Explicitly Correlated Gaussian Approach: Method Development and Application to
Ultracold Few-Fermion Systems

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Abstract

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Few-body physics plays an important role in quantum gases. For example, the lifetime of ultracold atomic gases is limited by atom losses. While atom losses are, in general, undesirable, they can be measured experimentally and analyzed in terms of three- and higher-body recombination processes. This dissertation takes a theoretical approach to discuss trapped and free-space few-fermion systems with emphasis on the development and implementation of numerical techniques.

To solve the Schrödinger equation for trapped few-body systems, we implement the explicitly correlated Gaussian technique, which is a basis set expansion-type approach. The technique is used to investigate equal-mass spin-balanced and spin-imbalanced four-body systems confined in a spherically symmetric trap. A large portion of the zero-range energy spectra for infinitely large interspecies s-wave scattering length are tabulated and analyzed. The results serve as a benchmark for other numerical techniques and are relevant for understanding few-body energy spectra, which can be measured experimentally using radio-frequency spectroscopy. The energies were used to calculate the fourth-order virial coefficient and to investigate inter-system degeneracies. In addition, we discuss unequal-mass four-body systems consisting of three identical fermions and one distinguishable impurity.

Experiments on ultracold Fermi gases cannot only realize three-dimensional few-body
systems but also effectively low-dimensional few-body systems. The properties of quasi one-dimensional systems can be described by effective one-dimensional model Hamiltonian. The explicitly correlated Gaussian technique is used to investigate the validity regime of different effective one-dimensional model Hamiltonian through direct comparison with three-dimensional results.

This thesis also develops a hyperspherical explicitly correlated Gaussian approach, which solves- within the hyperspherical framework- the hyperangular Schrödinger equation for few-body systems with finite angular momentum. One major advantage of this technique is that the hyperspherical framework provides access to bound states as well as to scattering states. As a first application, we solved and analyzed the energetically lowest-lying hyperangular eigenvalues of equal- and unequal-mass four-particle systems with infinitely large interspecies $s$-wave scattering length. The analysis can be extended to study interesting few-body phenomena like four-body resonances and Efimov physics.
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4.1 The solid and dashed lines show the free-space scattering lengths \(a_{3D}^{aa}\) and \(a_{1D}^{aa}\) for the Gaussian potential \(V_{tb}\) as a function of the well depth \(V_0\). The scattering lengths and depths are measured in the “natural units” of the free-space system, i.e., in units of \(r_0\) \([z_0]\) and \(\hbar^2/(2\mu^{aa} r_0^2)\) \([\hbar^2/(2\mu^{aa} z_0^2)]\) for the 3D \([1D]\) system, where \(\mu^{aa}\) denotes the reduced mass of the atom-atom system.
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5.1 Pair distribution function \( P_{13}(z) \) for the up-down distance of the energetically lowest-lying state of the \((2,1)\) system with even parity. The solid, dashed and dash-dotted lines correspond to the pair distribution functions at scattering lengths \( a_{1D}^a/a_z = 1.32654, 0.326537 \) and 0.126537, respectively. The black dash-dash-dotted line corresponds to the non-interacting case. The calculations are performed using \( z_0 = 0.005a_z \). The circles, squares and crosses show the pair distribution functions for the \((1,1)\) system with zero-range interactions and \( a_{1D}^{ad}/a_z = 1.32654, 0.326537 \) and 0.126537, respectively. The two-body pair distribution functions are normalized to 1/2.

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6.1 The first column shows the mass ratio $\kappa$. Columns 2 and 3 show the $s_{0,\text{unit}}^{Z\text{R}}$ values for the (3,1) system with $1^+$ symmetry at unitarity obtained by the HECG approach and from the extrapolated zero-range energies of the trapped system (see the text for details). For comparison, column 4 shows the results from Ref. [117]. The $\kappa = 1$ entry in the third column is taken from Ref. [39].
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Related Publications


Chapter 1

Introduction

The fundamental particles in nature can be divided into two different classes, fermions and bosons. The fundamental difference between these two kinds of particles is the spin angular momentum. The class of particles with integer spin angular momentum is called bosons (e.g. photon, gluon) and the class of particles with half-integer spin angular momentum is called fermions (e.g. electron, proton, neutron, quark) [1, 2]. Atoms consist of half-integer spin particles, namely electrons, neutrons and protons. In the low-energy regime the breakup of an atom into its constituents is not possible. In this regime, an atom can be classified as a composite fermion or a composite boson depending on its net spin [3, 4, 5, 6]. The net spin is determined by coupling the spin angular momenta of the constituent particles vectorially. If an atom is made up of an odd number of constituents, the resulting spin of the atom is a half-integer and, correspondingly, the atom is a composite fermion. If an atom is made up of an even number of constituents, the resulting spin of the atom is an integer and, correspondingly, the atom is a composite boson.

Fermionic particles obey Pauli’s exclusion principle, which forces the many-body wave function to be anti-symmetric under the exchange of two identical fermions [7]. As a result, two identical fermions are prohibited from occupying the same quantum state. The
wave function of a system of identical bosons has to be symmetric under the exchange of two identical bosons. As a consequence, identical bosons are allowed to occupy the same quantum state. Fermionic and bosonic particles follow the Fermi-Dirac statistics and the Bose-Einstein statistics, respectively [8]. These statistics depend on the temperature of the system and, in a single-particle picture, govern the mean occupation numbers of the single-particle energy states.

The thermal de Broglie wavelength $\lambda_{dB}$ reflects the quantum nature of a system. The de Broglie wavelength is defined through [2,9]

$$\lambda_{dB} = \frac{h}{\sqrt{2\pi mk_B T}},$$

(1.1)

where $h$ is the Planck constant, $m$ is the mass of the particle, $T$ is the temperature and $k_B$ is the Boltzmann constant. The de Broglie wave length increases with decreasing $T$. When the thermal de Broglie wavelength is much smaller than the interparticle distance, the particles can be treated classically. When the de Broglie wavelength becomes of the order of the average interparticle spacing, the system reaches the quantum degenerate regime. The degeneracy temperature $T_c$ can be determined from the condition $\rho \lambda_{dB}^3 \approx 1$, where $\rho$ is the number density [3]. Quantum degeneracy has distinctly different characteristics for bosons and fermions. Below $T_c$, a large fraction of the bosonic particles occupy the lowest quantum state. This new state of matter is known as Bose-Einstein condensate [10,11]. However, there is no such transition in the fermionic system due to the Pauli exclusion principle. Identical fermions occupy the available energy levels up to the Fermi energy $E_F$ even at zero temperature [8]. The Fermi energy is the energy of the highest single-particle state occupied by the fermions. In the regime of quantum degeneracy the particles have to be treated quantum mechanically. If the temperature is much lower than $T_c$, then a zero-temperature quantum picture should provide a good description.
To treat the particles quantum mechanically, we need to solve the Schrödinger equation. For atomic gases with sufficiently low densities, usually only two-body interactions are important [12]. In the degenerate regime, the short-range features of the two-body potential can not be resolved since the de Broglie wave length $\lambda_{dB}$ is much larger than the range of the two-body potential. As a result, the low-energy physics does not depend on the details of the underlying two-body potential but on a few atomic physics parameters such as the two-body $s$-wave scattering length or effective range. At the two-body level, the outcome of a scattering process depends, in general, on all partial waves [13, 14]. However, away from higher partial wave resonances, atom-atom collisions at very low scattering energies are dominated by the lowest partial wave due to the threshold law [9]. The $s$-wave scattering can be parameterized through the $s$-wave scattering length $a_{3D}^{aa}$ [12,15,16], which is described in the next paragraph.

We consider the scattering of two particles having coordinates $\vec{r}_1$ and $\vec{r}_2$, and masses $m_1$ and $m_2$. The particles interact via a central potential $V_{tb}(|\vec{r}_1 - \vec{r}_2|)$. We introduce the relative coordinate $\vec{r}$ and the center of mass coordinate $\vec{R}$, where $\vec{r} = \vec{r}_1 - \vec{r}_2$ and $\vec{R} = (m_1\vec{r}_1 + m_2\vec{r}_2)/(m_1 + m_2)$. The relative motion of the system is described by the wavefunction $\psi(\vec{r}) = R_l(r)Y_{l,m}(\hat{r})$, where $Y_{l,m}(\hat{r})$ is the spherical harmonic with angular momentum $l$ and projection quantum number $m$. We aim to find the stationary solution of the radial Schrödinger equation [9]:

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2} \right] u_l(r) = 0,$$

where $u_l(r) = R_l(r)/r$, $U(r) = [2\mu V_{tb}(r)]/\hbar^2$ and $k = \sqrt{(2\mu E)/\hbar}$. Here, $\mu$ is the reduced mass of the two interacting atoms and $E$ is the relative energy. The solution of Eq. (1.2) is...
subject to the boundary condition

\[
u_t(r) = 0 \quad (1.3)
\]

at \( r = 0 \). Assuming \( V_{ib}(r) \) vanishes at \( r = R_m \), the s-wave solution for \( r \gg R_m \) can be approximately written as [17]

\[
u_0(r) = \frac{A_0(k)}{k} \sin[kr + \delta_0(k)], \quad (1.4)
\]

where \( \delta_0(k) \) is the phase shift that is accumulated during the scattering process and \( A_0(k) \) is a normalization constant. The phase shift can be obtained by matching the logarithmic derivatives of the inner solution \((r < R_m)\) and the outer solution \((r > R_m)\) at \( r = R_m \). The s-wave scattering length \( a_{3D}^{aa} \) is defined through [9,18]

\[
a_{3D}^{aa} = -\lim_{k \to 0} \frac{\tan[\delta_0(k)]}{k}, \quad (1.5)
\]

and the scattering cross section \( \sigma \), in the s-wave dominated regime, is given by

\[
\sigma = 4\pi(a_{3D}^{aa})^2. \quad (1.6)
\]

Using Eqs. (1.4) and (1.5), one can show that in the zero-energy limit the asymptotic solution \( u_0(r) \) varies linearly with \( r \) and has a node when \( r = a_{3D}^{aa} \) [17],

\[
u_0(r) = A_0(0)(r - a_{3D}^{aa}). \quad (1.7)
\]

Figure 1.1 shows three s-wave scattering wave functions for a model potential, namely an attractive Gaussian potential \( V_{ib}(r) = -V_0 \exp[-r^2/(2\sigma_0^2)] \) with depth \( V_0 \) and range \( \sigma_0 \), as a function of \( r/\sigma_0 \). Dashed, solid and dotted lines show the scaled s-wave scattering wave function \( u_0(r) \) for \( V_0/E_{ref} = 1.157, 1.342 \) and 1.591, respectively, where the reference energy \( E_{ref} \) is defined through \( E_{ref} = \hbar^2/(2\mu\sigma_0^2) \). The linear behavior of \( u_0(r) \) for \( r \gg \sigma_0 \) can be
seen readily in Fig. 1.1. In general, depending on the potential parameters, the scattering length of an attractive potential can be positive, negative or diverging.

Experimentally, the $s$-wave scattering length can be tuned by applying an external magnetic field in the vicinity of a Fano-Feshbach resonance [14,19]. A Fano-Feshbach resonance exists when the binding energy of a closed channel molecule coincides with the scattering energy of the open channel. In the vicinity of a Fano-Feshbach resonance, the $s$-wave scattering length can be adjusted to any desired value by tuning the magnetic field around the resonance value. Dilute two-component Fermi gases are stable even for infinitely large interspecies $s$-wave scattering length since the Pauli exclusion principle stabilizes the system against collapse due to the attractive interspecies interactions [20,21,22]. For small negative scattering length [in the Bardeen-Cooper-Schrieffer (BCS) regime], the unlike fermions pair up to form Cooper pairs [5,23,24,25]. For small positive scattering length (in the BEC regime), the unlike fermions form tightly bound bosonic dimers. This evolution from Cooper pair to bosonic dimer is known as BCS-BEC crossover [5,25,26].

To conduct experiments on degenerate quantum gases it is necessary to confine the atoms
in an external potential. Ultracold atoms can be confined magnetically or optically [3, 4]. Magnetic traps depend on the interaction between the external magnetic field and the intrinsic magnetic moment of the atoms. Optical traps depend on the interaction between an induced dipole moment of the atoms and an external electric field from a laser [27, 28]. A one-dimensional periodic potential or optical lattice can be created by using a standing wave generated by two counterpropagating laser beams. Two- and three-dimensional optical lattices can be created as well by using more laser beams [27, 28]. The lattice depth and spacing can be manipulated by tuning the intensity and frequency of the lasers. The bottom of these lattice sites is approximately harmonic. Recently, the deterministic preparation of few-fermion systems consisting of one to ten particles in a well-defined quantum state has been achieved [29]. The approach involves a so-called microtrap, which uses a tightly focused laser beam. Applying an additional magnetic field gradient can control the number of atoms. This gradient leads to a tilt of the trap. The controlled spilling of atoms prepares a sample of few atoms. The atom number can be determined by using the absorption imaging technique.

A system is said to be fully universal when the system properties depend solely on the s-wave scattering length [15,16,30,31]. A necessary condition for universality is that \(a^{aa}_{3D} \gg r_0\). For example, if \(a^{aa}_{3D}\) is large and positive, two particles with reduced mass \(\mu\) form a loosely bound dimer in free space with binding energy \(E \approx -\hbar^2/[2\mu(a^{aa}_{3D})^2]\). There have been exciting developments in understanding universal aspects of three- and higher-body systems (see, e.g., Refs. [15, 16, 32, 33, 34, 35, 36, 37, 38]). Away from higher-partial wave resonances, for example, equal-mass two-component three- and higher-fermion systems are universal if the range \(r_0\) of the interaction potential is much smaller than the s-wave scattering length \(a^{aa}_{3D}\) and the harmonic oscillator length \(a_{ho}\). In the small-range limit, the system behavior is essentially independent of the shape of the potential. In the unequal-mass sector, universal three- and four-body bound states, which are fully determined by the s-wave scattering length, have been predicted to exist for the (2, 1) and (3, 1) Fermi systems,
respectively, consisting of a majority of heavy species and a single light impurity [30, 43].

A remarkable few-body phenomenon is the Efimov effect, which was originally studied by Vitaly Efimov [44, 45, 46]. Efimov considered the three-boson problem with large scattering length and predicted the appearance of an infinite series of geometrically spaced three-body bound states in the absence of any two-body bound state. Unlike the description of universal two-body bound states, the description of the Efimov effect requires an additional parameter, the three-body parameter $k_*$. The three-body parameter, which is typically believed to depend on the details of the interaction potential [15, 47], has been claimed to be universal for a certain class of interaction potentials such as van der Waals potentials [48, 49]. Evidence of the Efimov effect is found by probing the loss of atoms from the trap as a function of the scattering length [50]. An enhanced three-body loss of atoms from the trap was first observed experimentally for identical bosons by tuning the scattering length to a value where the binding energy of an Efimov state coincides with the energy of three free atoms [50, 51, 52]. Though equal mass (2, 1) systems consisting of two spin-up atoms and one spin-down atom do not exhibit the Efimov effect as a consequence of the Pauli exclusion principle, the Efimov effect exists in fermionic (2, 1) systems with large mass ratio and for three distinguishable equal-mass particles [32, 53, 54, 55, 56]. The four-body system has been predicted to exhibit the four-body Efimov effect [57].

Along with experimental achievements, enormous progress has been made in the theoretical description of the zero-temperature behavior of few-body systems. Progress has been made in analytical and numerical treatments. The two-body system with zero-range s-wave interactions under isotropic harmonic trap was solved analytically by Busch et al. [58]. At unitarity, i.e., for infinite scattering length, Werner and Castin calculated the complete three-body spectrum for three particles under external isotropic confinement semi-analytically [59]. Numerical efforts aimed at solving the few-particle Schrödinger equation have benefited from
growing computational resources and improved algorithms. The hyperspherical harmonics expansion method, which is based on the expansion of the wave function in terms of hyperspherical harmonic functions, has been applied to few-body systems \( n \leq 4 \) \[60, 61\], where \( n \) is number of particles. The adiabatic hyperspherical approach has been used extensively to study ultracold few-body collisions and Efimov physics \[48, 62, 63, 64, 65, 66\].

Another well established method to treat both bound and scattering states is based on the Faddeev equations \( n = 3 \) and Faddeev-Yakubovsky equations \( n = 4 \) \[67, 68, 69\]. Effective field theory has been a widely used approach for quantitative calculations of low-energy observables \[15\]. For example, effective field theory has been applied successfully to describe weakly-interacting systems \[70, 71\] and universal aspects of strongly-interacting few-body systems \[72, 73\]. Monte Carlo methods, which are particularly useful for simulating many-body systems, have been applied successfully to few-body systems \[34, 74\]. However, the results from Monte Carlo methods might be less accurate than some other few-body techniques. As Monte Carlo methods are usually designed to study ground states, they have limited applicability for the description of excited states.

One of the major goals of this dissertation is to determine bound states of few-body systems with high accuracy as a function of different parameters such as the trapping geometry, mass ratio, interaction strength, statistics and symmetry of the system. We implement the explicitly correlated Gaussian technique \[75, 76\], which is a basis set expansion-type approach. We utilize the variational principle to set an upper bound on the eigenenergies of two-component Fermi gases. We achieve high accuracy for the energies through controlled convergence using the stochastic variational method. The few-body energies, in principle, can be measured via radio-frequency spectroscopy. For instance, the binding energy of weakly bound \(^6\text{Li}_2\) molecules has been traced out \[19, 77, 78\]. Accurate calculations of few-body energy spectra provide access to the high-temperature dynamics of many-fermion systems \[79\]. The thermodynamic potential is expanded in terms of the fugacity \( z = \exp[\mu/k_B T] \), where
The chemical potential $\mu$ is the chemical potential. The expansion coefficients associated with the series in the small parameter are called virial coefficients $b_n$ [80, 81, 82]. The fugacity $z$ decreases with decreasing de Broglie wavelength $\lambda_{dB}$. At high temperature, $\lambda_{dB}$ is small and the fugacity $z$ is also a small parameter. As a result, the expansion at high temperature should work well if only the first and second virial coefficients are included. The determination of the $n^{th}$ order virial coefficient $b_n$ requires knowledge of the complete set of eigenenergies of all “subsystems” consisting of $i, i \leq n$, particles. In practice, only portions of the energy spectra are known. In this thesis we use the explicitly correlated Gaussian technique to obtain a large portion of the zero-range energy spectra at unitarity for the equal mass (3, 1) and (2, 2) Fermi systems. These energies are used to study the behavior of the fourth-order virial coefficient $b_4$ as a function of temperature. This is approach is unfortunately limited to fairly small temperatures, since the energy spectra can only be determined up to a fairly low energy.

In addition, we developed a hyperspherical explicitly correlated Gaussian (HECG) approach, which provides an alternative numerical technique to solving few-body systems within the hyperspherical framework. An earlier HECG approach was developed by von Stecher and Greene for three- and four-body systems with vanishing angular momentum and positive parity [65, 83, 84]. This thesis presents a major extension of this approach to finite angular momentum ($L = 1$) and positive or negative parity. The theoretical framework is valid for any number of particles. However, present day computational capabilities limit these calculations to $n \leq 5$. The $L^\Pi = 1^+$ case is particularly interesting since it supports universal four-body bound states and four-body Efimov states. Moreover, in addition to the bound state calculations, the developed framework provides access to scattering states [83, 84].

The remainder of the thesis is organized as follows. Chapter 2 describes the explicitly correlated Gaussian technique. The system Hamiltonian and the explicitly correlated
Gaussian basis functions with definite symmetry are introduced. The energy optimization procedure based on the stochastic variational method is discussed. Compact expressions for the required matrix elements are provided in Appendix A.

Chapter 3 considers small equal-mass two-component Fermi gases under spherically symmetric external harmonic confinement with large $s$-wave scattering length. The stochastic variational approach is used to calculate a large portion of the $(2, 2)$ and $(3, 1)$ eigenenergies as a function of the interaction range. The zero-range energies are obtained by extrapolating the finite-range energies. Applications of these zero-range energies are discussed. In addition, Ch. 3 analyzes the ground state energy of the trapped $(3, 1)$ system with unequal masses. The zero-range energies for the $(2, 2)$ and $(3, 1)$ system with different symmetries and infinitely large $s$-wave scattering length are provided in Appendix B. Chapter 3.2 is largely based on Ref. [39].

Chapter 4 contains the manuscript that has been published in Physical Review A [D. Blume and D. Rakshit, Phys. Rev. A 80, 013601 (2009)]. The chapter considers three- and four-body two-component Fermi gases under highly-elongated cigar-shaped confinement. We employ the explicitly correlated Gaussian approach to calculate the ground state energies and excitation frequencies within a full three-dimensional framework and within an effective one-dimensional framework. The comparison of the three-dimensional and one-dimensional calculations establishes the validity regimes of the one-dimensional Hamiltonian. In this work I contributed by implementing the explicitly correlated Gaussian approach, selecting the proper trial basis functions that are required for describing the system along the BCS-BEC crossover and by performing calculations for the three-body system. D. Blume performed the four-body calculations. The manuscript was prepared by D. Blume.

In Ch. 5 we employ the explicitly correlated Gaussian approach to look at selected structural properties of the energetically lowest-lying even parity state of the trapped one-dimensional $(2, 1)$ Fermi gas. The features of the structural properties as a function of the one-dimensional scattering length are discussed.
Chapter 6 contains the manuscript that has been published in Physical Review A [D. Rakshit and D. Blume, Phys. Rev. A 86, 062513 (2012)]. In this chapter we develop the hyperspherical explicitly correlated Gaussian (HECG) technique for few-body systems with finite angular momentum. This chapter develops a theoretical framework to calculate the effective potential and the associated coupling matrix elements for a \( n \)-particle system. The application of the method is demonstrated by considering the equal- and unequal-mass (2, 2) and (3, 1) systems. The development of the framework is a combined effort by myself and D. Blume. The numerical results presented in Chs. 6.5 and 6.6 were obtained by D. Blume, and the manuscript was prepared by D. Blume. An independent numerical implementation of this technique by myself analyzed four-body systems up to a mass ratio eight. However, numerical challenges restricted the calculations to larger \( r_0/R \), where \( R \) is the hyperradius, than those considered in Chs. 6.5 and 6.6 and thus the extrapolated zero-range results had larger uncertainties.

Finally, Ch. 7 concludes and discusses possible extensions of the work presented in this thesis.
Chapter 2

Explicitly correlated Gaussian technique

2.1 Introduction

The variational method has found extensive applications in describing quantum states of physical systems [60, 85, 86, 87, 88]. When solving the time-independent Schrödinger equation using a basis set expansion approach, an important aspect is the choice of the basis functions. The basis set has to be flexible enough to account for the correlations introduced by the interactions. Explicitly correlated Gaussian (ECG) basis functions, i.e., functions that contain an explicit dependence on the interparticle distances, can describe highly correlated few-body systems with great efficiency [75, 89, 90, 91]. Explicitly correlated functions were first used to calculate the energy of the helium atom and helium-like ions [92, 93, 94]. In the 1960s, Boys and Singer [95, 96] introduced the basis set of Gaussian-type geminals. These geminals were later proved to be complete [97, 98]. The stochastic variational method, which is a trial and error optimization procedure, helps in selecting the most suitable basis functions [75]. The stochastic variational method has been widely used to study few-body systems in different branches of physics like atomic, molecular and nuclear few-body physics [75, 90],
solid-state physics [75, 99] and quantum chemistry [100, 101].

Section 2.2 introduces the systems under study. Section 2.3 introduces the Jacobi coordinates and discusses the separation of the center of mass motion and the relative motion. Section 2.4 presents the variational principle and matrix representation of the Schrödinger equation. Section 2.5 discusses different types of explicitly correlated Gaussian basis functions. The symmetrization of the basis functions is discussed in Sec. 2.6 and Sec. 2.7 describes the stochastic variational scheme.

### 2.2 System under study

The quantum behavior of a $N$-particle system with masses $m_1, \ldots, m_N$ and position vectors $\vec{r}^T = \{\vec{r}_1, \ldots, \vec{r}_N\}$ is governed by the Schrödinger equation

$$H_{\text{tot}}^{3D} \Psi_{\text{tot}}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = E_{\text{tot}} \Psi_{\text{tot}}(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N), \quad (2.1)$$

where $H_{\text{tot}}^{3D}$ denotes the Hamiltonian of the $N$-particle system. The particles can be identical bosons, identical fermions, distinguishable particles, or any combination thereof. This thesis considers few-body systems under varying confinement. Throughout, the Hamiltonian $H_{\text{tot}}^{3D}$ of the system in three-dimensional space is assumed to have the form

$$H_{\text{tot}}^{3D} = T_{\text{tot}} + V_{\text{tr}}^{\text{tot}} + V_{\text{int}}, \quad (2.2)$$

where

$$T_{\text{tot}} = \sum_{i=1}^{N} -\hbar^2 \frac{\nabla^2_{\vec{r}_i}}{2m_i}, \quad (2.3)$$

$$V_{\text{tr}}^{\text{tot}} = \sum_{i=1}^{N} V_{\text{tr}}(\vec{r}_i), \quad (2.4)$$
and

\[ V_{\text{int}} = \sum_{j > i=1}^{N} V_{tb}(\vec{r}_{ij}). \]  \hspace{1cm} (2.5)

In Eq. (2.4), \( V_{tr}(\vec{r}_i) \) denotes the trapping potential of the \( i^{th} \) particle,

\[ V_{tr}(\vec{r}_i) = \frac{1}{2} m_i \omega^2 r_i^2, \]  \hspace{1cm} (2.6)

where \( r_i = |\vec{r}_i| \) and \( \omega \) is the angular trapping frequency of the spherically symmetric external confining potential. In Eq. (2.5), \( V_{tb}(\vec{r}_{ij}) \) denotes the interaction potential between the \( i^{th} \) and \( j^{th} \) particle, where \( \vec{r}_{ij} = \vec{r}_i - \vec{r}_j \).

The true interaction potential between two neutral atoms can, in the Born-Oppenheimer approximation, be described by a van der Waals potential. Asymptotically the van der Waals potential varies as \(-C_6/r_{ij}^6 + O(r_{ij}^{-7})\), where \( C_6 \) is a positive coefficient \([102, 103]\). The characteristic length scale between two neutral atoms is the van der Waals length \( l_{vdw} = (\mu C_6/\hbar^2)^{1/4} \) \([13]\), where \( \mu \) is the reduced mass of the two atoms. At low temperature, the de Broglie wavelength \( \lambda_{dB} \) is much larger than the van der Waals length \( l_{vdw} \). Consequently, the details of the interparticle interaction become, in many cases, negligible and the low energy scattering can be described by simple model potentials. For ultracold systems, the main contribution to the scattering cross section comes from the lowest partial wave \( (l = 0) \), i.e., from \( s \)-wave states \([12]\). However, for identical fermions, the Pauli exclusion principle excludes \( s \)-wave scattering as the wave function between spin polarized fermions has to be antisymmetric. In our numerical calculations, we model the atom-atom interaction \( V_{tb}(\vec{r}_{ij}) \) by a simple Gaussian potential,

\[ V_{tb}(\vec{r}_{ij}) = -V_0 \exp \left( \frac{-r_{ij}^2}{2r_0^2} \right). \]  \hspace{1cm} (2.7)

For a fixed range \( r_0 \), we adjust the depth \( V_0 \) \((V_0 > 0)\) to obtain the desired three-dimensionsional free-space \( s \)-wave atom-atom scattering length \( a_{3D}^{aa} \). The solid line in Fig. 2.1 shows \( a_{3D}^{aa} \) as a
Figure 2.1: The solid and dashed lines show the free-space scattering lengths $a_{3D}^{aa}$ and $a_{1D}^{aa}$ for the Gaussian potential $V_{tb}$ as a function of the well depth $V_0$. The scattering lengths and depths are measured in the natural units of the free-space system, i.e., in units of $r_0$ [$z_0$] and $\hbar^2/(2\mu r_0^2)$ [$\hbar^2/(2\mu z_0^2)$] for the 3D [1D] system. This figure has been adapted from Fig. 1 of Ref. [104].

function of the depth $V_0$. Starting from the noninteracting system, i.e., $V_0 = 0$, we increase $V_0$ to a small finite value. In this regime the scattering length $a_{3D}^{aa}$ is small and negative. For negative $a_{3D}^{aa}$ (and small $V_0$), the potential supports no two-body bound state. With increasing $V_0$ the scattering length $|a_{3D}^{aa}|$ increases. For infinitely large $|a_{3D}^{aa}|$, the two-body potential supports a single zero-energy bound state. If $V_0$ is increased further, $a_{3D}^{aa}$ takes on positive values. For positive $a_{3D}^{aa}$, the two-body potential supports a single s-wave bound state.

Similar to the three-dimensional space, the Hamiltonian $H_{tot}^{1D}$ in one-dimensional space is written as

$$H_{tot}^{1D} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i} \frac{\partial^2}{\partial z_i^2} + \sum_{i=1}^{N} V_{tr}(z_i) + \sum_{j>i=1}^{N} V_{tb}(z_{ij}), \quad (2.8)$$

where $z^T = \{z_1, z_2, \ldots, z_N\}$ are the position coordinates. The trapping potential $V_{tr}(z_i)$ is
given by

\[ V_{tr}(z_i) = \frac{1}{2}m_i \omega_z^2 z_i^2, \quad (2.9) \]

where \( \omega_z \) denotes the angular trapping frequency that characterizes the one-dimensional external confinement. The particles interact through the short-range Gaussian potential

\[ V_{tb}(z_{ij}) = -V_0 \exp \left( \frac{-z_{ij}^2}{2z_0^2} \right), \quad (2.10) \]

where \( z_0 \) is the range of the potential. The dotted line in Fig. 2.1 shows the 1D atom-atom scattering length \( a_{1D}^{aa} \) as a function of the depth \( V_0 \). The non-interacting one-dimensional system \( (V_0 = 0) \) is characterized by an infinitely large \( a_{1D}^{aa} \). This corresponds to a vanishing coupling constant \( g_{1D}^{aa} \) [105],

\[ g_{1D}^{aa} = -\frac{\hbar^2}{\mu a_{1D}^{aa}}. \quad (2.11) \]

### 2.3 Center of mass separation

The trapping potentials introduced in Eqs. (2.7) and (2.9) are harmonic. As we show below, it follows that the relative and center of mass motion separate. To separate the center of mass and relative motion, we introduce a set of Jacobi coordinates \( \vec{x}^T = \{\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N\} \), where \( \vec{x}_N \) is the center of mass coordinate and the rest of the coordinates describes the relative motion of the \( N \)-particle system. There are many ways to parameterize the relative coordinates of an \( N \)-particle system. Throughout this thesis, we use “standard Jacobi coordinates” [75]. Figure 2.2 illustrates the construction of the Jacobi vectors \( \vec{x}_1, \vec{x}_2 \) and \( \vec{x}_3 \) for the four-particle system. The Jacobi coordinates are related to the single particle coordinates \( \vec{r} \) by the linear transformation [75]

\[ \vec{x}_i = \sum_{k=1}^{N} T_{ik} \vec{r}_k \quad (2.12) \]
Figure 2.2: Jacobi coordinates of the four-particle system. The circles labeled 1, 2, 3 and 4 denote the particles. The label O denotes the origin. The arrows indicate the Jacobi vectors: the arrow that points from 2 to 1 is $\vec{x}_1$, the arrow that originates at 3 is $\vec{x}_2$, the arrow that originates at 4 is $\vec{x}_3$, and the arrow that originates at O is $\vec{x}_4$. The Jacobi coordinates are

\[
\vec{x}_1 = \vec{r}_1 - \vec{r}_2, \quad \vec{x}_2 = (m_1 \vec{r}_1 + m_2 \vec{r}_2)/(m_1 + m_2) - \vec{r}_3 \quad \text{and} \quad \vec{x}_3 = (m_1 \vec{r}_1 + m_2 \vec{r}_2 + m_3 \vec{r}_3)/(m_1 + m_2 + m_3) - \vec{r}_4.
\]

$\vec{x}_4$ is the center of mass vector, $\vec{x}_4 = (m_1 \vec{r}_1 + m_2 \vec{r}_2 + m_3 \vec{r}_3 + m_4 \vec{r}_4)/(m_1 + m_2 + m_3 + m_4)$.

or

\[
\vec{r}_i = \sum_{k=1}^{N} (T^{-1})_{ik} \vec{x}_k,
\]

where $i = 1, \cdots, N$. The explicit form of the transformation matrix $T$ and its inverse $T^{-1}$ are given by

\[
T = \begin{pmatrix}
1 & -1 & 0 & \cdots & 0 \\
\frac{m_1}{m_{12}} & \frac{m_2}{m_{12}} & -1 & \cdots & 0 \\
& \ddots & \ddots & \ddots & \ddots \\
& & \ddots & \ddots & \ddots \\
\frac{m_1}{m_{12\cdots N-1}} & \frac{m_2}{m_{12\cdots N-1}} & \frac{m_3}{m_{12\cdots N-1}} & \cdots & -1 \\
\frac{m_1}{m_{12\cdots N}} & \frac{m_2}{m_{12\cdots N}} & \frac{m_3}{m_{12\cdots N}} & \cdots & \frac{m_N}{m_{12\cdots N}}
\end{pmatrix}
\]

(2.14)
and

\[
T^{-1} = \begin{pmatrix}
\frac{m_2}{m_{12}} & \frac{m_3}{m_{123}} & \cdots & \frac{m_N}{m_{12\ldots N}} & 1 \\
\frac{-m_1}{m_{12}} & \frac{m_2}{m_{123}} & \cdots & \frac{m_N}{m_{12\ldots N}} & 1 \\
0 & \frac{m_{12}}{m_{123}} & \cdots & 1 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \frac{m_{12\ldots N-1}}{m_{12\ldots N}} & 1 \\
\end{pmatrix},
\]

(2.15)

where \(m_{12\ldots i} = m_1 + m_2 + \cdots + m_i\).

