Translationally Invariant Treatment of Light Nuclei

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Declaration

No portion of the work referred to in this thesis has been submitted in support of an application for another degree or qualification of this or any other university, or other institution of learning.

Abstract

One of the recent discoveries in nuclear physics is the existence of halo nuclei. These can be thought of as loosely bound systems where a nuclear core with normal nuclear density is surrounded by a region of dilute nuclear matter, referred to as the neutron halo. Such nuclei occur from light to heavy masses and have been the subject of a large number of theoretical studies to try and understand them. A number of theoretical models have been proposed over the years.

In this thesis the structure of light halo nuclei is examined through a fully microscopic variational model, where the Pauli exclusion principle is explicitly satisfied and semi-realistic nucleon-nucleon interactions are used. The model is an extension of previous work for closed shell nuclei. The wavefunction is obtained from a starting or 'reference' state, which includes the required symmetries and provides a translationally invariant description of the system in terms of several uncorrelated clusters. Medium- to long-range linear and short-range non-linear correlation operators are then applied to obtain a good wavefunction.

In order to evaluate the many-body matrix elements that occur in the linear eigenvalue problem associated with the variational approach, we make use of the variational Monte Carlo method. The numerical accuracy of the Monte Carlo method is thoroughly examined, paying particular attention to the specific requirements of the model. It is shown that the presence of correlations in the random walk must be taken into account for a reliable error estimate.

The model developed is then used to examine the nuclei ^{5}He, ^{6}He, ^{8}Be and ^{9}Be. By making use of one- and two-body density distributions a qualitative picture of the matter

distribution in the nucleus is obtained. The analysis provided indicates that for a bound state one requires spin-orbit force, something that we do not include. Nevertheless, working in the $L-S$ coupling scheme we have shown that our model is capable of producing bound states for open-shell systems by artificially altering the central term of the semi-realistic interactions in use. In general this model is a successful first step in extending past developments for closed-shell systems into the area of halo nuclei.

Contents

Chapter 1

The nuclear many-body problem and halo nuclei

1.1 Motivations for this research

Although nuclear physics has a long tradition the exact theory of nuclear forces is not yet known and thus a number of different phenomenological models are in use. At low energies (E$\sim$MeV) the nucleus behaves like a quantum object and has been the subject of theoretical studies since the birth of quantum mechanics. This thesis is aimed to an investigation of the low-energy nuclear many-body problem by making use of a number of quantum many-body techniques.

Recent advancements in experimental techniques have probed extreme types of nuclear structures not previously known, termed 'exotic nuclei'. Amongst such structures are the 'halo' nuclei and occur all over the periodic table, ranging from light to heavy nuclei. It has been the subject of a large number of theoretical studies to try to understand such structures and a number of theoretical models have been proposed in order to examine them. Up to now there has not been a single most successful model, but different models each have there own merits and shortcomings. This research is restricted to the case of light nuclei and in particular to the investigation of such exotic structures in a non-relativistic approximation. It is more or less an attempt to extend previously known techniques to the case of light halo nuclei.

1.1.1 The importance of correlations

One of the recent realizations in the nuclear problem is the effect of correlations (and in particular short range ones) in the nuclear properties. Such correlations arise when one uses 'realistic' nucleon-nucleon interactions contrary to the independent particle model where nucleons move independently in a mean field. An interaction is termed 'realistic' when it is designed to reproduce experimental data. They range form simple radial ones to potentials containing state dependence in terms of scalar and tensor operators (we give a brief description of these interactions in chapter 3). In order to adequately investigate such interactions is necessary to go beyond the simple mean-field approximation.

In the last few years the microscopic many-body theory of nuclei has reached a high level of accuracy. For example, Green's function Monte Carlo (GFMC) methods [1] have obtained a consistent description of nuclei up to a mass number A = 10, including the ground and the first few excited states. Furthermore, the realistic nucleon-nucleon interactions can be complemented by a partially phenomenological three-body force (whose contribution turns out to be small but essential) that can further increase the level of accuracy.

However, the solution of the bare nucleon-nucleon Hamiltonian is not an easy task when the number of particles increases, since the resulting configuration space can be considerably larger than in the case of a mean field. Apart from the size of the system, structures such as halo nuclei that exhibit extended spatial properties, are not yet adequately described. This requires the introduction of models that will take account of correlation effects in a way open to approximations. During the last years there have been a large number of developments in this area, in particular for light nuclei. Most of the methods used are essentially diagonalizing the many-body Hamiltonian in a set of basis states that are explicitly constructed to include correlation effects. In the next section we give a short description of some known models that can be used for the few-body problem, but first we give a more detailed description of halo nuclei.

1.1.2 Drip line Nuclei and the halo phenomenon

For each individual mass number A there are usually a few possible combinations of neutrons and protons that result in a stable nucleus. Both at the neutron rich and neu-

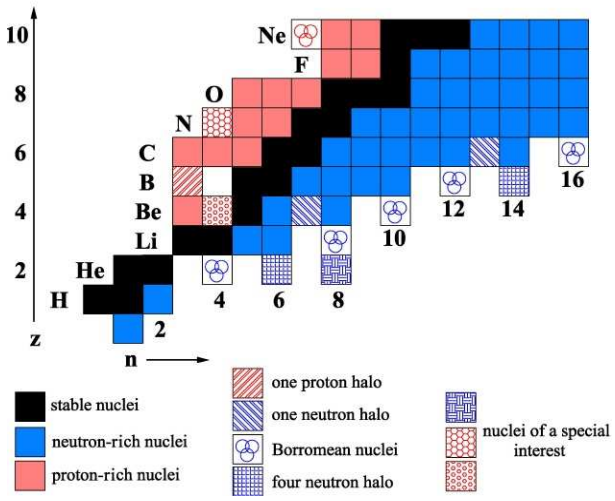


Figure 1.1: The lightest known halo nuclei.

tron deficient sides there is a limit of stability corresponding to zero binding energy for neutrons and protons. These two limits are referred to as the drip lines.

