} \leq 0.08\) and by then fitting these energies for the largest basis set considered by a linear function. The third column in Table I shows the slopes \(\chi\), which characterize the dependence of \(E_{\text{rel}}^{0\Omega}(r_0)\) on \(r_0\) at unitarity. We find that the slopes for states that are affected by \(s\)-wave interactions are positive. Table I shows that the slopes vary over nearly two orders of magnitude. The slopes can be related to the effective range \(r_{\text{eff}}\) using the relation \(r_{\text{eff}} = 2.032r_0\). This numerically determined relationship is specific to the Gaussian model potential employed in this paper and is quite accurate over the \(r_0\) values considered. It may be used to estimate the leading order dependence of the energies on the effective range for the Gaussian model potential.

The relative energies at unitarity for zero-range interactions can be written in the form \((2q+s_{L,\nu}+1)\hbar\Omega\) \([4, 40]\), where \(s_{L,\nu}\) is associated with the eigenvalue of the hyperangular Schrödinger equation and where the radial quantum number \(q\) takes the values 0, 1, \cdots (although the \(s_{L,\nu}\) depend on \(\Pi\), this dependence is not explicitly indicated for notational simplicity). The fourth column of Table I shows the \(s_{L,\nu}\) values determined from our energies for \(q = 0\), i.e., for the lowest rung of the ladder with \(2\hbar\Omega\) spacings. The extrapolated zero-range energies of states 2 and 7, e.g., lie 2.0001\hbar\Omega and 4.0006\hbar\Omega, respectively, above the energy of the ground state. Correspondingly, we assign the quantum numbers \(q = 1\) and \(q = 2\) to these states, i.e., we identify them as belonging to the same ladder as the ground state. The small deviations from the \(2q\hbar\Omega\) spacings can be interpreted as a measure of our numerical accuracy. For the states considered in Table I the \(2q\hbar\Omega\) spacing is fulfilled to better than 0.1 %. We find that the energies of states that belong to the same ladder are characterized by similar slopes.

For some symmetries, nearly degenerate states exist in the energy range \(E_{\text{rel}}^{\Omega} \leq 10.56\hbar\Omega\). Figure 4 shows the range dependence of the (3, 1) energies with \(3^-\) symmetry corresponding to states 15 and 16. This figure illustrates exemplarily that the “ordering” of states can change as a function of \(r_0\), i.e., that the energies of two or more states can cross at finite \(r_0\). Crossings like these can only be resolved by considering at least three different \(r_0\) values for each state.

Following the format of Table I the supplemental material tabulates the energies of the (2, 2) and (3, 1) systems. The results are obtained by analyzing the finite-range energies determined by the stochastic variational approach along the lines discussed above. For the (2, 2) and (3, 1) systems, there exist 286 and 164 states at unitarity with relative energy \(E_{\text{rel}}^{\Omega} \leq 10.56\hbar\Omega\) [not counting the \((2L + 1)\) multiplicity]. Of these states, respectively 52 and 46 are unshifted. The

| st. no. | \(E_{\text{rel}}^{(3)1}(r_0 = 0)/(\hbar\Omega)\) | \(\chi\) | \(s_{L,\nu}\) | \(s_{L,\nu}^{(1)}\) |
|--------|-----------------------------------|--------|-------------|-------------|
| 1      | 5.0819                            | 0.04   | 4.0819      | 5.5         |
| 2      | 7.0820                            | 0.03   |             |             |
| 3      | 7.6056                            | 0.51   | 6.6056      | 7.5         |
| 4      | 8.1456                            | 0.76   | 7.1456      | 7.5         |
| 5      | 8.9846                            | 1.19   | 7.9846      | 9.5         |
| 7      | 9.0825                            | 0.03   |             |             |
| 8      | 9.1324                            | 0.28   | 8.1324      | 9.5         |
| 9      | 9.4544                            | 0.46   | 8.4544      | 9.5         |
| 10     | 9.6060                            | 0.55   |             |             |
| 11     | 9.6847                            | 1.17   | 8.6847      | 9.5         |
| 12     | 10.147                            | 0.80   |             |             |
shifted energies are characterized by respectively 170 and 89 \( s_{L,\nu} \) values. Figures 3(a) and 3(b) show the density of states of the (2, 2) system and the (3, 1) system, respectively, at unitarity. The plots account for the (2, 2) -multiplicity of the energies. For the (2, 2) and (3, 1) systems, the convergence is slower than for the (2, 2) and (3, 1) systems.