We now transform the Hamiltonian, Eq. (2.2), from single particle coordinates \(\vec{r}\) to Jacobi coordinates \(\vec{x}\). To express the kinetic energy in terms of the Jacobi coordinates, we use the identity

\[
\nabla \vec{r}_i = \sum_{k=1}^{N} T_{ki} \nabla \vec{x}_k.
\]

(2.16)

Applying Eq. (2.16) twice to the kinetic energy operator [see Eq. (2.3)], we obtain

\[
T_{3D}^{tot} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i} \left( \sum_{k'=1}^{N} T_{k'i} \nabla \vec{x}_{k'} \right) \left( \sum_{k=1}^{N} T_{ki} \nabla \vec{x}_k \right).
\]

(2.17)

Rearranging the sums over \(k\) and \(k'\), Eq. (2.17) becomes

\[
T_{3D}^{tot} = \frac{-\hbar^2}{2} \sum_{i=1}^{N} \left[ \sum_{k=1}^{N-1} \sum_{k'=1}^{N-1} \left( \frac{T_{k'i} T_{ki}}{m_i} \right) \nabla \vec{x}_{k'} \nabla \vec{x}_k + 2 \sum_{k=1}^{N-1} \left( \frac{T_{ki} T_{Ni}}{m_i} \right) \nabla \vec{x}_k \nabla \vec{x}_N \right]
\]

(2.18)

The transformation matrix \(T\) satisfies the relations

\[
\sum_{i=1}^{N} \frac{T_{k'i} T_{ki}}{m_i} = \frac{1}{\mu_k} \delta_{k'k} \quad \text{and} \quad \sum_{i=1}^{N} \frac{T_{ki} T_{Ni}}{m_i} = \frac{1}{m_{12\ldots N}} \delta_{kN},
\]

(2.19)

where \(k, k' = 1, \cdots, N - 1\). In Eq. (2.16), \(\mu_k (k = 1, \cdots, N - 1)\) is the mass associated with
the \( k^{th} \) Jacobi vector,

\[
\mu_k = \frac{m_{k+1}m_{12-1}}{m_{12-1}+1}.
\]  \hspace{1cm} \text{(2.20)}

Due to Eq. (2.19), the mixed derivatives in the square bracket on the right hand side of Eq. (2.18) vanish and the kinetic energy can be expressed as

\[
T_{tot}^{3D} = T + T_{cm},
\]  \hspace{1cm} \text{(2.21)}

where the kinetic energy \( T \) associated with the relative motion is given by

\[
T = \sum_{k=1}^{N-1} \frac{-\hbar^2}{2\mu_k} \nabla^2_{\vec{x}_k}
\]  \hspace{1cm} \text{(2.22)}

and the center of mass kinetic energy \( T_{cm} \) reads

\[
T_{cm} = \frac{-\hbar^2}{2m_{12-N}} \nabla^2_{\vec{x}_N}.
\]  \hspace{1cm} \text{(2.23)}

Similarly, the external confining potential \( V_{tr}^{tot} \) can be separated into the center of mass contribution \( V_{tr}^{cm} \),

\[
V_{tr}^{cm} = \frac{1}{2} m_{12-N} \omega^2 \vec{x}_N^2,
\]  \hspace{1cm} \text{(2.24)}

and the relative contribution \( V_{tr} \),

\[
V_{tr} = \sum_{k=1}^{N-1} \frac{1}{2} \mu_k \omega^2 \vec{x}_k^2.
\]  \hspace{1cm} \text{(2.25)}

The interaction potential \( V_{int} \), Eq. (2.5), depends only on the interparticle distance vectors and is independent of the center of mass vector \( \vec{x}_N \). Equation (2.12) enables us to express the interparticle distance vectors \( \vec{r}_{ij} \) in terms of the Jacobi vectors \( \vec{x} \),

\[
\vec{r}_{ij} = \sum_{k=1}^{N-1} \left( (T^{-1})_{ik} - (T^{-1})_{jk} \right) \vec{x}_k.
\]  \hspace{1cm} \text{(2.26)}
Equation (2.14) can be compactly written as

$$\vec{r}_{ij} = (\vec{\varphi}_{ij})^T \vec{x},$$

(2.27)

if we define the kth component of the (N - 1)-dimensional vector $\vec{\varphi}_{ij}$ through Eq. (2.26).

Combining the above equations, the total Hamiltonian $H_{3D}^{tot}$ can be written as a sum of the relative Hamiltonian $H$ and the center of mass Hamiltonian $H_{cm},$

$$H_{3D}^{tot} = H + H_{cm},$$

(2.28)

where

$$H = \sum_{i=1}^{N-1} -\frac{\hbar^2}{2\mu_i} \nabla^2_{\vec{x}_i} + \sum_{i=1}^{N-1} \frac{1}{2} \mu_i \omega^2 x_i^2 + \sum_{j \geq 1}^{N} V_{tb}\left((\vec{\varphi}_{ij})^T \vec{x}\right),$$

(2.29)

and

$$H_{cm} = -\frac{\hbar^2}{2m_{12 \cdots N}} \nabla^2_{\vec{x}_N} + \frac{1}{2} m_{12 \cdots N} \omega^2 x_N^2.$$  

(2.30)

For notational convenience, the 3D superscript has been suppressed in writing the relative Hamiltonian $H$ and the center of mass Hamiltonian $H_{cm}$. Since $H_{3D}^{tot}$ separates, the total wave function $\Psi_{tot}$ can be written as a product of the center of mass wave function $\Psi_{cm}(\vec{x}_N)$ and the relative wave function $\Psi(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_{N-1}),$ i.e.,

$$\Psi_{tot}(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_N) = \Psi(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_{N-1}) \Psi_{cm}(\vec{x}_N).$$

(2.31)

Here, $\Psi_{cm}(\vec{x}_N)$ is the solution to the center of mass Schrödinger equation with Hamiltonian $H_{cm}$ and eigenenergy $E_{cm},$ and $\Psi(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_{N-1})$ is the solution to the relative Schrödinger equation

$$H \Psi(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_{N-1}) = E \Psi(\vec{x}_1, \vec{x}_2, \cdots, \vec{x}_{N-1}),$$

(2.32)

with $E_{tot} = E_{cm} + E.$

Analogously, the Jacobi coordinates $\vec{x}^{\prime T} = \{\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_N\}$ in one-dimensional space are
related to the single particle coordinates $\mathbf{z}^T = \{z_1, z_2, \cdots, z_N\}$ by the linear transformation

$$\bar{x}_i = \sum_{k=1}^{N} T_{ik} z_k. \quad (2.33)$$

Following the steps discussed above for the three-dimensional system, the relative Hamiltonian $H$ of the one-dimensional system reads

$$H = \sum_{i=1}^{N-1} -\frac{\hbar^2}{2\mu_i} \frac{\partial^2}{\partial \bar{x}_i^2} + \sum_{i=1}^{N-1} \frac{1}{2} \mu_i \omega_z^2 \bar{x}_i^2 + \sum_{j \geq i=1}^{N} V_{tb} \left( (\hat{\omega}_{ij})^T \bar{x} \right). \quad (2.34)$$

### 2.4 The variational principle

The variational principle is widely used to approximate the energies and wave functions of quantum mechanical systems [2, 17, 75, 106, 107]. In many cases, physical intuition or prior knowledge about the system is used to aid in choosing an appropriate variational ansatz. Let us consider a Hamiltonian $H$ with eigenenergies $\epsilon_1, \epsilon_2, \cdots$, where $\epsilon_1$ is the ground state energy and $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3 \cdots$. The variational principle [2, 17], in its simplest form, states that the expectation value of the Hamiltonian $H$ with respect to the wave function $\psi_{\text{var}}(\vec{p})$, where $\psi_{\text{var}}(\vec{p})$ is an arbitrary square integrable function that depends on the variational parameters $\vec{p}$, provides an upper bound to the exact ground state energy $\epsilon_1$, i.e.,

$$\frac{\langle \psi_{\text{var}}(\vec{p}) | H | \psi_{\text{var}}(\vec{p}) \rangle}{\langle \psi_{\text{var}}(\vec{p}) | \psi_{\text{var}}(\vec{p}) \rangle} = E_{\text{var}} \geq \epsilon_1. \quad (2.35)$$

The variational principle allows us to calculate an upper bound to the ground state energy by minimizing the variational energy $E_{\text{var}}$ with respect to the set of variational parameters $\vec{p}$, i.e., to estimate the energy by enforcing that $\frac{\partial E_{\text{var}}}{\partial p_j} = 0$, where the $p_j$ are the elements of the parameter vector $\vec{p}$. In this thesis, the variational principle is used, in generalized form, to find the eigenenergies of the relative Hamiltonian $H$ [see Eq. (2.29)].

The basic idea of the variational principle can be illustrated by considering the one-
Figure 2.3: Solid (red), dashed (green) and dotted (blue) lines show the expectation values \( \langle E \rangle / \hbar \omega_z \), \( \langle T \rangle / \hbar \omega_z \) and \( \langle V \rangle / \hbar \omega_z \), respectively, as a function of the variational parameter \( \alpha \) for a single particle confined in a one-dimensional harmonic trap, where \( a_z = \sqrt{\frac{\hbar}{m \omega_z}} \). The horizontal black line corresponds to the exact ground state energy.

dimensional harmonic oscillator. Equation (2.8) with \( N = 1 \) (no interactions) reduces to the Hamiltonian of the standard 1D harmonic oscillator. We consider the variational function \( \psi(\alpha) = \exp(-\frac{\alpha z^2}{2}) \), where \( \alpha \) is a variational parameter to be chosen such that the energy is minimized. The analytic expressions for the expectation values of the potential energy \( \langle V \rangle = \frac{\langle \psi(\alpha)|V|\psi(\alpha) \rangle}{\langle \psi(\alpha)|\psi(\alpha) \rangle} \), the kinetic energy \( \langle T \rangle = \frac{\langle \psi(\alpha)|T|\psi(\alpha) \rangle}{\langle \psi(\alpha)|\psi(\alpha) \rangle} \) and the total energy \( \langle E \rangle = \frac{\langle \psi(\alpha)|H|\psi(\alpha) \rangle}{\langle \psi(\alpha)|\psi(\alpha) \rangle} \) for this variational function are given by

\[
\langle V \rangle = \frac{m_1 \omega_z^2}{4\alpha}, \quad \langle T \rangle = \frac{\hbar^2 \alpha}{4m_1} \quad \text{and} \quad \langle E \rangle = \frac{m_1 \omega_z^2}{4\alpha} + \frac{\hbar^2 \alpha}{4m_1}.
\] (2.36)

Figure 2.3 shows the expectation values as a function of \( \alpha \). Enforcing \( \frac{d\langle E \rangle}{d\alpha} = 0 \), the minimum value of \( \langle E \rangle \) is found for \( \alpha = \frac{m \omega_z}{\hbar} \). The corresponding minimum energy \( \langle E \rangle_{\text{min}} \) happens to be equal to the exact ground state energy \( \frac{1}{2} \hbar \omega_z \). As expected from the variational principle, \( \langle E \rangle \) is greater than \( \frac{1}{2} \hbar \omega_z \) for all other \( \alpha \) values. \( \langle E \rangle \) monotonically approaches \( \langle E \rangle_{\text{min}} \) as the width \( \alpha^{-1/2} \) of the variational function approaches the harmonic oscillator length \( a_z \), where
We now consider variational wave functions that depend linearly on the variational parameters. Variational wave functions of this type are widely used throughout physics and chemistry to study few- and many-body systems [60, 75, 85]. In this context, the variational parameters are referred to as expansion coefficients and the different terms in the variational wave function as basis functions. The basis set expansion of the $n^{th}$ eigenstate $\Psi_n$ reads

$$\Psi_n = \sum_{j=1}^{N_b} c_j^{(n)} \psi_j(\vec{\alpha}_j),$$  \hspace{1cm} (2.37)

where the $c_j^{(n)}$'s are expansion coefficients and the $\vec{\alpha}_j$'s are a set of variational parameters. The unknown parameters $\vec{\alpha}_j$ and $c_j^{(n)}$ can be determined by minimizing the energy. In this case, the variational energy reads (note that the subscript “var” has been dropped for notational convenience)

$$E_n = \frac{\sum_{j,k=1}^{N_b} (c_j^{(n)})^* c_k^{(n)} H_{jk}}{\sum_{j,k=1}^{N_b} (c_j^{(n)})^* c_k^{(n)} O_{jk}},$$  \hspace{1cm} (2.38)

where $H_{jk} = \langle \psi_j | H | \psi_k \rangle$ and $O_{jk} = \langle \psi_j | \psi_k \rangle$.

We now derive a means to determine the expansion parameters $c_j^{(n)}$, assuming the parameters $\vec{\alpha}_j$ are fixed. The minimization of the energy $E_n$ with respect to the $c_i^{(n)}$ requires

$$\frac{\partial E_n}{\partial c_i^{(n)}} = 0 \text{ for all } i.$$  

Differentiating $E_n \langle \Psi_n | \Psi_n \rangle$ with respect to $c_i^{(n)}$ gives

$$\frac{\partial E_n}{\partial c_i^{(n)}} \sum_{j,k=1}^{N_b} (c_j^{(n)})^* c_k^{(n)} O_{jk} = -E_n \sum_{j,k=1}^{N_b} \left[ \frac{\partial (c_j^{(n)})^*}{\partial c_i^{(n)}} c_k^{(n)} + \frac{\partial c_k^{(n)}}{\partial c_i^{(n)}} (c_j^{(n)})^* \right] O_{jk}$$

$$+ \sum_{j,k=1}^{N_b} \left[ \frac{\partial (c_j^{(n)})^*}{\partial c_i^{(n)}} c_k^{(n)} + \frac{\partial c_k^{(n)}}{\partial c_i^{(n)}} (c_j^{(n)})^* \right] H_{jk}. \hspace{1cm} (2.39)$$

$$a_z = \sqrt{\frac{\hbar}{m_{1\omega_z}}}.$$
Since $\frac{\partial (c_i^{(n)})}{\partial c_1^{(n)}} = \delta_{ij}$, the condition $\frac{\partial E_n}{\partial c_i^{(n)}} = 0$ gives

$$\sum_{k=1}^{N_b} (H_{ik} - E_n O_{ik}) c_i^{(n)} = 0$$  \hspace{1cm} (2.40)

for $i = 1, 2, \cdots, N_b$. Equation (2.40) is a generalized eigenvalue equation for the $N_b$ energies $E_n$ and the $N_b$ eigenvectors $\vec{c}^{(n)}$ where $(\vec{c}^{(n)})^T = \{c_1^{(n)}, \cdots, c_{N_b}^{(n)}\}$. In matrix form, Eq. (2.40) becomes

$$H \vec{c}^{(n)} = E_n O \vec{c}^{(n)},$$  \hspace{1cm} (2.41)

where the Hamiltonian matrix $H$ is given by

$$H = \begin{pmatrix}
   \langle \psi_1 | H | \psi_1 \rangle & \langle \psi_1 | H | \psi_2 \rangle & \cdots & \langle \psi_1 | H | \psi_{N_b} \rangle \\
   \langle \psi_2 | H | \psi_1 \rangle & \langle \psi_2 | H | \psi_2 \rangle & \cdots & \langle \psi_2 | H | \psi_{N_b} \rangle \\
   & & \cdots & \cdots \\
   \langle \psi_{N_b} | H | \psi_1 \rangle & \langle \psi_{N_b} | H | \psi_2 \rangle & \cdots & \langle \psi_{N_b} | H | \psi_{N_b} \rangle 
\end{pmatrix}$$  \hspace{1cm} (2.42)

and the overlap matrix $O$ is given by

$$O = \begin{pmatrix}
   \langle \psi_1 | \psi_1 \rangle & \langle \psi_1 | \psi_2 \rangle & \cdots & \langle \psi_1 | \psi_{N_b} \rangle \\
   \langle \psi_2 | \psi_1 \rangle & \langle \psi_2 | \psi_2 \rangle & \cdots & \langle \psi_2 | \psi_{N_b} \rangle \\
   & & \cdots & \cdots \\
   \langle \psi_{N_b} | \psi_1 \rangle & \langle \psi_{N_b} | \psi_2 \rangle & \cdots & \langle \psi_{N_b} | \psi_{N_b} \rangle 
\end{pmatrix}$$  \hspace{1cm} (2.43)

The generalized eigenequation, Eq. (2.41), has $N_b$ independent eigenvalues $E_n$ ($n = 1, \cdots, N_b$) and corresponding eigenvectors $\vec{c}^{(n)}$. If we account for all the eigenvalues together, the
eigenvalue equation can be presented compactly as

\[
H \mathbf{C} = E \mathbf{O} \mathbf{C},
\]  

(2.44)

where the energy matrix \( E \) is given by

\[
E = \begin{pmatrix}
E_1 & 0 & \ldots & 0 \\
0 & E_2 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & E_{N_b}
\end{pmatrix}
\]

(2.45)

and

\[
C = \begin{pmatrix}
c_1^{(1)} & c_2^{(1)} & \ldots & c_{N_b}^{(1)} \\
c_1^{(2)} & c_2^{(2)} & \ldots & c_{N_b}^{(2)} \\
\vdots & \vdots & \ddots & \vdots \\
c_1^{(N_b)} & c_2^{(N_b)} & \ldots & c_{N_b}^{(N_b)}
\end{pmatrix}
\]

(2.46)

The \( n^{th} \) column of \( C \) corresponds to the eigenvector of the \( n^{th} \) eigenvalue of \( H \).

The variational principle introduced above for the ground state energy can be generalized so that it applies to all eigenenergies. In particular, the generalized Ritz variational principle states that the energies \( E_1, \ldots, E_{N_b} \), determined by solving the eigenvalue equation, Eq. (2.29), are upper bounds to the true or exact eigenenergies of \( H \), provided the basis set consists of well-behaved basis functions. If \( E_1 \leq E_2 \leq \ldots \leq E_{N_b} \) are the eigenvalues obtained from the restricted subspace spanned by the \( N_b \) basis functions, then

\[
E_1 \geq \varepsilon_1, E_2 \geq \varepsilon_2, \ldots, E_{N_b} \geq \varepsilon_{N_b}.
\]

(2.47)

The generalized variational principle allows us to use the generalized eigenvalue equation
[see Eq. (2.44)] to approximate the eigenenergies and eigenvectors, provided $O$ and $H$ are known. With increasing size of the basis set, the true energies are approached from above. In general, the true eigenenergies are obtained in the infinite basis size limit. In numerical implementations of the approach, we have to choose a maximum basis set size, and (i) ensure that the basis set is “sufficiently complete” and (ii) develop accurate means to estimate the basis set error.

The basis can be complete like the harmonic oscillator basis [107], where the basis functions are orthogonal and linearly independent, or overcomplete, where the basis functions are nonorthogonal. A given basis with basis functions $\psi_j(\vec{\alpha}_j)$, $j = 1, \cdots, N_b$, is linearly independent if

$$\sum_{j=1}^{N_b} c_j^{(n)} \psi_j(\vec{\alpha}_j) = 0$$  \hspace{1cm} (2.48)

only when $c_j^{(n)} = 0$ for all $j$. It can be shown [75] that if one or several of the eigenvalues of the overlap matrix are much smaller than the largest eigenvalues, the nonorthogonal basis set is linearly dependent. This can lead to numerical instabilities, preventing one from reliably solving the generalized eigenvalue problem. The problem of linear dependency can be mitigated if we perform an orthogonal transformation of the Hamiltonian matrix. In particular, a rotation of the basis allows one to exclude basis functions that have a particularly large overlap with other basis functions [83]. In practice, we solve the eigenvalue equation

$$O \: B = \lambda \: B,$$  \hspace{1cm} (2.49)

where $\lambda$ is a matrix whose diagonal elements $\lambda_i$ are the eigenvalues of $O$ and whose off-diagonal matrix elements are zero. $B$ is the matrix consisting of the eigenvectors of the overlap matrix $O$. Multiplying Eq. (2.49) from the left with $B^T$, we find

$$B^T \: \lambda \: B = O.$$  \hspace{1cm} (2.50)
where we have used the orthonormal property of the eigenfunctions of the overlap matrix

\[ B^T B = B B^T = I \]  \hspace{1cm} (2.51)

and the commutation relation

\[ [B, \lambda] = 0. \]  \hspace{1cm} (2.52)

In Eq. (2.51), \( I \) is the identity matrix. Rearranging Eq. (2.42), we have

\[ B \lambda B^T = 0. \]  \hspace{1cm} (2.53)

We use Eq. (2.53) and rewrite the generalized eigenvalue equation [see Eq. (2.44)] as

\[ H C = E B \lambda B^T C. \]  \hspace{1cm} (2.54)

We again utilize Eq. (2.51) to rewrite Eq. (2.54) as

\[ B (B^T H B) B^T C = B (E \lambda) B^T C, \]  \hspace{1cm} (2.55)

where we have utilized the commutation relation between \( E \) and \( B \). Multiplying Eq. (2.55) with \( B^T \) from the left, we obtain the eigenvalue equation

\[ \alpha v = E \lambda \beta, \]  \hspace{1cm} (2.56)

where

\[ \alpha = B^T H B \]  \hspace{1cm} (2.57)
The orthogonal transformation of the Hamiltonian matrix leaves the eigenvalues $E$ unchanged and rotates $C$ to $b$. We selectively throw out “bad basis functions” by removing the rotated basis vectors $B^T \vec{c}_j$ that correspond to eigenvalues $\lambda_j$ smaller than a preset cutoff value. The number of rotated basis functions removed is denoted by $N_{bad}$. If the eigenvalues $\lambda_i$ are ordered in decreasing order, the $N_b - N_{bad}$ eigenenergies are obtained by diagonalizing the “reduced” $(N_b - N_{bad}) \times (N_b - N_{bad})$-dimensional eigenvalue equation

$$a_{\text{red}} b_{\text{red}} = E_{\text{red}} \lambda_{\text{red}} b_{\text{red}},$$

(2.59)

where the matrices $a_{\text{red}}, b_{\text{red}}, E_{\text{red}}$ and $\lambda_{\text{red}}$ are obtained from the matrices $a, b, E$ and $\lambda$ by removing the last $N_b - N_{red}$ rows and columns. In practice, typical cutoff value for $\lambda_i$ are smaller than $10^{-10}$, and the maximum number of removed basis function $N_{bad}$ is restricted to be less than $N_b/2$; ideally, $N_{bad}$ is smaller than $N_b/20$.

### 2.5 Variational basis functions

To solve the relative Schrödinger equation, we expand the eigenstates $\Psi$ in terms of explicitly correlated Gaussian basis functions $\psi_k$. The explicitly correlated Gaussian basis functions are nonorthogonal and depend explicitly on the interparticle distance coordinates. It is generally advantageous to employ basis functions that are characterized by the same quantum numbers as the state of interest.

In our work, we consider systems in three spatial dimensions for which the relative angular momentum $L$, the corresponding projection quantum number $M$ and the parity $\Pi$ are conserved quantities. The explicitly correlated Gaussian basis functions $\psi_k(\vec{r})$ for vanishing
angular momentum and positive parity are given by

$$\psi_k(\vec{r}) = \exp \left[ -\frac{1}{2} \sum_{j>i=1}^{N} \alpha^k_{ij} (\vec{r}_i - \vec{r}_j)^2 \right],$$

(2.60)

where the $\alpha^k_{ij}$ are variational parameters. The variational parameter $\alpha^k_{ij}$ is the inverse of the square of the width $d^k_{ij}$ of the $k^{th}$ basis function, i.e., $d^k_{ij} = (\alpha^k_{ij})^{-1/2}$. The width $d^k_{ij}$ characterizes the correlations associated with the relative distance coordinate $r_{ij}$ and can be chosen according to physical considerations. For example, to understand how the widths of the basis functions appropriate for the Hamiltonian $H$ [see Eq. (2.2)] are distributed, we need to look into the physics of the eigenstates of the system. Whereas gaslike states require widths of the order of the harmonic oscillator length $a_{ho}$, molecules of size $r_0$ require widths of order $r_0$. For dimers, one small width is needed but for trimers, three small widths are required.

Using Eq. (2.26), we express the interparticle distances in Eq. (2.60) in terms of the Jacobi coordinates, yielding

$$\psi_k(\vec{x}, A^k) = \exp \left( -\frac{1}{2} \vec{x}^T A^k \vec{x} \right),$$

(2.61)

where $A^k$ is a symmetric $(N - 1) \times (N - 1)$ matrix,

$$A^k_{kl} = \sum_{j>i=1}^{N} \alpha^k_{ij} \omega_k^{(ij)} \omega_l^{(ij)}.$$  

(2.62)

Here, $A^k$ has to be positive-definite as the norm $\langle \Psi | \Psi \rangle$ of the wave function $\Psi$ becomes finite if and only if $A^k$ is a positive-definite matrix [75]. The positive-definiteness of the matrix $A$ is ensured by restricting the $\alpha^k_{ij}$’s to take positive values. If one of the $\alpha^k_{ij}$’s is negative, the corresponding basis function grows exponentially at large interparticle distances and the resulting wave function is not square integrable.

The explicitly correlated Gaussian basis functions of Eq. (2.61) can be modified to de-
scribe states with nonzero angular momentum $L$. To construct basis functions with finite relative angular momentum $L$ and projection quantum number $M$, one efficient approach is to multiply $\psi_k$ of Eq. (2.61) by the angular function $\theta_{LM}(\vec{x})$. $\theta_{LM}(\vec{x})$ can be expressed in terms of “global vectors” $\vec{v}_{jk}$ [75, 109, 110, 111] ($j = 1, 2$), where

$$\vec{v}_{jk} = \sum_{i=1}^{N-1} (u_{jk})_i \vec{x}_i = \vec{u}^T_{jk} \vec{x}.$$  

(2.63)

Here, $\vec{u}^T_{jk}$ is a $(N-1)$-dimensional vector containing the variational parameters $(u_{jk})_1, \cdots , (u_{jk})_{N-1}$. In terms of the global vectors, $\theta_{LM}(\vec{x}, \vec{u}_{1k}, \vec{u}_{2k})$ can be written as

$$\theta_{LM}(\vec{x}, \vec{u}_{1k}, \vec{u}_{2k}) = |\vec{v}_{1k}|^{L_1} |\vec{v}_{2k}|^{L_2} [Y_{L_1M_1}(\vec{v}_{1k}) \otimes Y_{L_2M_2}(\vec{v}_{2k})]_{LM}.$$  

(2.64)

Here, the two spherical harmonics $Y_{L_1M_1}(\vec{v}_{1k})$ and $Y_{L_2M_2}(\vec{v}_{2k})$ are coupled to form a function with angular momentum $L$ and projection quantum number $M$. Finally, the basis function with finite relative angular momentum $L$ and projection quantum number $M$ can be written as

$$\psi^{LM}_k(\vec{x}, \vec{A}_k, \vec{u}_{1k}, \vec{u}_{2k}) = \exp \left( -\frac{1}{2} \vec{x}^T \vec{A}^k \vec{x} \right) \theta_{LM}(\vec{x}, \vec{u}_{1k}, \vec{u}_{2k}).$$  

(2.65)

For states with natural parity, i.e., $\Pi = (-1)^L$, we choose $L_1 = L$ and $L_2 = 0$ [75, 109, 110, 112]. For states with finite angular momentum and unnatural parity, i.e., $= (-1)^{L+1}$, we choose $L_1 = L$ and $L_2 = 1$ [111,113]. To describe states with $L = 0$ and unnatural parity, i.e., $\Pi = -1$, one has to introduce a third global vector as this particular state requires coupling of three spherical harmonics with non-zero angular momenta $L_1, L_2$ and $L_3$ [111,113].

The good quantum number in one-dimensional space is the parity $\Pi_z$. Consequently we construct one-dimensional basis functions with definite parity. The explicitly correlated Gaussian basis functions for even parity ($\Pi_z = +1$) are given by

$$\psi_k(\vec{x},\vec{A}_z^k) = \exp \left( -\frac{1}{2} \vec{x}^T \vec{A}_z^k \vec{x} \right),$$  

(2.66)
where the matrix $A^k_z$ is symmetric and has dimension $(N - 1) \times (N - 1)$. The $N(N - 1)/2$ independent elements of the matrix $A^k_z$ are treated as variational parameters. The explicitly correlated Gaussian basis functions for odd parity ($\Pi_z = -1$) are given by

$$
\psi_k(\vec{x}, A^k_z, \vec{u}_{1k}) = (\vec{u}_{1k}^T \vec{x}) \exp \left( -\frac{1}{2} \vec{x}^T A^k_z \vec{x} \right). \tag{2.67}
$$

The benefits of using explicitly correlated Gaussian basis functions are multiple. Since the basis functions are correlated, they are capable of providing accurate descriptions of strongly interacting systems. Moreover, the relatively simple form of the basis functions allows one to derive analytical expressions for the matrix elements. Appendix A contains the analytical expressions for the matrix elements. This enables us to achieve very accurate values for the matrix elements and makes the calculations comparatively fast. Lastly, the use of explicitly correlated Gaussian basis functions in the stochastic variational approach provides a fairly reliable means to optimize the variational parameters $\alpha^k_{ij}$ (see Sec. 2.7 for details).

The basis functions discussed so far are not symmetric or anti-symmetric with respect to the exchange of identical particles. The next section discusses how to impose the proper exchange symmetry on the basis functions.

### 2.6 Imposing proper exchange symmetry of basis functions

The eigenstate $\Psi$ is expanded in terms of the symmetrized or anti-symmetrized basis functions,

$$
\Psi = \sum_{k=1}^{N_b} c_k \hat{S} \psi_k, \tag{2.68}
$$

where the operator $\hat{S}$ is a symmetrization operator that acts like an antisymmetrizer for identical fermions and a symmetrizer for identical bosons. The eigen state has to be either
symmetric for bosons or antisymmetric for fermions under the interchange of identical particles. The operator $\hat{S}$ is the combination of contributions from all possible permutation operators $\hat{P}_{ij}$ associated with a sign that depends on the symmetry under the exchange of identical particles. $\hat{P}_{ij}$ exchanges the position vectors of the particles $i$ and $j$, i.e.,

$$\hat{P}_{ij}\{\cdots, \vec{r}_i, \cdots, \vec{r}_j, \cdots\} = \{\cdots, \vec{r}_j, \cdots, \vec{r}_i, \cdots\}. \quad (2.69)$$

The associated sign is positive or negative for the exchange of two identical bosons or two identical fermions. For example, $\hat{P}_{12}$ exchanges the coordinates of particles 1 and 2 and correspondingly for two identical bosons and fermions and we have $\hat{S} = \hat{I} + \hat{P}_{12}$ and $\hat{S} = \hat{I} - \hat{P}_{12}$, respectively, where $\hat{I}$ is the identity operator. For a system of three identical fermions we have $\hat{S} = \hat{I} - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{12}\hat{P}_{23} + \hat{P}_{23}\hat{P}_{12}$. The operator $\hat{P}_{ij}$ transforms the Jacobi coordinates as

$$\hat{P}_{ij}\vec{x} = T_{P_{ij}}\vec{x}, \quad (2.70)$$

where, using Eq. (2.12), the matrix elements $(T_{P_{ij}})_{mn}$ are given by [75]

$$(T_{P_{ij}})_{mn} = \sum_{k=1}^{N} T_{mk}(T^{-1})_{pk}n, \quad (2.71)$$

where $m, n = 1, \cdots, N - 1$. In Eq. (2.71), $(p_1, \cdots, p_N)$ are the set of integers that correspond to the new arrangement of the particles after permutation, i.e., the permutation transforms the single-particle coordinates as $\vec{r}_k \rightarrow \vec{r}_{p_k} \ (k = 1, \cdots, N)$. Property (2.70) facilitates the evaluation of matrix elements between “permuted basis functions”. As we show below, Eq. (2.70) ensures that the form of the matrix elements is retained under permutations.

To look for the effect of $\hat{P}_{ij}$ on the explicitly correlated Gaussian basis functions, we operate the permutation operator $\hat{P}_{ij}$ on the function from Eq. (2.61),

$$\hat{P}_{ij}\psi_k(\vec{x}, \vec{A}^k) = \exp\left(-\frac{1}{2}(T_{P_{ij}}\vec{x})^T \vec{A}^k(T_{P_{ij}}\vec{x})\right), \quad (2.72)$$
or, equivalently,

\[ \hat{P}_{ij} \psi_k(\vec{x}, A^k) = \psi_k(\vec{x}, T^T_{P_{ij}} A^k T_{P_{ij}}). \]  \tag{2.73} 

Similarly, under permutation the explicitly correlated Gaussian from Eq. (2.65) changes as

\[ \hat{P}_{ij} \psi^L_{k}(\vec{x}, A^k, \vec{u}_{1k}, \vec{u}_{2k}) = \psi^L_{k}(\vec{x}, T^T_{P_{ij}} A^k T_{P_{ij}}, T^T_{P_{ij}} \vec{u}_{1k}, T^T_{P_{ij}} \vec{u}_{2k}). \]  \tag{2.74} 

Hence, by redefining the quantities \( A^k, \vec{u}_{1k} \) and \( \vec{u}_{2k} \), we can impose the proper symmetry on the basis functions.

The operators \( T, V_{tr}, \) and \( V_{tb} \) relevant for the determination of the energy are unchanged under permutations of any two identical particles. If a given operator \( \hat{B} \) is invariant under the interchange of the particles \( i \) and \( j \), then the permutation operator \( \hat{P}_{ij} \) and the operator \( \hat{B} \) commute, i.e.,

\[ [\hat{P}_{ij}, \hat{B}] = 0. \]  \tag{2.75} 

This property can be used for the determination of the energy to reduce the numerical effort of evaluating matrix elements containing symmetrized basis functions [83]. As an example, we look at the system consisting of two identical fermions. The matrix element associated with the hermitian operator \( \hat{B} \) reads

\[ \langle \hat{S} \psi_k | \hat{B} | \hat{S} \psi_{k'} \rangle = \langle (\hat{I} - \hat{P}_{12}) \psi_k | \hat{B} | (\hat{I} - \hat{P}_{12}) \psi_{k'} \rangle. \]  \tag{2.76} 

We use the commutation relation from Eq. (2.75) and rewrite Eq. (2.76) as

\[ \langle \hat{S} \psi_k | \hat{B} | \hat{S} \psi_{k'} \rangle = \langle \psi_k | \hat{B} | \psi_{k'} \rangle - \langle \psi_k | \hat{B} | \hat{P}_{12} \psi_{k'} \rangle - \langle \hat{P}_{12} \psi_k | \hat{B} | \psi_{k'} \rangle + \langle \hat{P}_{12} \psi_k | \hat{P}_{12} \hat{B} | \psi_{k'} \rangle. \]  \tag{2.77}
We further utilize \( \langle \hat{S}\psi_k|\hat{B}|\hat{S}\psi_{k'} \rangle = \langle \hat{S}\psi_k|\hat{B}|\hat{S}\psi_{k'} \rangle^* \) and get

\[
\langle \hat{S}\psi_k|\hat{B}|\hat{S}\psi_{k'} \rangle = \langle \psi_k|\hat{B}|\psi_{k'} \rangle - 2\langle \psi_k|\hat{B}|\hat{P}_{12}\psi_{k'} \rangle + \langle \hat{P}_{12}^T\hat{P}_{12}\psi_k|\hat{B}|\psi_{k'} \rangle, \tag{2.78}
\]

i.e.,

\[
\langle \hat{S}\psi_k|\hat{B}|\hat{S}\psi_{k'} \rangle = 2\langle \psi_k|\hat{B}|\left(\hat{I} - \hat{P}_{12}\right)\psi_{k'} \rangle, \tag{2.79}
\]

as \( \hat{P}_{12}^T\hat{P}_{12} = \hat{I} \).