A very interesting discovery [2] in the neutron drip-line regions is the existence of nuclei that can be described as a nuclear core with normal nuclear density, surrounded by a dilute region of nuclear matter, referred to as the neutron halo [3]. The main characteristic feature of the halo phenomenon is the large reaction radius. This is observed when a radioactive beam collides with a target nucleus. In general halo structures are characterized by a very small neutron separation energy ($<$1 MeV) and a large spatial extension, the latter observed in the neutron density distribution as a large extension or as a narrow momentum distribution for the last neutron [2]. The most weakly bound nuclei are the most interesting cases since they have the most extreme halos. Halo nuclei have opened studies for the weakly bound nuclear system, which was not freely accessible before. A schematic of the lightest nuclei with halo structures is shown in figure 1.1.

Only recently has the picture for the lightest halo nuclei become clear. The nucleus ^{11}Li, which has two weakly bound neutrons, was the first observed case of neutron halo and is often described as a ^{9}Li plus two outlying neutrons. This nucleus has been called Borromean because none of the subsystems (n+n, ^{9}Li+n) are bound, but the three-body system is. Other examples of nuclei known to have neutron halos are ^{6}He and ^{11}Be.

The Borromean structure is a genuine structure of a non-mean-field phenomenon [4]. As an example, in the case of ^{6}He the core+n+n system cannot be described as a neutron

in the mean field of the core+n subsystem, since such a subsystem (^{5}He) is not bound. Assuming an alpha-particle core, ^{6}He can be described by a model involving the effect of at least three interactions, namely the interaction of each of the two weakly-bound neutrons with the alpha-particle and the interaction between the two neutrons. In this thesis we will develop a cluster model for studying light nuclei, where our main objective is its application to light borromean systems.

1.2 Some methods of the nuclear many-body problem

As a result of the complexity of the many-body problem it is usually only approximately solved. There is a large number of methods available for attacking the many-body problem and it is beyond our scope to give a general description of such methods. As stated earlier we wish to examine light nuclear systems that exhibit strong correlations, by making use of realistic nucleon-nucleon interactions. We give a brief description of some of the main methodologies that make use of realistic interactions. In general these are methods that can be used to solve the many-body Schrödinger equation in a non-relativistic approximation.

1.2.1 The generator coordinate method (GCM) and the resonating-group method (RGM)

Although its original purpose was to examine collective phenomena, the generator coordinate method (GCM) is a fully quantum-mechanical method and consists of the construction of a linear superposition of many different wavefunctions [5]. It was originally proposed by Griffin and Wheeler [6] as a way of 'generating' the full wavefunction ψ through

$$\psi(x_1, ..., x_n) = \int \phi(x_1, ..., x_n; a) f(a) da. \tag{1.1}$$

The wavefunctions ϕ, come from the solution (or approximate solution) of a model problem depending on the generator coordinate a, while $f(a)$ is a collective wavefunction or 'generator function'. In the integration the generator coordinate disappears, yielding a wavefunction that depends only upon the coordinates of the particles.

The function $f(a)$ can be determined using the variational principle, where variation

of the hamiltonian expectation value with respect to $f(a)$ gives the integral equation

$$\int da' \phi^*(x_1, ..., x_n; a) \hat{H} \phi(x_1, ..., x_n; a') = E \int da' \phi(x_1, ..., x_n; a) \phi^*(x_1, ..., x_n; a') f(a'), \tag{1.2}$$

that is known as the 'Hill-Wheeler equation'. The function $f(a)$ is usually approximated through some linear expansion. This method is particularly useful for introducing collective behaviour in the many-body wavefunction, through the function $f(a)$, without explicitly introducing collective coordinates, since the Hamiltonian used for the energy of the system is the full n-particle Hamiltonian. This method has been extensively used for describing exotic nuclei in a cluster model [7, 8, 9, 10], where the $f(a)$ was approximated through a linear expansion, while the set of parameters a assigned separations between the different clusters.

The resonating-group method (RGM) [11, 12] is another microscopic method which explicitly takes cluster correlations into account. It provides a wavefunction that has a number of important features that classify it a fully microscopic method. Specifically it employs totally antisymmetric wavefunctions and thus takes the Pauli exclusion principle fully into account, it utilizes a semi-realistic nucleon-nucleon potential and it treats correctly the motion of the total center-of-mass. The RGM is sometimes referred to as the cluster model [12]. In general the wavefunction Ψ is given as an antisymmetrized product of all the different correlated cluster configurations:

$$\begin{aligned} \Psi = \ & \mathcal{A} \ \{ \sum_i \phi(A_i)\phi(B_i)F_i(R_i) + \sum_j \phi(A_j)\phi(B_j)\phi(C_j)F_j(R_{j1}, R_{j2}) \\ & + \ \sum_k \phi(A_k)\phi(B_k)\phi(C_k)\phi(D_k)F_k(R_{k1}, R_{k2}, R_{k2}) + ... \\ & + \ \sum_m c_m \zeta_m \} Z(R_{\text{cm}}), \end{aligned} \tag{1.3}$$

where the functions ϕ describe the internal behaviour of the different clusters while $Z(R_{\text{cm}})$ is a normalizable function describing the total center-of-mass motion. The functions $F_i(R_i)$, $F_j(R_{j1}, R_{j2})$, $F_k(R_{k1}, R_{k2}, R_{k3})$, and so on are relative motion functions correlating two, three-, four- and more-cluster configurations, with the R_i representing the set of Jacobi coordinates defined with respect to the centers-of-mass of the various clusters. The functions ζ_i are chosen to include the short-range effects of the nuclear-

force and vanish over long distances.

The above wavefunction is used to solve

$$\langle \delta\Psi | \hat{H} - E | \Psi \rangle = 0, \tag{1.4}$$

where the variations are taken over the linear functions F_i and the linear amplitudes c_m. This provides a set of coupled integral equations. The computation will in general become quite complicated if the function space is taken to be rather large (particularly because of the antisymmetrization). Thus, in practise, relatively simple forms of Ψ are used, usually chosen according to physical intuition.

We are not primarily interested in either the GCM or RGM method but we shall later on make use of a from of 'reference function' of very similar nature to that of the RGM wavefunction. However, our method shares more similarities with the correlated basis-functions discussed later on.