The supplemental material also tabulates results for the (3, 2) and (4, 1) systems. For these systems, the convergence is slower than for the \( n = 4 \) systems, and we choose the size of our basis sets such that the basis set extrapolation error is smaller than 1 \% . Since the calculations for \( n = 5 \) are significantly more demanding than for \( n = 4 \), we restrict ourselves to states with \( E_{\text{rel}}^{(n_1,n_2)} \leq 17\Omega /2 \). We first extrapolate the energy for a given \( r_0 \) to the infinite basis set limit, and then determine the zero-range energy from these extrapolated energies. For the (3, 2) and (4, 1) systems, there exist 19 and 4 states with energies \( E_{\text{rel}}^{(n_1,n_2)} \leq 17\Omega /2 \) at unitarity [not counting the \((2L+1)\) multiplicity and excluding, for technical reasons, (3, 2) states with 0 \(^{-}\) symmetry]. All of these energies correspond to shifted states. One of the (3, 2) energies corresponds to a “repeated state” with hyperradial quantum number \( q = 1 \).

IV. 4\(^{th}\)-ORDER VIRIAL COEFFICIENT

This section uses the (2, 2) and (3, 1) energies to determine the fourth-order virial coefficient \( b_4 \) of the \( s \)-wave interacting two-component Fermi gas under spherically symmetric harmonic confinement at unitarity in the low-temperature regime. We also summarize a few results for the low-temperature behavior of the higher-order virial coefficients.

The virial coefficients \( b_n \) enter into the virial equation of state, which describes the finite temperature behavior of trapped two-component Fermi gases [20–27, 29, 41–43]. We work in the grand canonical ensemble and denote the fugacities of component 1 and component 2 by \( z_1 \) and \( z_2 \), respectively, where the \( z_i \) are defined in terms of the chemical potentials \( \mu_i \) of the \( i \)th component and the temperature \( T \),

\[
z_i = \exp[\mu_i/(k_B T)].
\] (6)

The thermodynamic potential \( \Omega^{(2)} \) of the harmonically trapped Fermi gas can be written in terms of the thermodynamic potentials \( \Omega_1^{(1)} \) and \( \Omega_2^{(1)} \) of the non-interacting components 1 and 2, and an “interaction piece” \( \Delta \Omega^{(2)} \) that accounts for the interactions between the atoms of component 1 and the atoms of component 2 [23, 25, 41–43],

\[
\Delta \Omega^{(2)} = -k_BTQ_1 \left( \sum_{n_1=1}^{\infty} \sum_{n_2=1}^{\infty} b_{n_1,n_2} z_1^{n_1} z_2^{n_2} \right). 
\] (7)
TABLE II: The second and third columns show the expressions for $Q_n$, $\Delta b_n$, and $b_n^{ref}$, $n = 2 - 5$, for the trapped system. In deriving these expressions, we used that $\Delta Q_{n_1,n_2} = \Delta Q_{n_2,n_1}$ for the systems considered in this paper.