The result in Eq. (2.79) can be written in general as

\[
\langle \hat{S}\psi_k(\vec{x},\vec{A}^k)|\hat{B}|\hat{S}\psi_k(\vec{x}',\vec{A}'^k) \rangle = n_p\langle \psi_k(\vec{x},\vec{A}^k)|\hat{B}|\hat{S}\psi_k(\vec{x}',\vec{A}'^k) \rangle, \tag{2.80}
\]

where \( n_p \) is the total number of permutations. This property reduces the numerical effort of the determination of the energy by a factor of \( n_p \).

It is important to note that one cannot take advantage of the property given in Eq. (2.79) for the calculation of structural properties like density profiles and pair-correlation functions as they involve delta function operators which are not, in general, invariant under the application of \( \hat{P}_{ij} \).

### 2.7 The stochastic variational method

The simplest approach to obtain the variational solution is to solve the secular equation (2.56). However, the variational approach becomes numerically efficient only if the matrix elements \( H_{ij} \) and \( O_{ij} \) are calculated analytically. The use of correlated Gaussian basis functions, as discussed in Sec. 2.5, allows us to obtain analytical expressions for the matrix elements (see appendix A for the expressions). If the non-linear variational parameters are
not optimized carefully, it is in most cases necessary to include a relatively large number of basis functions to reach convergence. The approach without optimization of the non-linear parameters suffers from certain limitations. A subset of the basis functions $\psi_k$ may be undesirable as they are not useful to describe the eigenstates and a portion of the basis functions may need to be removed using the orthogonolization scheme introduced in Sec. 2.5 to avoid linear dependency. For a large basis set size $N_b$, the calculations of the matrix elements and the diagonalization of generalized eigenvalue problem are numerically expensive.

To select the most useful basis functions, we need to perform a basis set optimization. The flexibility of the basis functions $\psi_k$ is determined by the “correct” choice of their parameters $A_k, \vec{u}_{1k}$ and $\vec{u}_{2k}$. To find “good” basis functions, one has to optimize the parameters. This can be done by minimizing the relative energy. Minimization of the energy with respect to the parameters is complicated as the number of the parameters increases with the size of the basis set and the number of particles. Another disadvantage is that the energy surface, with the parameters as variables, can have several local minima [7].

A semi-systematic energy minimization is possible by selecting the basis functions via the stochastic variational method. The stochastic optimization of the parameters of explicitly correlated Gaussians was first proposed by Kukulin and Kranopolsky [86]. In the stochastic variational method we increase the basis set size by selectively adding new basis functions, which reduce the energy of the system notably. The basis functions added to the basis set are selected from a large number of trial basis functions. The optimization strategy of the stochastic variational method is the following [75, 114]:

1. Let us assume that the generalized eigenvalue equation Eq. (2.41) has been solved in the $K$-dimensional space for the basis set consisting of the basis functions $\psi_1, \cdots, \psi_K$ with eigenvalues $E_1, \cdots, E_K$ and corresponding eigenvectors $\vec{c}^{(1)}, \cdots, \vec{c}^{(K)}$ satisfying $(\vec{c}^{(j)})^T \mathbf{Q} \vec{c}^{(j)} = 1$ ($j = 1, \cdots, K$). Let $\phi_1, \cdots, \phi_K$ be the orthonormalized basis set
corresponding to the eigenvalues $E_1, \cdots , E_K$, i.e.,

$$\langle \phi_j | H | \phi_i \rangle = E_i \delta_{ij}, \quad (2.81)$$

where $i, j = 1, \cdots , K$. $\phi_j$ is expressed in terms of the basis functions $\psi_i$ as

$$\phi_j = \sum_{i=1}^{K} c_i^{(j)} \psi_i, \quad (2.82)$$

where $j = 1, \cdots , K$.

2. We now expand the basis by adding a single basis function $\psi_{K+1}$. The Gram-Schmidt method [115] allows us to construct $\phi_{K+1}$ from $\psi_{K+1}$. $\phi_{K+1}$, which needs to be orthogonal to all other $\phi_k$’s, is given by

$$\phi_{K+1} = \frac{\psi_{K+1} - \sum_{i=1}^{K} \phi_i \langle \phi_i | \psi_{K+1} \rangle}{\sqrt{\mathcal{N}}}, \quad (2.83)$$

where $\mathcal{N} = \langle \psi_{K+1} | \psi_{K+1} \rangle - \sum_{i=1}^{K} |\langle \phi_i | \psi_{K+1} \rangle|^2$. Using the basis $\phi_1, \cdots , \phi_{K+1}$, the generalized eigenvalue problem reduces to finding the roots of the function

$$D(\beta) = \sum_{j=1}^{K} \frac{h_j^2}{E_j - \beta} - \beta + h_{K+1}, \quad (2.84)$$

where $h_j = \langle \phi_j | H | \phi_{K+1} \rangle$. Using Eq. (2.83) we get

$$h_j = \frac{1}{\sqrt{\mathcal{N}}} \left( \langle \phi_j | H | \psi_{K+1} \rangle - \sum_{i=1}^{K} \langle \phi_i | \psi_{K+1} \rangle \langle \phi_j | H | \phi_i \rangle \right). \quad (2.85)$$

Using Eqs. (2.81) and (2.82) in Eq. (2.85), we find

$$h_j = \frac{1}{\sqrt{\mathcal{N}}} \left( \mathcal{H}_j - E_j \mathcal{O}_j \right), \quad (2.86)$$
where
\[ \mathcal{H}_j = \sum_{i=1}^{K} (d_i^{(j)})^* H_{ij} \] (2.87)
and
\[ \mathcal{O}_j = \sum_{i=1}^{K} (c_i^{(j)})^* O_{i,K+1} \] (2.88)
with \( j = 1, \ldots, K \). The \( h_{K+1} \) is given by
\[ h_{K+1} = \langle \phi_{K+1} | H | \phi_{K+1} \rangle. \] (2.89)

Using Eqs. (2.81)-(2.83) and Eqs. (2.87)-(2.88), the final form of \( h_{K+1} \) can be shown to be
\[ h_{K+1} = \frac{1}{N} \left( H_{K+1,K+1} + \sum_{j=1}^{K} E_j |O_j|^2 - 2 \sum_{j=1}^{K} O_j \mathcal{H}_j \right). \] (2.90)

\( D(\beta) \) is a polynomial of order \((K + 1)\) [see Eq. (2.84)]. The \((K + 1)\) roots of \( D(\beta) \), \( \beta_1, \ldots, \beta_{K+1} \), are the new energies of the system described by the basis set of size \( K + 1 \).
The advantage here is that we do not need to diagonalize the \((K + 1)\)-dimensional matrix. Another advantage is that we need to calculate only one single row with \( K + 1 \) elements \( h_i \) instead of recalculating all the \((K + 1) \times (K + 1)\) matrix elements. The variational principle ensures that the eigenvalues of the \((K + 1)\)-dimensional basis are always lower than those of the \( K \)-dimensional basis.

3. We repeat the second step for several trial basis functions \( \psi_{K+1}^{(m)} \), each having a different set of parameters, to calculate the energies \( \beta_{K+1}^{(m)} \)'s. The quality of each trial function is determined by comparing one or more of the \( K+1 \) energies \( \beta_{j}^{(m)} \) for all \( m \). The parameter set that corresponds to the lowest energy is selected as the \((K + 1)^{th}\) parameter set and the rest of the functions is discarded.

4. We increase the basis set size and follow steps 1 to 3 until we reach the desired accuracy.

We look at the rate of convergence of the energy as a function of number of the basis
functions to examine the accuracy. The rate of convergence is quantified by the quantity
\[
\Delta E/\Delta N_{(n_1,n_2)} = [E(n_1) - E(n_2)] / (n_2 - n_1),
\]
where \( E(n_1) \) and \( E(n_2) \) are the energies corresponding to the basis sets of size \( n_1 \) and \( n_2 \), respectively (\( n_1 < n_2 \)). For a given \( \Delta N \), where \( \Delta N = n_2 - n_1 \), \( \Delta E/\Delta N_{(n_1,n_2)} \) decreases with increasing basis set size. The basis set error can be estimated by the quantity
\[
\Delta \epsilon = E(N_b) - E(N_b \to \infty) / E(N_b \to \infty),
\]
(2.91)
where \( E(N_b \to \infty) \) is the extrapolated energy corresponding to the infinite number of basis functions. Figure 2.4 shows an example of a typical basis set optimization for the ground state of the harmonically trapped three-body system consisting of two spin-up fermions and one spin-down fermion at unitary \( (a^{3D}_s = \infty) \). The system is described by the Hamiltonian given in Eq. (2.29) with interspecies but no intraspecies interactions.

Figure 2.4 considers the \( L^\Pi = 0^+ \) subspace. The range \( r_0 \) of the Gaussian interaction potential [see Eq. (2.7)] is set to \( r_0 = 0.01a_{ho} \). The circles show the relative energy \( E(2,1) \) as a function of \( 1/N_b \). Here, \( \Delta E/\Delta N_{(150,200)}, \Delta E/\Delta N_{(200,250)}, \Delta E/\Delta N_{(250,300)} \) are \( 2.86 \times 10^{-7} \hbar \omega, 4.4 \times 10^{-8} \hbar \omega \) and \( 1.1 \times 10^{-8} \hbar \omega \), respectively. The basis set error \( \Delta \epsilon \) for this example
Figure 2.5: Range-dependence of the relative energy for the ground state with $0^+$ symmetry of the $(2,1)$ system at unitarity ($a_{3D}^{3a} = \infty$). The circles show the relative energies $E(2,1)$, obtained by the stochastic variational approach, as a function of range $r_0$ of the Gaussian two-body potential; for each $r_0$, the energy for the largest basis set is shown (no extrapolation to the $N_b \to \infty$ limit has been performed). The solid line shows a quadratic fit to the stochastic variational energies.

is approximately 0.001%.

The zero-range three-body system at unitarity in a harmonic trap can be solved analytically [59]. To obtain the zero-range energy using the stochastic variational method, we calculate the relative energies as a function of the range $r_0$ and extrapolate to the $r_0 \to 0$ limit. Figure 2.5 shows the range dependence for the ground state relative energy of the $(2,1)$ system with $0^+$ symmetry at unitarity. The energy varies approximately linearly for small $r_0/a_{ho}$. The extrapolated zero-range energy, obtained by performing a quadratic fit, is $E(r_0 \to 0) = 3.16618\hbar\omega$, whereas the exact energy from the analytical treatment is $E_{\text{ext}} = 3.16622\hbar\omega$. The fractional difference in the energies, $(E_{\text{ext}} - E(r_0 \to 0))/E_{\text{ext}} \times 100\% \approx 0.0013\%$, is less than the combined errors due to the basis set extrapolation and the zero-range extrapolation. The example demonstrates that the energy obtained using the stochastic variational method converges to the correct value with high accuracy.
Chapter 3

Natural and unnatural parity states of small trapped two-component Fermi gases at unitarity

3.1 Introduction

In this chapter we consider equal- and unequal-mass two-component Fermi gases under spherically symmetric external harmonic confinement with large s-wave scattering length. This chapter presents extensive benchmark results for the (2, 2) and (3, 1) energies of natural and unnatural parity states at unitarity. Specifically, using the stochastic variational approach, we determine the lowest 286 and 164 relative eigenenergies of the equal mass (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 $r_0 \to 0$ limit. Our calculations include all states with vanishing and finite angular momentum $L$ (and natural and unnatural parity II) 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.

In addition, we use the explicitly correlated Gaussian approach to characterize the
trapped unequal-mass systems consisting of three heavy fermions and one light fermion at unitarity. Using the explicitly correlated Gaussian technique and employing basis functions that are neither eigenfunctions of the angular momentum operator $L$ nor the parity operator $\Pi$, it has been predicted that four-body systems with the angular momentum $L = 1$ and the parity $\Pi = +1$ exhibit four-body resonances [116,117]. Here, we employ basis functions that are characterized by good quantum numbers $L$ and $\Pi$ to improve these results. Though our results agree in general with those of Ref. [116], the present work significantly improves the accuracy of the unequal-mass energies. In Ch. 6, the improved unequal-mass results are used to benchmark a new numerical scheme, which, within a hyperspherical coordinate approach, solves the hyperangular Schrödinger equation.

Section 3.2 discusses the energy spectrum of trapped equal-mass Fermi gases with vanishing and finite angular momentum as well as natural and unnatural parity. Section 3.3 considers two-component Fermi gas with unequal masses. Section 3.4 summarizes the results and provides an outlook.

3.2 Energies of small trapped equal-mass Fermi gases

This section discusses the solution to the generalized eigenvalue equation [see Eq. (2.44)] for the two component Fermi gas. We consider a two-component Fermi gas with $n_1$ spin-up and $n_2$ spin-down atoms of mass $m$ with $N = n_1 + n_2$. The Hamiltonian is given in Eq. (2.2). The kinetic energy and the trap potentials are given in Eqs. (2.3) and (2.4), respectively. We assume that the spin-up and spin-down atoms interact through a short-range potential $V_{tb}(r_{pq})$ and the atoms with like spin do not interact. Thus, the interaction potential is given by

$$V_{\text{int}} = \sum_{q=n_1+1}^{N} \sum_{p=1}^{n_1} V_{tb}(r_{pq}),$$

(3.1)

where $V_{tb}(r_{pq})$ is given in Eq. (2.7).
Figure 3.1: Illustration of convergence for the (3, 1) system at unitarity with $1^+$ symmetry and $r_0 = 0.04a_{ho}$. Solid and dashed lines show the quantity $\Delta \epsilon_{3,1}$, where $\Delta \epsilon_{3,1} = [E_{3,1}(N_b) - E_{3,1}(N_b \to \infty)] / E_{3,1}(N_b \to \infty)$, for states 1 and 12 as a function of $1/N_b$. 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. This figure is taken from Fig. 1 of Ref. [39].

One key purpose of this chapter is to elucidate how we determine a large portion of the energy spectrum of trapped two-component Fermi systems with $N = 4$. We tabulate the extrapolated zero-range energies in Appendix B. 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 accuracy and validity regime of alternative approaches. We anticipate that the tabulated energies will also prove useful in other applications.

Figure 3.1 shows an example of our basis set optimization for the (3, 1) system with $1^+$ symmetry and $r_0 = 0.04a_{ho}$ at unitarity. Solid and dashed lines show the fractional difference $\Delta \epsilon_{3,1}$ for the ground state (state 1) and state 12, respectively, between the relative energy $E_{3,1}$ for a basis set of size $N_b$ and the energy for an infinite basis set. Here, the states are counted separately for each $L^\Pi$ symmetry. In counting the states, we do include the unshifted states (see below for a definition of the term “unshifted states”) but we do not account for the $2L + 1$ degeneracy of the energies (see column 1 of Table 1 for the state
The dotted lines in Fig. 6.1 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 $E_{3,1}(r_0 = 0.04a_{ho}) = 5.08294\hbar\omega$ for state 1 and $E_{3,1}(r_0 = 0.04a_{ho}) = 10.1788\hbar\omega$ 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 respectively 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 $N_b$. The convergence is slower for most other states and, 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 3.2 exemplarily illustrates the range dependence for the relative energy of the $(3, 1)$ system with $1^+$ symmetry. Figure 3.2(a) shows the range dependence of the ground state energy, Fig. 3.2(b) shows the range dependence of the energy associated with state 12, and Fig. 3.2(c) shows the range dependence of the energy for a state that depends comparatively weakly on $r_0$ (state 5). In Figs. 3.2(a) and 3.2(b), the energies vary to a very good approximation linearly with $r_0$ for sufficiently small $r_0/a_{ho}$. This finding is in agreement with earlier work [31,118,119]. For the ground state [see Fig. 3.2(a)], the range dependence is quite weak and linear behavior is only observed for $r_0 \lesssim 0.03a_{ho}$.

In Fig. 3.2(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. [118,119], which utilizes zero-range contact interactions. For the $(3, 1)$ system with $L^\Pi = 1^+$ 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
Figure 3.2: Illustration of finite-range dependence for the $(3,1)$ system with $1^+$ symmetry at unitarity. Squares show the relative eigenenergies $E_{3,1}(N_b)$ for various ranges $r_0$ of the underlying two-body interaction potential for (a) the ground state (state 1), (b) state 12, and (c) state 5; $N_b$ is the largest basis set considered. The energies provide variational upper bounds and the estimated basis set extrapolation error is indicated by errorbars; in panels (a) and (b), the basis set extrapolation error is smaller than the symbol size and thus not visible. In panels (a) and (b), solid lines show linear fits to the energies $E_{3,1}(N_b)$ [the fit shown in panel (a) includes the energies for the five smallest $r_0$ values]. This figure is taken from Fig. 2 of Ref. [39].
Table 3.1: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 1^+$ symmetry [only states that are affected by $s$-wave interactions are included; each energy is $(2L + 1)$-fold degenerate]. The first column indicates the state number (st. no.). The second column shows the extrapolated zero-range energy $E_{3,1}(r_0 = 0)$ at unitarity; the uncertainty is estimated to be 0.1% or smaller. The third column indicates the dependence of the energy at unitarity on the range $r_0$ of the Gaussian potential $V_g$. We assume a linear dependence and write $E_{3,1}(r_0) = E_{3,1}(r_0 = 0) + \chi(r_0/a_{ho})\hbar\omega$. The fourth column shows the $s_{L,\nu}$ value determined from the energy; the value of $s_{L,\nu}$ is only shown for the lowest rung of a ladder, i.e., for states with $q = 0$. The last column shows $s_{L,\nu}^{ni}$ of the non-interacting state. There exist 1 and 6 unshifted states with energy $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

<table>
<thead>
<tr>
<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar\omega)$</th>
<th>$\chi$</th>
<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{ni}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.0819</td>
<td>0.04</td>
<td>4.0819</td>
<td>5.5</td>
</tr>
<tr>
<td>2</td>
<td>7.0820</td>
<td>0.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>7.6056</td>
<td>0.51</td>
<td>6.6056</td>
<td>7.5</td>
</tr>
<tr>
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<td>8.1456</td>
<td>0.76</td>
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<td>7.5</td>
</tr>
<tr>
<td>5</td>
<td>8.9846</td>
<td>1.19</td>
<td>7.9846</td>
<td>9.5</td>
</tr>
<tr>
<td>7</td>
<td>9.0825</td>
<td>0.03</td>
<td></td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>9.1324</td>
<td>0.28</td>
<td>8.1324</td>
<td>9.5</td>
</tr>
<tr>
<td>9</td>
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<td>0.46</td>
<td>8.4544</td>
<td>9.5</td>
</tr>
<tr>
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<td>0.55</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>1.17</td>
<td>8.6847</td>
<td>9.5</td>
</tr>
<tr>
<td>12</td>
<td>10.147</td>
<td>0.80</td>
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<td></td>
</tr>
</tbody>
</table>

six states with relative energy $21\hbar\omega/2$ that are independent of the $s$-wave scattering length $a_{3d}^{aa}$.

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 [59, 119]. 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 $0^-\text{symmetry}$ can be affected by $s$-wave interactions since the system is characterized by one more Jacobi vector than angular momenta needed to ensure the $0^-\text{symmetry}$. Indeed, this prediction is in agreement with our results from the perturbative and stochastic variational calculations.

Table 3.1 summarizes our extrapolated zero-range energies $E_{3,1}(r_0 = 0)$, $E_{3,1}(r_0 = 0) \leq 10.5\hbar\omega$, for states with $1^+\text{symmetry}$ 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 $0.0025 \leq r_0/a_{\hbar\omega} \leq 0.08$ and by then fitting these energies for the largest basis set considered by a linear function. The third column in Table 3.1 shows the slopes $\chi$, which characterize the dependence of $E_{3,1}$ on $r_0$ at unitarity. We find that the slopes for states that are affected by $s$-wave interactions are positive. Table 3.1 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 our calculations 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 $(2q + s_{L,\nu} + 1)\hbar\omega$ [42, 59], where $s_{L,\nu}$ is associated with the eigenvalue of the hyperangular Schrödinger equation and where the radial quantum number $q$ takes the values $0, 1, \ldots$ (although the $s_{L,\nu}$ depend on $\Pi$, this dependence is not explicitly indicated for notational simplicity). The fourth column of Table 3.1 shows the $s_{L,\nu}$ values determined from our energies for $q = 0$, i.e., for the lowest rung of the ladder with $2q\hbar\omega$ 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
Figure 3.3: Illustration of finite-range dependence for $(3,1)$ system with $3^-\,$ symmetry at unitarity. Circles and squares show the relative eigenenergies $E_{3,1}(N_b)$ for states 15 and 16, respectively, for three different ranges $r_0$ of the underlying two-body interaction potential; $N_b$ is the largest basis set considered (typically, $N_b$ increases with decreasing $r_0/a_{ho}$). The energies provide variational upper bounds and the estimated basis set extrapolation error is indicated by errorbars. Solid lines show linear fits to the energies $E_{3,1}(N_b)$. This figure is taken from Fig. 3 of Ref. [39].

numerical accuracy. For the states considered in Table 3.1, 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 $E_{3,1} \leq 10.5\hbar\omega$. Figure 3.3 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. When optimizing a state whose energy is nearly degenerate 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
Figure 3.4: Panels (a) and (b) show the density of states for the $(2, 2)$ and $(3, 1)$ systems at unitarity; only the relative degrees of freedom are accounted for. The histograms show the number of energies corresponding to shifted states per $\hbar \omega/4$ while the crosses show the number of energies corresponding to unshifted states. The histograms and the crosses account for the $(2L + 1)$-multiplicity of the energies. This figure is taken from Fig. 4 of Ref. [39].
accurate description of the lower lying part of the energy spectrum. The advantage of our optimization procedure is that the basis set is optimized for a particular state or a particular subset of states. Correspondingly, we work with comparatively small basis sets. The energies of the (2, 2) and (3, 1) systems at unitarity (see Table 3.1 and Appendix B) are obtained using basis sets that consist of 700-3400 basis functions.

Following the format of Table 3.1, Appendix B 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 \( E_{n_1,n_2} \) smaller or equal to \( 10.5\hbar\omega \) [not counting the \((2L + 1)\) multiplicity]. Of these states, respectively 52 and 46 are unshifted. The shifted energies are characterized by respectively 170 and 89 \( s_{L,\nu} \) values. Figures 3.4(a) and 3.4(b) show the density of states of the (2, 2) system and the (3, 1) system, respectively, at unitarity. The plots account for the \((2L + 1)\)-multiplicity, and the density of states is shown separately for the shifted and unshifted states. It can be seen that the density of states increases significantly with increasing energy for both the (2, 2) and (3, 1) systems.

3.3 Two-component unequal-mass Fermi gases at unitarity

This section extends the equal-mass calculations presented in the previous section to unequal-mass systems. We focus on the energetically lowest-lying state of the two-component system with three spin-up atoms (mass = \( m_1 \)) and one spin-down atom (mass = \( m_2 \)), which has \( L^\Pi = 1^+ \) symmetry. For each mass ratio \( \kappa \), where \( \kappa = m_1/m_2 \), we use the stochastic variational method to calculate the energies for different \( r_0 \) values.

Symbols in Fig. 3.5 show the ground state energy of the (3, 1) system as a function of
Figure 3.5: Illustration of the range dependence for the (3, 1) system with 1+ symmetry at unitarity. (a) Circles, squares, diamonds, triangles and crosses show $E_{3,1}/E_{ho}$ as a function of $r_0/a_{ho}^\mu$, where $a_{ho}^\mu = \sqrt{\hbar/(\mu \omega)}$, for the mass ratios $\kappa = 1/10, 1, 4, 8$ and 9, respectively. The solid lines show three-parameter fits to the relative energies for $\kappa < 8$ and four-parameter fits to the relative energies for $\kappa \geq 8$. (b) Pluses, squares, diamonds, circles and down triangles show the relative energies as a function of $r_0/a_{ho}^\mu$ for $\kappa = 10.5, 10.525, 10.55, 10.575$ and 10.6, respectively. The dotted lines are shown as a guide to the eye. The errorbars indicate the estimated basis set extrapolation errors. The basis set extrapolation errors are not visible in panel (a) as they are smaller than the symbol size. The black line shows the function $c_0 + c_{-2} r_0^{-2}$ with $c_0 = 0.2131 E_{ho}$ and $c_{-2} = -7.02 \times 10^{-5} (a_{ho}^\mu)^2 E_{ho}$, where $c_0$ and $c_{-2}$ are determined by fitting the relative energies for $\kappa = 10.575$ with $r_0/a_{ho}^\mu \leq 0.019$. 

50
For $\kappa \leq 9$, we obtain the zero-range energies by extrapolating the finite-range energies of the trapped system to the $r_0/a_{ho}^\kappa \to 0$ limit. Table 3.2 summarizes the extrapolated zero-range energies $E_{3,1}(r_0 = 0)$ for the $(3, 1)$ system with $L^\Pi = 1^+$ symmetry for $1/10 \leq \kappa \leq 9$. The solid lines in Fig. 3.5(a) show the fits to the relative energies using the fitting function $E_{3,1}(r_0 = 0)/\hbar \omega + \sum_{i=1}^k c_i x^i$, where $x = r_0/a_{ho}^\kappa$ and $k = 2$ for $\kappa < 8$ and $k = 3$ for $\kappa \geq 8$. The range dependence is comparatively small for $\kappa < 1$ and the energies approach the zero-range limit approximately linearly from above. For $\kappa > 1$, the range dependence increases with increasing $\kappa$ and the energies approach the zero-range limit from below. Figure 3.6 shows the extrapolated zero-range energies as a function of $\kappa$ for $1/10 \leq \kappa \leq 9$. The extrapolated zero-range energies decrease monotonically with increasing mass ratio $\kappa$. The change of the energy with $\kappa$ increases with increasing $\kappa$.

Figure 3.5(b) shows the range dependence for $\kappa > 9$. The dependence of the energies on the range $r_0$ becomes comparatively small for $\kappa \approx 10.55$. For yet larger $\kappa$, the energy varies roughly as $1/r_0^2$ and approaches large negative values for small $r_0$. For $9 < \kappa < 10.55$, the extrapolation to the zero-range limit based on the energies for $r_0 > 0.01a_{ho}$ is difficult. Ideally, one would want to perform additional calculations for smaller $r_0$. Such calculations with the explicitly correlated Gaussian approach are, however, numerically extremely demanding. In this regime, the dependence on $r_0$ indicates non-universal physics. The diverging nature of the energy as a function of the range around $\kappa \approx 10.55$ is interpreted as evidence for the appearance of a four-body resonance. The four-body resonance occurs at a lower mass ratio than the three-body resonance, which is located at $\kappa \approx 12.314$ [116].

### 3.4 Summary and outlook

This chapter considered the energy spectra of small trapped two-component Fermi gases with vanishing and finite angular momentum as well as natural and unnatural parity. Large portions of the energy spectra of the $(2, 2)$ and $(3, 1)$ systems at unitarity were determined
as a function of the range of the underlying two-body model potential and extrapolated to the zero-range limit. The extrapolated zero-range energies are expected to be universal, i.e., independent of the underlying Gaussian model potential. The energies were determined by solving the relative Schrödinger equation using the stochastic variational approach. Compact expressions for the relevant matrix elements were presented in Appendix A. The eigen frequencies corresponding to the calculated eigenenergies can, in principle, be measured experimentally via radio-frequency spectroscopy [56]. The four-body energies were further used to calculate the fourth-order virial coefficient $b_4$ [39] and stimulated the work on previously unobserved inter-system degeneracies [120].

One motivation for calculating such large portions of the $(2, 2)$ and $(3, 1)$ energies at unitarity was to calculate the fourth-order virial coefficient $b_4$ of the trapped Fermi gas. The high-temperature limit of the fourth-order virial coefficient enters into the universal virial equation of state, which allows for the determination of the universal thermodynamics of two-component Fermi gases. Using the $(2, 2)$ and $(3, 1)$ energies determined in this thesis (see Ch. 3.2), the calculation of $b_4$ was carried out by K. Daily. The main findings of the analysis are [39]: At low-temperature the fourth-order virial coefficient $b_4$ of the trapped
system is negative and decreases monotonically with increasing temperature. Assuming $b_4$ changes monotonically as a function of temperature throughout the medium to high temperature regime, an extrapolation to the high-temperature limit, combined with the application of the local density approximation, results in a negative value for the fourth-order virial coefficient of the homogeneous system in the high temperature limit. Recent results, based on the equation of state, determined both experimentally [121,122] and calculated via a diagrammatic Monte Carlo technique [123], suggest that the fourth-order virial coefficient of the homogeneous system is positive. Thus, we speculate that the virial coefficient $b_4$ of the trapped system changes sign (i.e., behaves non-monotonically) in the medium- or high-temperature regime. We conclude that much larger portions of the energy spectra are needed to predict the high-temperature limit of $b_4$.

The relative four-body energies for the equal-mass system were also used to identify intersystem degeneracies, where the eigen energies $E_{n_1-1,n_2+1}$ of the less spin balanced system are degenerate with the energies $E_{n_1,n_2}$ of the more spin balanced system for any $s$-wave scattering length $a_{aa}^{ssdd}$, including infinitely large, positive and negative $a_{aa}^{ssdd}$. The intersystem degeneracies were “discovered” as follows: We analyzed the extrapolated zero-range energies of the $(3, 1)$ and $(2, 2)$ systems at unitarity for all states with relative energy $E_{n_1,n_2}$ equal to or
smaller than 21 $\hbar \omega / 2$, which have an accuracy of 0.1 % or better. There are 89 and 170 states corresponding to (3, 1) and (2, 2), respectively, that are affected by the interactions. Each of these is characterized by a $s_{L,\nu}$ value (see Sec. 3.2). Quite surprisingly, every $s_{L,\nu}$ value of the (3, 1) system, within the numerical accuracy, appears in the sequence of $s_{L,\nu}$ values of the (2, 2) system. In addition to the four-body system, evidence for analogous degeneracies were also found in equal-mass five- and six-body systems [120]. It has been shown [120] that a new Hamiltonian $H'$, which accounts for interactions between all particle pairs regardless of the particle statistics, reproduces the energies of the Hamiltonian $H$ in the zero-range limit. It follows that the Hamiltonian $H'$ can be used to understand the intersystem degeneracies between the $(n_1 + 1, n_2 - 1)$ and $(n_1, n_2)$ systems in the zero-range limit. The introduction of the Hamiltonian $H'$ is important as it treats all particle pairs on an equal footing. Since the Hamiltonian $H'$ is invariant under the permutation of any pair of atoms, the inter-system degeneracies, which are a manifestation of an underlying symmetry, are found to be related to the symmetric group $S_N$. A group theoretical analysis [120] shows that the intersystem degeneracies are not specific to the $N = 4$ system, but rather an inherent property of two-component equal-mass Fermi gases with zero-range interactions, regardless of the number of particles.

In addition to the equal-mass system, we considered small fermionic two-component systems with unequal masses. We focused on the trapped (3, 1) system with $1^+$ symmetry at unitarity. We find that the range dependence of the energy increases notably with increasing mass ratio $\kappa$. Around $\kappa \approx 10.55$, the energy changes sign and approaches a large negative value. This prohibits us from extracting the $s_{1,0}$ value from the finite-range energies of the trapped system. It would be interesting to solve the hyperangular Schrödinger equation which yields $s_{1,0}$ directly. Such calculations can be carried out by generalizing the explicitly correlated Gaussian to solve the hyperangular Schrödinger equation, which depends parametrically on the hyperradius. The resulting approach is referred to as the hyperspherical explicitly correlated Gaussian approach. The underlying theoretical framework and first
proof-of-principle calculations are presented in Ch. 6.
Chapter 4

Excitation spectrum and effective interactions of highly-elongated Fermi gas

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Full 3D calculations of small two-component Fermi gases under highly-elongated confinement, in which unlike fermions interact through short-range potentials with variable atom-atom s-wave scattering length, are performed using the correlated Gaussian approach. In addition, microscopic 1D calculations are performed for effective “atomic” and “molecular” 1D model Hamiltonian. Comparisons of the 3D and 1D energies and excitation frequencies establish the validity regimes of the effective 1D Hamiltonian. Our numerical results for three- and four-particle systems suggest that the effective 1D atom-dimer and dimer-
dimer interactions are to a good approximation determined by simple analytical expressions. Implications for the description of quasi-1D Fermi gases within strict 1D frameworks are discussed.

4.1 Introduction

Ultracold atomic and molecular gases are considered nearly ideal model systems since their confining geometry, size and interaction strength can be varied with unprecedented control [12, 28]. A key goal of ongoing research activities is to experimentally determine the complete phase diagram of cold atom systems [124]. The successful demonstration of this task would provide a first step towards utilizing cold atom systems as quantum emulators. The determination of phase diagrams of quasi-1D systems has received considerable attention since these systems can, under certain circumstances, be described by 1D model Hamiltonian whose properties have been studied extensively in the literature [125, 126, 127, 128]. For this class of systems, the challenge is to establish which aspects of quasi-1D cold atom experiments can be described by 1D model Hamiltonian.

Naively, the 1D scattering strength between two particles in a waveguide geometry may be estimated by integrating out the tightly-confined transverse degrees of freedom. However, while the result is accurate in the weakly-interacting regime, Olshanii’s seminal work [129] shows that the 1D scattering strength $g_{1D}^{aa}$ depends in general non-trivially on the 3D $s$-wave atom-atom scattering length $a_{3D}^{aa}$ and the transverse angular frequency $\omega_\rho$. The coupling constant $g_{1D}^{aa}$ determined by Olshanii is now widely used in many-body studies of Bose and Fermi gases. The applicability of an effective atomic 1D Hamiltonian whose two-body interactions are parameterized in terms of $g_{1D}^{aa}$ has, e.g., been confirmed for a Bose gas under highly elongated harmonic confinement by comparing the results of 3D and 1D Monte Carlo calculations [130, 131].

Over the past few years, an effective atomic 1D Hamiltonian has also been applied exten-
sively to two-component Fermi gases under highly-elongated confinement \[41, 132, 133, 134, 135, 136\]; in this case, however, the validity regime of the effective atomic 1D Hamiltonian has not yet been assessed carefully. It is clear that an effective atomic 1D Hamiltonian description breaks down when tightly-bound molecules form. In this case, the system may be described by an effective molecular 1D Hamiltonian that treats each tightly-bound molecule as a composite boson. While the functional form of such an effective molecular Hamiltonian is generally agreed upon, the parametrization of the effective atom-dimer and dimer-dimer interactions varies \[134, 135, 136\]. Reference \[135\], e.g., assumes that the atom-atom and dimer-dimer resonance positions coincide. Reference \[136\], in contrast, finds by solving the few-body problem explicitly that these resonance positions do not coincide.