1.2.2 No-core shell models

Historically shell-model calculations have been made assuming a closed, inert core of nucleons with only a few active valence nucleons. In the simplest form of the shell model [5], the valence nucleons exist in atom-like discrete energy levels in a time-averaged nuclear potential well, i.e. the many-body Schrödinger equation is approximated by the sum of single-body hamiltonians and the wavefunction is a Slater determinant of single-particle functions that are eigenfunctions of the single-body hamiltonians. A residual interaction can then be added between the valence nucleons, which can be either 'derived' through some method such as the Hartree-Fock method or phenomenologically obtained through fitting experimental data. The effect of such interaction can be then treated as a perturbation. However, conventional shell-model calculation cannot account for the halo structure [13]. This is due to many-body correlations that are a result of the realistic nucleon-nucleon interaction which in practise can be very different from the residual and time-averaged interactions. A realistic nucleon-nucleon interaction cannot be used in the traditional shell-model to describe the interaction of the valence nucleons with the core and with other valence nucleons, since such interactions have been developed for 'bare' few-body systems.

The no-core shell model [14, 15, 16, 17] is a method of using effective interactions and operators in a truncated Hilbert space that will take into account the many-body correlation effects. In the no-core shell model approach one begins with a purely intrinsic A-particle hamiltonian [14] that can be written as

$$H_A = \hat{T}_{\rm rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j}\frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i<j} V_{NN}(ij), \tag{1.5}$$

where V_{NN} can be any realistic nucleon-nucleon potential that can be either coordinate or momentum dependent. The hamiltonian is then modified by adding to it a harmonic oscillator (HO) center-of-mass hamiltonian, $H^{\rm HO}_{\rm cm}$, where

$$H^{\rm HO}_{\rm cm} = \frac{\vec{P}^2}{2Am} + \frac{1}{2}Am\Omega^2\vec{R}^2 \;\;;\;\; \vec{R}^2 = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i \;\;,\;\; \vec{P} = Am\dot{\vec{R}}. \tag{1.6}$$

The contribution of the HO hamiltonian will be subtracted in the final many-body calculation so the intrinsic properties of the many-body system are not influenced. This procedure yields a new hamiltonian with a pseudodependence on the HO frequency Ω that has the general form

$$H^{\Omega}_A = \sum_i h_i + \sum_{i<j} V^{\Omega}_{NN}(ij). \tag{1.7}$$

The modified hamiltonian facilitates the use of the convenient HO basis. The strong correlations of the bare nucleon-nucleon interaction, however, lead to slowly converging results in the HO basis. This problem can be solved by deriving an effective A-body hamiltonian, $H_{\rm eff}$ in a truncated 'model' space from the full HO space. The model space and the excluded space are such that $H_{\rm eff}$ does not have any matrix elements between the two. For practical purposes $H_{\rm eff}$ must be further approximated. There is a systematic way of obtaining the effective hamiltonian as a result of the fact that the no-core shell model assumes that all nucleons are active. The no-core shell model has been applied to ^{12}C using large-basis calculations [17], where a two-body effective interaction was derived microscopically from modern nucleon-nucleon potentials.

In general the no-core shell model is a microscopic approach for calculating nuclear properties and for A=3 and A=4 it reproduces the results obtained by other exact ap-

proaches such as the GFMC. However as the model space size increases the approximated effective interaction can yield results that are not fully convergent.

1.2.3 Correlation-based approximations

There exist a family of theoretical models, where the many-body wavefunction Ψ is explicitly constructed by making use of a correlation operator $\hat{F}$ that acts on some starting function Φ_0:

$$\Psi = \hat{F}\Phi_0. \tag{1.8}$$

Such an approach is the coupled cluster method (CCM). Here the wavefunction is expanded in terms of an exponentiated correlation operator acting on a model state. We give a more thorough description of this method in the next chapter (chapter 2). The important property of the CCM is that is open to a variety of approximation schemes and in particular to a linearized one that leads to a variational problem for the ground state energy. Another approach is the Jastrow variational method, [18], also described in chapter 2. The Jastrow variational wavefunction is in general composed of the product of a non-linear state-dependent correlation operator and a reference function that describes the uncorrelated wavefunction (usually a Slater determinant). The correlation operator contains a number of non-linear variational parameters. An admixture of the linearized version of CCM and that of the Jastrow method can yield a highly accurate method for the case of light nuclei and is the one we shall make use of.

The same approach also exists under a different name of the 'correlated basis functions' (CBF) method [19, 20, 21], which was extended up to medium-heavy mass nuclei with the use of semi-realistic interactions. Furthermore, the CBF with state-dependent correlations was used to investigate the ground-state properties of the closed shell nuclei ^{16}O and ^{40}Ca [22] using realistic nucleon-nucleon interaction including tensor components. CBF is a more complicated method that systematically improves the wavefunction.

1.2.4 Monte-Carlo methods

The first approach of Monte Carlo methods to nuclei interacting with realistic potentials was through the variational Monte Carlo (VMC) calculation [23]. This is essentially a method of statistically evaluating the integrals involved in the variational problem. We

describe this method in some detail in chapter 4. Strictly speaking the VMC is not a method on its own but a means of evaluating expectation values. However, it allows the application of some advanced correlation mechanisms, that would otherwise lead to practically impossible analytic evaluations. These involve both state-dependent and state-independent correlation mechanisms involving both linear and non-linear terms. We shall make use of such correlations in the next chapter.