| $n$ | $Q_n$ | $\Delta b_n$ | $b_n^{ref}$ |
|-----|-------|--------------|-------------|
| 2   | $\Delta Q_{1,1}/2$ | - | 0 |
| 3   | $\Delta Q_{2,1}$ | -2b2Q1 | |
| 4   | $\Delta Q_{3,1} + \Delta Q_{2,2}/2$ | $-b2[(Q1)2 + b2Q1 + 2Q2] - 2b3Q1$ | |
| 5   | $\Delta Q_{4,1} + \Delta Q_{3,2}$ | $-2b2[(Q2)2 + Q1Q2 + Q3]$ | $-b2[(Q1)2 + 2Q2 + 2b2Q1] - 2b3Q1$ |

In Eq. (7), $Q_1$ denotes the canonical partition function of a single particle in a spherically symmetric harmonic trap with angular frequency $\Omega$,

$$Q_1 = e^{\omega/2}(e^{\tilde{\omega}} - 1)^{-3},$$

where $\tilde{\omega}$ denotes a dimensionless inverse temperature,

$$\tilde{\omega} = \frac{\hbar \Omega}{k_B T}.$$

If we restrict ourselves to spin-balanced systems with equal masses, the fugacities $z_1$ and $z_2$ are equal, $z = z_1 = z_2$, and Eq. (7) reduces to

$$\Delta \Omega(2) = -2k_B TQ_1 \left( \sum_{n=2}^{\infty} b_n z_n^n \right),$$

where $b_2 = b_{1,1}/2$, $b_3 = (b_{1,2} + b_{2,1})/2$, $b_4 = (b_{1,3} + b_{3,1} + b_{2,2})/2$, and so on.

We find it convenient to write the virial coefficients $b_n$ as

$$b_n = \Delta b_n + b_n^{ref},$$

where $b_n^{ref}$ is determined by the virial coefficients $b_j$ and the canonical partition functions $Q_j$ with $j < n$. The interaction piece $\Delta b_n$, in contrast, accounts for the “new” physics introduced by the interacting $(n_1,n_2)$ clusters with $n = n_1 + n_2$. Explicit expressions for $\Delta b_n$ and $b_n^{ref}$ are given in Table II where the $\Delta Q_{n_1,n_2}$ are defined in terms of the canonical partition functions $Q_{n_1,n_2}$ of the interacting $(n_1,n_2)$ and single-component system with $n_1$ atoms, respectively,

$$\Delta Q_{n_1,n_2} = Q_{n_1,n_2}^{int} - Q_{n_1}Q_{n_2}.\tag{11}$$

The temperature-dependent canonical partition functions $Q_{n_1,n_2}^{int}$ are determined by the total energies $E_{n_1,n_2}^{int,j}$ and $E_{n_1}^{int,j}$ of the interacting two-component and non-interacting single-component systems, respectively. It is important to note that the energies $E_{n_1,n_2}^{int,j}$ and $E_{n_1}^{int,j}$ contain the center of mass energy. The summation over $j$ in Eqs. (13) and (14) extends over all states allowed by symmetry. For $n_1 = 1$, the sum in Eq. (14) can be performed analytically, yielding Eq. (8). In the high-temperature limit, one finds for systems with zero-range interactions at unitarity that

$$b_n = b_n^{(0)} + b_n^{(2)} \tilde{\omega}^2 + b_n^{(4)} \tilde{\omega}^4 + \cdots .$$

The second-order virial coefficient of the trapped system at unitarity takes the simple form

$$b_2 = \Delta b_2 = \lim_{q_{max} \to \infty} \sum_{q=0}^{q_{max}} \frac{1}{2} \left[ e^{-(2q+1)2\tilde{\omega}} - e^{-(2q+3)2\tilde{\omega}} \right].$$

or, performing the infinite sum,

$$b_2 = \frac{1}{2} e^{-\tilde{\omega}/2} (1 + e^{-\tilde{\omega}})^{-1}. \tag{15}$$