This work presents 3D and 1D zero-temperature \textit{ab initio} calculations for small two-component Fermi gases with up to \(N = 4\) atoms under highly-elongated confinement and assesses the validity regimes of effective atomic and molecular 1D Hamiltonian. Our main findings are: \textit{i}) The 3D energies are reproduced well by an effective atomic 1D Hamiltonian for small \(|a_{\text{3D}}^{aa}/a_\rho| (a_{\text{3D}}^{aa} < 0)\), where \(a_\rho\) denotes the oscillator length in the tight confinement direction [see Eq. (4.5)]. \textit{ii}) For small positive \(a_{\text{3D}}^{aa}/a_\rho\), the 3D energies are reproduced well by an effective molecular 1D Hamiltonian that depends on the effective 1D atom-dimer and dimer-dimer scattering lengths \(a_{\text{1D}}^{ad}\) and \(a_{\text{1D}}^{dd}\); analytical expressions for \(a_{\text{1D}}^{ad}\) and \(a_{\text{1D}}^{dd}\) are presented. \textit{iii}) For two of the energy curves considered (see below), the descriptions based on the effective atomic and molecular 1D Hamiltonian join fairly smoothly in the strongly-interacting regime, defined through \(|a_{\text{3D}}^{aa}| \gtrsim a_\rho\); not surprisingly, the dependence of the energies on the aspect ratio is largest in the strongly-interacting regime.

Our assessment of the validity regimes of the effective atomic and molecular 1D Hamiltonian for small systems is expected to provide guidelines for larger systems, and is thus of great importance for realizing condensed matter and materials analogs as well as for exploiting cold atom systems for quantum computation and quantum simulation. Quasi-1D few-fermion systems can be prepared by loading a gas of ultracold fermions into an optical
lattice [77, 137]. Measurements of the excitation spectrum as a function of the interaction strength would provide a stringent test of our microscopic predictions.

Section 4.2 introduces the 3D model Hamiltonian, discusses the numerical techniques employed to solve the corresponding Schrödinger equation and presents the resulting 3D energies. Section 4.3 introduces the effective atomic and molecular 1D Hamiltonian and presents detailed comparisons between the 3D and 1D energies. Section 4.4 discusses the excitation spectrum of strongly-interacting two-component Fermi gases under highly-elongated cylindrically-symmetric confinement. Finally, Sec. 4.5 concludes.

4.2 Full 3D treatment: Energetics

This section introduces the 3D model Hamiltonian and the numerical techniques employed to solve the corresponding Schrödinger equation. 3D energies are presented for $N = 2 - 4$ fermions under highly-elongated confinement.

Our 3D model Hamiltonian $H_{3D}$ for the trapped two-component Fermi gas with $N_1$ spin-up and $N_2$ spin-down fermions, where $N = N_1 + N_2$, reads

$$H_{3D} = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m} \nabla_{\vec{r}_i}^2 + V_{\text{tr}}(\vec{r}_i) \right] + \sum_{i=1}^{N_1} \sum_{j=N_1+1}^{N} V_{tb}(r_{ij}). \quad (4.1)$$

Here, $m$ and $\vec{r}_i$ denote the atom mass and the position vector of the $i$th atom, $\vec{r}_i = (x_i, y_i, z_i)$. The trapping potential $V_{\text{tr}}(\vec{r}_i)$ is given by

$$V_{\text{tr}}(\vec{r}_i) = \frac{1}{2} m \omega_z^2 (\lambda^2 \rho_i^2 + z_i^2), \quad (4.2)$$

where $\rho_i$ and $\lambda$ are defined through $\rho_i = \sqrt{x_i^2 + y_i^2}$ and

$$\omega_\rho = \lambda \omega_z, \quad (4.3)$$
and $\omega_\rho$ and $\omega_z$ denote the transverse and axial angular frequencies. Unlike atoms interact through a spherically symmetric short-range Gaussian potential $V_{tb}$,

$$V_{tb}(r_{ij}) = -V_0 \exp \left( -\frac{r_{ij}^2}{2r_0^2} \right),$$  \hspace{1cm} (4.4)

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$. We take the range $r_0$ to be much smaller than the oscillator lengths $a_z$ and $a_\rho$ in the $z$- and $\rho$-directions,

$$a_{z,\rho} = \sqrt{\frac{\hbar}{m\omega_{z,\rho}}},$$  \hspace{1cm} (4.5)

and adjust the depth $V_0$ ($V_0 > 0$) so that the free-space 3D $s$-wave atom-atom scattering length $a_{3D}^{aa}$ takes the desired value. A solid line in Fig. 4.1 shows $a_{3D}^{aa}$ as a function of the well depth $V_0$. To realize different negative $a_{3D}^{aa}$, we start with a non-interacting (NI) system ($V_0 = 0$) and increase the depth $V_0$ till $|a_{3D}^{aa}|$ becomes infinitely large; at this point, the free-space two-particle system supports a single zero-energy $s$-wave bound state. To realize different positive $a_{3D}^{aa}$, we increase $V_0$ further. In general, $V_{tb}$ can lead not only to $s$-wave scattering but also to higher partial wave scattering. We have checked that the generalized $p$-wave scattering length and generalized scattering lengths corresponding to other higher partial waves are negligible over the range of well depths considered in this paper. This implies that $H_{3D}$ effectively describes an $s$-wave interacting system.

To solve the time-independent Schrödinger equation for $H_{3D}$, we separate off the center-of-mass motion and numerically solve the resulting Schrödinger equation in the relative coordinates. For $N_1 = N_2 = 1$, we expand the relative wave function in terms of two-dimensional B-splines and diagonalize the Hamiltonian matrix. For the three- and four-particle systems, we employ a correlated Gaussian (CG) approach [75,138,139] that expands
Figure 4.1: The solid and dashed lines show the free-space scattering lengths $a_{3D}^{aa}$ and $a_{1D}^{aa}$ for the Gaussian potential $V_{tb}$ as a function of the well depth $V_0$. The scattering lengths and depths are measured in the “natural units” of the free-space system, i.e., in units of $r_0$ [$z_0$] and $\hbar^2/(2\mu^{aa} r_0^2)$ [$\hbar^2/(2\mu^{aa} z_0^2)$] for the 3D [1D] system, where $\mu^{aa}$ denotes the reduced mass of the atom-atom system.
the relative wave function $\psi$ in terms of Gaussian basis functions $f_k^{(\rho)} f_k^{(z)}$,

$$\psi = \sum_{k=1}^{N_b} c_k \mathcal{A} \left[ f_k^{(\rho)}(\rho_{12}, \cdots, \rho_{N-1,N}) f_k^{(z)}(z_{12}, \cdots, z_{N-1,N}) \right],$$

(4.6)

where

$$f_k^{(\rho)}(\rho_{12}, \cdots, \rho_{N-1,N}) \equiv \exp \left[ -\sum_{i<j}^N \left( \frac{\rho_{ij}}{\sqrt{2} d_{ij,k}^{(\rho)}} \right)^2 \right]$$

(4.7)

and $f_k^{(z)}$ is defined analogously. The relative coordinates $\rho_{ij}$ and $z_{ij}$ are defined as $\rho_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$ and $z_{ij} = z_i - z_j$ ($i, j = 1, \cdots, N$ with $i < j$). The widths $d_{ij,k}^{(\rho)}$ and $d_{ij,k}^{(z)}$ are chosen semi-stochastically for each pair $ij$ and $k$th basis function, and the total number of basis functions is denoted by $N_b$. In Eq. (4.6), the $c_k$ denote expansion coefficients and $\mathcal{A}$ denotes an anti-symmetrizer that ensures the proper symmetry of the two-component Fermi gas under exchange of identical fermions. For $N = 3$ ($N_1 = 2$ and $N_2 = 1$), $\mathcal{A}$ can be conveniently written as $1 - P_{12}$, where $P_{12}$ permutes the two up-fermions. For $N = 4$ ($N_1 = N_2 = 2$), $\mathcal{A}$ can be written as $1 - P_{12} - P_{34} + P_{12}P_{34}$.

For the interaction and confining potentials chosen, the Hamiltonian and overlap matrix elements (the basis functions $f_k^{(\rho)} f_k^{(z)}$ do not form an orthogonal set) can be constructed analytically. The diagonalization of the eigenvalue equation is then performed using standard techniques. The resulting eigenenergies, whose accuracy can be systematically improved by increasing the number of basis functions and by optimizing the widths $d_{ij,k}^{(\rho)}$ and $d_{ij,k}^{(z)}$ of the Gaussian functions, provide upper bounds to the exact eigenenergies.

The 2D functions $f_k^{(\rho)}$ are eigenfunctions of the $z$-component $L_z$ of the orbital angular momentum operator with eigenvalues $\hbar m_l$, $m_l = 0$ [75], while the 1D functions $f_k^{(z)}$ have even parity $P_z = +1$. For the $N = 4$ system, the energetically lowest-lying state has $m_l = 0$ and $P_z = +1$ for all 3D scattering lengths $a_{3D}$ and the basis functions $f_k^{(\rho)} f_k^{(z)}$ defined in and below
Eq. (4.6) have the proper symmetry. The ground state of the NI $N = 3$ system, in contrast, has $m_l = 0$ and odd parity ($P_z = -1$), which cannot be described by the basis functions $f^{(\rho)}_k f^{(z)}_z$. To describe states with odd parity, we add a spectator atom that does not interact with the $N$-fermion system of interest; the energy of the NI spectator atom follows from its $m_l$ quantum number and from its parity, and is subtracted at the end of the calculation. Since the basis functions of the $(N + 1)$-system have even parity, the spectator atom and the $N$-fermion system either both have even parity or both have odd parity. In the following, we label our solutions by the parity $P_z$; if a spectator atom is added for computational purposes, we report the parity of the physical system of interest. Furthermore, since all energetically lowest-lying states of two-component Fermi gases under highly-elongated confinement have $m_l = 0$, we frequently omit the $m_l$ label.

Figures 4.2(a) and (b) show the relative 3D energies for $N = 2–4$ and $\lambda = 10$ as a function of the inverse 3D scattering length $a_\rho/a_{3D}^{na}$. Solid lines in Figs. 4.2(a) and (b) show the relative $s$-wave ground state energy $E_s(1, 1) - E_{CM,0}$ of the two-body system. For later convenience, the energy $E_s(1, 1)$ as well as the energies $E(N_1, N_2)$ (see below) include the center-of-mass ground state energy $E_{CM,0}$, $E_{CM,0} = \hbar \omega_\rho + \hbar \omega_z/2$. In the NI limit, $E_s(1, 1) - E_{CM,0}$ equals $10.5 \hbar \omega_z = 1.05 \hbar \omega_\rho$. In the absence of the confining potential in the $z$-direction, the relative two-body energy is always smaller than $\hbar \omega_\rho$, indicating the existence of a quasi-1D bound state for all 3D scattering lengths $a_{3D}^{na}$ [129, 140]. The confining potential in the $z$-direction pushes the energy up; in the NI limit, the up-shift is given by the zero-point energy $\hbar \omega_z/2$.

For the $N = 3$ system, the relative energies $E(2, 1) - E_{CM,0}$ of the energetically lowest-lying states with $P_z = +1$ and $-1$ are shown by dotted and dashed lines, respectively. The $P_z = -1$ state has lower energy for small $|a_{3D}^{na}|$, $a_{3D}^{na} < 0$ [see Fig. 4.2(a)], while the $P_z = +1$ state has lower energy for small positive $a_{3D}^{na}$ [the crossover of the two states is not visible on the scale shown in Fig. 4.2(b); it occurs at $a_{\rho}/a_{3D}^{na} \approx 2$ (see also Fig. 6.2)]. The relative three-particle energies are just slightly larger than the relative two-body $s$-wave energies in the limit of small positive $a_{3D}^{na}$, indicating that the three-particle system can be thought of
Figure 4.2: (Color online) Relative 3D energies calculated using $H_{3D}$ as a function of $a_\rho/a_{3D}^{aa}$ for (a) negative $a_{3D}^{aa}$ and (b) positive $a_{3D}^{aa}$ for $\lambda = 10$ [$r_0 = 0.03a_z$ for $a_{3D}^{aa} < 0$ and $N = 4$, and $0.01a_z$ otherwise]. Solid lines show the s-wave energy $E_s(1,1) - E_{CM,0}$ of the two-particle system, dashed lines show the lowest three-particle energy $E(2,1) - E_{CM,0}$ with $P_z = -1$, dotted lines show the lowest three-particle energy $E(2,1) - E_{CM,0}$ with $P_z = +1$ and dash-dotted lines show one half of the lowest four-particle energy $E(2,2) - E_{CM,0}$ with $P_z = +1$. The horizontal solid lines on the left side of panel (a) indicate the relative energies of the NI systems: $E_s(1,1) - E_{CM,0} = 10.5\hbar\omega_z$, $E(2,1) - E_{CM,0} = 22\hbar\omega_z$ ($P_z = -1$), $E(2,1) - E_{CM,0} = 23\hbar\omega_z$ ($P_z = +1$), and $[E(2,2) - E_{CM,0}]/2 = 16.75\hbar\omega_z$. 
as consisting of an $s$-wave dimer and an unpaired atom. The relative ground state energy $E(2,2) - E_{CM,0}$ of the four-particle system has $P_z = +1$ for all 3D scattering lengths $a_{3D}^{aa}$; to ease comparisons between the energies of the two- and four-particle systems, dash-dotted lines in Figs. 4.2(a) and (b) show one half of the relative four-particle energy. For small positive $a_{3D}^{aa}$, the four-particle energy approaches approximately twice the energy of the two-particle system, indicating that the four-particle system can be thought of as consisting of two $s$-wave molecules. No tightly-bound trimers or tetramers are formed in the $a_{3D}^{aa} \rightarrow 0^+$ limit, in agreement with results for zero-range interactions [32,33,141,142].

The 3D energies can be combined to define the universal energy curve $\Lambda_{N_1,N_2}$ for a two-component Fermi gas under external cylindrically symmetric confinement,

$$\Lambda_{N_1,N_2} = \frac{E(N_1, N_2) - N_d E_s(1,1) - N_f \hbar \left( \omega_p + \frac{1}{2} \omega_z \right)}{E_{NI}(N_1, N_2) - N \hbar \left( \omega_p + \frac{1}{2} \omega_z \right)},$$

(4.8)

where $N_d = \min\{N_1, N_2\}$ and $N_f = |N_1 - N_2|$. In Eq. (4.8), $E_{NI}(N_1, N_2)$ denotes the energy of the NI system, and the energies $E_{NI}(N_1, N_2)$, $E(N_1, N_2)$ and $E_s(1,1)$ include the center-of-mass ground state energy $E_{CM,0}$. To remove dependencies of the total energy $E(N_1, N_2)$ of the trapped system on $V_{tb}$, the $s$-wave ground state energy $E_s(1,1)$ of the trapped two-particle system is subtracted on the right hand side of Eq. (4.8). If $E(N_1, N_2)$ corresponds to the energetically lowest-lying state of the NI system, the universal energy curve $\Lambda_{N_1,N_2}$ equals one. Conversely, if $\Lambda_{N_1,N_2}$ equals zero in the $a_{3D}^{aa} \rightarrow 0^+$ limit, then this indicates that the system is effectively NI and that induced interactions are absent. The definition of the universal energy curve presented in Eq. (4.8) for cylindrically-symmetric two-component Fermi systems constitutes a straightforward generalization of that previously introduced for spherically-symmetric two-component systems [118,143].

Figure 6.2 shows the 3D energy curves $\Lambda_{N_1,N_2}$ as a function of $a_{\rho}/a_{3D}^{aa}$ for $\lambda = 10$; the energies used to calculate the $\Lambda_{N_1,N_2}$ are the same as those shown in Fig. 4.2. A thick dotted line shows $\Lambda_{2,2}$ calculated using the four-body energies $E(2,2)$ that correspond to states with
Figure 4.3: (Color online) $\Lambda_{N_1,N_2}$ as a function of $a_\rho/a_{3D}^{aa}$. Panel (a) covers a large scattering length range while panel (b) shows an enlargement of the strongly-interacting regime. Thick dotted, dashed and solid lines show $\Lambda_{2,2}$ ($P_z = +1$), $\Lambda_{2,1}$ ($P_z = +1$) and $\Lambda_{2,1}$ ($P_z = -1$) calculated using $H_{3D}$ for $\lambda = 10$ [$r_0 = 0.03a_z$ for $a_{3D}^{aa} < 0$ and $N = 4$, and $0.01a_z$ otherwise]. Thin dash-dash-dotted and dash-dot-dotted lines show the corresponding 1D energy curves calculated using $H_{1D}^a$ and $H_{1D}^m$. 

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$m_l = 0$ and $P_z = +1$. The energy curve $\Lambda_{2,2}$ decreases monotonically from 1 to approximately 0 as $a_\rho/a_{3D}^{aa}$ increases from small negative to large positive values. Thick dashed and solid lines in Fig. 6.2 show the energy curves $\Lambda_{2,1}$ for the energetically lowest-lying $N = 3$ states with $P_z = +1$ and $-1$, respectively. It can be seen that these $N = 3$ energy curves cross at $a_\rho/a_{3D}^{aa} \approx 1.9$. For $a_{3D}^{aa} \rightarrow 0^-$ (NI limit), the ground state has $m_l = 0$ and $P_z = -1$: One spin-up and one spin-down atom occupy the ground state harmonic oscillator orbital while the second up-atom occupies the first excited state harmonic oscillator orbital. For $a_{3D}^{aa} \rightarrow 0^+$, in contrast, the ground state for $N = 3$ has $m_l = 0$ and $P_z = +1$: The system consists of a tightly-bound dimer and an atom, which both occupy the lowest trap state. In this limit, the energy of the state with $P_z = -1$ is about $\hbar \omega_z$ larger than the energy of the $P_z = +1$ state [note that the energy difference is too small to be visible on the scale shown in Fig. 4.2(b)]. This suggests that the tightly-bound molecule and the unpaired atom interact through effective 1D potentials that lead to even and odd parity scattering for $P_z = +1$ and $-1$, respectively (see also the next section).

### 4.3 1D treatment: Energetics and effective interactions

This section considers effective atomic and molecular 1D Hamiltonian, which assume that the motion in the $\rho$-direction is frozen, and compares the resulting 1D energies with the 3D energies discussed in the previous section. The applicability of the 1D model Hamiltonian and their parametrizations are discussed in detail.

If the system behaves like an atomic gas, the effective atomic 1D Hamiltonian $H_{1D}^a$ is given by

$$H_{1D}^a = \sum_{i=1}^{N} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z_i^2} + V_{tr}(z_i) \right] + \sum_{i=1}^{N_1} \sum_{j=N_1+1}^{N} V_{tb}(z_{ij}), \quad (4.9)$$
where

\[ V_{tr}(z_i) = \frac{1}{2} m \omega_z^2 z_i^2. \]  

(4.10)

In Eq. (4.9), the spin-up and spin-down fermions interact through the two-body potential \( V_{tb}(z_{ij}) \) and, as in the 3D Hamiltonian \( H_{3D} \) [see Eq. (6.1)], like atoms do not interact. The two-body potential \( V_{tb} \) is chosen such that its 1D even parity atom-atom scattering length \( a_{aa}^{1D} \) is given by [129]

\[ a_{aa}^{1D} = -\frac{\hbar^2}{2\mu_{aa}\omega_{\rho}} \left( \frac{1}{a_{aa}^{3D}} - 1.4603 \frac{\mu_{aa}\omega_{\rho}}{\hbar} \right), \]  

(4.11)

where \( \mu_{aa} \) denotes the reduced mass of the atom-atom system. The 1D even parity scattering length \( a_{aa}^{1D} \) [solid lines in Figs. 6.1(a) and (b)] is large for large \( |a_{\rho}/a_{3D}^{aa}| \) \( (a_{3D}^{aa} < 0) \), decreases linearly with increasing \( a_{\rho}/a_{3D}^{aa} \), and crosses zero at \( a_{\rho}/a_{3D}^{aa} = 1.0326 \). Since the 1D coupling constant \( g_{1D}^{aa} \),

\[ g_{1D}^{aa} = -\frac{\hbar^2}{\mu_{aa}a_{aa}^{1D}}, \]  

(4.12)

diverges when \( a_{aa}^{1D} \) vanishes, the quasi-1D system is infinitely strongly-interacting for a finite \( a_{aa}^{1D} \). Furthermore, a large positive \( a_{aa}^{1D} \) indicates the presence of a weakly-bound even parity two-body bound state. In the literature, the effective 1D atom-atom potential \( V_{tb} \) is frequently modeled by a 1D zero-range \( \delta \)-function potential. For numerical convenience, we use instead a 1D Gaussian potential [Eq. (4.4) with \( r_{ij} \) and \( r_0 \) replaced by \( z_{ij} \) and \( z_0 \)] with a small width \( z_0 \) \( (z_0 = 0.005a_z) \) and a depth adjusted so as to obtain the desired \( a_{aa}^{1D} \). We have checked that the resulting 1D energies depend only very weakly on \( z_0 \) and that the odd parity atom-atom scattering length is negligibly small over the range of well depths considered. The 1D even parity atom-atom scattering length \( a_{aa}^{1D} \) for the 1D Gaussian potential is shown in Fig. 4.1 by a dashed line as a function of the well depth \( V_0 \).
Figure 4.4: (Color online) 1D even parity atom-atom scattering length $a_{1D}^{aa}/a_\rho$ (solid line) and corresponding 1D scattering strength $g_{1D}^{aa}/(\hbar \omega a_\rho)$ (dashed line) as a function of the inverse 3D atom-atom scattering length $a_\rho/a_{3D}^{aa}$: Panel (a) covers a large 3D scattering length range while panel (b) shows an enlargement of the strongly-interacting regime. The 1D coupling constant $g_{1D}^{aa}$ changes from about $-\hbar \omega a_\rho$ to about $-60 \hbar \omega a_\rho$ as $a_\rho/a_{3D}^{aa}$ increases from $-1$ to $1$ (i.e., in the strongly-interacting regime).
For the 3D energy curves considered in Fig. 6.2, the effective atomic 1D Hamiltonian is expected to provide an accurate description if the size of the 1D dimer is much larger than the oscillator length $a_\rho$ (see, e.g., Refs. [134, 135]). Approximating the size of the dimer by $|a_1^{a_1}|$ and using $|a_1^{a_1}| \approx |a_\rho^2/a_3^{a_3}|$ [i.e., using the first part on the right hand side of Eq. (4.11)], the validity condition $a_\rho \gg |a_3^{a_3}|$ is obtained. Relaxing the disparity of length scales, we have $a_\rho \gtrsim |a_3^{a_3}|$ with $a_3^{a_3} < 0$.

To obtain the 1D energies of the effective atomic 1D Hamiltonian $H_{1D}^a$, we first separate off the center-of-mass motion and then solve the resulting Schrödinger equation in the relative coordinates using the B-spline approach for the two-particle system and the CG approach for the three- and four-particle systems. Our CG implementation for the 1D system parallels that discussed above for the 3D system. The main difference is that the basis functions are now given by $f_k^{(z)}$ instead of by $f_k^{(\rho)} f_k^{(z)}$. Systems with odd parity are, similarly to the 3D case, treated by adding a NI spectator atom. For large positive $a_1^{a_1}$, we find that the energetically lowest-lying 1D states accurately model the corresponding 3D states. For small positive $a_1^{a_1}$, however, the effective atomic 1D Hamiltonian supports a sequence of tightly-bound three- and four-particle states, which have no analog in the 3D system (as discussed above, tightly-bound three- and four-particle states are not supported by $H_{3D}$); these 1D states are excluded from our analysis. The 1D energy states of interest to us are those that smoothly evolve from a NI gas-like state in the $a_1^{a_1} \rightarrow \infty$ limit to states that describe a weakly-bound molecule and an atom or two weakly-bound molecules for $N = 3$ and $N = 4$, respectively, in the $a_1^{a_1} \rightarrow 0^+$ limit. Our last 1D energies are reported for $a_\rho/a_3^{a_3} \approx 1$ for $N = 3$ with $P_z = +1$, and for $a_\rho/a_3^{a_3} = 0$ for $N = 3$ with $P_z = -1$ and $N = 4$ with $P_z = +1$. We note that tightly-bound $N$-body states also exist for negative $a_1^{a_1}$. Their existence can be traced back to the finite range of the Gaussian two-body interaction potential; an effective atomic 1D Hamiltonian with zero-range δ-function potentials and negative $a_1^{a_1}$ does not support tightly-bound $N$-body states.

The 1D energies determine the 1D energy curves $\Lambda_{N_1,N_2}$, which are given by Eq. (4.8)
with $\omega_\rho = 0$, $E_{e}(1,1)$ denoting the 1D even parity two-particle energy, and $E(N_1, N_2)$ and $E_{N1}(N_1, N_2)$ interpreted as 1D energies. Thin dash-dash-dotted lines in Fig. 6.2 show the 1D energy curves obtained using $H_{1D}^a$ for $N = 3$ and 4. The agreement between the 1D energy curves and the corresponding 3D quantities (thick lines) in the weakly-attractive regime is excellent. For $P_z = +1$, the agreement between the 1D and 3D energy curves extends into the strongly-interacting, large positive $a_{3D}^{aa}$ regime. The 1D energy curve for $N = 3$ with $P_z = -1$, in contrast, starts deviating from the corresponding 3D energy curve for somewhat less strong interactions ($|a_\rho/a_{3D}^{aa}| \lesssim 2$ with $a_{3D}^{aa} < 0$). We have checked that these deviations are not due to the finite range of $V_{tb}$.

In addition to an effective atomic 1D Hamiltonian $H_{1D}^a$, we consider an effective molecular 1D Hamiltonian $H_{1D}^m$. We show in the following that the 3D energy curves with $P_z = +1$ can be reproduced well for $a_{3D}^{aa} > 0$ by treating the $N = 3$ and 4 systems as effective two-particle systems that consist of an atom and a tightly-bound molecule and of two tightly-bound molecules, respectively. To this end, we model the atom-dimer and dimer-dimer interactions through a $\delta$-function potential. The effective two-particle 1D Hamiltonian for the relative coordinate $z$ then reads

$$H_{1D}^m = -\frac{\hbar^2}{2\mu_j} \frac{d^2}{dz^2} + \frac{1}{2} \mu_j \omega_z^2 z^2 + g_{1D}^{1D} \delta(z), \quad (4.13)$$

where $j = ad$ and $dd$ for the atom-dimer and dimer-dimer system, respectively, and where the 1D coupling strengths $g_{1D}^{ad}$ and $g_{1D}^{dd}$ are related to the 1D scattering lengths $a_{1D}^{ad}$ and $a_{1D}^{dd}$ [Eq. (4.12) with aa replaced by ad and dd, respectively]. We approximate the effective 1D atom-dimer and dimer-dimer scattering lengths $a_{1D}^{ad}$ and $a_{1D}^{dd}$ by the right hand side of Eq. (4.11) with superscripts aa replaced by ad and dd, respectively. The 3D atom-dimer and dimer-dimer scattering lengths $a_{3D}^{ad}$ and $a_{3D}^{dd}$, in turn, are approximated by their free-space values [32,118,141,142,144],

$$a_{3D}^{ad} = 1.18 a_{3D}^{aa} \quad (4.14)$$
and \[33,118,143\]

\[a_{3D}^{dd} = 0.608 a_{3D}^{aa}. \quad (4.15)\]

Physically, this implies that molecules are formed in 3D and that their effective 3D interactions with atoms and other molecules are renormalized by the quasi-1D confinement.

The validity regime of the effective molecular 1D Hamiltonian \(H_{1D}^m\), with the parametrization of the effective interactions discussed above, is expected to be determined by three conditions: \(i\) Since the 3D free-space atom-dimer and dimer-dimer scattering lengths are derived assuming that \(a_{3D}^{aa} \gg r_0\), the above parametrization is expected to break down when \(a_{3D}^{aa}\) approaches \(r_0\). \(ii\) For three- and four-particle systems under spherically symmetric confinement, it has been shown [118] that the full 3D energies on the BEC side (positive \(a_{3D}^{aa}\)) are well described by effective 3D atom-molecule and molecule-molecule models if \(a_{3D}^{aa}\) is much smaller than the harmonic oscillator length. Correspondingly, since our parametrization of the effective interactions given in Eqs. (4.13)-(4.15) for the highly-elongated system assumes that the molecules are formed in 3D, the validity regime of \(H_{1D}^m\) is expected to be given by \(a_{3D}^{aa} \ll a_{3D}\). \(iii\) The effective 1D model treats the dimer as a point particle. This treatment is justified if the atom-dimer and dimer-dimer distances are much larger than the size of the dimer, i.e., if \(a_z \gg a_{3D}^{aa}\) (see, e.g., Refs. [134, 135]). Combining the three criteria, we find that \(H_{1D}^m\) is expected to provide an accurate description if \(a_{3D}^{aa} \gg a_{3D}^{aa} \gg r_0\) or, employing less stringent criteria, if \(a_{3D}^{aa} \gg a_{3D}^{aa} \gg r_0\). Combining this with the expected validity regime of \(H_{1D}^m\) (see above), the strongly-interacting regime is defined through \(|a_{3D}^{aa}| \gtrsim a_{3D}\). If the exact effective 1D atom-dimer and dimer-dimer scattering lengths were known, condition \(ii\) would not apply and the expected validity regime of the molecular 1D Hamiltonian would be larger \((a_z \gtrsim a_{3D}^{aa} \gtrsim r_0)\).

The Hamiltonian \(H_{1D}^m\) given in Eq. (4.13) parametrizes the effective interactions through a \(\delta\)-function potential and thus assumes that the effective 1D atom-dimer and dimer-dimer
interactions lead to even parity scattering. Consequently, the Hamiltonian $H_{1D}^m$ does not describe the $P_z = -1$ energy curve for $N = 3$. An effective molecular 1D model for the $N = 3$ system with $P_z = -1$ would include an effective 1D interaction that leads to odd parity scattering such as a so-called zero-range $\delta'$-potential [105, 145, 146, 147]. Although interesting, an effective molecular 1D description of the energy curve with $P_z = -1$ is not pursued in this work.

Calculating the eigenenergies of $H_{1D}^m$ from the known quantization condition [58], we find that the energy of the energetically lowest-lying state with gas-like character agrees well with the 3D quantities $E(2, 1) - E_s(1, 1) - \hbar \omega_\rho$ and $E(2, 2) - 2E_s(1, 1)$ for the atom-dimer and dimer-dimer systems with $P_z = +1$ and $a_{3D}^a \gtrsim 0$. Dash-dot-dotted lines in Fig. 6.2 show the energy curves for $P_z = +1$ calculated using the effective 1D molecule model. These 1D energy curves agree well with the corresponding 3D energy curves in the weakly-interacting regime. Deviations are visible for $N = 3$ for $a_\rho / a_{3D}^a \lesssim 1$ and for $N = 4$ for $a_\rho / a_{3D}^a \lesssim 0$. The agreement of the 1D and 3D energy curves over a wide range of interaction strengths a posteriori justifies our parameterization of the effective 1D atom-dimer and dimer-dimer scattering lengths (see also Sec. 4.4), which differs from that employed in earlier work [134, 135, 136, 141, 142]. Notably, the 1D energy curves for the effective molecular 1D Hamiltonian connect nearly smoothly with those for the effective atomic 1D Hamiltonian in the strongly-interacting regime.

4.4 Excitation spectrum

This section discusses the behavior of the excitation frequency $\omega_0$ for systems with $P_z = +1$. Within our 3D framework, the excitation energy $\hbar \omega_0$ is defined as the difference between the first excited and the lowest $P_z = +1$ states. The corresponding 1D excitation energy is defined as the difference between the energies of the corresponding 1D states.

Circles in Fig. 6.4 show the 3D excitation frequency $\omega_0$ for $N = 3$ with $P_z = +1$ and
Figure 4.5: (Color online) Excitation frequency $\omega_0/\omega_z$ for $N = 3$ with $P_z = +1$ and $r_0 = 0.01a_z$. (a) $\omega_0/\omega_z$ as a function of $a_\rho/a_{3D}^{aa}$ for $\lambda = 10$. Circles show the 3D excitation frequency, while solid and dotted lines show the corresponding 1D quantities calculated using $H_{1D}^{a}$ and $H_{1D}^{m}$, respectively. Panels (b), (c) and (d) show the strongly-interacting regime in more detail. (b) $\omega_0/\omega_z$ as a function of $-a_{1D}^{aa}/a_z$. Circles, squares and diamonds show the 3D excitation frequency for $\lambda = 10, 15$ and 20. A solid line shows the corresponding 1D quantities calculated using $H_{1D}^{a}$. (c) $\omega_0/\omega_z$ as a function of $-a_{1D}^{ad}/a_z$. Circles, squares and diamonds show the 3D excitation frequency for $\lambda = 10, 15$ and 20. A dotted line shows the corresponding 1D quantities calculated using $H_{1D}^{m}$. (d) Enlargement of panel (a).
\( \lambda = 10 \). Panels (a) and (d) show \( \omega_0 \) as a function of \( a_\rho/a_{3D}^{\text{aa}} \). The excitation frequency \( \omega_0 \) equals \( 2\omega_z \) in the NI limit (\( a_{3D}^{\text{aa}} \rightarrow 0^- \)), reaches its maximum for infinitely large \( a_{3D}^{\text{aa}} \) and its minimum for \( a_\rho/a_{3D}^{\text{aa}} \approx 5 \), and increases monotonically towards \( 2\omega_z \) as \( 1/a_{3D}^{\text{aa}} \) increases further. To illustrate the dependence of \( \omega_0 \) on the aspect ratio, squares and diamonds in Figs. 6.4(b) and (c) show the 3D excitation frequency \( \omega_0 \) for two larger aspect ratios, i.e., for \( \lambda = 15 \) and 20. Small dependencies of \( \omega_0 \) on \( \lambda \) are visible in the strongly-interacting regime.

To ease comparisons between the 3D excitation frequencies and those based on the 1D Hamiltonian, Figs. 6.4(b) and (c) show enlargements of the strongly-interacting regime as functions of \( -a_{1D}^{\text{aa}}/a_z \) and \( -a_{1D}^{\text{ad}}/a_z \). These scales are chosen since \( a_{1D}^{\text{aa}} \) and \( a_{1D}^{\text{ad}} \) determine the properties of \( H_{1D}^{\text{aa}} \) and \( H_{1D}^{\text{ad}} \), respectively. Solid lines in Fig. 6.4 show the excitation frequencies calculated using the effective atomic 1D Hamiltonian. These 1D excitation frequencies reproduce the 3D excitation frequencies well in the weakly-attractive regime (\( a_{1D}^{\text{aa}} \) large). In the strongly-interacting regime, the agreement improves with increasing \( \lambda \) [see Fig. 6.4(b)]. Dotted lines in Fig. 6.4 show the 1D excitation frequencies calculated using \( H_{1D}^{\text{ad}} \). For large \( |a_{1D}^{\text{ad}}| \) (\( a_{1D}^{\text{ad}} < 0 \)), the 3D excitation frequencies are independent of \( \lambda \) and reproduced well by the 1D molecular model. For smaller \( |a_{1D}^{\text{ad}}| \), the agreement improves with increasing \( \lambda \) [see Fig. 6.4(c)].