The next step after the VMC is the Green's function Monte Carlo method (GFMC) [1]. This shares a lot of similarities with the older method of diffusion Monte Carlo that has been used in the past [24] for some model calculations. While the VMC finds an upper bound to the eigenvalue of some hamiltonian, the GFMC projects out the lowest-energy eigenstate from a trial wavefunction (usually found using VMC) Ψ_T. The full wavefunction Ψ_0 for the ground state is obtained through the propagation of the trial function

$$\Psi_0 = \lim_{\tau\to\infty} \exp[-(\hat{H} - E_0)\tau]\Psi_\tau, \tag{1.9}$$

At the above limit the GFMC can provide a statistically exact value for the ground state. However, in practise the evaluation of $\exp[-(\hat{H} - E_0)\tau]$ is made by introducing a small time step, $\Delta\tau = \tau/n$, giving

$$\Psi(\tau) = \{\exp[-(\hat{H} - E_0)\Delta\tau]\}^n \Psi_T = G^n \Psi_T \tag{1.10}$$

The GFMC has been used up to A=10 nuclei [25, 26], although beyond $A = 4$ calculations suffer significantly from the well-know fermion sign problem. It must be noted that the calculations for $A = 10$ require ≈10000 processor hours on modern massively parallel computers.

In general, Monte Carlo methods is a rapidly growing area of nuclear physics and particular for the evaluation of semi-realistic interactions but at the time being are restricted to light nuclei due to the complexity of the many-body problem.

1.3 Existing models for halo nuclei

Different kinds of theoretical models are currently being used to investigate the halo structure. One of the early works on halo nuclei was an intermediate between shell

model calculations and fully microscopic ones, is the so called *cluster-orbital shell model* [27, 28, 29]. This model employs a wave function of the alpha-cluster form but uses a Hamiltonian which is not fully microscopic. In such a model the nucleus is described as a system of valence nucleons weakly coupled to the core. The motion of the valence nucleons is described in terms of radius vectors measured from the CM of the core, obtained by the use a non-orthogonal transformation. This results in a translationally invariant formalism where the Hamiltonian is broken into three parts: the core Hamiltonian, a single particle part for the valence nucleons, and the interaction part between valence nucleons. The interaction between valence nucleons and the core is described by a single particle effective potential, adjusted to fit experimental results. In the case of a core and a weakly bound nucleon [27], the general form of the wave function is

$$\Psi = \mathcal{A}\{\Phi^{\text{core}}(\rho_c\sigma_c\tau_c)u_{lj}(x)[Y^l_{m_l}(\hat{\mathbf{x}})\otimes\chi_{1/2}]^j_m\} \tag{1.11}$$

where ρ_c represents the core relative coordinates, while $\vec{x}$ the coordinates of the additional nucleon with respect to the core center-of-mass. The 'relative motion' function u_{ij} assigns the radial dependence of the additional nucleon while $[Y^l_{m_l}(\hat{\mathbf{x}})\otimes\chi_{1/2}]^j_m$ assigns angular dependence in the spin-orbit coupling scheme. Applications of this model include the isotopes ^{6}He and ^{8}He of ^{4}He [27, 28], as well as ^{11}Li [29]. In general the binding energies obtained are lower than the experimental values by an amount between 0.5 and 1.4 MeV, while the matter radii are in reasonable agreement with experimental values.

When shell model calculations are considered, single particle wave functions are provided from a certain mean field potential assuming stable single particle motion. The shell model calculation is then carried out to treat the residual interaction between nucleons moving on such stable single particle orbits. In neutron rich nuclei where the last neutrons are forced to occupy loosely bound or even unbound orbits of the mean potential, the validity of shell model calculations can be questioned. T. Otsuka et al [30], proposed a variational shell model in order to describe the structure of such nuclei. The model was applied to ^{11}Be, where by using a Skyrme interaction the observed ground state of this nucleus was reproduced correctly. In general mean field approximations proved to be of restricted validity because of the weak binding of the halo neutrons. It was realized that a more realistic approach to the halo structure would rely on microscopic many-body mod-

els. After about 1991 a large amount of theoretical research treating halo structure in such a manner has been going on. An account of all of the current research is impossible, but an outline of the main type of models used is described in the rest of this section.

In one of the early models, the main features of ^{11}Li were qualitatively reproduced based on three body calculations [31]. This was based on a simple model with an inert ^{9}Li core interacting with two mutually interacting neutrons. The Faddeev three-body equations in coordinate space were solved, using realistic neutron-neutron interactions for the halo neutrons and an effective neutron-core interaction where parameters were fixed to reproduce experimental data. A fully microscopic calculation for ^{6}He was performed [32], where the Afnan and Tang S3 potential was used, supplemented by a tensor term. The model treated the nucleus as a three-body system, involving different configurations of spin-orbit coupling. A thick neutron halo was found, which was not far from experimental data.

The neutron halo structure of ^{6}He and of ^{8}He was studied in a microscopic three-body and five-body model, respectively (alpha particle and single neutrons) by Varga et al [33]. A stochastic variational calculation was used to determine an adequate set of basis functions for an RGM like intercluster wave function, taking account for various relative angular momentum arrangements. The spin of the clusters and angular momenta (belonging to independent Jacobi coordinates) were coupled to a total spin and total angular momentum. A central effective nucleon-nucleon interaction was used, were a parameter was adjusted to give the nearly correct ground state energy of ^{6}He. Zero total spin and angular momentum were considered. The ground state energy of ^{8}He was reproduced with fair accuracy. The wave function and some physical properties were calculated such as the neutron, proton and the point matter rms radii. The model gave an excellent estimate for the neutron skin, but it gave a larger rms radius for ^{6}He than for ^{8}He.

Following the above formalism another paper, [34], mainly by the same authors, discussed extensions of the multicluster model. These were aimed to describe non-uniform density distributions characteristic of the halo structure. Clusters such as the alpha particle, triton, ^{3}He, proton and neutron were used. The additional nuclei studied were ^{8}Li, ^{9}Li, ^{8}B, ^{9}C and ^{6}Li. The obtained wave functions were used to discuss spatially extended halo structures, where in the case of ^{6}Li it was argued that the halo structure may appear even in stable nuclei as the isospin increases.

The GCM was applied to the ^{17}B nucleus [7], using a three cluster model. This involved a wave function composed by different ^{13}B + dineutron + dineutron configurations corresponding to different spatial arrangements, where projections over total angular momentum and parity of ^{17}B were performed. The ^{13}B wave functions were constructed in the HO model with all possible configurations in the 1p shell, so that core excitations could be taken into account. The radius and quadrupole moment and densities of the ^{17}B ground state were investigated. It was found that the neutron density extends very far outside the ^{13}B core, supporting the picture of a halo structure in ^{17}B. Further work based on the same method was performed by the same author concerning the ^{14}Be, ^{11}Be and ^{11}N nuclei [8, 9].