The solid line in Fig. 5 shows the second-order virial coefficient $b_2$, Eq. (17), as a function of $\tilde{\omega}$. In the high-temperature (small $\tilde{\omega}$) limit, $b_2$ approaches the constant $b_2^{(0)} = 1/4$ (solid horizontal line in Fig. 5), which can be obtained by Taylor-expanding Eq. (17). To illustrate the convergence of $b_2$ with increasing energy cutoff, dash-dot-dotted, dash-dotted and dashed lines show $b_2$ obtained by setting $q_{max}$ in Eq. (16) to 0, 1 and 10, respectively. For a finite energy cutoff, it can be seen that $b_2$ goes to 0 in the small $\tilde{\omega}$ region as opposed to $b_2^{(0)} = 1/4$. The temperature-dependent canonical partition functions $Q_{n_1,n_2}$ and $Q_{n_1}$,

$$Q_{n_1,n_2}^{int} = \sum_j \exp[-E_{n_1,n_2}^{int,j} / (k_B T)],$$

and

$$Q_{n_1} = \sum_j \exp[-E_{n_1}^{int,j} / (k_B T)].$$
As expected, a larger energy cutoff provides an accurate description of $b_2$ over a larger temperature range, i.e., down to a smaller inverse temperature $\tilde{\omega}$.

The relative three-body energies at unitarity and for vanishing s-wave scattering length $a_s$ can be written as $(2q + s_{L,\nu} + 1)\hbar\Omega$ (see Sec. III and (2q + $s_{L,\nu}^n + 1)\hbar\Omega$, respectively. Performing the sum over $q$ analytically, the interaction piece $\Delta b_3$ of the trapped three-body system at unitarity takes the form

$$\Delta b_3 = \lim_{\nu_{\text{max}}, L_{\text{max}} \to \infty} e^{2\tilde{\omega}}(e^{2\tilde{\omega}} - 1)^{-1} \times \sum_{\nu = 0}^{\nu_{\text{max}}} \sum_{L = 0}^{L_{\text{max}}} (2L + 1)[e^{-(s_{L,\nu} + 1)\tilde{\omega}} - e^{-(s_{L,\nu}^n + 1)\tilde{\omega}}]. \quad (18)$$

Using large $L_{\text{max}}$ and $\nu_{\text{max}}$, a fully converged pointwise representation of $b_3$ is obtained (see solid line in Fig. 4). Using the analytical forms for $Q_1$ and $b_2$, Eqs. (13) and (17), we find that $b_3^{\text{ref}}$ diverges as $-\tilde{\omega}^{-3/2} + \tilde{\omega}^{-1}/8$ in the high-temperature limit. This divergence is cancelled by a divergence of $\Delta b_3$ of opposite sign. As a result, $b_3$ is well behaved in the small $\tilde{\omega}$ (high $T$) limit. A careful analysis of the high-temperature behavior gives

$$b_3^{(0)} = -0.0683396093112849(1) \quad (19)$$

(see horizontal solid line in Fig. 4).

To illustrate the convergence of $b_3$, we calculate $b_3^{\text{ref}}$ and $b_3$ with increasing $L_{\text{max}}$ and $\nu_{\text{max}}$ [see Eq. (18)], and find that $b_3^{\text{ref}}$ converges with $L_{\text{max}}$ and $\nu_{\text{max}}$ chosen such that $s_{L,\nu} \leq 11/5, \leq 19/2$ and $\leq 50$, respectively. No cutoff is imposed in calculating $b_3^{\text{ref}}$. In these calculations, we include the same number of $s_{L,\nu}$ and $s_{L,\nu}^n$ in evaluating $\Delta b_3$, i.e., each interacting $s_{L,\nu}$ value is paired with the corresponding non-interacting $s_{L,\nu}^n$ value. Figure 4 shows that the cutoff introduces a divergence in $b_3$. This divergence arises because the cutoff alters the high-temperature behavior of $\Delta b_3$, which implies that the divergencies of $b_3^{\text{ref}}$ and $\Delta b_3$ no longer cancel. Importantly, $b_3$ is converged in the low-temperature (large $\tilde{\omega}$) regime even for a relatively small cutoff. This allows us to use the converged low-temperature tail to constrain $b_3$ in the high-temperature regime. Extrapolating $b_3$ (calculated using a cutoff of 9) to the high-temperature limit, we find $b_3^{(0)} \approx -0.068(1)$, which deviates by less than 2% from the exact value.