The effective molecular 1D Hamiltonian \( H_{1D}^{\text{ad}} \) predicts that a subset of the \( P_z = +1 \) energy spectrum of the three- and four-particle systems coincides with that of a two-particle Tonks-Girardeau (TG) gas for \( a_{1D}^{\text{ad}} = 0 \) [129]. For this atom-dimer scattering length, the effective molecular 1D Hamiltonian predicts \( \Lambda_{2,1} = 1 \), \( \Lambda_{2,2} = 1/2 \) and \( \omega_0 = 2\omega_z \). Assuming that the behavior of the effective dimer system is indeed governed by \( a_{1D}^{\text{ad}} \) (i.e., assuming that effective range and other corrections are negligible), the condition \( a_{1D}^{\text{ad}} = 0 \) signals an atom-dimer resonance. Our 3D calculations for the three-particle system with \( P_z = +1 \) show that the ground state energy corresponds to that of a TG gas for \( a_\rho/a_{3D}^{\text{aa}} \approx 1.54 - 1.58 \) and that \( \omega_0 \) equals \( 2\omega_z \) for \( a_\rho/a_{3D}^{\text{aa}} \approx 1.1 - 1.4 \) for \( \lambda = 10 - 20 \), in fairly good agreement with the prediction based on the 1D model, \( a_\rho/a_{3D}^{\text{aa}} = 1.4069 \). The good agreement between our
3D results and those based on the effective molecular 1D Hamiltonian, which is based on a simple empirical parametrization of the effective 1D atom-dimer and dimer-dimer scattering lengths, suggests that the molecular 1D model employed in this work provides a viable and fairly accurate description of the system.

The atom-dimer s-wave resonance of quasi-1D systems found here, \( a_\rho/a^{aa}_{3D} \approx 1.5 \), is somewhat smaller than that found by Mora et al. [141, 142] by solving a set of integral equations for zero-range interactions, \( a_\rho/a^{aa}_{3D} \approx 1.85 \) [148]. The 3D Hamiltonian employed by Mora et al. accounts for the same physics as our 3D Hamiltonian and the determination of the effective 1D atom-dimer scattering length should, at least in principle, be exact [141,142]. It is not clear at present why our empirical molecular 1D Hamiltonian provides a seemingly better description than Mora et al.’s results for \( a^{ad}_{1D} \approx 0 \).

We also analyzed the ground state energy and excitation spectrum for \( N = 4 \). The four-particle 3D energies are harder to converge than the three-particle 3D energies, and comparisons between the full 3D excitation frequencies and the corresponding 1D quantities are accompanied by non-negligible uncertainties. We find that our 3D results are consistent with the dimer-dimer s-wave resonance value predicted by \( H_{1D}^{m} \) [Eq. (4.13) with \( j = dd \), and \( a_{dd} \) given by Eq. (4.11) with \( aa \) replaced by \( dd \)], \( a_\rho/a^{aa}_{3D} = 0.89 \) [148].

### 4.5 Conclusions

In summary, we have presented highly-accurate, microscopic 3D calculations for small highly-elongated Fermi gases with \( N = 2 - 4 \) atoms and reported the energies as a function of the interaction strength, covering the weakly-attractive and weakly-repulsive regimes as well as the strongly-interacting regime. In addition, the dependence of the energies on the aspect ratio was investigated for selected cases. While the role of the aspect ratio is negligible in the weakly-interacting regimes, its role becomes more important in the strongly-interacting regime, possibly indicating that virtual excitations of transverse modes become relevant. The
full 3D energy curves with $P_z = +1$ are reproduced to a good approximation by effective atomic and molecular 1D models whose effective interactions are given by simple analytical expressions that depend on the atom-atom $s$-wave scattering length $a_{3D}^{aa}$, the aspect ratio $\lambda$ and the atom mass $m$. We find that the energies obtained from these effective atomic and molecular 1D Hamiltonian join fairly smoothly in the strongly-interacting regime. Assuming that the effective 1D atom-dimer and dimer-dimer scattering lengths govern the behavior of the highly-elongated system, we deduced the positions of confinement-induced atom-dimer and dimer-dimer resonances from our energies. Whether the effective 1D models also connect fairly smoothly for larger systems is a pressing questions, in particular since the determination of the phase diagram of highly-elongated systems often times relies on strictly 1D treatments.

In the future, it will be interesting to extend the studies presented here to larger population-balanced and population-imbalanced two-component Fermi gases. While some microscopic calculations exist for strictly 1D systems, microscopic 3D treatments that accurately account for the dynamics along the tight and loose confining directions are challenging. Furthermore, it will be interesting to compare the 1D results obtained here for small systems with those obtained within the local density approximation and to extend analogous comparisons to larger systems.

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Chapter 5

Structural properties of harmonically trapped one-dimensional two-component Fermi gases

5.1 Introduction

Chapters 3 and 4 discussed the determination of few-fermion spectra using the explicitly correlated Gaussian technique. This chapter utilizes the explicitly correlated Gaussian technique to determine structural properties of the one-dimensional trapped (2, 1) system with even parity. In particular, we consider the pair distribution function, the radial density and the one-body density matrix [83, 118, 149]. The structural properties provide crucial insights into the system dynamics throughout the BCS-BEC crossover. We determine the momentum distribution function associated with an atom. The momentum distribution function can be determined from the one-body density matrix.

The pair distribution functions and radial densities are discussed in Sec. 5.2. Section 5.3 describes the one-body density matrix and the momentum distribution function. Finally, Sec. 5.4 concludes.
Figure 5.1: Pair distribution function $P_{13}(z)$ for the up-down distance of the energetically lowest-lying state of the $(2, 1)$ system with even parity. The solid, dashed and dash-dotted lines correspond to the pair distribution functions at scattering lengths $a_{1d}^a/a_z = 1.32654$, 0.326537 and 0.126537, respectively. The black dash-dash-dotted line corresponds to the non-interacting case. The calculations are performed using $z_0 = 0.005a_z$. The circles, squares and crosses show the pair distribution functions for the $(1, 1)$ system with zero-range interactions and $a_{1d}^a/a_z = 1.32654$, 0.326537 and 0.126537, respectively. The two-body pair distribution functions are normalized to $1/2$.

### 5.2 Pair distribution function and radial density

The pair distribution function determines the probability of finding two particles at a given separation distance. If the positions of particles $i$ and $j$ are $z_i$ and $z_j$, respectively, and the separation distance is $z_{ij}$, $z_{ij} = z_i - z_j$, then the pair distribution function $P_{ij}(z)$ is defined as

$$P_{ij}(z) = \frac{\int \delta(z - z_{ij})|\Psi_{tot}(z_1, z_2, \cdots, z_N)|^2 dz_1 \cdots dz_N}{\int |\Psi_{tot}(z_1, z_2, \cdots, z_N)|^2 dz_1 \cdots dz_N}. \quad (5.1)$$

The pair distribution function is normalized such that

$$\int_{-\infty}^{\infty} P_{ij}(z) dz = 1. \quad (5.2)$$

Figure 5.1 shows the pair distribution functions $P_{13}(z)$ of the up-down pair for the $(2, 1)$ system with one-dimensional scattering lengths $a_{1d}^a/a_z = 1.32654$ (solid line), 0.326537
Figure 5.2: Pair distribution function $P_{12}(z)$ for the up-up distance of the energetically lowest-lying state of the $(2, 1)$ system with even parity. The solid, dashed and dash-dotted lines correspond to the pair distribution functions at scattering lengths $a_{1D}^{aa}/a_z = 1.32654$, 0.326537 and 0.126537, respectively. The calculations are performed using $z_0 = 0.005a_z$.

(dashed line) and 0.126537 (dash-dotted line). The black dash-dash-dotted line shows the pair distribution for the non-interacting $(2, 1)$ system. The pair distribution function $P_{13}(z)$ is characterized by a two-peak structure. While the width of the peak at small $z$ changes notably with $a_{1D}^{aa}$, the peak at $z \approx 1.5 - 2a_z$ depends comparatively weakly on $a_{1D}^{aa}$. The peak at small $z$ becomes more pronounced with decreasing $a_{1D}^{aa}/a_z$. This can be explained by realizing that the size of the pair decreases with increasing interaction strength and that the system can, for sufficiently small pair size, be thought of as consisting of a dimer and an atom. For small $a_{1D}^{aa}$, the peak at $z \approx 1.5 - 2a_z$ roughly corresponds to the atom-dimer distance.

To investigate the atom-dimer picture quantitatively, we use the two-body wavefunction [58] for the zero-range pseudopotential [see Eq. (4.13)] to calculate the $(1, 1)$ pair distribution functions of the $(1, 1)$ ground state for the same set of scattering lengths as those used in Fig. 5.1. Since the $(2, 1)$ system has two up-down distances while the $(1, 1)$ system has only one up-down distance, the relative importance of the $(1, 1)$ pair is adjusted by normalizing the pair distribution function of the $(1, 1)$ system to $1/2$. Circles, squares and crosses show the $(1, 1)$ pair distribution functions for $a_{1d}^{aa}/a_z = 1.32654$, 0.326537 and 0.126537, respectively.
The radial densities (a) $\rho_1(z)$ of the spin-up particle and (b) $\rho_2(z)$ of the spin-down particle for the ground state with even parity of the $(2, 1)$ system as a function of the distance from the center of the trap. The calculations are performed using $r_0 = 0.005a_z$. The solid, dashed and dash-dotted lines correspond to the radial densities at scattering lengths $a_{1D}^a/a_z = 1.32654, 0.326537$ and $0.126537$, respectively. The black dash-dash-dotted line corresponds to the non-interacting case.

The small $z$ behavior of the pair distribution functions of the $(2, 1)$ and $(1, 1)$ systems agrees well when the dimer is sufficiently small.

Figure 5.2 shows the pair distribution functions $P_{12}(z)$ for the up-up distance of the $(2, 1)$ system with one-dimensional scattering lengths $a_{1D}^a/a_z = 1.32654, 0.326537$ and $0.126537$. The vanishing of the pair distribution function $P_{12}(z)$ at zero separation distance signifies that no two identical particles are allowed to sit on top of each other. The peak at $z \approx 1.5a_z$ shifts towards smaller separation distance with decreasing $a_{1D}^a/a_z$. Although the identical particles are non-interacting, they are being pulled together because of the attractive interactions between the fermions with opposite spins.

In addition, we calculate the radial density $\rho_i(z)$, where $z$ is the distance from the center
of the trap. The radial density gives us the probability of finding the $i^{th}$ particle at the distance $z$ from the trap center. The radial density $\rho_i(z)$ is defined through

$$\rho_i(z) = \frac{\int \delta(z - z_i) |\Psi_{\text{tot}}(z_1, \cdots, z_N)|^2 dz_1 \cdots dz_N}{\int |\Psi_{\text{tot}}(z_1, \cdots, z_N)|^2 dz_1 \cdots dz_N}. \quad (5.3)$$

The radial density is normalized such that

$$\int_{-\infty}^{\infty} \rho_i(z) dz = 1. \quad (5.4)$$

For the (2, 1) system, the radial densities for the spin-up and spin-down particles are different. Figure 5.3 shows the radial density of the spin-up and the spin-down particles for $a_{1D}/a_z = 1.32654$ (solid line), $0.326537$ (dashed line) and $0.126537$ (dash-dotted line). The functions are characterized by one peak on each side of the trap center. The analytically known non-interacting densities are shown by dash-dash-dotted lines in panels (a) and (b) of Fig. 5.3. Since the relative wave function has to be anti-symmetric with respect to the exchange of the identical particles, the $z_{12}$ distance coordinate has to be associated with an odd function. Since the relative wave function considered has even parity, the wave function in the second Jacobi coordinate also has to be odd. For the interacting systems shown in Fig. 5.3, the maxima of the radial densities for the spin-up and spin-down particles is located at finite $z$ values. As $a_{1D}/a_z$ decreases, the density becomes more compact due to the attractive interspecies interactions.

### 5.3 One-body density matrix and momentum distribution function

We calculate the one-body density matrix in coordinate space and its Fourier transform in momentum space. The one-body density matrix $\rho(z, z')$ for the spin-up atoms is defined
Figure 5.4: Contour plot of the one-body density matrix $\rho_1(z,z')$ of the spin-up particle for the ground state of the $(2,1)$ system with scattering length $a_{1D}^{aa}/a_z = 0.326537$. The crosses show the contours corresponding to $0.3a_z^{-1}$ (red), $0.2a_z^{-1}$ (blue) and $0.1a_z^{-1}$ (yellow). The calculations are performed using $z_0 = 0.005a_z$.

through

$$
\rho_1(z, z') = \frac{\int \Psi_{tot}^*(z', z_2, \ldots, z_N) \Psi_{tot}(z, z_2, \ldots, z_N) dz_2 \ldots dz_N}{\int \Psi_{tot}^*(z_1, \ldots, z_N) \Psi_{tot}(z_1, \ldots, z_N) dz_1 \ldots dz_N}. \quad (5.5)
$$

Appendix D provides analytical expressions for the matrix elements for $\rho_1(z, z')$ for the basis functions with even parity [see Eq. (2.66)]. Note that the diagonal element $\rho_1(z, z)$ coincides with the radial density $\rho_1(z)$. Physically, $\rho_1(z, z')$ gives us the probability of finding the particle at the position $z'$ while removing it from the position $z$. Figure 5.4 shows an example, where we plot the contour of the one-body density matrix of the spin-up particle for $a_{1D}^{aa}/a_z = 0.326537$. If we remove the particle at the trap center ($z/a_z = 0$) and move along the $z'$ axis, then $\rho_1(0, z')$ decreases monotonically.

Lastly, we consider the momentum distribution function $n_1(k)$ of the spin-up particle. The momentum distribution function is obtained by Fourier transforming the one-body density matrix,

$$
n_1(k) = \frac{1}{2\pi} \int \rho_1(z, z') \exp\{ik(z - z')\} dz' dz. \quad (5.6)
$$

Appendix D provides analytical expressions for the matrix elements for $n_1(k)$ for the even
parity basis functions. Figure 5.5 shows the momentum distribution function $n_1(k)$ of the spin-up particle for the even parity ground state of the (2, 1) system. The momentum distribution function is maximal at momentum $\hbar k = 0$. The momentum distribution function complements our understanding obtained by analyzing the other structural properties. The tail of the momentum distribution function broadens with increasing interaction strength. Since the particles become more localized with increasing interaction strength, the tails of the corresponding momentum distribution functions extend to larger $k$. For the interacting system in the large $k$ limit, the tail of the momentum distribution function varies approximately as $1/k^4$. The $1/k^4$ dependence of the momentum distribution for large $k$ has been discussed in earlier works in the context of larger two-component Fermi systems [74] and hardcore bosons (Tonks-Girardeau gas) [150] in one-dimensional harmonic traps.
5.4 Conclusions

This chapter discussed selected structural properties of the energetically lowest-lying even parity state of the trapped one-dimensional (2, 1) Fermi gas. We discussed the features of the structural properties as a function of $a_{ld}$. The analytical expressions for the one-body density matrix and momentum distribution function for even parity basis functions are presented in Appendix D. These expressions apply to any number of particles $N$ and can be used to study larger systems.
Chapter 6

Hyperspherical explicitly correlated Gaussian approach for few-body systems with finite angular momentum

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Within the hyperspherical framework, the solution of the time-independent Schrödinger equation for a $n$-particle system is divided into two steps: the solution of a Schrödinger-type equation in the hyperangular degrees of freedom and the solution of a set of coupled Schrödinger-type hyperradial equations. The solutions to the former provide effective potentials and coupling matrix elements that enter into the latter set of equations. This paper
develops a theoretical framework to determine the effective potentials, as well as the associated coupling matrix elements, for few-body systems with finite angular momentum $L = 1$ and negative and positive parity $\Pi$. The hyperangular channel functions are expanded in terms of explicitly correlated Gaussian basis functions, and relatively compact expressions for the matrix elements are derived. The developed formalism is applicable to any $n$; however, for $n \geq 6$, the computational demands are likely beyond present-day computational capabilities. A number of calculations relevant to cold-atom physics are presented, demonstrating that the developed approach provides a computationally efficient means to solving four-body bound and scattering problems with finite angular momentum on powerful desktop computers. Details regarding the implementation are discussed.

6.1 Introduction

Few-body phenomena play important roles across all disciplines of physics, including atomic and molecular physics, chemical physics, nuclear and particle physics, and condensed matter physics. Progress in solving and understanding the quantum mechanical few-body problem has been driven, roughly speaking, by one or more of the following three aspects: (i) Using well-established algorithms, the steady increase of computational resources has made it possible to tackle problems that were impossible to tackle a decade or even just a few years ago. (ii) A number of model systems have been investigated analytically, semi-analytically, or numerically, providing crucial insights into some of the low-energy processes that govern the few-body dynamics. (iii) More efficient numerical schemes that are not only applicable to the three-body problem but also to four- and higher-body problems have been developed.

This paper extends the correlated Gaussian hyperspherical (CGHS) or hyperspherical explicitly correlated Gaussian (HECG) approach [65,83,84]. In earlier work, von Stecher and Greene [65,83,84] considered three- and four-body systems with vanishing angular momentum $L$ and positive parity $\Pi$. Here, we extend the approach to systems with finite angular

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momentum \( L \). Although the overall scheme developed for systems with \( L = 0^+ \) symmetry carries over to systems with finite angular momentum, the determination of compact expressions for the matrix elements associated with finite angular momentum states is significantly more involved than that for states with \( L = 0^+ \) symmetry.

The HECG approach provides an efficient numerical scheme for solving few-body problems. It is a basis-set expansion-type approach, which combines elements of the aspects (i)-(iii) mentioned above. In particular, the use of hyperspherical coordinates \([65,151,152,153,154,155,156,157,158,159,160,161,162]\) within the framework of explicitly correlated Gaussian (ECG) basis functions \([75]\) allows us to take advantage of the machinery developed for bound-state calculations while it at the same time enables us to describe the scattering continuum. Although significant progress has been made \([65,84,163,164,165,166]\), in general, the determination of scattering quantities is significantly more involved than that of bound state quantities, and the four-, five-, and higher-body scattering continua are comparatively poorly understood. Thus, the framework developed in this work for systems with \( 1^- \) and \( 1^+ \) symmetry provides a promising step forward.

The HECG approach is quite general and applicable to a wide range of few-body systems. As an application, we consider the four-particle system consisting of three identical fermions and an impurity whose mass is lighter than that of the majority species. We assume interspecies short-range \( s \)-wave interactions and investigate the system properties of the energetically lowest-lying \( 1^+ \) state as a function of the mass ratio \( \kappa \) between the majority particles and the impurity particle. These finite angular momentum states are interesting since universal four-body bound states have been predicted to exist if the two-body \( s \)-wave scattering length is positive and \( \kappa \gtrsim 9.5 \) \([30]\). Moreover, for \( 13.38 \lesssim \kappa \lesssim 13.61 \), the \((3,1)\) system with \( 1^+ \) symmetry has been predicted to support four-body Efimov states \([57]\); in this mass ratio regime, three-body Efimov states are absent \([15,32,44,45]\). This work determines and interprets the hyperangular eigen value of the \((3,1)\) system with infinitely large interspecies \( s \)-wave scattering length in the limit that the hyperradius is much larger than
the range of the underlying two-body potential.

The remainder of this paper is organized as follows. Section 6.2 introduces the system Hamiltonian and the hyperspherical framework, while Sec. 6.3 introduces the ECG basis functions used to expand the hyperangular channel functions. Section 6.4 discusses the matrix elements, applicable to any \( n \), needed to calculate the effective hyperradial potential curves and associated coupling matrix elements. Details regarding the numerical implementation of the HECG approach and a set of proof-of-principle calculations for the four- and five-particle system are discussed in Sec. 6.5. Section 6.6 applies the HECG framework to the \((3,1)\) system with \(1^+\) symmetry and diverging interspecies \(s\)-wave scattering length for various mass ratios \(\kappa\). Lastly, Sec. 6.7 summarizes and concludes. Details regarding the derivation of and final results for the fixed hyperradius matrix elements are presented in three appendixes. Appendix 6.8 defines a number of auxiliary quantities that depend on the symmetry considered. Appendix 6.9 outlines exemplarily how to derive the matrix elements for the three-body system with \(1^-\) symmetry. Appendix 6.10 summarizes our expressions for a number of quantities that enter into the final equations for the matrix elements; these equations apply to all symmetries considered in this paper.

### 6.2 System Hamiltonian and hyperspherical framework

We consider an \(n\)-particle system with position vectors \(\vec{r}_j\) described by the Hamiltonian \(H\),

\[
H = \sum_{j=1}^{n} -\frac{\hbar^2}{2m_j} \nabla_{\vec{r}_j}^2 + V_{\text{int}},
\]

where \(m_j\) denotes the mass of the \(j\)th particle. The interaction potential \(V_{\text{int}}\) is written as a sum of two-body potentials \(V_{jk}(\vec{r}_{jk})\),

\[
V_{\text{int}} = \sum_{j<k}^{n} V_{jk}(\vec{r}_{jk}),
\]
where \( \vec{r}_{jk} = \vec{r}_j - \vec{r}_k \) (\( r_{jk} = |\vec{r}_{jk}| \)). To separate off the center-of-mass degrees of freedom, we define \( n \) mass-scaled Jacobi vectors \( \vec{\rho}_j \):

\[
\vec{\rho}_j = \sum_{k=1}^{n} T_{jk} \vec{r}_k. \tag{6.3}
\]

The elements \( T_{jk} \) form an \( n \times n \) matrix. The explicit forms for \( n = 3 \) and \( 4 \) read as

\[
T_{n=3} = \begin{pmatrix}
\sqrt{\mu_1} & -\sqrt{\mu_1} & 0 \\
\frac{\sqrt{\mu_2 m_1}}{m_1 + m_2} & \frac{\sqrt{\mu_2 m_2}}{m_1 + m_2} & -\sqrt{\mu_2} \\
m_1/\sqrt{\mu_3} & m_2/\sqrt{\mu_3} & m_3/\sqrt{\mu_3}
\end{pmatrix}, \tag{6.4}
\]

and

\[
T_{n=4} = \begin{pmatrix}
\sqrt{\mu_1} & -\sqrt{\mu_1} & 0 & 0 \\
\frac{\sqrt{\mu_2 m_1}}{m_1 + m_2} & \frac{\sqrt{\mu_2 m_2}}{m_1 + m_2} & -\sqrt{\mu_2} & 0 \\
\frac{\sqrt{\mu_2 m_1}}{m_1 + m_2 + m_3} & \frac{\sqrt{\mu_2 m_2}}{m_1 + m_2 + m_3} & \frac{\sqrt{\mu_2 m_3}}{m_1 + m_2 + m_3} & -\sqrt{\mu_3} \\
m_1/\sqrt{\mu_4} & m_2/\sqrt{\mu_4} & m_3/\sqrt{\mu_4} & m_4/\sqrt{\mu_4}
\end{pmatrix}, \tag{6.5}
\]

where \( \mu_j \) denotes the mass associated with the \( j^{th} \) Jacobi vector,

\[
\mu_j = \frac{\left( \sum_{k=1}^{j} m_k \right) m_{j+1}}{\sum_{k=1}^{j+1} m_k} \quad \text{for } j = 1, \ldots, n - 1 \tag{6.6}
\]

and

\[
\mu_n = \sum_{k=1}^{n} m_k. \tag{6.7}
\]

The generalization to \( n \geq 5 \) is straightforward. By definition, the \( n^{th} \) Jacobi vector coincides with the “mass-scaled” center of mass vector of the \( n \)-particle system. Although the mass-
scaling is not needed to separate off the center of mass motion, the use of mass-scaled Jacobi vectors—as opposed to the use of non-mass-scaled Jacobi vectors—simplifies the derivation of the fixed-$R$ matrix elements for the ECG basis functions (here, $R$ denotes the hyperradius; see below and Sec. 6.4). The Hamiltonian $H$ can now be written as a sum of the relative Hamiltonian $H_{\text{rel}}$ and the center of mass Hamiltonian $H_{\text{cm}},$

$$H = H_{\text{rel}} + H_{\text{cm}}$$  \hfill (6.8)

with

$$H_{\text{rel}} = T_{\text{rel}} + V_{\text{int}},$$ \hfill (6.9)

$$T_{\text{rel}} = \sum_{j=1}^{n-1} \frac{-\hbar^2}{2} \nabla^2_{\vec{\rho}_j}$$ \hfill (6.10)

and

$$H_{\text{cm}} = -\frac{\hbar^2}{2} \nabla^2_{\vec{\rho}_n}.$$ \hfill (6.11)

In the following, we seek solutions to the relative Schrödinger equation

$$H_{\text{rel}} \psi_E = E \psi_E,$$ \hfill (6.12)

i.e., we seek to determine $\psi_E$ and $E$. The energy $E$ can be negative or positive, i.e., we consider both bound state and scattering solutions.

We employ the hyperspherical coordinate approach [65, 154, 155, 162], which has proven to provide critical physical insights that, in some cases, are more difficult or even impossible to unravel in alternative approaches. The solution to the relative Hamiltonian is divided into two steps: \(i\) the solution of a Schrödinger like equation in the hyperangular coordinates
and (ii) the solution of a Schrödinger-like equation in the hyperradial coordinate. More specifically, the idea is to expand the relative wave function \( \psi_E(\vec{\rho}_1, \cdots, \vec{\rho}_{n-1}) \) in terms of a complete set of hyperangular channel functions \( \Phi_\nu(R; \vec{\Omega}) \) that depend parametrically on the hyperradius \( R \) and hyperradial weight functions \( F_\nu E(R) \) [65, 154, 155, 162],

\[
\psi_E = R^{-(3n-4)/2} \sum_\nu F_{\nu E}(R) \Phi_\nu(R; \vec{\Omega}). \tag{6.13}
\]

Here, \( R \) denotes the hyperradius,

\[
R^2 = \sum_{k=1}^{n-1} \rho_k^2, \tag{6.14}
\]

which has, as the components of \( \vec{\rho}_j \), units of “mass\(^{1/2}\) times length”. The mass-scaled hyperradius \( R \) can be related to the “conventional unscaled hyperradius” by pulling out a factor of \( \sqrt{\mu} \), where \( \mu \) is the hyperradial mass. In Eq. (6.13), \( \vec{\Omega} \) collectively denotes the \( 3n - 4 \) hyperangles. The hyperangles \( \vec{\Omega} \) can be defined in different ways (see Sec. 6.4 for the definition employed in this work).

The channel functions \( \Phi_\nu(R; \vec{\Omega}) \) form a complete set in the \((3n-4)\)-dimensional Hilbert space associated with the hyperangular degrees of freedom [65, 154, 155, 162],

\[
\int [\Phi_{\nu'}(R; \vec{\Omega})]^* \Phi_\nu(R; \vec{\Omega}) d^{3n-4} \vec{\Omega} = \delta_{\nu'\nu}. \tag{6.15}
\]

The \( \Phi_\nu(R; \vec{\Omega}) \) are chosen to solve the fixed-\( R \) hyperangular Schrödinger equation

\[
\left[ H_{\text{adia}} + V_{\text{int}}(R; \vec{\Omega}) \right] \Phi_\nu(R; \vec{\Omega}) = U_\nu(R) \Phi_\nu(R; \vec{\Omega}), \tag{6.16}
\]

where

\[
H_{\text{adia}} = T_{\Omega} + V_{\text{eff}}(R) \tag{6.17}
\]
with

\[ T_{\Omega} = \frac{\hbar^2 \Lambda^2}{2R^2} \tag{6.18} \]

and

\[ V_{\text{eff}}(R) = \frac{\hbar^2(3n - 4)(3n - 6)}{8R^2}. \tag{6.19} \]

The grandangular momentum operator \( \Lambda \) [65,161] accounts for the kinetic energy associated with the hyperangular degrees of freedom. For our purposes, it proves advantageous to define \( T_{\Omega} \) through

\[ T_{\Omega} = T_{\text{rel}} - T_R, \tag{6.20} \]

where

\[ T_R = -\frac{\hbar^2}{2} \frac{1}{R^{3n-4}} \frac{\partial}{\partial R} R^{3n-4} \frac{\partial}{\partial R}. \tag{6.21} \]

Inserting Eq. (6.13) into Eq. (6.12), we find that the weight functions \( F_{\nu E}(R) \) and the relative energy \( E \) are obtained by solving a set of coupled hyperradial equations

\[ \left[ -\frac{\hbar^2}{2} \frac{\partial^2}{\partial R^2} + U_\nu(R) \right] F_{\nu E}(R) + V_{c,\nu}(R) = EF_{\nu E}(R), \tag{6.22} \]

where the coupling term \( V_{c,\nu} \) is given by

\[ V_{c,\nu}(R) = \sum_{\nu'} \left[ -2P_{\nu \nu'}(R) \frac{\partial F_{\nu' E}(R)}{\partial R} - Q_{\nu \nu'}(R)F_{\nu' E}(R) \right] \tag{6.23} \]
with
\[
P_{\nu\nu'}(R) = \frac{\hbar^2}{2} \int \left[ \Phi_{\nu}(R; \vec{\Omega}) \right]^* \frac{\partial \Phi_{\nu'}(R; \vec{\Omega})}{\partial R} d^{3n-4} \vec{\Omega}
\] (6.24)

and
\[
Q_{\nu\nu'}(R) = \frac{\hbar^2}{2} \int \left[ \Phi_{\nu}(R; \vec{\Omega}) \right]^* \frac{\partial^2 \Phi_{\nu'}(R; \vec{\Omega})}{\partial R^2} d^{3n-4} \vec{\Omega}.
\] (6.25)

To reiterate, the hyperspherical framework consists of two steps: In the first step, the \((3n - 4)\)-dimensional hyperangular Schrödinger equation is solved, yielding \(U_\nu(R), P_{\nu\nu'}(R)\) and \(Q_{\nu\nu'}(R)\). In the second step, the coupled set of one-dimensional hyperradial equations is solved, yielding \(F_{\nu E}(R)\) and \(E\). This paper focuses primarily on solving the hyperangular Schrödinger equation. Expressions for the relevant matrix elements, valid for any \(n\), are derived and applications to systems with \(n = 4\) are presented.

### 6.3 Functional form of the basis functions

To solve the hyperangular Schrödinger equation, we expand the channel functions \(\Phi_\nu(R; \vec{\Omega})\) for fixed \(R\) in terms of ECG basis functions \(\psi_k(A^{(k)}, \vec{u}_1^{(k)}, \vec{u}_2^{(k)}, \vec{x})|_R\),

\[
\Phi_\nu(R; \vec{\Omega}) = \sum_{k=1}^{N_B} c_k \psi_k(A^{(k)}, \vec{u}_1^{(k)}, \vec{u}_2^{(k)}, \vec{x})|_R,
\] (6.26)

where \(\vec{x}\) collectively denotes the \(3n - 3\) Jacobi vectors, \(\vec{x} = (\vec{p}_1, \cdots, \vec{p}_{n-1})\). In Eq. (6.26), the notation “|\(R\)” indicates that \(\psi_k\) is evaluated at a fixed hyperradius \(R\). The \((n - 1) \times (n - 1)\) dimensional matrices \(A^{(k)}\) are symmetric and positive definite. The \(n(n - 1)/2\) independent elements of \(A^{(k)}\) are treated as variational parameters of the \(k\)th basis function. The elements of the \((n - 1)\)-dimensional vectors \(\vec{u}_1^{(k)}\) and \(\vec{u}_2^{(k)}\) are also treated as variational parameters. The optimization scheme employed to determine the values of these variational parameters
is discussed in Sec. 6.5. In Eq. (6.26), \( S \) denotes an operator that imposes the proper symmetry under exchange of identical particles. For the three-body system consisting of two identical fermions and an impurity, e.g., we have \( S = 1 - P_{12} \). For the four-body system consisting of three identical fermions and an impurity (see Sec. 6.6), we have \( S = 1 - P_{12} - P_{13} - P_{23} + P_{12}P_{23} + P_{13}P_{32} \).

The functional form of the basis functions depends on the \( L^\Pi \) symmetry considered. We consider ECG basis functions of the form \[ \psi(\mathbf{A}, \mathbf{u}_1, \mathbf{u}_2, \mathbf{x}) = N_{L^\Pi} |\mathbf{v}_1|^{l_1} |\mathbf{v}_2|^{l_2} [Y_{l_1}(\hat{v}_1) \otimes Y_{l_2}(\hat{v}_2)]_{LM_L} \exp \left(-\frac{\mathbf{x}^T A \mathbf{x}}{2}\right), \] (6.27)

which can be used to describe states with \( 0^+, 1^+, 1^- \), \( 2^+, \cdots \) symmetry but not states with \( 0^- \) symmetry \[168\]. The three-dimensional vectors \( \mathbf{v}_j, j = 1 \) and 2, are defined through

\[ \mathbf{v}_j = (\mathbf{u}_j)^T \mathbf{x} = \sum_{k=1}^{n-1} u_{j,k} \mathbf{\rho}_k, \] (6.28)

where \( u_{j,k} \) denotes the \( k\)th component of the vector \( \mathbf{u}_j \). We denote the elements of the vector \( \mathbf{v}_j \) by \( v_{j,1} \), \( v_{j,2} \) and \( v_{j,3} \). In Eq. (6.27), the notation \( [Y_{l_1} \otimes Y_{l_2}]_{LM_L} \) indicates that the two spherical harmonics \( Y_{l_j m_j} \) are coupled to a function with total angular momentum \( L \) and projection quantum number \( M_L \), and \( N_{L^\Pi} \) denotes a normalization constant.

In the following, we write the basis functions out for \( M_L = 0 \); in writing the basis functions for a specific symmetry, we choose the normalization constant \( N_{L^\Pi} \) in Eq. (6.27) conveniently. Throughout this paper, we restrict ourselves to states with \( 0^+, 1^- \) and \( 1^+ \) symmetry. The \( L^\Pi = 0^+ \) basis functions, obtained by setting \( l_1 \) and \( l_2 \) to 0, are independent of \( \mathbf{u}_1 \) and \( \mathbf{u}_2 \) (or, equivalently, of \( \mathbf{v}_1 \) and \( \mathbf{v}_2 \)),

\[ \psi(\mathbf{A}, \mathbf{x}) = \exp \left(-\frac{\mathbf{x}^T A \mathbf{x}}{2}\right). \] (6.29)

The \( L^\Pi = 1^- \) basis functions, obtained by setting \( l_1 \) to 1 and \( l_2 \) to 0, depend on \( \mathbf{u}_1 \) but not
on $\vec{u}_2$,

$$
\psi(A, \vec{u}_1, \vec{x}) = 3^{1/2} v_{1,3} \exp \left( -\frac{\vec{x}^T A \vec{x}}{2} \right). \quad (6.30)
$$

Lastly, the $L^\Pi = 1^+$ basis functions, obtained by setting $l_1$ and $l_2$ to 1, depend on both $\vec{u}_1$ and $\vec{u}_2$,

$$
\psi(A, \vec{u}_1, \vec{u}_2, \vec{x}) = \frac{3}{2^{1/2}} (v_{1,2} v_{2,1} - v_{1,1} v_{2,2}) \exp \left( -\frac{\vec{x}^T A \vec{x}}{2} \right). \quad (6.31)
$$

The next section presents relatively compact expressions for the fixed-$R$ matrix elements between two basis functions $\psi = \psi(A, \vec{u}_1, \vec{u}_2, \vec{x})$ and $\psi' = \psi(A', \vec{u}_1', \vec{u}_2', \vec{x})$. Throughout, we assume that $\psi$ and $\psi'$ are characterized by the same $L$, $M_L$ and $\Pi$ quantum numbers. For systems with finite angular momentum, neither the fixed-$R$ overlap matrix element nor the fixed-$R$ matrix elements for $T_\Omega$, $P_{\nu\nu'}$, $Q_{\nu\nu'}$, and $V_{\text{int}}$ have, to the best of our knowledge, been reported in the literature.