More resent work on ^{6}He involves the improvement of the RGM three-cluster wave function, to an "extended three-cluster model" [35]. The aim is to improve the description of the alpha-particle core, by assuming that is composed of a three-cluster 0s state and a single nucleon. This results in the inclusion of a t-t (triton-triton) configuration in the initial α+n+n model (pure three cluster model) allowing for a core breakup configuration caused by the halo neutrons. The main conclusion of this paper was that the precise value of the energy as well as other properties of a halo nucleus require a realistic treatment of the core. This was based upon showing that a t-t inclusion affects the tail behaviour of the core thus effecting the binding of the halo nucleons.

1.4 General remarks

The number of existing many-body methods and models for the few-body problem is too large to summarize in just one chapter. We have mentioned only a few and in particular those related to our problem. The numerical accuracy and sophistication of the various methods and models used is constantly improving.

The main drawback of cluster models is a partial implementation of the Pauli exclusion principle, and the use of not very realistic interactions. The model we are going to develop in a way follows the multi-cluster models described, but implements the Pauli principle completely. We shall make use of a variational approximation of the many-body Scrödinger equation. We aim to investigate the structure of the lightest neutron-halo states as an extension of previously existing work for the alpha-particle. For this purpose we do

not aim at sophistication but in a consistent model that is easy to apply and at the same time can be extended to more complicated approximations. We shall introduce a cluster structure by restricting the symmetry of the subspace used and at the same time keep the fully microscopic nature of the wavefunction.

In the next chapter (chapter 2) we examine the coupled cluster method and its truncation to a linearized version. This is enhanced by the addition of central Jastrow correlations. We pay attention in the inclusion of state-dependent correlations. The method is examined by applying it to the alpha-particle, where comparison can be made with other methods.

Chapter 3 describes the cluster model that we shall make use of. Particular emphasis is given to the inclusion of the correct symmetry properties and in particular permutation symmetry. Some types of semi-realistic nucleon-nucleon interactions are described.

Chapter 4 deals with the numerical method. This is a rather technical chapter. The fact that we are using the VMC to calculate the matrix elements, implies that the error estimate is statistical. We ensure that the statistics are ‘healthy’, in the sense that we get a reliable error estimate. Furthermore, we examine possibilities of improving this method.

The results of the cluster model for a few light nuclei are given in chapter 5, while chapter 6 contains the conclusions and a discussion for possible extensions of this research.

Chapter 2

Linearized trial wavefunctions

In this thesis we are concerned with the approximation of the few-body Schrödinger equation in terms of a linear variational problem. The most basic ingredient in such an approximation is the construction of the trial wavefunction. One way of doing this is by appropriately approximating some rather complicated, usually non-linear, parametrization. One type of such a parametrization is given by the Coupled Cluster Method (CCM). The first part of this chapter gives a brief description of the CCM wavefunction and the ways of performing approximations appropriate to our study.

Another type of non-linear parametrization of the many-body wavefunction that is variational in nature is the Jastrow method [18, 36, 37]. We also provide a brief discussion of this technique and ways of approximating it. The final form of the wavefunction that we shall make use of is obtained by combining these two methods in a way appropriate for a linear variational method.

The effectiveness of the approximation scheme is illustrated by considering the calculation for the ground-state of the alpha-particle. For this purpose we quote results from a number of authors as well as our own. Apart from the ground-state energy, we also examine the calculation of the one- and two-body density distributions that can be used to provide qualitative information about the wavefunction.

Later on our objective will be to apply the approximation described in this chapter to light halo nuclei beyond the alpha particle. Therefore, the method illustrated in this chapter will be central to the whole thesis.

2.1 Basic Elements of the Coupled Cluster Method

The Coupled Cluster Method (CCM) is a non-perturbative microscopic method for approaching the many-body problem. Detailed reviews of this method can be found in a number of places such as [38, 39, 40]. Although we are not primarily interested in the formalism of the CCM we shall make use of an approximation of the wavefunction provided by this method and particularly a linearized translationally-invariant form in coordinate representation.

2.1.1 Reference states

In the case of many-body problems it is often convenient to introduce the idea of reference states. In general a set of reference states, $\{|\Phi_i\rangle; i = 0, 1, ..., D\}$, is used, where the orthonormality condition $\langle\Phi_i|\Phi_j\rangle = \delta_{ij}$ can be assumed to be satisfied (since it can always be imposed). The reference states form the basis of a D-dimensional subspace of the full Hilbert space, referred to as the 'model space'.

In the case of the Coupled Cluster Method (CCM) the reasoning behind the introduction of these reference states is that the set $\{|\Phi_i\rangle\}$ can act as starting functions, from which we can construct the full wavevefunction by the action of correlation operators. A non-degenerate ground state corresponds to the case of a single reference state ($D = 0$) and is referred to as the 'single-reference' version of the CCM.

The reference state should be constructed to obey the symmetries of the exact ground-state, while the correlation operators of CCM can be scalar operators that do not carry any quantum numbers (this is not necessary but is the simplest case). Furthermore, it is always convenient for such a state to have an analytic description, since a large part of the CCM will require calculations involving the reference function alone. When considering a many-fermion system, a non-interacting many body wave function or ground state can often be described by a Slater determinant. Such a state can serve as the reference state. It is well known that in the language of second quantization a Slater determinant can be written as

$$|\Phi_0\rangle = \prod_{i=1}^{N} a^\dagger_{\nu_i}|0\rangle \ , \tag{2.1}$$

where N is the number of particles and the $a^\dagger_{\nu_i}$ are fermion creation operators that obey

the usual anticommutation relations and are defined by their action on the vacuum state $|0\rangle$. The occupied single particle states $\{|\nu_i\rangle;\ i = 1, 2, ..., N\}$ are referred to as hole states, while the set $\{|\rho_i\rangle;\ i = 1, 2, ...\}$ corresponds to states unoccupied in $|\Phi_0\rangle$ and orthogonal to the hole states $\{|\nu_i\rangle\}$, referred to as particle states.