The validity of the employed extrapolation scheme crucially hinges on the fact that the functional form of $b_3$ changes “predictably” as $\tilde{\omega}$ changes from the low- to the medium- to the high-temperature regime. For example, if $b_3$ changed sign in the medium- or high-temperature regime, as is the case for the coefficient $b_{2,1}$ that characterizes the behavior of two identical fermions and one lighter fermion (with a mass ratio from 3.11 to 8.62) [29], the extrapolation employed above would predict the incorrect high-temperature limit of $b_{2,1}$.

The interaction piece $\Delta b_4$ of the fourth-order virial coefficient can be expressed analogously to $\Delta b_3$. In particular, we write the energies at unitarity in terms of the $s_{L,\nu}$ (see Sec. III and the supplemental material for a listing of the $s_{L,\nu}$ values) and perform, as in the three-body case above, the sum over the hyperradial quantum number $q$ analytically. Since both natural and unnatural parity states of the four-body systems are affected by the s-wave interactions, the $s_{L,\nu}$ values corresponding to both natural and unnatural parity states need to be included when evaluating $\Delta b_4$. The reference piece $b_4^{\text{ref}}$ diverges as

$$b_4^{\text{ref}} = -\frac{1}{2} \tilde{\omega}^{-6} + \frac{3}{16} \tilde{\omega}^{-4} - \frac{1 + 64b_3^{(0)}}{32} \tilde{\omega}^{-3} - \frac{149}{3840} \tilde{\omega}^{-2} + \frac{1 + 64b_3^{(0)} + 512b_4^{(0)}}{256} \tilde{\omega}^{-1} \quad (20)$$

in the high-temperature limit. This divergence must be cancelled by a divergence of $\Delta b_4$ of opposite sign.

Dash-dot-dotted, dash-dotted and dashed lines in Fig. 7 show $b_4$ at unitarity obtained by using the full expression for $b_4^{\text{ref}}$ and by limiting the sums over $q$ and $L$ in $\Delta b_4$ such that $s_{L,\nu} \leq 11/2, \leq 15/2$ and $\leq 19/2$, respectively. For the largest cutoff, our calculation includes 169 and 89 $s_{L,\nu}$ values associated with shifted states [not counting the $(2L + 1)$-multiplicity] of the harmonically trapped (2,2) and (3,1) systems with zero-range interactions, respectively. Figure 7 shows that $b_4$ is negative in the low-temperature (large $\tilde{\omega}$) regime and that neither $b_4$ nor its first or second derivatives with respect to $\tilde{\omega}$ change sign in the regime where $b_4$ is converged. This motivates us to extrapolate the converged part of $b_4$ to the medium- and high-temperature regime (see dotted line in Fig. 7), yielding $b_4^{(0)} = -0.0020(5)$.

The LDA predicts that the virial coefficient $b_{n,\text{hom}}^{\text{LDA}}$ of the homogeneous system is related to the high-temperature limit of the $n$th order virial coefficient of the trapped
FIG. 7: (Color online) Virial coefficient $b_4$ of the trapped two-component Fermi gas at unitarity as a function of the inverse temperature $\tilde{\omega}$. The dash-dot-dotted, dash-dotted and dashed lines show $b_4$ obtained by limiting $s_{L,\omega}$ to be smaller than $11/2, 15/2$ and $19/2$, respectively. The dotted line shows our attempt to extrapolate to the high-temperature limit; this extrapolation assumes that $b_4$ changes “predictably” from the low- to the medium- to the high-temperature regime. The inset shows the same data as the main figure. In addition, the solid horizontal line shows the high-temperature limit $b_4^{\text{hom}}$ determined by applying the LDA to the fourth-order virial coefficient predicted for the homogeneous system.\[23\]