### 6.4 Matrix elements for hyperspherical explicitly correlated Gaussians

We introduce the short-hand notation

$$
\langle \psi' | \psi \rangle_R = \int \left[ \psi(A', \vec{u}_1', \vec{u}_2', \vec{x}) \right]^* \psi(A, \vec{u}_1, \vec{u}_2, \vec{x}) d^{3n-4} \vec{\Omega}, \quad (6.32)
$$

$$
\langle \psi' | P | \psi \rangle_R = \frac{\hbar^2}{2} \int \left[ \psi(A', \vec{u}_1', \vec{u}_2', \vec{x}) \right]^* \frac{\partial^2 \psi(A, \vec{u}_1, \vec{u}_2, \vec{x})}{\partial R^2} d^{3n-4} \vec{\Omega}, \quad (6.33)
$$

$$
\langle \psi' | Q | \psi \rangle_R = \frac{\hbar^2}{2} \int \left[ \psi(A', \vec{u}_1', \vec{u}_2', \vec{x}) \right]^* \frac{\partial^2 \psi(A, \vec{u}_1, \vec{u}_2, \vec{x})}{\partial R^2} d^{3n-4} \vec{\Omega}, \quad (6.34)
$$
and

$$
\langle \psi'| T_\Omega | \psi \rangle_R = \frac{1}{2} \int \left[ \psi(A', \vec{u}', \vec{v}, \vec{x}) | R \right]^* \! T_\Omega \psi(A, \vec{u}, \vec{v}, \vec{x}) | R \! \! d^{3n-4} \vec{\Omega} + \frac{1}{2} \int \left[ \psi(A, \vec{u}, \vec{v}, \vec{x}) | R \right]^* \! T_\Omega \psi(A', \vec{u}', \vec{v}, \vec{x}) | R \! \! d^{3n-4} \vec{\Omega}. \tag{6.35}
$$

As in Refs. [65,83,84], Eq. (6.35) explicitly symmetrizes the matrix element associated with the hyperangular kinetic energy.

To evaluate the fixed-$R$ matrix elements defined in Eqs. (6.32)-(6.35), we introduce a new set of coordinates $\vec{y}, \vec{\bar{y}} = (\vec{y}_1, \ldots, \vec{y}_{n-1})$, through $\vec{y} = (U_B)^T \vec{x}$. The matrix $U_B$ is chosen such that the matrix $(U_B)^T B U_B$, where

$$
B = A + A',
$$

is diagonal with diagonal elements $\beta_1, \ldots, \beta_{n-1}$, i.e., such that $\vec{x}^T B \vec{x} = \sum_{j=1}^{n-1} \beta_j \vec{y}_j^2$. It follows that the arguments of the exponentials in the integrals defined in Eqs. (6.32)-(6.35) reduce to quadratic forms. Since the coordinate transformation from $\vec{x}$ to $\vec{y}$ is orthogonal, we have

(i) $R^2 = \sum_{j=1}^{n-1} \vec{y}_j^2$ and (ii) $\int \cdots d^{3(n-1)} \vec{x} = \int \cdots d^{3(n-1)} \vec{y}$.

To perform the integration over $\vec{\Omega}$, we need to specify the $3n - 4$ hyperangles. Following Refs. [65,83,84,169,170], we define $2(n-1)$ angles as the polar and azimuthal angles $\vartheta_j$ and $\varphi_j$ of the $n-1$ vectors $\vec{y}_j$. The remaining $n-2$ hyperangles $\gamma_1, \ldots, \gamma_{n-2}$ are defined in terms of the direction of the $(n-1)$-dimensional vector $\vec{s}$, where $\vec{s} = (y_1, \ldots, y_{n-1})$ and $y_j = |\vec{y}_j|$. 

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Specifically, we write

\begin{align*}
y_1 &= R \sin \gamma_1 \sin \gamma_2 \cdots \sin \gamma_{n-2}, \\
y_2 &= R \cos \gamma_1 \sin \gamma_2 \cdots \sin \gamma_{n-2}, \\
y_3 &= R \cos \gamma_2 \sin \gamma_3 \cdots \sin \gamma_{n-2}, \\
&\quad \cdots, \\
y_{n-2} &= R \cos \gamma_{n-3} \sin \gamma_{n-2}, \\
y_{n-1} &= R \cos \gamma_{n-2},
\end{align*}

(6.37)

where \(\gamma_j \in [0, \pi/2]\). This restriction on the range of the angles ensures that the \(y_j\) are non-negative. Correspondingly, we have [169,170]

\[
\int \cdots d^{3n-4}\bar{\Omega} = \int \cdots \left( \prod_{j=1}^{n-1} d^2\hat{y}_j \right) \left( \prod_{k=1}^{n-2} \sin^{3k-1} \gamma_k \cos^2 \gamma_k d\gamma_k \right),
\]

(6.38)

where \(d^2\hat{y}_j\) denotes the “usual” angular piece of the volume element in spherical coordinates, \(d^2\hat{y}_j = \sin \vartheta_j d\vartheta_j d\varphi_j\).

In general, the expressions for the matrix elements defined in Eqs. (6.32)-(6.35) depend on the functional form of the basis functions \(\psi(A, \vec{u}_1, \vec{u}_2, \vec{x})\) (see Sec. 6.3). For the basis functions defined in Eqs. (6.29)-(6.31), the integrations involving the angles \(\vartheta_j\) and \(\varphi_j\) \((j = 1, \cdots, n-1)\) can be performed analytically, yielding

\[
\langle \psi' | \psi \rangle_R = (4\pi)^{n-1} \int f_o(\vec{s}) \exp \left( -\frac{1}{2} \sum_{j=1}^{n-1} \beta_j y_j^2 \right) \left( \prod_{k=1}^{n-2} \sin^{3k-1} \gamma_k \cos^2 \gamma_k d\gamma_k \right),
\]

(6.39)

\[
\langle \psi' | P | \psi \rangle_R = -\frac{\hbar^2(4\pi)^{n-1}}{2} \int f_P(\vec{s}) \exp \left( -\frac{1}{2} \sum_{j=1}^{n-1} \beta_j y_j^2 \right) \left( \prod_{k=1}^{n-2} \sin^{3k-1} \gamma_k \cos^2 \gamma_k d\gamma_k \right),
\]

(6.40)
\[ \langle \psi' | Q | \psi \rangle |_R = -\frac{\hbar^2 (4\pi)^{n-1}}{2} \int f_Q(\vec{s}) \exp \left(-\frac{1}{2} \sum_{j=1}^{n-1} \beta_j y_j^2 \right) \left( \prod_{k=1}^{n-2} \sin^{3k-1} \gamma_k \cos^2 \gamma_k d \gamma_k \right), \quad (6.41) \]

and

\[ \langle \psi' | T \Omega | \psi \rangle |_R = -\frac{\hbar^2 (4\pi)^{n-1}}{4} \int f_{\Omega}(\vec{s}) \exp \left(-\frac{1}{2} \sum_{j=1}^{n-1} \beta_j y_j^2 \right) \left( \prod_{k=1}^{n-2} \sin^{3k-1} \gamma_k \cos^2 \gamma_k d \gamma_k \right). \quad (6.42) \]

The matrix elements \( \langle \psi' | \psi \rangle |_R \), \( \langle \psi' | P | \psi \rangle |_R \), \( \langle \psi' | Q | \psi \rangle |_R \) and \( \langle \psi' | T \Omega | \psi \rangle |_R \), Eqs. (6.39)-(6.42), have been written such that \( f_o(\vec{s}) \), \( f_P(\vec{s}) \), \( f_Q(\vec{s}) \) and \( f_{\Omega}(\vec{s}) \) have analogous functional forms.

We write

\[ f_o(\vec{s}) = d^{(0)} + \sum_{j=1}^{n-1} \left[ d^{(2)}(j) y_j^2 + d^{(4)}(j) y_j^4 + d^{(6)}(j) y_j^6 \right] + \]

\[ \sum_{k>j=1}^{n-1} \left[ d^{(22)}_{j,k} y_j^2 y_k^2 + d^{(44)}_{j,k} y_j^4 y_k^4 \right] + \]

\[ \sum_{j=1, k=1, k \neq j}^{n-1} \left[ d^{(24)}_{j,k} y_j^2 y_k^4 + d^{(26)}_{j,k} y_j^2 y_k^6 \right] + \]

\[ \sum_{k>j=1; j \neq k}^{n-1} \left[ d^{(222)}_{j,k,i} y_j^2 y_k^2 y_i^2 + d^{(224)}_{j,k,i} y_j^2 y_k^4 y_i^4 \right] + \]

\[ \sum_{k>j=1; j \neq k}^{n-1} \left[ d^{(2222)}_{j,k,l,m} y_j^2 y_k^2 y_l^2 y_m^2 \right]. \quad (6.43) \]

In writing \( f_o(\vec{s}) \), we dropped terms that contain odd powers of \( y_j \) since these terms average to zero when integrating over the remaining hyperangles. The quantities \( f_{p}(\vec{s}) \), \( f_{Q}(\vec{s}) \) and \( f_{\Omega}(\vec{s}) \) are obtained by replacing the \( d \)'s in Eq. (6.43) by \( p \)'s, \( q \)'s and \( b \)'s, respectively. The super- and subscripts of the \( d \), \( p \), \( q \) and \( b \) coefficients indicate the polynomial in the \( y \)'s that the coefficients are associated with. The \( d \), \( p \), \( q \) and \( b \) coefficients depend on the symmetry of the wave function, and are listed in Appendix 6.8 for states with \( L^\Pi = 0^+, 1^- \) and \( 1^+ \) symmetry. It should be noted that, depending on the symmetry and number of particles, a varying number of the \( d \), \( p \), \( q \) and \( b \) coefficients vanish. Appendix 6.9 exemplarily illustrates
how to obtain Eq. (6.39) for the three-body system with $L^{II} = 1^-$ symmetry. We emphasize that Eqs. (6.39)-(6.43), together with the expressions given in Appendix 6.8, apply to any number of particles. For states with $L > 1$ and $L^{II} = 0^-$, the definitions of the $d$, $p$, $q$ and $b$ coefficients contained in $f_o$, $f_P$, $f_Q$ and $f_\Omega$ change and polynomials in the $y$’s of higher power than those considered in Eq. (6.43) may appear.

The integration over $\gamma_1$ in Eqs. (6.39)-(6.42) can also be done analytically. To perform this integration, we recognize that the hyperangle $\gamma_1$ enters into $y_1$ and $y_2$ but not into $y_j$ with $j \geq 3$. Using Eq. (6.37), we write $y_1^2 = R^2 \sin^2 \gamma_1 H(\gamma_2, \ldots, \gamma_{n-2})$ and $y_2^2 = R^2 \cos^2 \gamma_1 H(\gamma_2, \ldots, \gamma_{n-2})$, where $H(\gamma_2, \ldots, \gamma_{n-2}) = 1$ for $n = 3$ and

$$H(\gamma_2, \ldots, \gamma_{n-2}) = \sin^2 \gamma_2 \times \cdots \times \sin^2 \gamma_{n-2}$$

for $n > 3$. In the following, we suppress the dependence of $H$ on the angles $\gamma_j$ ($j \geq 2$) and rewrite $f_o(\vec{s})$ such that the dependence on $\gamma_1$ is “isolated”,

$$f_o(\vec{s}) = sc_{00} + sc_{20} HR^2 \sin^2 \gamma_1 + sc_{02} HR^2 \cos^2 \gamma_1 +$$
$$sc_{40}(HR^2)^2 \sin^4 \gamma_1 + sc_{04}(HR^2)^2 \cos^4 \gamma_1 +$$
$$sc_{60}(HR^2)^3 \sin^6 \gamma_1 + sc_{06}(HR^2)^3 \cos^6 \gamma_1 +$$
$$sc_{22}(HR^2)^2 \sin^2 \gamma_1 \cos^2 \gamma_1 +$$
$$sc_{44}(HR^2)^4 \sin^4 \gamma_1 \cos^4 \gamma_1 +$$
$$sc_{24}(HR^2)^3 \sin^2 \gamma_1 \cos^4 \gamma_1 +$$
$$sc_{42}(HR^2)^3 \sin^4 \gamma_1 \cos^2 \gamma_1 +$$
$$sc_{26}(HR^2)^4 \sin^2 \gamma_1 \cos^6 \gamma_1 +$$
$$sc_{62}(HR^2)^4 \sin^6 \gamma_1 \cos^2 \gamma_1.$$  

(6.45)

The coefficients $sc_{jk}$ depend on the hyperangles $\gamma_l$ with $l \geq 2$ and the $d$ coefficients, and are defined in Appendix 6.10. The subscripts $j$ and $k$ of the $sc$-coefficients denote respectively
the powers of \( \sin \gamma_1 \) and \( \cos \gamma_1 \) that the coefficients \( sc_{jk} \) are associated with. Using Eq. (6.45), we find

\[
\int_0^{\pi/2} f_o(\vec{s}) \exp \left( -\frac{1}{2} \sum_{j=1}^{n-1} \beta_j y_j^2 \right) \sin^2 \gamma_1 \cos^2 \gamma_1 d\gamma_1 = \frac{\pi}{16z} \exp \left( -\frac{1}{4} HR^2 (\beta_1 + \beta_2) - \frac{1}{2} \sum_{j=3}^{n-1} \beta_j y_j^2 \right) \left[ M_1 \frac{I_1(\zeta)}{\zeta} + M_2 \frac{I_2(\zeta)}{\zeta} \right],
\]

(6.46)

where \( I_1 \) and \( I_2 \) denote Bessel functions and \( \zeta \) is defined through

\[
\zeta = \frac{1}{4} (\beta_1 - \beta_2) HR^2.
\]

(6.47)

The quantities \( M_1 \) and \( M_2 \) can be written in terms of \( RH^2 \), \( \zeta \) and the \( sc \)-coefficients; \( M_1 \) and \( M_2 \) depend on \( \gamma_2, \ldots, \gamma_{n-2} \) since \( H \) and the \( sc \)-coefficients depend on these angles. Explicit expressions for \( M_1 \) and \( M_2 \) are given in Appendix 6.10. Using Eq. (6.46) in Eq. (6.39), the matrix element \( \langle \psi | \psi \rangle |_R \) is known fully analytically for \( n = 3 \) and reduces to a \((n-3)\)-dimensional integral for \( n > 3 \). For \( n = 4 \) and 5, the remaining one- and two-dimensional integrations can, as discussed in Sec. 6.5, be performed numerically with high accuracy. Expressions (6.45) and (6.46) also apply to \( f_P(\vec{s}) \), \( f_Q(\vec{s}) \) and \( f_O(\vec{s}) \) if the \( d \) coefficients are replaced by the \( p \), \( q \), and \( b \) coefficients, respectively.

For \( L^{II} = 0^+ \), our results obtained using the above expressions agree with those reported in Refs. [83, 84] for \( n = 3 \) and 4. Motivated by our desire to express the various matrix elements for different number of particles \( n \) and \( L^{II} \) symmetries in a unified framework, we adopted a notation that differs notably from the notation adopted in Refs. [65, 83, 84, 171].

We now turn to the evaluation of the interaction matrix element. We define

\[
\langle \psi' | V_{kl}(\vec{r}_{kl}) | \psi \rangle |_R = \int [\psi(A', \vec{u}_1', \vec{u}_2', \vec{x})]_R^* V_{kl}(\vec{r}_{kl}) \psi(A, \vec{u}_1, \vec{u}_2, \vec{x}) |_R d^{3n-4(\vec{\Omega})}.
\]

(6.48)

If the two-body potential \( V_{kl}(\vec{r}_{kl}) \) is parameterized by a spherically symmetric short-range
Gaussian $V_g(r_{kl})$ with depth $D_{kl}$ and range $r_{0,kl}$,

$$V_g(r_{kl}) = -D_{kl} \exp \left[ -\left( \frac{r_{kl}}{\sqrt{2}r_{0,kl}} \right)^2 \right],$$  \hspace{1cm} (6.49)

then $\langle \psi' | V_g(r_{kl}) | \psi \rangle |_R$ is equivalent to $-D_{kl} \langle \psi' | \psi \rangle |_R$ if $A$ and $A'$ are replaced by $A + W^{(kl)}/(2r_{0,kl}^2)$ and $A' + W^{(kl)}/(2r_{0,kl}^2)$, respectively. Here, the matrix $W^{(kl)}$ is defined as

$$W^{(kl)} = \bar{\omega}^{(kl)} \left( \bar{\omega}^{(kl)} \right)^T,$$  \hspace{1cm} (6.50)

where the vector $\bar{\omega}^{(kl)}$ provides the transformation from the Jacobi coordinates $\bar{x}$ to the interparticle distance vector $\bar{r}_{kl}$,

$$\bar{r}_{kl} = \left( \bar{\omega}^{(kl)} \right)^T \bar{x}.$$  \hspace{1cm} (6.51)

It follows that we can use Eq. (6.39) [see also Eqs. (6.43)-(6.47)] if $\zeta$ is replaced by $\zeta^{(kl)}$ and if the $\beta_j$ are replaced by $\beta_j^{(kl)}$. Similar to $\zeta$, $\zeta^{(kl)}$ is defined through

$$\zeta^{(kl)} = \frac{1}{4} (\beta_1^{(kl)} - \beta_2^{(kl)}) HR^2$$  \hspace{1cm} (6.52)

and the $\beta_j^{(kl)}$ denote the eigenvalues of the matrix $B + W^{(kl)}/r_{0,kl}^2$.

### 6.5 Implementation details of the HECG approach and proof-of-principle applications

As discussed in the previous sections, the determination of the effective hyperradial potential curves and coupling matrix elements requires that the hyperangular Schrödinger equation be solved for several hyperradii $R$. For each fixed $R$, the determination of the linear and non-linear variational parameters is accomplished following approaches very similar to those
employed in the “standard” (non fixed $R$) ECG approach [75]. For a given set of basis functions, and thus for a given set of non-linear variational parameters, the expansion coefficients $c_k$, $k = 1, \cdots, N_b$ [see Eq. (6.26)], are determined by diagonalizing the generalized eigenvalue problem defined by the fixed-$R$ Hamiltonian matrix and the fixed-$R$ overlap matrix. According to the generalized Ritz variational principle, the $N_b$ eigenvalues provide variational upper bounds to the exact eigenvalues of the hyperangular Schrödinger equation.

The non-linear variational parameters are collected in $\mathbf{A}^{(k)}$, $\mathbf{u}_1^{(k)}$ and $\mathbf{u}_2^{(k)}$, where $k = 1, \cdots, N_b$, and determined using the stochastic variational approach [86], i.e., through a trial and error procedure. For concreteness, we consider the situation where we aim to determine the energetically lowest lying hyperangular eigenvalue $U_0(R)$ for a given $R$ value. We start with a small basis set (typically consisting of just one basis function). To add the next basis function, we semi-randomly generate $N_T$ trial basis functions ($N_T$ is typically of the order of a few thousand), yielding $N_T$ trial basis sets. We determine the eigenvalue for each of these trial basis sets and choose the trial basis set that yields the smallest eigenvalue as the new basis set. Following the same selection process, we continue to enlarge the basis set one basis function at a time. This procedure is repeated until the basis set is sufficiently complete and the desired accuracy of the energetically lowest-lying eigenvalue is reached. The optimization of excited states proceeds analogously. If nearly degenerate states exist, it is advantageous to simultaneously minimize the eigenvalues of multiple states.

Since the trial and error procedure “throws out” most of the trial basis functions generated, the resulting basis set is typically comparatively small. For the four-body systems discussed below, e.g., we achieve convergence for $N_b$ of the order of 100. Moreover, we have found that a carefully constructed basis set avoids a number of problems that can arise from the fact that the basis functions are not orthogonal. In particular, the minimization scheme that underlies the trial and error procedure tends to select basis functions that have relatively small overlaps among each other, i.e., that are “fairly linearly independent.” In some cases, however, the trial and error procedure does not fully eliminate numerical issues
arising from the linear dependence of the basis functions. Thus, we add another check and reject a given trial basis function $\psi_T$ if its overlap with one or more of the basis functions already selected is too large, i.e., if the quantity $\langle \psi_T | \psi_k \rangle |_R$ is larger than a preset value $\epsilon$, where we normalize $\psi_T$ and $\psi_k$ such that $\langle \psi_T | \psi_T \rangle |_R = \langle \psi_k | \psi_k \rangle |_R = 1$. We have used $\epsilon = 0.9$ or 0.95 in most of the calculations reported below. A similar criterion is employed in the HECG approach of Ref. [84] and in the standard ECG approach [75].

We now discuss the determination of the non-linear parameters that characterize the basis functions. The selection of the parameters of the matrices $A^{(k)}$ is guided by physical considerations. The fact that the basis functions have to be “compatible” with the value of the hyperradius considered implies that the parameters of the matrices $A^{(k)}$ have to be chosen such that the quantity $\sum_{j<l}^n (d^{(k)}_{jl})^2$ is of the order of $R^2/\mu$. The width parameters $d^{(k)}_{jl}$ are related to the parameter matrix $A^{(k)}$ via

$$\vec{x}^T A^{(k)} \vec{x} = \sum_{j<l} \frac{r_{jl}^2}{(d^{(k)}_{jl})^2}. \quad (6.53)$$

Moreover, the basis functions have to govern the dynamics that occurs at the length scale of the two-body interaction potential. Correspondingly, we consider different types of basis functions: The first type is characterized by all $d^{(k)}_{jl}$ being of the order of $R/(n\sqrt{\mu})$; the second type is characterized by one $d^{(k)}_{jl}$ being of the order of the range of the underlying two-body potential (we use $r_0$ to denote the smallest of the $r_{0,ji}$’s) and all other $d^{(k)}_{jl}$ being of the order of $R/(n\sqrt{\mu})$; the third type is characterized by two $d^{(k)}_{jl}$ being of the order of $r_0$ and all other $d^{(k)}_{jl}$ being of the order of $R/(n\sqrt{\mu})$; and so on. The exact values of the $d^{(k)}_{jl}$ are chosen stochastically from pre-defined parameter windows, which are chosen according to the above considerations. We have found that the convergence of the hyperangular eigenvalues for strongly interacting systems with large $R/(\sqrt{\mu}r_0)$ depends quite sensitively on the choice of the parameter windows. As in Ref. [84], we allow for basis functions with positive and negative widths. The elements of the parameter vectors $\vec{u}_1^{(k)}$ and $\vec{u}_2^{(k)}$ are chosen to lie
between $-1$ and $1$.

The quantity $|\xi|$, [see Eq. (6.47)], takes on large values if $|\beta_1| \gg |\beta_2|$ or $|\beta_2| \gg |\beta_1|$. This situation arises quite frequently if the hyperradius $R$ is much larger than $\sqrt{\mu r_0}$ and causes numerical difficulties when evaluating the Bessel functions. We mitigate these difficulties as follows. For concreteness, we consider the $n = 4$ case and the integral involving $I_1(\xi)$. For large $|\xi|$, we write the integral over the hyperangle $\gamma_2$ [see Eqs. (6.39) and (6.46)] as

$$\int_0^1 \xi^{-1} \exp \left[ -\frac{1}{4} (\beta_1 + \beta_2) R^2 (1 - x^2) - \frac{1}{2} \beta_3 R^2 x^2 \right] \times M_1(x) \frac{I_1(\xi)}{\xi} (1 - x^2)^2 x^2 dx \approx (2\pi)^{-1/2} \times \int_0^1 \xi^{-1} \exp \left[ -\frac{1}{2} \min(\beta_1, \beta_2) R^2 (1 - x^2) - \frac{1}{2} \beta_3 R^2 x^2 \right] \times \left( \frac{1}{|\xi|^{3/2}} - \frac{3}{8|\xi|^{5/2}} - \frac{15}{128|\xi|^{7/2}} - \frac{105}{1024|\xi|^{9/2}} \right) \times M_1(x) (1 - x^2)^2 x^2 dx, \quad (6.54)$$

where $x = \cos \gamma_2$ [implying $H(\gamma_2) = 1 - x^2$]. We use the right hand side of Eq. (6.54) when $|\xi| > 50$. An analogous expansion is done for the part of the integrand that involves $I_2(\xi)$.

Although $M_1$ depends on $x$, the overall behavior of the integrand in Eq. (6.54) is determined by the exponential. In particular, depending on the signs of $\min(\beta_1, \beta_2)$ and $\beta_3$, the integrand can be sharply peaked at $x \approx 0$ or $x \approx 1$. To perform the integration over $x$ (i.e., the integration over the hyperangle $\gamma_2$) numerically, we divide the integral into three sectors: the left, middle, and right sectors. The sector boundaries $x_{\text{mid},1}$ and $x_{\text{mid},2}$ are determined dynamically depending on the behavior of the integrand. The default values are $x_{\text{mid},1} = 0.3$ and $x_{\text{mid},2} = 0.7$. However, if $\beta_3 R^2 > \delta$ or $\min(\beta_1, \beta_2) R^2 < -\delta$, we choose $x_{\text{mid},1} = 1/\sqrt{\max(\beta_3 R^2, |\min(\beta_1, \beta_2)| R^2)}$. Similarly, if $\beta_3 R^2 < -\delta$ or $\min(\beta_1, \beta_2) R^2 > \delta$, we choose $x_{\text{mid},2} = 1 - 1/\sqrt{\max(\beta_3 R^2, \min(\beta_1, \beta_2) R^2)}$. Our calculations reported below use $\delta = 20$. The numerical integration for each sector is performed using a standard Gauss-
Laguerre integration scheme [172]. Typically, we choose the same order $N_{\text{order}}$ for all three sectors [the value of $N_b$ depends on the ratio $R/(\sqrt{\mu r_0})$]. We note that the integration scheme employed has not been optimized carefully and can possibly be refined further. For the five-body system, appropriate generalizations are introduced.

To demonstrate that the developed framework works, we consider four-body systems consisting of two identical spin-up fermions and two identical spin-down fermions. Such systems can be realized experimentally by occupying two different hyperfine states of ultracold atomic $^6\text{Li}$ or $^{40}\text{K}$ samples [12,16,28]. We assume that the identical fermions do not interact. This is a good assumption since $s$-wave interactions between identical fermions are forbidden by the Pauli exclusion principle and $p$-wave interactions are, in most experimental realizations, highly suppressed by the threshold law. Furthermore, we assume that the interspecies interactions have been tuned so that the interspecies free-space $s$-wave scattering length $a_s$ is infinitely large. This regime is referred to as the unitary regime and can be realized experimentally by applying an external magnetic field in the vicinity of a Fano-Feshbach resonance [14]. In our calculations, we describe the interspecies two-body interactions using a Gaussian two-body potential with depth $D$ and range $r_0$ adjusted such that the two-body potential supports a single zero-energy $s$-wave bound state. We calculate the energetically lowest-lying hyperangular eigenvalue $U_0(R)$ for various $\sqrt{\mu r_0}/R$ values.

To present our results, we rewrite $U_0(R)$ in terms of the quantity $s_0(R)$,

$$U_0(R) = \frac{\hbar^2\{[s_0(R)]^2 - 1/4\}}{2R^2}. \tag{6.55}$$

The scaling introduced in Eq. (6.55) is motivated by the fact that $s_0(R)$ becomes independent of $R$ in the non-interacting limit and if $r_0 \ll |a_s|$ [59]. The latter regime is realized if the $s$-wave scattering length diverges and if the quantity $\sqrt{\mu r_0}$ is much smaller than $R$.

Circles in Fig. 6.1 show the quantity $s_{0,\text{unit}}(R)$ for the $(2,2)$ system at unitarity as a function of $\sqrt{\mu r_0}/R$ for (a) $L^\Pi = 0^+$ symmetry, (b) $L^\Pi = 1^-$ symmetry, and (c) $L^\Pi = 1^+$.
symmetry. The basis set extrapolation error is smaller than the symbol size. Dotted lines show a fit to the data using the fitting function $s_{0,\text{unit}}^{\text{ZR}} + c_1 x + c_2 x^2$, where $x = \sqrt{\mu r_0}/R$. The coefficient $s_{0,\text{unit}}^{\text{ZR}}$ is found to be 2.510(1), 4.600(3), and 4.081(3) for $L^\Pi = 0^+$, $1^-$ and $1^+$, respectively. For the $(2, 2)$ system with $0^+$ symmetry, our results compare well with the value 2.5092 obtained by von Stecher and Greene [84] using the same approach as that employed here. For the $(2, 2)$ systems with $1^-$ and $1^+$ symmetry, the $s_{0,\text{unit}}^{\text{ZR}}$ value has, to the best of our knowledge, not been calculated within the hyperspherical coordinate approach. However, using scale invariance arguments [59], $s_{0,\text{unit}}^{\text{ZR}}$ can be extracted from the energy spectrum of the harmonically trapped $(2, 2)$ system. The $s_{0,\text{unit}}^{\text{ZR}}$ values for the zero-range system at unitarity, obtained by analyzing the energy spectrum of the trapped system, are $s_{0,\text{unit}}^{\text{ZR}} = 4.5978$ for $L^\Pi = 1^-$ symmetry and $s_{0,\text{unit}}^{\text{ZR}} = 4.0820$ for $L^\Pi = 1^+$ symmetry [39]. Our values reported above are in very good agreement with these literature values, indicating that the HECG approach is capable of reliably describing strongly-correlated few-body systems with finite angular momentum and positive and negative parity.

To illustrate the convergence of the HECG approach with the number of basis functions, we consider the $(3, 1)$ system with $1^+$ symmetry ($\kappa = 1$ and $1/a_s = 0$). Solid and dashed lines in Fig. 6.2 show the scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ as a function of the number of basis functions $N_b$ for $\sqrt{\mu r_0}/R = 0.02$ and $\sqrt{\mu r_0}/R = 0.005$, respectively. For these calculations, we considered $N_T = 4800$ and 6000 trial functions, respectively, for each new basis function selected. Figure 6.2 shows that the description of the system becomes more challenging as the separation of length scales increases, i.e., as the ratio $\sqrt{\mu r_0}/R$ decreases. Moreover, it can be seen that $s_{0,\text{unit}}(R)$ shows a few “shoulders,” suggesting that there is room to improve upon the selection of the basis functions. Possible improvements may include gradient optimization techniques, which have been successfully employed in electronic structure calculations [173], or a refined trial and error procedure. Nevertheless, the HECG approach in its present implementation yields good convergence for basis sets consisting of around 100 basis functions for the systems under study. The $s_{0,\text{unit}}(R)$ for the largest
Figure 6.1: (Color online) Scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ for the (2, 2) system with $\kappa = 1$ at unitarity. Circles show the scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ as a function of $\sqrt{\mu r_0}/R$ for (a) $L^\Pi = 0^+$ symmetry, (b) $L^\Pi = 1^-$ symmetry, and (c) $L^\Pi = 1^+$ symmetry. The dotted lines show three-parameter fits (using a second-order polynomial). The solid horizontal line in panel (a) shows the result from Ref. [84] for $s^{\text{ZR}_{0,\text{unit}}}$ while the solid horizontal lines in panels (b) and (c) show the results from Ref. [39] for $s^{\text{ZR}_{0,\text{unit}}}$ (see the text for details). The agreement between our results and those from the literature is very good.
Figure 6.2: (Color online) Convergence of the scaled hyperangular eigenvalue with increasing number of basis functions $N_b$. Solid and dashed lines show the scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ as a function of $N_b$ for the $(3,1)$ system with $1^+$ symmetry and $\kappa = 1$ at unitarity for $\sqrt{\mu r_0}/R = 0.02$ and $\sqrt{\mu r_0}/R = 0.005$, respectively. The inset shows a blowup.

The corresponding basis set errors are estimated to be smaller than 0.00002 and 0.0002, respectively. The dependence of $s_{0,\text{unit}}(R)$ on $r_0$ is relatively weak for the $(3,1)$ system with $1^+$ symmetry and we find the extrapolated value $s_{0,\text{unit}}^{\text{ZR}} = 4.0820(3)$. This result agrees well with the value of $s_{0,\text{unit}}^{\text{ZR}} = 4.0819$ extracted from the trap energies [39].

Circles in Fig. 6.3 show the scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ for the $(3,1)$ system with $\sqrt{\mu r_0}/R = 0.005$ and $1^+$ symmetry ($\kappa = 1$ and $1/a_s = 0$) as a function of the order $N_{\text{order}}$ used to perform the numerical integration over the hyperangle $\gamma_2$. As discussed above, the numerical integral is divided dynamically into three sectors, yielding a total of $3N_{\text{order}}$ integration points. For the calculations shown in Fig. 6.3, we used a basis set with $N_b = 95$. Figure 6.3 shows that the scaled hyperangular eigenvalue $s_{0,\text{unit}}(R)$ is, for the system considered, accurate to better than 0.1% for $N_{\text{order}} \gtrsim 60$. It is important to note, though, that while $N_{\text{order}} = 60$ yields quite accurate results, $N_{\text{order}} = 50$ yields completely unreliable results for the parameter combination and basis set considered. In practice, we perform the optimization of the basis set for fixed $N_{\text{order}}$. At the end of the construction of the basis
Figure 6.3: (Color online) Convergence of the scaled hyperangular eigenvalue with increasing number of grid points. The circles show the scaled hyperangular eigenvalue $s_{0, \text{unit}}(R)$, calculated for a basis set consisting of $N_b = 95$ basis functions, as a function of the order $N_{\text{order}}$ per sector used to perform the numerical integration over the angle $\gamma_2$; as discussed in the text, the numerical integration is divided into three sectors. For $N_{\text{order}} = 50$ (not shown), the numerical integration breaks down (it yields a value that deviates by 10% from the exact value). The calculations are performed for the $(3, 1)$ system with $1^+$ symmetry, $1/a_s = 0$, $\kappa = 1$ and $\sqrt{\mu r_0}/R = 0.005$. The dotted line is shown as a guide to the eye.