Once a reference state is provided in terms of a slater determinant with respect to a set of hole states $\{|\nu_i\rangle\}$, a more general determinant that mixes particle and hole states is provided by Thouless theorem [41], where

$$|\Phi_0^{'}\rangle \ = \ e^{\hat{S}_1}|\Phi_0\rangle \ . \tag{2.2}$$

The operator $\hat{S}_1$ is a one-body operator which acts on $|\Phi_0\rangle$ to produce a one-particle/one-hole (1p-1h) excitation. In the notation of particle/hole states it has the explicit form

$$\hat{S}_1 = \sum_{l=N+1} \sum_{k=1}^{N} \langle \rho_l | \hat{S}_1 | \nu_k \rangle a_{\rho_l}^{\dagger} a_{\nu_K} \ . \tag{2.3}$$

The new reference state $|\Phi_0^{'}\rangle$ is non-orthogonal to the original state $|\Phi_0\rangle$.

2.1.2 The exp(S) expansion

The time-independent Schrödinger equation for the ground state wave function $|\Psi_0\rangle$ is

$$H|\Psi_0\rangle = E_0|\Psi_0\rangle \ , \tag{2.4}$$

where H is a many-body Hamiltonian. As described in the previous section the exact ground state $|\Psi_0\rangle$ can be expanded in terms of a model state $|\Phi_0\rangle$ and states orthogonal to $|\Phi_0\rangle$, resulting from the dynamical correlations induced by H. Thouless theorem allows the inclusion of the simplest correlations in terms of 1p-1h excitations. A correlation operator describing a general mp-mh correlation is

$$\hat{S}_m = \frac{1}{(m!)^2} \sum_{\rho_1,...,\rho_m} \sum_{\nu_1,...,\nu_m} \langle \rho_1, ..., \rho_m | \hat{S}_m | \nu_1, ..., \nu_m \rangle_A a_{\rho_1}^{\dagger} ... a_{\rho_m}^{\dagger} a_{\nu_m} ... a_{\nu_1} \ , \tag{2.5}$$

where the subscript A denotes an antisymmetric state. As a result of the fermionic anti-commutation properties

$$\{a^{\dagger}_{\rho_i}, a_{\nu_j}\} = \delta_{ij}\delta_{\rho\nu}, \quad \{a_{\rho_i}, a_{\nu_j}\} = 0, \tag{2.6}$$

correlation operators involving different number of particles commute with each other, i.e. $[\hat{S}_m, \hat{S}_n] = 0$. Furthermore, the successive application of the same correlation operators will result in terms involving each particle label only once (otherwise repetitive applications of the same creation/distraction operator will give zero). Therefore, application of the operator $(\hat{S}_m)^n$ will result in all possible $n!$ terms that involve $n \times m$ distinct particle labels.

In the CCM formalism the exact ground state wave function is expanded over a set of states that contains all possible correlated independent particle clusters. For example in the case of only two-body correlation operators, the expansion takes the form of

$$|\Psi_0\rangle \simeq \left(1 + \hat{S}_2 + \frac{1}{2!}(\hat{S}_2)^2 + \frac{1}{3!}(\hat{S}_2)^3 + ...\right)|\Phi_0\rangle \tag{2.7}$$

$$= \exp(\hat{S}_2)|\Phi_0\rangle \tag{2.8}$$

where the expansion can be written as an exponential regardless of the number of occupied states in the reference state, since all terms involved with a number of operators greater than the number of occupied states will give a zero result. When all possible cluster sizes are taken into account, an N-body ground state wave function can be constructed from the reference state as

$$|\Psi_0\rangle = \left(\exp(\hat{S}_1)\exp(\hat{S}_2)...\exp(\hat{S}_N)\right)|\Phi_0\rangle \tag{2.9}$$

$$= \exp(\hat{S})|\Phi_0\rangle \ , \tag{2.10}$$

where

$$\hat{S} = \sum_{i=1}^{N} \hat{S}_i \ . \tag{2.11}$$

The exponential character of equation (2.10) is an important characteristic of the CCM. As a result of the commutation of the operators in (2.11) the CCM exponential parametrization obeys size-extensivity. A size-extensive method ensures that a calculation on a com-

pound system consisting of a number of non-interacting sub-systems yields a calculated value that is the same as that of the individual subsystem values. An important advantage of a size-extensive method is that it allows straightforward comparisons between calculations involving variable numbers of components, e.g. ionization processes or calculations using different numbers of active electrons. Lack of size-extensivity implies that errors from the exact energy increase as more components enter the calculation.

2.1.3 Ground state energy

After a choice for the model state $|\Phi_0\rangle$ is made, the CCM parametrization for the exact ground state is

$$|\Psi_0\rangle \;=\; \exp(\sum_{I\neq 0} s_I c_I^\dagger)|\Phi_0\rangle, \tag{2.12}$$

with $\{c_I^\dagger\}$ representing a complete set of multiconfigurational creation operators, and s_I the CCM coefficients:

$$c_1 = a_{\rho_1}^\dagger a_{\nu_1}; \qquad s_1 = \langle\rho_1|S_1|\nu_1\rangle, \tag{2.13}$$

$$c_2 = a_{\rho_1}^\dagger a_{\rho_2}^\dagger a_{\nu_2} a_{\nu_1}; \qquad s_2 = \langle\rho_1\rho_1|S_1|\nu_1\nu_2\rangle, \tag{2.14}$$

$$\ldots \quad .$$

By inserting this parametrization into the ground state Schrödinger equation, and by projecting either onto the model state or onto the states orthogonal to it ($c_I^\dagger|\Phi_0\rangle$), we obtain an equation for the ground state energy

$$E_0 \;=\; \langle\Phi_0|e^{-\hat{S}}\hat{H}e^{\hat{S}}|\Phi_0\rangle, \tag{2.15}$$

and a set of coupled nonlinear equations for the unknown coefficients s_I

$$\langle\Phi_0|c_I e^{-\hat{S}}\hat{H}e^{\hat{S}}|\Phi_0\rangle \;=\; 0 \;\;, \forall I \neq 0. \tag{2.16}$$