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Appendix A: Matrix elements

This appendix summarizes the expressions for the overlap, kinetic energy, trap potential, and interaction potential matrix elements for states with natural parity (any $L$) and unnatural parity ($L > 0$). For notational simplicity, we omit the subscripts of the matrix $A_k$ and the vectors $\vec{u}_1k$ and $\vec{u}_{2k}$, and consider the matrix elements between the unsymmetrized basis functions $\psi$ and $\psi'$ characterized by $(A, \vec{u}_1, \vec{u}_2)$ and $(A', \vec{u}_1', \vec{u}_2')$, respectively [see Eq. (5) of Sec. III]. The matrix elements have been derived in the literature \[32–37\] and are summarized here for completeness.

Before providing explicit expressions for the matrix elements, we introduce a number of auxiliary quantities that are utilized in Subsecs. A1 and A2. The product of $\psi'$ and $\psi$ can be conveniently written in terms of the matrix $B$.

$$B = A' + A. \quad \text{(A1)}$$

We further define the scalars $C$ and $\rho_{ij}$ ($i, j = 1$ or 2),

$$C = \left(\frac{(2\pi)^{n-1}}{\det(B)}\right)^{3/2} \rho_{11}^{L-2} \quad \text{(A2)}$$

and

$$\rho_{ij} = (\vec{u}_i')^T B^{-1} \vec{u}_j; \quad \text{(A3)}$$

note that the order of the primed and unprimed vectors $\vec{u}_i'$ and $\vec{u}_j$ matters. We further define the scalars $R$ and $S_{ij}$ ($i, j = 1$ or 2),

$$R = 3\text{Tr}(B^{-1} A A A') \quad \text{(A4)}$$

and

$$S_{ij} = (\vec{u}_i')^T B^{-1} A A' B^{-1} \vec{u}_j, \quad \text{(A5)}$$

where the diagonal elements of the matrix $A$ are given by the inverse of the masses associated with the Jacobi vectors and the off-diagonal elements of $A$ are zero. In Eq. (A4), $\text{Tr}$ denotes the trace operator. The scalars $\tilde{R}^{(pq)}$ and $\tilde{C}^{(pq)}$ ($p = 1, \ldots, n$ and $q = p + 1, \ldots, n$) have a similar structure to $R$ and $S_{ij}$,

$$\tilde{R}^{(pq)} = 3\text{Tr}(B^{-1} Q^{(pq)}) \quad \text{(A6)}$$

and

$$\tilde{S}^{(pq)}_{ij} = (\vec{u}_i')^T B^{-1} Q^{(pq)} B^{-1} \vec{u}_j. \quad \text{(A7)}$$

The matrix $Q^{(pq)}$ is defined as

$$Q^{(pq)} = \tilde{C}^{(pq)} \left(\tilde{C}^{(pq)}\right)^T, \quad \text{(A8)}$$

where $\tilde{C}^{(pq)}$ is the $(n - 1)$-dimensional vector that relates the distance vectors $\vec{r}_{pq}^p$ to the Jacobi vectors $\vec{x} = (\vec{r}_{11}, \ldots, \vec{r}_{n-1})$,

$$\vec{r}_{pq}^p = \left(\tilde{C}^{(pq)}\right)^T \vec{x}. \quad \text{(A9)}$$

Lastly, we define the total mass $M_{tot}$,

$$M_{tot} = \sum_{p=1}^{n} m_p. \quad \text{(A10)}$$

1. Natural parity

For natural parity states, we use $l_1 = L$ and $l_2 = 0$ in Eq. (3), which implies that $\psi'$ and $\psi$ are independent of $\vec{u}_2'$ and $\vec{u}_2$, respectively. In the following, we assume that $\psi'$ and $\psi$ are characterized by the same $L$ and II values.