As pointed out in Sec. 6.4, the expressions for the matrix elements presented in the Appendixes apply to any number of particles. To explicitly confirm this, we performed calculations for the non-interacting five-body systems with $0^+$, $1^-$, and $1^+$ symmetry and found hyperangular eigenvalues consistent with what is expected. Since the matrix elements for the two-body interactions are of the same form as those for the overlaps, treatment of the non-interacting systems suffices for testing the analytical expressions presented in this paper. The computational demands will, of course, increase as the interactions are turned on. Assessing the performance of the outlined formalism for strongly correlated five-body systems is beyond the scope of this paper.
Figure 6.4: (Color online) $s_{0, \text{unit}}(R)$ as a function of $\sqrt{\mu} r_0 / R$ for the $(3, 1)$ system with $1^+$ symmetry at unitarity for $\kappa = 1$ (circles), $\kappa = 4$ (pluses), $\kappa = 8$ (squares), $\kappa = 9.5$ (diamonds), and $\kappa = 10$ (triangles). Dotted lines show three-parameter fits to the data.

6.6 $(3, 1)$ system with $1^+$ symmetry

This section considers the $(3, 1)$ system with $1^+$ symmetry at unitarity for various mass ratios. The $s_{0, \text{unit}}^{ZR}$ value for these systems has been determined previously [116,117] by investigating the $(3, 1)$ system under spherically symmetric harmonic confinement using the stochastic variational approach combined with geminal-type basis functions, which are neither characterized by good angular momentum and corresponding projection quantum numbers nor good parity. As a result, the earlier calculations were restricted to comparatively large $r_0/a_{\text{ho}}$ values, where $a_{\text{ho}}$ denotes the harmonic oscillator length of the external confinement. The present work determines $s_{0, \text{unit}}^{ZR}$ for various mass ratios $\kappa$ by employing the HECG approach.

For comparative purposes, we repeat the trap calculations using the standard ECG approach; however, instead of using geminal type basis functions, we employ basis functions which are characterized by good $L$, $M_L$, and $\Pi$ quantum numbers, thereby allowing us to reduce the basis-set extrapolation error and to treat systems with smaller $r_0/a_{\text{ho}}$ than considered earlier.

Symbols in Fig. 6.4 show $s_{0, \text{unit}}(R)$ [see Eq. (6.55)], obtained by the HECG approach, as a function of $\sqrt{\mu} r_0 / R$ for $\kappa = 1, 4, 8, 9.5$, and 10. Dotted lines show three-parameter
Table 6.1: The first column shows the mass ratio \( \kappa \). Columns 2 and 3 show the \( s_{0,\text{unit}}^{Z\!R} \) values for the \((3,1)\) system with \( 1^+ \) symmetry at unitarity obtained by the HECG approach and from the extrapolated zero-range energies of the trapped system (see the text for details). For comparison, column 4 shows the results from Ref. [117]. The \( \kappa = 1 \) entry in the third column is taken from Ref. [39].

<table>
<thead>
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<th>( \kappa )</th>
<th>( s_{0,\text{unit}}^{Z!R} ) (HECG)</th>
<th>( s_{0,\text{unit}}^{Z!R} ) (trap, this work)</th>
<th>( s_{0,\text{unit}}^{Z!R} ) (trap, Ref. [117])</th>
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<td>2/5</td>
<td>4.2735(1)</td>
<td></td>
<td></td>
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<tr>
<td>3/5</td>
<td>4.2000(1)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>4/5</td>
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<td></td>
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</tr>
<tr>
<td>1</td>
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<td>4.0819(1)</td>
<td>4.08</td>
</tr>
<tr>
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<tr>
<td>3</td>
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<tr>
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fits. The resulting \( s_{0,\text{unit}}^{Z\!R} \) values are summarized in column 2 of Table 6.1. The errorbars are primarily due to the extrapolation to the \( \sqrt{\mu} r_0 / R \to 0 \) limit and only secondarily due to the basis set extrapolation error of the \( s_{0,\text{unit}}(R) \) for each \( R \). Figure 6.4 suggests that the leading-order correction to \( s_{0,\text{unit}}^{Z\!R} \) is proportional to \( 1/R \) for the \( \kappa \) values considered (\( \kappa > 1 \)). This is in agreement with what has been found analytically for the \((2,1)\) system with \( 1^- \) symmetry [43]. Figure 6.4 also shows that the range dependence of \( s_{0,\text{unit}}(R) \) increases with increasing \( \kappa \). For larger \( \kappa \), the range dependence appears to be more complicated and the determination of the corresponding \( s_{0,\text{unit}}(R) \) values is beyond the scope of this paper.

Circles in Fig. 6.5 show the \( s_{0,\text{unit}}^{Z\!R} \) values obtained from the HECG approach as a function of \( \kappa \). For comparison, crosses show the \( s_{0,\text{unit}}^{Z\!R} \) values obtained by extrapolating the finite-range energies of the trapped system to the \( r_0 / a_{ho} \to 0 \) limit. These \( s_{0,\text{unit}}^{Z\!R} \) values are reported in column 3 of Table 6.1 and are calculated following the procedure discussed in Ref. [39] for equal masses. The agreement between the two sets of calculations is very good. Column 4 of Table 6.1 shows the \( s_{0,\text{unit}}^{Z\!R} \) values obtained earlier [117]; these earlier calculations were
Figure 6.5: (Color online) $s_{0,\text{unit}}^{\text{ZR}}$ as a function of $\kappa$ for the (3, 1) system with 1$^+$ symmetry at unitarity. The circles show the $s_{0,\text{unit}}^{\text{ZR}}$ values determined using the HECG approach while the crosses show the $s_{0,\text{unit}}^{\text{ZR}}$ values determined by extrapolating the trap energies obtained by the standard ECG approach to the zero-range limit. The errorbars increase with increasing $\kappa$. The agreement between the $s_{0,\text{unit}}^{\text{ZR}}$ values determined by the two different approaches is very good. The main panel and inset show the same data on different scales; the main panel and inset use respectively logarithmic and linear scales for $\kappa$.

Following the discussion of Refs. [32, 59, 116, 117, 174], the $s_{0,\text{unit}}^{\text{ZR}}$ value indicates whether the system behaves universal or not. For two-component Fermi gases with zero-range $s$-wave interactions, e.g., the $s_{0,\text{unit}}^{\text{ZR}}$ value is larger than 1 and, correspondingly, the system properties are fully determined by $a_s$. If $s_{0,\text{unit}}^{\text{ZR}} < 1$, the solution to the hyperradial Schrödinger equation, which is a second order differential equation, can—at least in principle—contain contributions of the “regular” and “irregular” solutions. If the irregular solution contributes, the system is said to behave non-universal since its properties depend not only on the $s$-wave scattering length but additionally on a second parameter. Applying these arguments to the (3, 1) system with 1$^+$ symmetry and using that $s_{0,\text{unit}}^{\text{ZR}} > 1$ for the mass ratios considered, the present study supports the finding that the four-body bound states found in Ref. [30] for $\kappa \gtrsim 9.5$ and positive $s$-wave scattering length are universal.
6.7 Conclusions

This paper extended the HECG approach, which had previously been formulated for and applied to three- and four-particle systems with $L^\Pi = 0^+$ symmetry [65, 83, 84], to states with $1^-$ and $1^+$ symmetry. The developed framework is applicable to systems with any $n$; realistically, though, applications in the not too distant future will likely be limited to systems with up to five particles. This paper emphasized a unified formulation for solving the hyperangular Schrödinger equation. In particular, many of the resulting equations apply to any particle number and $L^\Pi$ symmetry, suggesting a numerical implementation in which most subroutines can be used for any particle number $n$ and any $L^\Pi$ symmetry; only a few subroutines specific to the values of $n$, $L$, and $\Pi$ are needed.

As a first application, we considered the $(2, 2)$ and $(3, 1)$ systems at unitarity. In particular, we solved the hyperangular Schrödinger equation for the energetically lowest-lying eigenvalue in the small-$\sqrt{\mu r_0}/R$ regime and extracted the corresponding $s_{0,\text{unit}}^{ZR}$ values. Our results are in very good agreement with results from the literature and with results determined by an alternative approach. The $s_{0,\text{unit}}^{ZR}$ values for the $(3, 1)$ system at unitarity with $1^+$ symmetry consisting of three heavy identical fermions and one light impurity particle are relevant to the $(3, 1)$ system with positive $a_s$. In particular, the results obtained in this paper lend strong support that the bound states of the $(3, 1)$ system with positive $s$-wave scattering length found in Ref. [30] are universal, i.e., fully determined by $a_s$. While we were able to reliably describe four-body systems for which the hyperradius $R$ is 200 times larger than the scaled range $\sqrt{\mu r_0}$ of the two-body potential, pushing this ratio to much larger values may be challenging.

In the future, it will be interesting to combine, as done in Refs. [65, 83, 84], the developed framework with a standard $R$-matrix approach and to describe the scattering properties of four-particle systems with finite angular momentum. The generalization of the developed formalism to states with other $L^\Pi$ symmetries, which amounts to determining the corresponding $d$, $b$, $p$, and $q$ coefficients, is tedious but straightforward. Other possible extensions...
include the generalization of the approach to cold-atom systems in a wave guide geometry.

6.8 Appendix A: Definition of (symmetry-dependent) auxiliary quantities

We first introduce a number of auxiliary quantities and then define quantities specific to the basis functions with $L^\Pi = 0^+, 1^-$ and $1^+$ symmetry.

The matrix $S$ is defined as

$$S = A_B A_B' + A_B' A_B,$$  \hspace{1cm} (6.56)

where

$$A_B = (U_B)^T A U_B$$  \hspace{1cm} (6.57)

and

$$A_B' = (U_B)^T A' U_B.$$  \hspace{1cm} (6.58)

Similarly, we define

$$B_B = A_B + A_B'.$$  \hspace{1cm} (6.59)

We define the vectors $\vec{u}_{j,B}$ and $\vec{u}_{j,B}'$ ($j = 1$ and 2),

$$\vec{u}_{j,B} = (U_B)^T \vec{u}_j$$  \hspace{1cm} (6.60)
and

\[ u'_{j,B} = (U_B) \cdot u'_j, \] (6.61)

Lastly, we define

\[ a(j, k) = u_{1,B}(j)u'_{1,B}(k), \] (6.62)

\[ \bar{a}(j, k) = u_{2,B}(j)u'_{2,B}(k), \] (6.63)

\[ g(j, k, l) = a(j, j)\bar{a}(l, k) + a(l, k)\bar{a}(j, j) - a(l, j)\bar{a}(j, k) - a(j, k)\bar{a}(l, j), \] (6.64)

\[ \bar{g}(j, k, l) = g(j, l, k), \] (6.65)

\[ h(j, k, l) = g(l, j, k) + \bar{g}(l, j, k), \] (6.66)

\[ F(j, k, l, m) = a(j, k)\bar{a}(l, m) + a(k, j)\bar{a}(l, m) + a(j, k)\bar{a}(m, l) + a(k, j)\bar{a}(m, l), \] (6.67)

\[ G(j, k, l, m) = a(j, l)\bar{a}(m, k) + a(j, m)\bar{a}(l, k) + a(k, l)\bar{a}(m, j) + a(k, m)\bar{a}(l, j), \] (6.68)

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\[ f(j,k,l,m) = F(j,k,l,m) + F(l,m,j,k) - G(j,k,l,m) - G(l,m,j,k). \] (6.69)

Sections 6.8.1-6.8.3 give explicit expressions for the \(d, p, q,\) and \(b\) coefficients for the basis functions with \(0^+, 1^-\) and \(1^+\) symmetry, respectively. In what follows, the elements of the vector \(\vec{u}_{j,B}\) are denoted by \(u_{j,B}(k), k = 1, \cdots, n - 1;\) the same notation is adopted for the elements of other vectors. The elements of the matrix \(S\) are denoted by \(S(k,l)\) with \(k\) and \(l = 1, \cdots, n - 1;\) the same notation is adopted for the elements of other matrices.

### 6.8.1 \(0^+\) symmetry

The only non-zero \(d\) coefficient is

\[ d^{(0)} = 1. \] (6.70)

The only non-zero \(p\) coefficient is

\[ p_j^{(2)} = \Delta_B(j, j)R^{-1}. \] (6.71)

The non-zero \(q\) coefficients are

\[ q_j^{(2)} = R^{-1}p_j^{(2)}, \] (6.72)

\[ q_j^{(4)} = -\Delta_B^2(j, j)R^{-2}; \] (6.73)
and

\[ q^{(22)}_{j,k} = - \left[ 2A_B(j,j)A_B(k,k) + \frac{4}{3}A_B^2(j,k) \right] R^{-2}. \quad (6.74) \]

Here, \( A_B^2(j,k) \) denotes the square of the matrix element \( A_B(j,k) \).

The non-zero \( b \) coefficients are \( b^{(4)}_j \) and \( b^{(22)}_{j,k} \):

\[ b^{(0)}_j = -3 \text{Tr}(B_B), \quad (6.75) \]

\[ b^{(2)}_j = \beta^2_j - S(j,j) + (3n - 3)\beta_j R^{-2}, \quad (6.76) \]

\[ b^{(4)}_j = \left[ -\beta^2_j + 2A_B(j,j)A'_B(j,j) \right] R^{-2}, \quad (6.77) \]

and

\[ b^{(22)}_{j,k} = -2\beta_j \beta_k R^{-2} + 2A_B(j,j)A'_B(k,k)R^{-2} + \]
\[ 2A_B(k,k)A'_B(j,j)R^{-2} + \frac{8}{3}A_B(j,k)A'_B(j,k)R^{-2}. \quad (6.78) \]

### 6.8.2 \( 1^- \) symmetry

The only non-zero \( d \) coefficient is

\[ d^{(2)}_j = a(j,j). \quad (6.79) \]

The non-zero \( p \) coefficients are

\[ p^{(2)}_j = -a(j,j)R^{-1}, \quad (6.80) \]
\[ p_j^{(4)} = A_B(j,j) a(j,j) R^{-1}, \] (6.81)

and

\[ p_{j,k}^{(22)} = A_B(j,j) a(k,k) R^{-1} + A_B(k,k) a(j,j) R^{-1} + \]
\[ \frac{2}{3} A_B(j,k) [a(j,k) + a(k,j)] R^{-1}. \] (6.82)

The non-zero \( q \) coefficients are

\[ q_j^{(4)} = 3 R^{-1} p_j^{(4)}, \] (6.83)

\[ q_{j,k}^{(22)} = 3 R^{-1} p_{j,k}^{(22)}, \] (6.84)

\[ q_j^{(6)} = -A_B^2(j,j) a(j,j) R^{-2}, \] (6.85)

\[ q_{j,k}^{(24)} = -A_B^2(k,k) a(j,j) R^{-2} - 2 A_B(j,j) A_B(k,k) a(k,k) R^{-2} - \]
\[ \frac{4}{3} A_B^2(j,k) a(k,k) R^{-2} - \frac{4}{3} A_B(k,k) A_B(j,k) [a(j,k) + a(k,j)] R^{-2}. \] (6.86)
and

\[
q_{j,k,l}^{(22)} = \left[ -2A_B(j,j)A_B(k,k)a(l,l) - \frac{4}{3}A_B^2(j,k)a(l,l) \right] R^{-2} + \left[ -\frac{4}{3}A_B(j,k)A_B(l,l) - \frac{8}{9}A_B(j,l)A_B(k,l) \right] \times [a(j,k) + a(k,j)] R^{-2}. \tag{6.87}
\]

The non-zero \(b\) coefficients are

\[
b_j^{(2)} = -2(3n - 4)a(j,j)R^{-2} - \\
2 \sum_{k=1}^{n-1} [A_B(j,k)a(k,j) + A'_B(j,k)a(j,k)] - 3\text{Tr}(B_B)a(j,j), \tag{6.88}
\]

\[
b_j^{(4)} = [\beta_j^2 - S(j,j) + (3n - 1)\beta_j R^{-2}] a(j,j), \tag{6.89}
\]

\[
b_j^{(6)} = [-\beta_j^2 + 2A_B(j,j)A'_B(j,j)] a(j,j) R^{-2}, \tag{6.90}
\]

\[
b_{j,k}^{(22)} = [\beta_j^2 - S(j,j) + (3n - 1)\beta_j R^{-2}] a(k,k) + \\
[\beta_k^2 - S(k,k) + (3n - 1)\beta_k R^{-2}] a(j,j) - \\
\frac{1}{3} [S(j,k) + S(k,j)] [a(j,k) + a(k,j)], \tag{6.91}
\]
\[ b_{j,k}^{(24)} = \left[ -\beta_k^2 + 2A_B(k,k)A'_B(k,k) \right] a(j,j)R^{-2} + \\
\left[ -2\beta_j\beta_k + 2A_B(j,j)A'_B(k,k) + 2A_B(k,k)A'_B(j,j) + \frac{8}{3}A_B(j,k)A'_B(j,k) \right] \times \\
a(k,k)R^{-2} + \\
\frac{4}{3} \left[ A_B(j,k)A'_B(k,k) + A_B(k,k)A'_B(j,k) \right] \times \\
\left[ a(j,k) + a(k,j) \right] R^{-2} \]  
\( (6.92) \)

and

\[ b_{j,k,l}^{(222)} = \left[ -2\beta_j\beta_k + 2A_B(j,j)A'_B(k,k) + 2A_B(k,k)A'_B(j,j) + \frac{8}{3}A_B(j,k)A'_B(j,k) \right] \times \\
a(l,l)R^{-2} + \\
\frac{4}{3} \left[ A_B(j,k)A'_B(l,l) + A_B(l,l)A'_B(j,k) \right] \times \\
\left[ a(j,k) + a(k,j) \right] R^{-2} + \\
\frac{8}{9} \left[ A_B(j,l)A'_B(k,l) + A_B(k,l)A'_B(j,l) \right] \times \\
\left[ a(j,k) + a(k,j) \right] R^{-2}. \]  
\( (6.93) \)

### 6.8.3 \( 1^+ \) symmetry

The only non-zero \( d \) coefficient is

\[ d_{j,k}^{(22)} = a(j,j)\bar{a}(k,k) + a(k,k)\bar{a}(j,j) - \\
a(j,k)\bar{a}(k,j) - a(k,j)\bar{a}(j,k). \]  
\( (6.94) \)

The non-zero \( p \) coefficients are

\[ p_{j,k}^{(22)} = -2R^{-1}d_{j,k}^{(22)}. \]  
\( (6.95) \)
\[ p_{j,k}^{(24)} = R^{-1} d_{j,k}^{(22)} A_B(k,k), \quad (6.96) \]

and

\[ p_{j,k,l}^{(222)} = R^{-1} d_{j,k}^{(22)} A_B(l,l) + \frac{2}{3} R^{-1} A_B(j,k)h(j,k,l). \quad (6.97) \]

The non-zero \( q \) coefficients are

\[ q_{j,k}^{(22)} = R^{-1} p_{j,k}^{(22)}, \quad (6.98) \]

\[ q_{j,k}^{(24)} = 5 R^{-1} p_{j,k}^{(24)}, \quad (6.99) \]

\[ q_{j,k,l}^{(222)} = 5 R^{-1} p_{j,k,l}^{(222)}, \quad (6.100) \]

\[ q_{j,k}^{(26)} = -d_{j,k}^{(22)} A_B^2(k,k)R^{-2}, \quad (6.101) \]

\[ q_{j,k}^{(44)} = -2d_{j,k}^{(22)} A_B(j,j) A_B(k,k)R^{-2} - \frac{4}{5} d_{j,k}^{(22)} A_B^2(j,k)R^{-2}, \quad (6.102) \]
\[ q^{(224)}_{j,k,l} = - \left[ \mathcal{A}_B(j,j) \mathcal{A}_B(l,l) + \frac{2}{3} \mathcal{A}_B^2(j,l) \right] 2R^{-2}d^{(22)}_{k,l} - \\
\left[ \mathcal{A}_B(k,k) \mathcal{A}_B(l,l) + \frac{2}{3} \mathcal{A}_B^2(k,l) \right] 2R^{-2}d^{(22)}_{j,l} - \\
\mathcal{A}_B^2(l,l) R^{-2}d^{(22)}_{j,k} - \\
\frac{4}{3} \left[ \mathcal{A}_B(j,k) \mathcal{A}_B(l,l) h(j,k,l) + \right. \\
\mathcal{A}_B(j,l) \mathcal{A}_B(l,l) h(j,l,k) + \\
\left. \mathcal{A}_B(k,l) \mathcal{A}_B(l,l) h(k,l,j) \right] R^{-2}, \]  
(6.103)

and

\[ q^{(2222)}_{j,k,l,m} = - \left[ 2\mathcal{A}_B(l,l) \mathcal{A}_B(m,m) + \frac{4}{3} \mathcal{A}_B^2(l,m) \right] R^{-2}d^{(22)}_{j,k} - \\
\left[ 2\mathcal{A}_B(j,j) \mathcal{A}_B(k,k) + \frac{4}{3} \mathcal{A}_B^2(j,k) \right] R^{-2}d^{(22)}_{l,m} - \\
\frac{4}{3} \left[ \mathcal{A}_B(j,k) \mathcal{A}_B(m,m) h(j,k,l) + \right. \\
\mathcal{A}_B(j,k) \mathcal{A}_B(l,l) h(j,k,m) \right] R^{-2} - \\
\frac{4}{3} \left[ \mathcal{A}_B(l,m) \mathcal{A}_B(k,k) h(l,m,j) + \right. \\
\mathcal{A}_B(l,m) \mathcal{A}_B(j,j) h(l,m,k) \right] R^{-2} - \\
\frac{8}{9} \left[ \mathcal{A}_B(l,k) \mathcal{A}_B(k,m) h(l,m,j) + \right. \\
\mathcal{A}_B(l,j) \mathcal{A}_B(j,m) h(l,m,k) \right] R^{-2} - \\
\frac{8}{9} \left[ \mathcal{A}_B(j,m) \mathcal{A}_B(m,k) h(j,k,l) + \right. \\
\mathcal{A}_B(j,l) \mathcal{A}_B(l,k) h(j,k,m) \right] R^{-2} - \\
\frac{8}{9} \left[ \mathcal{A}_B(j,k) \mathcal{A}_B(l,m) \right] f(j,k,l,m) R^{-2}. \]  
(6.104)
The non-zero $b$ coefficients are

\begin{align*}
b_{j,k}^{(22)} &= -5 \text{Tr}(B_B) d_{j,k}^{(22)} - 4(3n - 3) R^{-2} d_{j,k}^{(22)} - \\
&\quad 2 \sum_{l \neq j,k}^{n-1} \left[ A_B(j, l) g(k, j, l) + A_B'(j, l) \bar{g}(k, j, l) + A_B(k, l) g(j, k, l) + A_B'(k, l) \bar{g}(j, k, l) - \beta_l d_{j,k}^{(22)} \right], \\
&= [\beta_j - \mathcal{S}(j, k)] d_{j,k}^{(22)} + \beta_k (3n + 1) R^{-2} d_{j,k}^{(22)}, \quad (6.105) \\

b_{j,k}^{(24)} &= [\beta^2_k - \mathcal{S}(k, k)] d_{j,k}^{(22)} + \beta_k (3n + 1) R^{-2} d_{j,k}^{(22)}, \quad (6.106) \\

b_{j,k,l}^{(222)} &= [\beta^2_l - \mathcal{S}(l, l)] d_{j,k}^{(22)} - \\
&\quad \frac{2}{3} h(j, k, l) \mathcal{S}(j, k) + \beta_l (3n + 1) R^{-2} d_{j,k}^{(22)}, \quad (6.107) \\

b_{j,k}^{(44)} &= [- \beta_j \beta_k + A_B(j, j) A_B'(k, k) + \\
&\quad A_B(k, k) A_B'(j, j) + \frac{4}{5} A_B(j, k) A_B'(j, k)] 2 R^{-2} d_{j,k}^{(22)}, \quad (6.108) \\

b_{j,k}^{(26)} &= [- \beta^2_k + 2 A_B(k, k) A_B'(k, k)] R^{-2} d_{j,k}^{(22)}, \quad (6.109)
\end{align*}
\[ b_{j,k,l}^{(224)} = \left[ -\beta_j \beta_l + A_B(j, j) \dot{A}'_B(l, l) + A_B(l, l) \dot{A}'_B(j, j) + \right. \\
\left. \frac{4}{3} A_B(j, l) \dot{A}'_B(j, l) \right] 2R^{-2} d_{k,l}^{(22)} + \\
\left[ -\beta_k \beta_l + A_B(k, k) \dot{A}'_B(l, l) + A_B(l, l) \dot{A}'_B(k, k) + \right. \\
\left. \frac{4}{3} A_B(k, l) \dot{A}'_B(k, l) \right] 2R^{-2} d_{j,l}^{(22)} + \\
\left[ -\beta_l^2 + 2 A_B(l, l) \dot{A}'_B(l, l) \right] R^{-2} d_{j,k}^{(22)} - \\
\frac{4}{3} \left[ A_B(j, k) \dot{A}_B(l, l) + A'_B(j, k) A'_B(l, l) \right] R^{-2} h(j, k, l) - \\
\frac{4}{3} \left[ A_B(j, l) \dot{A}_B(l, l) + A'_B(j, l) A'_B(l, l) \right] R^{-2} h(j, l, k) - \\
\frac{4}{3} \left[ A_B(k, l) \dot{A}_B(l, l) + A'_B(k, l) A'_B(l, l) \right] R^{-2} h(k, l, j), \right. \]

(6.110)
and

$$b_{j,k,l,m}^{(2222)} =$$

$$- \left\{ 2 A_B(l, l) A_B(m, m) + 2 A'_B(l, l) A'_B(m, m) + \right.$$

$$\frac{4}{3} \left[ A_B^2(l, m) + A_B^2(l, m) \right] R^{-2} d_{jk}^{(22)} -$$

$$\left\{ 2 A_B(j, j) A_B(k, k) + 2 A'_B(j, j) A'_B(k, k) + \right.$$

$$\frac{4}{3} \left[ A_B^2(j, k) + A_B^2(j, k) \right] R^{-2} d_{lm}^{(22)} -$$

$$\frac{4}{3} \left[ A_B(j, k) A_B(m, m) + A'_B(j, k) A'_B(m, m) \right] \times$$

$$h(j, k, l) R^{-2} -$$

$$\frac{4}{3} \left[ A_B(j, k) A_B(l, l) + A'_B(j, k) A'_B(l, l) \right] \times$$

$$h(j, k, m) R^{-2} -$$

$$\frac{4}{3} \left[ A_B(l, m) A_B(k, k) + A'_B(l, m) A'_B(k, k) \right] \times$$

$$h(l, m, j) R^{-2} -$$

$$\frac{4}{3} \left[ A_B(l, m) A_B(j, j) + A'_B(l, m) A'_B(j, j) \right] \times$$

$$h(l, m, k) R^{-2} -$$

$$\frac{8}{9} \left[ A_B(l, k) A_B(k, m) + A'_B(l, k) A'_B(k, m) \right] \times$$

$$h(l, m, j) R^{-2} -$$

$$\frac{8}{9} \left[ A_B(l, j) A_B(j, m) + A'_B(l, j) A'_B(j, m) \right] \times$$

$$h(l, m, k) R^{-2} -$$

$$\frac{8}{9} \left[ A_B(j, m) A_B(m, k) + A'_B(j, m) A'_B(m, k) \right] \times$$

$$h(j, k, l) R^{-2} -$$

$$\frac{8}{9} \left[ A_B(j, l) A_B(l, k) + A'_B(j, l) A'_B(l, k) \right] \times$$

$$h(j, k, m) R^{-2} -$$

$$\frac{8}{9} \left[ A_B(j, k) A_B(l, m) + A'_B(j, k) A'_B(l, m) \right] \times$$

$$f(j, k, l, m) R^{-2}. \quad (6.111)$$
6.9 Appendix B: Sketch of derivation of matrix elements for \( n = 3 \) and \( L^\Pi = 1^- \) symmetry

This appendix derives the overlap matrix element for \( n = 3 \) and \( L^\Pi = 1^- \). To evaluate the overlap matrix element, we write, using Eq. (6.30),

\[
\psi(A', \vec{u}'_1, \vec{x})\psi(A, \vec{u}_1, \vec{x}) = 3v'_{1,3}v_{1,3}\exp\left(-\frac{\vec{x}^T B \vec{x}}{2}\right),
\]

(6.112)

where \( B \) is defined in Eq. (6.36). Using the transformation \( \vec{y} = U_B^T \vec{x} \), we find

\[
v'_{1,3}v_{1,3} = a(1,1)y^2_{1,3} + [a(1,2) + a(2,1)]y_{1,3}y_{2,3} + a(2,2)y^2_{2,3},
\]

(6.113)

where \( a(i,j) \) is defined in Eq. (6.62) and where \( y_{j,3} \) denotes the \( z \)-component of the vector \( \vec{y}_j \). Using \( y_{1,3} = y_1 \cos \vartheta_1 \) and \( y_{2,3} = y_2 \cos \vartheta_2 \) in Eqs. (6.112) and (6.113), we have

\[
\psi'\psi = 3\left\{a(1,1)y^2_1 \cos^2 \vartheta_1 + [a(1,2) + a(2,1)]y_1y_2 \cos \vartheta_1 \cos \vartheta_2 + a(2,2)y^2_2 \cos^2 \vartheta_2\right\}\exp\left[-\frac{1}{2} \left(\beta_1 y^2_1 + \beta_2 y^2_2\right)\right],
\]

(6.114)

where the \( \beta_j \) denote, as before, the eigenvalues of the matrix \( B \). When integrating over \( \hat{y}_1 \hat{y}_2 \), the cross term averages to zero and we have

\[
\int_0^{2\pi} \int_{-1}^1 \int_0^{2\pi} \int_{-1}^1 (\psi'\psi) |_{Rd} \cos \vartheta_1 d\varphi_1 d \cos \vartheta_2 d \varphi_2 = (4\pi)^2 \left[a(1,1)y^2_1 + a(2,2)y^2_2\right] \times \\
\times \exp\left[-\frac{1}{2} \left(\beta_1 y^2_1 + \beta_2 y^2_2\right)\right].
\]

(6.115)

Comparison of Eq. (6.115) with Eq. (6.39) shows that \( d^{(2)}_j = a(j,j) \) and that all other \( d \)-coefficients are zero. This agrees with the expressions given in Appendix 6.8.2.

Next, we consider the integration over \( \vartheta_2 \). To this end, we replace \( y_1 \) and \( y_2 \) in Eq. (6.115)
by \( R \sin \gamma_1 \) and \( R \cos \gamma_1 \), respectively. According to the discussion in Sec. 6.4, \( \gamma_1 \) can take values between 0 and \( \pi/2 \). Multiplying both sides of Eq. (6.115) by \( \sin^2 \gamma_1 \cos^2 \gamma_1 \) [see Eq. (6.38)] and integrating over \( \gamma_1 \), we find

\[
\int (\psi' \psi) |_R d^3 \Omega = (4\pi)^2 \frac{\pi}{16\zeta} \exp \left[ -\frac{1}{4} R^2 (\beta_1 + \beta_2) \right] \times \\
\left\{ [a(1,1) + a(2,2)] R^2 I_1(\zeta) + [-a(1,1) + a(2,2)] R^2 I_2(\zeta) \right\}.
\]

Applying the definitions from Appendix 6.8 and 6.10, it can be verified that Eq. (6.116) agrees with Eq. (6.46) [note that Eq. (6.46) does not contain a factor of \((4\pi)^2\) while Eq. (6.116) does; the reason is that \( f_o \) is defined without this prefactor].