A very important property of (2.15) and (2.16), arising from the exponential representation employed by the CCM, is that the expansion of the terms within the expectation value is of finite order. This is a result of the nested commutator expansion for the term

$e^{-\hat{S}}\hat{H}e^{\hat{S}}$ which has the form

$$e^{-\hat{S}}\hat{H}e^{\hat{S}} = \hat{H} + [\hat{H},\hat{S}] + \frac{1}{2!}[[\hat{H},\hat{S}],\hat{S}] + ... \ . \tag{2.17}$$

The above expansion is of finite order due to the fact that $\hat{H}$ is finite. Although the equations for the ground state energy are of finite order it is necessary for practical purposes to further approximate due to the complexity of the many-body problem. The simplest way of doing this is by performing a SUB(n) truncation. This implies that all parameters $\{s_I\}$, which describe correlations of clusters of more than n particles-hole pairs, are set to zero. Thus equation (2.11), would be approximated in the SUB(3) truncation by

$$\hat{S} \ \approx \ \hat{S}_1 \ + \ \hat{S}_2 \ + \ \hat{S}_3 \ . \tag{2.18}$$

The SUB(n) truncation when applied to an A-particle system, will still contain the excitation of multiple independent kp-kh pairs (with k ranging up to n), as a result of the exponential expansion that involves higher powers of $\hat{S}$. Therefore instead of solving for the full equations (2.15) and (2.16) which contain the exact g.s. wave-function, the resulting truncated equations are used. Such an approximation scheme has the property that it maintains size extensivity.

2.1.4 Translational invariance

A problem that can arise in the CCM formalism when performing a SUB(n) truncation is due to possible symmetry violations. In general the symmetries obeyed by the exact system should also be present in the approximated system, unless the effect on the calculated quantity is within some accepted limits. For example, violating translational invariance in medium- to heavy-mass nuclei might not greatly effect the binding energy, while violating permutation symmetry will result in a bosonic rather than a fermionic system. Such symmetry violations may result either from the construction of the model state (reference state) or from the action of the cluster operators $\{\hat{S}_n\}$. A symmetry-conserving calculation must involve a model state which satisfies the required symmetry and cluster operators which commute with the generators of the transformation.

The problem of preserving translational invariance is of particular importance in ap-

proximate solutions for light nuclei, since it can contribute substantially to the expectation value of the hamiltonian for the binding energy. One way of dealing with this problem is to construct a reference state depending only upon the system relative coordinates. This, however, might result in unwanted complexity. An alternative way is to construct a reference state $|\Phi\rangle$ that can be separated into the product relative and center-of-mass parts, i.e.

$$\Phi = |\Phi_{\rm rel}\rangle|\Phi_{\rm CM}\rangle, \tag{2.19}$$

where $\Phi_{\rm rel}$ represents the relative and $\Phi_{\rm CM}$ the center-of-mass part. The expectation value for the ground state energy becomes

$$\begin{aligned} E &= \frac{\langle\Phi|H|\Phi\rangle}{\langle\Phi|\Phi\rangle} && (2.20)\\ &= \frac{\langle\Phi_{\rm rel}|H_{\rm rel}|\Phi_{\rm rel}\rangle\langle\Phi_{\rm CM}|\Phi_{\rm CM}\rangle + \langle\Phi_{\rm CM}|H_{\rm CM}|\Phi_{\rm CM}\rangle\langle\Phi_{\rm rel}|\Phi_{\rm rel}\rangle}{\langle\Phi_{\rm rel}|\Phi_{\rm rel}\rangle\langle\Phi_{\rm CM}|\Phi_{\rm CM}\rangle} && (2.21)\\ &= \frac{\langle\Phi_{\rm rel}|H_{\rm rel}|\Phi_{\rm rel}\rangle}{\langle\Phi_{\rm rel}|\Phi_{\rm rel}\rangle} + \frac{\langle\Phi_{\rm CM}|H_{\rm CM}|\Phi_{\rm CM}\rangle}{\langle\Phi_{\rm CM}|\Phi_{\rm CM}\rangle} = E_{\rm rel} + E_{\rm CM}, && (2.22) \end{aligned}$$

with $H_{\rm rel}$ and $H_{\rm CM}$ representing the hamiltonian relative and CM, respectively, while $E_{\rm rel}$ and $E_{\rm CM}$ are the contributions to the energy from the relative and CM. This alternative approach will require the subtraction of the CM contribution, $E_{\rm CM}$, from the system's expectation value E.

Furthermore, the reference state alone cannot account for the conservation of translational symmetry, due to the fact that application of $(\hat{S})$ on the reference state will not necessarily result in a correlated state that preserves such symmetry. Further adjustment of the CCM parametrization is required.

Harmonic oscillator reference state

A choice for the model state that can be separated into the product of center-of-mass and relative parts is to consider products of harmonic-oscillator (HO) single-particle wave functions. These are defined in terms of creation operators acting on the vacuum state

$$|\Phi\rangle \;=\; \prod_{nlm} a^{\dagger}_{nlm}|0\rangle \;\;, \tag{2.23}$$

where the subscripts refer to the usual HO quantum numbers. In the case of an N-boson system the reference state can be written as

$$|\Phi\rangle \;=\; \frac{1}{\sqrt{N!}}(a^{\dagger}_{000})^{N}|0\rangle \;. \tag{2.24}$$

The fact that the set of quantum numbers (n, l, m) are all set to zero corresponds to a boson-condensate, where all particles are allowed to occupy the same state. Such a reference state can also be used for a number of fermion systems that can be approximated or described by spin-isospin saturated systems (such as the alpha-particle to be introduced shortly). In coordinate representation the resultant wave function is the product of N oscillator wave functions given by

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \;=\; \prod_{i=1}^{N} \Phi_{000}(\mathbf{r}_i) \;\; . \tag{2.25}$$

In general the single particle HO wave function is a product of a radial part and an angular part, which can be represented as

$$\langle \mathbf{r}|nlm\rangle \;=\; u_{nl}(\mathbf{r})Y_{lm}(\theta, \varphi) \tag{2.26}$$

In the above equation the function $u_{nl}(\mathbf{r})$ is given in terms of a Laguerre polynomial, while $Y_{lm}(\theta, \varphi)$ is a spherical harmonic.