Under these assumptions the overlap matrix element is given by

$$\langle \psi' | O | \psi \rangle = N_L^{\text{nat}} C \rho_{11}, \quad \text{(A11)}$$

where $N_L^{\text{nat}}$ is a $L$-dependent constant that enters into all matrix elements and thus cancels when calculating expectation values. The kinetic energy matrix element reads

$$\langle \psi' | T_{\text{rel}} | \psi \rangle = N_L^{\text{nat}} \frac{h^2}{2} C (R \rho_{11} + 2 L S_{11}) \rho_{11}. \quad \text{(A12)}$$

The matrix element for the trapping potential reads

$$\langle \psi' | V_{\text{trap}} | \psi \rangle = N_L^{\text{nat}} \sum_{p=1, q > p}^{n} \frac{1}{2} \left(\frac{m_p m_q}{M_{tot}}\right) \Omega^2 C \times \left(\tilde{R}^{(pq)} \rho_{11} + 2 L \tilde{C}^{(pq)} \right) \rho_{11}. \quad \text{(A13)}$$

Lastly, the interaction matrix element for the Gaussian potential can be written as

$$\langle \psi' | V_{\text{int}} | \psi \rangle = -V_0 \sum_{p=1}^{n_1} \sum_{q=n_1+1}^{n} \langle \psi' | \exp[-r_{pq}^2/(2 \sigma_0^2)] | \psi \rangle. \quad \text{(A14)}$$

The expression for the matrix element $\langle \psi' | \exp[-r_{pq}^2/(2 \sigma_0^2)] | \psi \rangle$ reduces to that for the overlap matrix element if the matrices $A'$ and $A$ are replaced by $A' + Q^{(pq)}/(2 \sigma_0^2)$ and $A + Q^{(pq)}/(2 \sigma_0^2)$, respectively.
2. Unnatural parity ($L > 0$)

For unnatural parity states with $L > 0$, we use $l_1 = L$ and $l_2 = 1$ in Eq. (3). In the following, we assume that $\psi'$ and $\psi$ are characterized by the same $L$ and $H$ values. Under these assumptions the overlap matrix element is given by

$$\langle \psi' | O | \psi \rangle = N_L^{\text{unnat}} C \rho_{11} (\rho_{11} \rho_{22} - \rho_{12} \rho_{21}),$$

(A15)

where $N_L^{\text{unnat}}$ is a $L$-dependent constant that enters into all matrix elements and thus cancels when calculating expectation values. The kinetic energy matrix element reads

$$\langle \psi' | T^{\text{rel}} | \psi \rangle = N_L^{\text{unnat}} \frac{\hbar^2}{2} C$$

$$\left\{ [R \rho_{11} + 2(L - 1) S_{11}] (\rho_{11} \rho_{22} - \rho_{12} \rho_{21}) + 2 \rho_{11} (\rho_{11} S_{22} + \rho_{22} S_{11} - \rho_{12} S_{21} - \rho_{21} S_{12}) \right\}. \quad \text{(A16)}$$

The matrix element for the trapping potential reads

$$\langle \psi' | V^{\text{trap}} | \psi \rangle = N_L^{\text{unnat}} \sum_{p=1,q>p}^{n} \frac{1}{2} \left( \frac{m_p m_q}{M_{\text{tot}}} \right) \Omega^2 C \times$$

$$\left\{ [\tilde{R}(pq) \rho_{11} + 2(L - 1) \tilde{S}_{11}(pq)] (\rho_{11} \rho_{22} - \rho_{12} \rho_{21}) + 2 \rho_{11} (\rho_{11} \tilde{S}_{22}(pq) + \rho_{22} \tilde{S}_{11}(pq) - \rho_{12} \tilde{S}_{21}(pq) - \rho_{21} \tilde{S}_{12}(pq)) \right\}. \quad \text{(A17)}$$

As in the natural parity case, the expression for the interaction matrix element for the Gaussian potential can be related to that of the overlap matrix element by making the appropriate substitutions.

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