The derivation sketched above for the overlap matrix element can be fairly straightforwardly generalized to arbitrary \( n \). To calculate the matrix element \( \langle \psi | T_\Omega | \psi \rangle |_R \), we use Eq. (6.20), i.e., we separately calculate the matrix elements \( \langle \psi | T_{\text{rel}} | \psi \rangle |_R \) and \( \langle \psi | T_R | \psi \rangle |_R \). The evaluation of these matrix elements is not fundamentally difficult but somewhat tedious and lengthy.
6.10 Appendix C: Definitions of \(sc\)-coefficients, \(M_1\) and \(M_2\)

The \(sc\)-coefficients entering into \(f_o\) are given by

\[
sc_{00} = d_1^{(0)} + \sum_{j=3}^{n-1} \left[ d_1^{(2)} y_j^2 + d_1^{(4)} y_j^4 + d_1^{(6)} y_j^6 \right] + \sum_{k>j; k \neq 1,2}^{n-1} \left[ d_1^{(22)} y_j^2 y_k^2 + d_1^{(44)} y_j^4 y_k^4 \right] + \sum_{j=3, k=3 \atop k \neq j}^{n-1} \left[ d_1^{(24)} y_j^2 y_k^4 + d_1^{(26)} y_j^6 y_k^2 \right] + \sum_{k>j; l \neq j, k \neq l \neq 1,2}^{n-1} \left[ d_1^{(222)} y_j^2 y_k^2 y_l^2 + d_1^{(224)} y_j^2 y_k^4 y_l^2 \right] + \sum_{k>j; l>j; m>l; k \neq l \neq m; k, l, m \neq 1,2}^{n-1} \left[ d_1^{(2222)} y_j^2 y_k^2 y_l^2 y_m^2 \right], \quad (6.117)
\]

\[
sc_{20} = d_2^{(2)} + \sum_{j=3}^{n-1} \left[ d_2^{(22)} y_j^2 y_j^2 + d_2^{(24)} y_j^4 + d_2^{(26)} y_j^6 \right] + \sum_{j=3, k=3 \atop k \neq j}^{n-1} \left[ d_2^{(22)} y_j^2 y_k^2 y_j^2 + d_2^{(24)} y_j^2 y_k^4 y_j^2 \right] + \sum_{j<k; j, k \neq 1,2}^{n-1} d_2^{(222)} y_j^2 y_j^2 y_k^2 + \sum_{l>k; j \neq l \neq k \neq 1,2}^{n-1} d_2^{(2222)} y_j^2 y_j^2 y_k^2 y_j^2, \quad (6.118)
\]

\[
sc_{02} = d_2^{(2)} + \sum_{j=3}^{n-1} \left[ d_2^{(22)} y_j^2 y_j^2 + d_2^{(24)} y_j^4 + d_2^{(26)} y_j^6 \right] + \sum_{j=3, k=3 \atop k \neq j}^{n-1} \left[ d_2^{(22)} y_j^2 y_k^2 y_j^2 + d_2^{(24)} y_j^2 y_k^4 y_j^2 \right] + \sum_{j<k; j, k \neq 1,2}^{n-1} d_2^{(222)} y_j^2 y_j^2 y_k^2 + \sum_{l>k; j \neq l \neq k \neq 1,2}^{n-1} d_2^{(2222)} y_j^2 y_j^2 y_k^2 y_j^2, \quad (6.119)
\]

\[
sc_{40} = d_1^{(4)} + \sum_{j=3}^{n-1} \left[ d_1^{(44)} y_j^4 + d_1^{(24)} y_j^2 y_j^2 \right] + \sum_{j<k; j, k \neq 1,2}^{n-1} d_1^{(224)} y_j^2 y_j^2 y_k^2, \quad (6.120)
\]
$$sc_{04} = d_2^{(4)} + \sum_{j=3}^{n-1} \left[ d_{2,j}^{(44)} y_j^4 + d_{j,2}^{(24)} y_j^2 \right] + \sum_{j<k; j, k \neq 1, 2}^{n-1} d_{j,k,2}^{(224)} y_j^2 y_k^2, \quad (6.121)$$

$$sc_{06} = d_1^{(6)} + \sum_{j=3}^{n-1} d_{j,1}^{(26)} y_j^2, \quad (6.122)$$

$$sc_{06} = d_2^{(6)} + \sum_{j=3}^{n-1} d_{j,2}^{(26)} y_j^2, \quad (6.123)$$

$$sc_{22} = d_{1,2}^{(22)} + \sum_{j=3}^{n-1} \left\{ \left[ d_{1,2,j}^{(222)} + d_{1,j,2}^{(222)} + d_{2,j,1}^{(222)} \right] y_j^2 + d_{1,2,j}^{(224)} y_j^4 \right\} + \sum_{j<k; j, k \neq 1, 2}^{n-1} d_{12jk}^{(222)} y_j^2 y_k^2 + \sum_{j<k; j, k \neq 1, 2}^{n-1} d_{1j2k}^{(222)} y_j^2 y_k^2, \quad (6.124)$$

$$sc_{44} = d_{1,2}^{(44)}, \quad (6.125)$$

$$sc_{24} = d_{1,2}^{(24)} + \sum_{j=3}^{n-1} d_{1,j,2}^{(224)} y_j^2, \quad (6.126)$$

$$sc_{42} = d_{2,1}^{(24)} + \sum_{j=3}^{n-1} d_{2,j,1}^{(224)} y_j^2, \quad (6.127)$$

$$sc_{26} = d_{1,2}^{(26)}, \quad (6.128)$$

130
and

$$sc_{62} = d_{2,1}^{(26)}.$$  \hfill (6.129)

Equation (6.117)-(6.129) also apply to $f_P$, $f_Q$ and $f_\Omega$ if the $d$-coefficients are replaced by the $p$-, $q$- and $b$-coefficients, respectively. The quantities $M_1$ and $M_2$ are defined through

$$M_1 = -\frac{1}{4} M_{aux} + \left[ 2sc_{60} + (sc_{20} + sc_{02})HR^2 + (sc_{40} + sc_{04})(HR^2)^2 + (sc_{60} + sc_{06})(HR^2)^3 \right] \zeta$$  \hfill (6.130)

and

$$M_2 = \zeta^{-1} M_{aux} + \frac{3}{4} \left[ -2sc_{40} - 2sc_{04} + 2sc_{22} + (-3sc_{60} - 3sc_{06} + sc_{24} + sc_{42})HR^2 + (sc_{26} + sc_{62})(HR^2)^2 \right] (HR^2)^2 + \left[ -sc_{20} + sc_{02} + (-sc_{40} + sc_{04})HR^2 + (-sc_{60} + sc_{06})(HR^2)^2 \right] HR^2 \zeta,$$  \hfill (6.131)

where

$$M_{aux} = -\frac{15}{2} (-sc_{26} + sc_{44} - sc_{62})(HR^2)^4 \zeta^{-1} + 3 \left[ -sc_{60} + sc_{06} - sc_{24} + sc_{42} + (-sc_{26} + sc_{62})HR^2 \right] (HR^2)^3.$$  \hfill (6.132)

### 6.11 Acknowledgments

We thank Javier von Stecher for fruitful discussions and correspondence. Support by the ARO and NSF through grant PHY-1205443 is gratefully acknowledged. This work was
additionally supported by the National Science Foundation through a grant for the Institute for Theoretical Atomic, Molecular and Optical Physics at Harvard University and Smithonian Astrophysical Observatory.
Chapter 7

Summary and outlook

This thesis considered two-component fermionic few-body systems under spherically and anisotropic external harmonic confinement. One of the primary objectives of this work was to develop numerical techniques that can accurately describe few-body systems along the BCS-BEC crossover. Our interest has been to describe universal features along the crossover curve, i.e., properties that are determined by just a few parameters such as the $s$-wave scattering length. In addition, we identified regimes where non-universal physics comes into play.

We implemented the explicitly correlated Gaussian method and used this technique to treat trapped fermionic four-body systems in a spherically symmetric trap with vanishing or finite angular momentum and natural or unnatural parity. A large portion of the zero-range equal-mass energy spectra at unitarity were calculated with uncertainty $\leq 0.1\%$. The energies were used to calculate the fourth-order virial coefficient and to investigate intersystem degeneracies. In addition to equal-mass systems, the explicitly correlated Gaussian approach was used to investigate the trapped unequal-mass (3, 1) system with $1^+$ symmetry at unitarity. Compared to Ref. [116], this work significantly improved the accuracy of the unequal-mass energies. Our study showed, in general agreement with Ref. [116], that a non-universal four-body bound state is supported for $\kappa \approx 10.55$, signaling the presence...
of a four-body resonance. It should be noted that the estimate of the critical mass ratio hinges on the extrapolation to the zero-range limit. The strong range dependence makes this extrapolation challenging. It would be desirable to develop more accurate approaches in the future.

The explicitly correlated Gaussian approach was employed to treat small two-component Fermi gases under highly-elongated cigar-shaped confinement along the BCS-BEC crossover. The system was treated within a full three-dimensional framework and within an effective one-dimensional framework. Comparisons of the three-dimensional and one-dimensional energies and excitation frequencies established the validity regimes of the effective one-dimensional Hamiltonian.

In addition, we developed the hyperspherical explicitly correlated Gaussian (HECG) technique for finite angular momentum states. This technique provides access to the bound states as well as the scattering states. Within the HECG framework, the solution of the time-independent Schrödinger equation is divided into two steps, the solution of the Schrödinger like equation in the hyperangular degrees of freedom, which yields effective potential curves and coupling matrix elements, and the solution of the coupled Schrödinger like hyperradial equations. We developed a theoretical framework to calculate the effective potentials as well as the associated coupling matrix elements for few-body systems with finite angular momentum \( L = 1 \) and negative and positive parity. A number of proof-of-principle calculations were presented, demonstrating that the developed approach provides a computationally efficient means to treating equal- and unequal-mass four-body systems. In the future, there is still room for improving the method further like pushing the calculations to larger \( R/(\sqrt{\mu r_0}) \) values. A natural extension of the HECG formalism for \( L = 0^+, 1^+ \) and \( 1^- \) will be the generalization to other \( L^\Pi \) symmetries.

Our unequal-mass results at unitarity support the claim [30] that the bound state found for the \((3, 1)\) system with \( 1^+ \) symmetry, positive scattering length and \( \kappa \gtrsim 9.5 \) is universal. In the future, it will be interesting to apply the HECG formalism to the \((3, 1)\) system with
finite scattering length. In particular, the positive s-wave scattering length results obtained within the HECG framework will provide an alternative means to analyze these universal four-body bound states.

The HECG method also provides a platform for performing scattering calculations. The asymptotic behavior of the effective potential curves describes different dissociation pathways. In the future, it will be interesting to combine the HECG approach with a standard $R$-matrix calculation to analyze few-body collisions.

The explicitly correlated Gaussian and the HECG techniques can readily be applied to multi-component fermionic and bosonic systems and as well as Bose-Fermi mixtures to study the rich physics that arises due to the interplay of statistics and interactions. These systems support Efimov states, which have been studied extensively in the three-body sector. In the four-body sector, many open questions exist.
Appendix A

Matrix elements for three-dimensional explicitly correlated Gaussians

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 ($L > 0$). We consider the matrix elements between the unsymmetrized basis functions $\psi_k^{LM}(\vec{x}, A^k, \vec{u}_1, \vec{u}_2)$ and $\psi_k'^{LM}(\vec{x}, A'^k, \vec{u}_{1'}, \vec{u}_{2'})$ [see Eq. (2.64)]. The matrix elements are derived in the literature [75,109,110,111,112,113] 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. A.1 and A.2. The product of $\psi_{k'}^{LM}$ and $\psi_k^{LM}$ can be conveniently written in terms of the matrix $B$, 

$$ B = A^{k'} + A^k. \quad (A.1) $$

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

$$ C = \left( \frac{(2\pi)^{N-1}}{\det(B)} \right)^{3/2} \rho_{11}^{L-2} \quad (A.2) $$
and

\[ \rho_{ij} = (\bar{u}_{ik'})^T B^{-1} \bar{u}_{jk}; \]  

(A.3)

note that the order of the primed and unprimed vectors \( \bar{u}_{ik'} \) and \( \bar{u}_{jk} \) matters. We further define the scalars \( R \) and \( S_{ij} \) \( (i,j = 1 \text{ or } 2) \),

\[ R = 3 \text{Tr}(B^{-1} A^k \Lambda A^{k'}) \]  

(A.4)

and

\[ S_{ij} = (\bar{u}_{ik'})^T B^{-1} A^k \Lambda A^{k'} B^{-1} \bar{u}_{jk}, \]  

(A.5)

where the diagonal elements of the matrix \( \Lambda \) are given by the inverse of the masses associated with the Jacobi vectors and the off-diagonal elements of \( \Lambda \) are zero. In Eq. (C.3), \( \text{Tr} \) denotes the trace operator. The scalars \( \tilde{R}^{(pq)} \) and \( \tilde{S}_{ij}^{(pq)} \) \( (p = 1, \cdots, n \text{ and } q = p + 1, \cdots, n) \) have a similar structure to \( R \) and \( S_{ij} \),

\[ \tilde{R}^{(pq)} = 3 \text{Tr}(B^{-1} Q^{(pq)}) \]  

(A.6)

and

\[ \tilde{S}_{ij}^{(pq)} = (\bar{u}_{ik'})^T B^{-1} Q^{(pq)} B^{-1} \bar{u}_{jk}. \]  

(A.7)

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

\[ Q^{(pq)} = \bar{\omega}^{(pq)} (\bar{\omega}^{(pq)})^T, \]  

(A.8)

where the \( (n - 1) \)-dimensional vector \( \bar{\omega}^{(pq)} \) is defined in Eq. (2.27). Lastly, we define the
total mass $M_{\text{tot}}$,

$$M_{\text{tot}} = \sum_{p=1}^{n} m_p.$$  \hfill (A.9)

### A.1 Natural parity

For natural parity states, we use $l_1 = L$ and $l_2 = 0$ in Eq. (2.64), which implies that $\psi_{L'M}^L$ and $\psi_{L'M}^L$ are independent of $\vec{u}_{2k}$ and $\vec{u}_{2k}$, respectively. In the following, we assume that $\psi_{L'M}^L$ and $\psi_{L'M}^L$ are characterized by the same $\Pi$ value. Under these assumptions the overlap matrix element is given by

$$\langle \psi_{L'M}^L | \psi_{L'M}^L \rangle = N^\text{nat}_L C \rho_{11}^2,$$  \hfill (A.10)

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

$$\langle \psi_{L'M}^L | T_{\text{rel}} | \psi_{L'M}^L \rangle = N^\text{nat}_L \frac{\hbar^2}{2} C \left(R \rho_{11} + 2 L S_{11}\right) \rho_{11}.$$  \hfill (A.11)

The matrix element for the trapping potential reads

$$\langle \psi_{L'M}^L | V_{\text{trap}} | \psi_{L'M}^L \rangle = N^\text{nat}_L \sum_{p=1,q>p}^{n} \frac{1}{2} \left( \frac{m_p m_q}{M_{\text{tot}}} \right) \omega^2 C \left( \tilde{R}(pq) \rho_{11} + 2 L \tilde{S}(pq) \right) \rho_{11}.$$  \hfill (A.12)

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

$$\langle \psi_{L'M}^L | V_{\text{int}} | \psi_{L'M}^L \rangle = -V_0 \sum_{p=1}^{n} \sum_{q=n_1+1}^{n} \langle \psi_{L'M}^L | \exp[-r_{pq}^2/(2r_0^2)] | \psi_{L'M}^L \rangle.$$  \hfill (A.13)

The expression for the matrix element $\langle \psi_{L'M}^L | \exp[-r_{pq}^2/(2r_0^2)] | \psi_{L'M}^L \rangle$ reduces to that for the overlap matrix element if the matrices $A^{K'}$ and $A^k$ are replaced by $A^{K'} + Q^{(pq)}/(2r_0^2)$ and $A^k + Q^{(pq)}/(2r_0^2)$, respectively.
A.2 Unnatural parity \((L > 0)\)

For unnatural parity states with \(L > 0\), we use \(l_1 = L\) and \(l_2 = 1\) in Eq. (2.64). In the following, we assume that \(\psi_{k'}^{LM}\) and \(\psi_{k}^{LM}\) are characterized by the same \(\Pi\) value. Under these assumptions the overlap matrix element is given by

\[
\langle \psi_{k'}^{LM} | \psi_{k}^{LM} \rangle = N_L^{\text{unnat}} C \rho_{11} (\rho_{11} \rho_{22} - \rho_{12} \rho_{21}),
\]

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

\[
\langle \psi_{k'}^{LM} | T^{\text{rel}} | \psi_{k}^{LM} \rangle = N_L^{\text{unnat}} \frac{\hbar^2}{2} C \sum_{p \neq q \neq p} \frac{1}{2} \left( \frac{m_p m_q}{M_{\text{tot}}} \right) \omega^2 C \times \]

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

The matrix element for the trapping potential reads

\[
\langle \psi_{k'}^{LM} | V^{\text{rel}}_{\text{trap}} | \psi_{k}^{LM} \rangle = N_L^{\text{unnat}} \sum_{p=1, q > p}^{n} \frac{1}{2} \left( \frac{m_p m_q}{M_{\text{tot}}} \right) \omega^2 C \times \]

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

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.
Appendix B

Tabulation of four-body energy spectra at unitarity

Section B.1 tabulates the relative energies of the $(3,1)$ system at unitarity with $E_{3,1} \leq 21\hbar\omega/2$ and Sec. B.2 tabulates the relative energies of the $(2,2)$ system at unitarity with $E_{2,2} \leq 21\hbar\omega/2$.

B.1 Energy spectrum of the $(3,1)$ system at unitarity

This appendix tabulates the energies of the $(3,1)$ system at unitarity with $E_{3,1} \leq 21\hbar\omega/2$. The notation follows that introduced in Ch. 2 and Ch. 3.

For $(3,1)$ states with $0^{-}$ symmetry, there exist 1 and 2 unshifted states with energy $15\hbar\omega/2$ and $19\hbar\omega/2$, respectively.

The $(3,1)$ energies for states with $1^{+}$ symmetry are reported in Sec. 3.2.

There are no states with $7^{+}$ symmetry with energy $\leq 21\hbar\omega/2$. 
Table B.1: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^{\Pi} = 0^+$ symmetry (only states that are affected by $s$-wave interactions are included; each energy is $(2L + 1)$-fold degenerate). The first column indicates the state number (st. no.). The second column shows the extrapolated zero-range energy $E_{3,1}(r_0 = 0)$ at unitarity; the uncertainty is estimated to be 0.1 % or smaller. The third column indicates the dependence of the energy at unitarity on the range $r_0$ of the Gaussian potential $V_g$. We assume a linear dependence and write $E_{3,1}(r_0) = E_{3,1}(r_0 = 0) + \chi (r_0/a_0) \hbar \omega$. The fourth column shows the $s_{L,\nu}$ value determined from the energy (the value of $s_{L,\nu}$ is only shown for the lowest rung of a ladder, i.e., for states with $q = 0$). The last column shows the $s_{L,\nu}^{ni}$ of the non-interacting state that is “paired” with the interacting state when determining $\Delta Q_{3,1}$ (see Ref. [39] for details). There exist 2 unshifted states for $21 \hbar \omega/2$.

<table>
<thead>
<tr>
<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar \omega)$</th>
<th>$\chi$</th>
<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{ni}$</th>
</tr>
</thead>
<tbody>
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Table B.2: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^{\Pi} = 1^-$ symmetry. For details see caption of Table B.1. There exists 1 unshifted state for $19 \hbar \omega/2$.

<table>
<thead>
<tr>
<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar \omega)$</th>
<th>$\chi$</th>
<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{ni}$</th>
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Table B.3: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 2^+$ symmetry. For details see caption of Table B.1. There exist 1 and 6 unshifted states for $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

<table>
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<th>$s_{L,\nu}$</th>
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</table>

Table B.4: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 2^-$ symmetry. For details see caption of Table B.1. There exist 4 unshifted states for $19\hbar\omega/2$.

<table>
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<th>$s_{L,\nu}$</th>
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Table B.5: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 3^+$ symmetry. For details see caption of Table B.1. There exist 1 and 8 unshifted states for $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

<table>
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<tr>
<th>st. no.</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{\text{ni}}$</th>
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Table B.6: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 3^-$ symmetry. For details see caption of Table B.1. There exist 2 unshifted states for $19\hbar\omega/2$.

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<th>$s_{L,\nu}^{\text{ni}}$</th>
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Table B.7: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 4^+$ symmetry. For details see caption of Table B.1. There exist 5 unshifted states for $21 \hbar \omega/2$.

<table>
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<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar \omega)$</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{\mu}$</th>
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</thead>
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<td>7.6481</td>
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</tr>
<tr>
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</table>

Table B.8: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 4^-$ symmetry. For details see caption of Table B.1. The state with energy 10.501$\hbar \omega$ is identified as a state with hyperradial quantum number $q = 1$; it is included in the table since accounting for the basis set extrapolation error will likely push the energy below 10.5$\hbar \omega$. There exist 2 unshifted states for $19\hbar \omega/2$.

<table>
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<tr>
<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar \omega)$</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{\mu}$</th>
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</thead>
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Table B.9: Relative energies $E_{3,1}$ for the $(3, 1)$ system with $L^\Pi = 5^+$ symmetry. For details see caption of Table B.1. There exist 3 unshifted states for $21\hbar \omega/2$.

<table>
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<tr>
<th>st. no.</th>
<th>$E_{3,1}(r_0 = 0)/(\hbar \omega)$</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{\mu}$</th>
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</table>
Table B.10: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 5^-$ symmetry. For details see caption of Table B.1. There exist no unshifted states for $\leq 21\hbar\omega/2$.

<table>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{ni}$</th>
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<tr>
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<td>0.44</td>
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</table>

Table B.11: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 6^+$ symmetry. For details see caption of Table B.1. There exists 1 unshifted states for $21\hbar\omega/2$.

<table>
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<th>st. no.</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{ni}$</th>
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<td>0.43</td>
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</table>

Table B.12: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 6^-$ symmetry. For details see caption of Table B.1. There exist no unshifted states for $\leq 21\hbar\omega/2$.

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<th>st. no.</th>
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<th>$s_{L,\nu}$</th>
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</table>

Table B.13: Relative energies $E_{3,1}$ for the (3, 1) system with $L^\Pi = 7^-$ symmetry. For details see caption of Table B.1. There exist no unshifted states for $\leq 21\hbar\omega/2$.

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B.2 Energy spectrum of (2,2) system at unitarity

This appendix tabulates the energies of the (2, 2) system at unitarity with $E_{2,2} \leq 21\hbar\omega/2$. The notation follows that introduced in Ch. 2 and Ch. 3.

The energies for states with natural parity ($L \leq 6$) and $E_{2,2} \leq 17\hbar\omega/2$ as well as the energies of states 1 and 2 with $7^{-}$ symmetry and the energy of state 1 with $8^{+}$ symmetry are taken from K. M. Daily and D. Blume, Phys. Rev. A 81, 053615 (2010); in some cases, this paper reports four and not five significant figures.

Our $s_{L,v}$ values for states with $0^{+}$ symmetry agree with those reported in J. von Stecher and C. H. Greene, Phys. Rev. A 80, 022504 (2009).

For the (2, 2) system with $0^{-}$ symmetry, there exist 1 and 3 unshifted states with energy $15\hbar\omega/2$ and $19\hbar\omega/2$, respectively.

There are no states with $7^{+}$ symmetry with energy $\leq 21\hbar\omega/2$. 
Table B.14: Relative energies $E_{2,2}$ for the $(2,2)$ system with $L^\Pi = 0^+$ symmetry (only states that are affected by $s$-wave interactions are included; each energy is $(2L + 1)$-fold degenerate). The first column indicates the state number (st. no.). The second column shows the extrapolated zero-range energy $E_{2,2}(r_0 = 0)$ at unitarity; the uncertainty is estimated to be 0.1 % or smaller. The third column indicates the dependence of the energy at unitarity on the range $r_0$ of the Gaussian potential $V_g$. We assume a linear dependence and write $E_{2,2}(r_0) = E_{2,2}(r_0 = 0) + \chi(r_0/a_\omega)\hbar\omega$. The fourth column shows the $s_{L,\nu}$ value determined from the energy (the value of $s_{L,\nu}$ is only shown for the lowest rung of a ladder, i.e., for states with $q = 0$). The last column shows the $s_{L,\nu}^{ni}$ of the non-interacting state that is “paired” with the interacting state when determining $\Delta Q_{2,2}$ ($\Delta Q_{2,2}$ enters into the determination of the fourth-order virial coefficient; see Ref. [39] for details). There exist 2 unshifted states for $21\hbar\omega/2$.

<table>
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Table B.15: Relative energies $E_{2,2}$ for the $(2, 2)$ system with $L^\Pi = 1^+$ symmetry. For details see caption of Table B.14. There exist 1 and 7 unshifted states for $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

<table>
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<th>st. no.</th>
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<th>$s_{L,\nu}$</th>
<th>$s_{L,\nu}^{\text{ni}}$</th>
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Table B.17: Relative energies $E_{2,2}$ for the $(2, 2)$ system with $L^\Pi = 2^+$ symmetry. For details see caption of Table B.14. There exist 1 and 7 unshifted states for $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

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Table B.18: Relative energies $E_{2,2}$ for the (2, 2) system with $L^\Pi = 2^-$ symmetry. For details see caption of Table B.14. There exist 4 unshifted states for $19\hbar\omega/2$.

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Table B.19: Relative energies $E_{2,2}$ for the $(2, 2)$ system with $L^{\Pi} = 3^+$ symmetry. For details see caption of Table B.14. There exist 1 and 9 unshifted states for $17\hbar\omega/2$ and $21\hbar\omega/2$, respectively.

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Table B.20: Relative energies $E_{2,2}$ for the (2, 2) system with $L^\Pi = 3^-$ symmetry. For details see caption of Table B.14. The state with energy $10.502\hbar\omega$ is not included when reporting the number of states with energy $\leq 10.5\hbar\omega$; we note, however, that the energy may drop below $10.5\hbar\omega$ when the basis set extrapolation error is corrected for. There exist 2 unshifted states for $19\hbar\omega/2$.

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Table B.21: Relative energies $E_{2,2}$ for the (2, 2) system with $L^\Pi = 4^+$ symmetry. For details see caption of Table B.14. There exist 6 unshifted states for $2\hbar\omega/2$.

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Table B.22: Relative energies $E_{2,2}$ for the $(2, 2)$ system with $L^\Pi = 4^-$ symmetry. For details see caption of Table B.14. The state with energy 10.505$\hbar\omega$ is not included when reporting the number of states with energy $\leq 10.5\hbar\omega$; we note, however, that the energy may drop below 10.5$\hbar\omega$ when the basis set extrapolation error is corrected for. There exist 2 unshifted states for 19$\hbar\omega$/2.

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Table B.23: Relative energies $E_{2,2}$ for the $(2, 2)$ system with $L^\Pi = 5^+$ symmetry. For details see caption of Table B.14. There exist 4 unshifted states for 21$\hbar\omega$/2.

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Table B.24: Relative energies $E_{2,2}$ for the (2, 2) system with $L^I = 5^-$ symmetry. For details see caption of Table B.14. The state with energy $10.504 \hbar \omega$ is not included when reporting the number of states with energy $\leq 10.5 \hbar \omega$; we note, however, that the energy may drop below $10.5 \hbar \omega$ when the basis set extrapolation error is corrected for. There exist no unshifted states for $\leq 21 \hbar \omega/2$.

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Table B.25: Relative energies $E_{2,2}$ for the (2, 2) system with $L^I = 6^+$ symmetry. For details see caption of Table B.14. There exists 1 unshifted state for $21 \hbar \omega/2$.

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Table B.26: Relative energies $E_{2,2}$ for the (2, 2) system with $L^I = 6^-$ symmetry. For details see caption of Table B.14. The state with energy $10.504 \hbar \omega$ is not included when reporting the number of states with energy $\leq 10.5 \hbar \omega$; we note, however, that the energy may drop below $10.5 \hbar \omega$ when the basis set extrapolation error is corrected for. There exist no unshifted states for $\leq 21 \hbar \omega/2$.

<table>
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Table B.27: Relative energies $E_{2,2}$ for the (2, 2) system with $L^\Pi = 7^-$ symmetry. For details see caption of Table B.14. There exist no unshifted states for $\leq 21\hbar\omega/2$.

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Table B.28: Relative energies $E_{2,2}$ for the (2, 2) system with $L^\Pi = 8^+$ symmetry. For details see caption of Table B.14. There exist no unshifted states for $\leq 21\hbar\omega/2$.

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Appendix C

Matrix elements for one-dimensional explicitly correlated Gaussians

Section 4.2 discusses that one can choose to work with even parity basis functions and yet successfully describe states with odd parity via the introduction of a spectator atom. A more direct approach is to evaluate the matrix elements using the odd parity basis functions whose functional form is given in Eq. (2.66). The derivation of the even parity matrix elements is discussed in the literature [75]. We take an analogous approach to derive the expressions for the odd parity matrix elements. This appendix summarizes the expressions for the overlap, kinetic energy, trap potential, and interaction potential matrix elements for the one-dimensional system with even and odd parity.

We first introduce the auxiliary quantities that enter into the expressions of the matrix elements. We define the scalars $C$ and $\rho$,

$$C = \left( \frac{(2\pi)^{N-1}}{\det(B)} \right)^{1/2} \quad \text{(C.1)}$$

and

$$\rho = (\bar{u}_{1k'})^T B^{-1} \bar{u}_{1k}, \quad \text{(C.2)}$$
where \( B \) is defined in Eq. (A.1). We further define the scalars \( R \) and \( S \),

\[
R = \text{Tr}(B^{-1}A^k\Lambda A^k')
\]

(C.3)

and

\[
S = (\vec{u}_{1k}')^T B^{-1}A^k\Lambda A^k' B^{-1}\vec{u}_{1k},
\]

(C.4)

where the diagonal elements of the matrix \( \Lambda \) are given by the inverse of the masses associated with the Jacobi vectors and the off-diagonal elements of \( \Lambda \) are zero. In Eq. (C.3), \( \text{Tr} \) denotes the trace operator. The scalars \( \tilde{R}^{(pq)} \) and \( \tilde{S}^{(pq)} \) (\( p = 1, \cdots, N \) and \( q = p + 1, \cdots, N \)) have a similar structure to \( R \) and \( S \),

\[
\tilde{R}^{(pq)} = \text{Tr}(B^{-1}Q^{(pq)})
\]

(C.5)

and

\[
\tilde{S}^{(pq)} = (\vec{u}_{1k'})^T B^{-1}Q^{(pq)} B^{-1}\vec{u}_{1k},
\]

(C.6)

where the matrix \( Q^{(pq)} \) is defined in Eq. (A.8).

### C.1 Even parity

In the following, we assume that \( \psi_{k'} \) and \( \psi_k \) are characterized by \( \Pi_z = +1 \). Under this assumption the overlap matrix element is given by

\[
\langle \psi_{k'} | \psi_k \rangle = C.
\]

(C.7)
The kinetic energy matrix element reads

$$\langle \psi_{k'} | T^{\text{rel}} | \psi_k \rangle = \frac{\hbar^2}{2} C R.$$  \hfill (C.8)

The matrix element for the trapping potential reads

$$\langle \psi_{k'} | V^{\text{rel}}_{\text{trap}} | \psi_k \rangle = \sum_{p=1, q>p}^{n} \frac{1}{2} \left( \frac{m_p m_q}{M_{\text{tot}}} \right) \omega^2 C \tilde{R}^{(pq)}.$$  \hfill (C.9)

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

$$\langle \psi_{k'} | V_{\text{int}} | \psi_k \rangle = -V_0 \sum_{p=1}^{n_1} \sum_{q=n_1+1}^{n} \langle \psi_{k'} | \exp[-z_{pq}^2/(2z_0^2)] | \psi_k \rangle.$$  \hfill (C.10)

The expression for the matrix element $\langle \psi_{k'} | \exp[-z_{pq}^2/(2z_0^2)] | \psi_k \rangle$ reduces to that for the overlap matrix element if the matrices $\mathbf{A}^{k'}$ and $\mathbf{A}^k$ are replaced by $\mathbf{A}^{k'} + Q^{(pq)}/(2z_0^2)$ and $\mathbf{A}^k + Q^{(pq)}/(2z_0^2)$, respectively.

### C.2 Odd parity

In the following, we assume that $\psi_{k'}$ and $\psi_k$ are characterized by $\Pi_z = -1$. Under these assumptions the overlap matrix element is given by

$$\langle \psi_{k'} | \psi_k \rangle = C \rho.$$  \hfill (C.11)

The kinetic energy matrix element reads

$$\langle \psi_{k'} | T^{\text{rel}} | \psi_k \rangle = \frac{\hbar^2}{2} C (R \rho + 2S).$$  \hfill (C.12)
The matrix element for the trapping potential reads

$$\langle \psi_{k'}|V_{\text{rel}}^{\text{trap}}|\psi_k \rangle = \sum_{p=1,q>p}^n \frac{1}{2} \left( \frac{m_pm_q}{M_{\text{tot}}} \right) \omega^2 C \left( \tilde{R}^{(pq)} \rho + 2 \tilde{S}^{(pq)} \right). \quad (C.13)$$

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

$$\langle \psi_{k'}|V_{\text{int}}|\psi_k \rangle = -V_0 \sum_{p=1}^{n_1} \sum_{q=n_1+1}^n \langle \psi_{k'}|\exp[-z_{pq}^2/(2z_0^2)]|\psi_k \rangle. \quad (C.14)$$

The expression for the matrix element $\langle \psi_{k'}|\exp[-z_{pq}^2/(2z_0^2)]|\psi_k \rangle$ reduces to that for the overlap matrix element if the matrices $A^{k'}$ and $A^k$ are replaced by $A^{k'} + Q^{(pq)}/(2z_0^2)$ and $A^k + Q^{(pq)}/(2z_0^2)$, respectively.
Appendix D

Matrix elements of one-body density matrix and momentum distribution function for one-dimensional even parity basis function

The expressions for the three-dimensional one-body density matrix and the momentum distribution function are derived for basis functions with angular momentum $L = 0$ and natural parity in Ref. [149]. Similarly, analogous expressions can be derived for the one-dimensional basis functions. This appendix provides compact expressions for the one-body density matrix and the momentum distribution function for the one-dimensional basis functions with even parity.

To determine the one-body density matrix, we multiply the basis functions for the relative coordinates by the unnormalized center of mass ground state wave function. The functional form of the total basis function $\psi_{\text{tot}}(\vec{r}, A)$ is similar to that given in Eq. (2.66). However, due to the inclusion of center of mass, $A$ is now a $N \times N$ dimensional symmetric matrix. The matrix elements $(A)_{j\ell} = (N/a_N^2) \delta_{jN}$, where $j = 1, \cdots, N$ and the rest of the $(N-1)(N-2)/2$ matrix elements are the optimized parameters obtained through the energy minimization (see Ch. 2 for details).

We first introduce the auxiliary quantities that enter into the expressions for the matrix
elements. We define the scalars $c_1$, $c$, $c'$ and $a$,

\begin{align}
    c_1 &= \left( \frac{(2\pi)^{N-1}}{\det(D^T + D)} \right)^{\frac{1}{2}}, \\
    c &= b_1 - \vec{b}^T D \vec{b}, \\
    c' &= b'_1 - \vec{b}'^T D \vec{b}'
\end{align}

and

\begin{align}
    a &= \vec{b}^T D \vec{b} + \vec{b}'^T D \vec{b}.
\end{align}

where

\[ D = (A_T + A'_T)^{-1}. \]

In Eq. (D.5), the $(N - 1) \times (N - 1)$ dimensional matrix $A_T$ is defined as $T^T A T$ with the first row and column removed, the scalar $b_1$ is given by $(T^T A T)_{11}$ and the $(N - 1)$-dimensional vector $\vec{b}'$ is defined as $((T^T A T)_{12}, \cdots, (T^T A T)_{1N})$. Here, $T$ is the transformation matrix [see Eq. (2.14)]. The quantities $b'_1$, $\vec{b}'$ and $A'_T$ are defined analogously to $b_1$, $\vec{b}$, and $A_T$ with $A$ replaced by $A'$.

Assuming $\psi_{tot}(\vec{x}, A')$ and $\psi_{tot}(\bar{x}, A)$ are both even parity basis functions, the one-dimensional one-body density matrix is given by

\[ \rho_1(z, z') = C^{-1} c_1 \exp \left( -\frac{c'}{2} z'^2 - \frac{c}{2} z^2 + \frac{a}{2} z' z \right), \]

(D.6)
where $C$ is given in Eq. (C.1). The momentum distribution function is given by

$$n_1(k) = C^{-1} \frac{c_1}{(df)^{1/2}} \exp\left( -\frac{k^2}{2d} \right),$$  \hspace{1cm} (D.7)$$

where $f = c' + c - a$, $d = c' - g^2/(4f)$ and $g = a - 2c'$. The derivation assumes $d > 0$ and $f > 0$. 

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[148] Eq. (4.11) predicts an atom-dimer [dimer-dimer] resonance at $a_{\rho}/a_{3D}^{aa} = 1.4603 \times \sqrt{2/3} \times 1.18 = 1.4069$ [$a_{\rho}/a_{3D}^{aa} = 1.4603 \times 0.608 = 0.8879$], which is smaller [larger] than $a_{\rho}/a_{3D}^{aa} = -\zeta(1/2, 2.2)/\sqrt{2} = 1.8503$ [$a_{\rho}/a_{3D}^{aa} = -\zeta(1/2, 0.3)/\sqrt{2} = -0.0079$] [136,141,142].


To construct basis functions with $0^-$ symmetry, one has to couple three spherical harmonics; see Refs. [113, 167].


[171] We note that the equations reported in Refs. [83, 84] for $n = 3$ and 4 with $L^I = 0^+$ symmetry contain a number of non-trivial typos; this has been confirmed by J. von Stecher in a private communication in 2011.