TICC

As mentioned earlier the choice of the model state alone will not satisfy the translational invariance. Extensive work has been done [42, 43], regarding the inclusion of translational invariance in the $\exp(\hat{S})$ expansion. This involves the inclusion of cluster operators that will not excite the CM of the system. The methods used are based upon a particular SUB(n) approximations of the CC expansion. In the particular case of the SUB(2) approximation, applied to a four-boson system, two basic results were obtained for the cluster operators [39], with the requirement of both translational and rotational invariance. These are:

(i)The S_1 operator cannot occur on its own, otherwise it would violate translational invariance. This requires the coefficients $\{s_1\}$ and $\{s_2\}$ to be coupled, resulting in the

transformation of the cluster operator as

$$S \approx S_1 + S_2 \;\rightarrow\; S^{(1,2)} = \frac{1}{2!}\sum_{\beta_1}\sum_{\beta_2} a^{\dagger}_{\beta_1} a^{\dagger}_{\beta_2} a^{2}_{000} \;\;, \tag{2.27}$$

with β_1 and β_2 representing the quantum numbers (nlm)and ranging over all the possible values, but with only one of them having the index (000) at a particular time.
(ii)The final CCM wave function at the SUB(2) level of approximation $|\Psi_2\rangle$ is given by

$$|\Psi_2\rangle \;=\; :\exp(S^{(1,2)}):|\Phi\rangle \;. \tag{2.28}$$

The reason for the inclusion of the normal order, is due to the fact that higher powers of $S^{(1,2)}$ occurring in the exponential would otherwise excite the CM.

The above formulation based on the SUB(2) level of approximation can be extended to higher order approximations [44]. Such reformulation of the CCM is called Translationally Invariant coupled cluster (TICC) method.

2.1.5 Generalized coordinate representation of the TICC method

The cluster operators used in CCM were originally introduced by using the notation of second quantization. In the case of translational invariance, these cluster operators were shown to have a general representation in coordinate space, depending only on the relative coordinates of the involved particles. For the particular case of TICC(2) (SUB(2) level for TICC), the coordinate representation of the cluster operator (equation (2.27)), for a four-boson system is given by [42]

$$\langle \mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4|S^{(1,2)}|\Phi_0\rangle \;=\; 2\left(\sum_{i<j=1}^{4} S_{1,2}(r_{ij})\right)\langle \mathbf{r}_1\mathbf{r}_2\mathbf{r}_3\mathbf{r}_4|\Phi_0\rangle, \quad r_{ij} = |\mathbf{r}_i - \mathbf{r}_j| \;. \tag{2.29}$$

In the above equation the coordinate dependence of the cluster correlation function $S_{1,2}$ is only on the relative coordinates r_{ij}, where the explicit form is given in terms of HO coefficients. Although the functional form of the correlation operators could be derived for this simple case, it is by no means guaranteed that this will be possible for the general case, due to the complexity of the many-body problem. However we can generalize the result obtained as an approximation for the coordinate representation of cluster operators

[43, 45, 46], that will preserve translational invariance .

By considering the case of TICC_2 we can express the effect of the operator $\exp(S^{(1,2)})$ as a general expansion in coordinate space of the form

$$\Psi(\mathbf{r}_1,...,\mathbf{r}_N) = \left(1 + \sum_{i<j} f(r_{ij}) + \frac{1}{2!}\sum_{i<j}\sum_{k<l}{}' f(r_{ij})f(r_{kl}) + ...\right)\Phi(\mathbf{r}_1,...,\mathbf{r}_N)\ . \quad (2.30)$$

This equation preserves the essential features of the TICC by an additional constraint imposed on summation and denoted by a prime, indicating that no repeated indices can occur when multiple summations are required. The $f(r_{ij})$ are the coordinate representations of the correlation operators with the requirement that they depend on the relative coordinates of the system and preserve the overall symmetry of the reference function. The above correlation functions can be viewed as producing independent clusters in coordinate space. It is furthermore important to note that equation (2.30) is finite, the number of terms depending on the number of particles. For the case of a four-particle system only the first three term shown will appear.

This structure can be generalized beyond the SUB(2) approximation for the full TICC wavefunction [45, 47]. In the most general case the N particle wavefunction looks likes

$$\Psi(\{r_{ij}\},\mathbf{R}) = \hat{C}(\{r_{ij}\})\Phi_{\text{int}}(\{r_{ij}\})\Phi_{\text{CM}}(\mathbf{R}), \quad (2.31)$$

where

$$\hat{C}(\{r_{ij}\}) = 1 + \sum_{i<j}^{N}\hat{C}_2(r_{ij}) + \sum_{i<j<k}^{N}\hat{C}_3(r_{ij},r_{ik},r_{jk}) + \sum_{i<j<k<L}^{N}\hat{C}_4(r_{ij},...,r_{kl}) + ..., \quad (2.32)$$

with $\{r_{ij}\}$ representing the set of relative coordinates. A possible extension that can improve the computation of the ground state energy is the inclusion of state dependence in the representation of the correlation operators [48, 49]. This can be achieved by the spin, isospin and tensor operators, at the cost of greatly complicating the evaluation of matrix elements and is discussed later on in section 2.4.

The benefit in using the above formalism is in the freedom it provides for approximately choosing the functional form of the correlation operators, according to the problem in question. For example in the case of (2.30) the easiest method is to approximate

the two body correlation functions $f(r_{ij})$ in terms of gaussian non-orthogonal functions, [43, 45], of the form

$$f(r_{ij}) = \sum_{n=1}^{n_{\max}} A_n \exp(-b_n r_{ij}^2). \tag{2.33}$$

The finite value $n_{\max}$ indicates a truncation, as necessary for practical calculations. The coefficients A_n can now be determined by a numerical calculation or in the case of a linear approximation as the linear coefficients of a generalized eigenvalue problem. The parameters b_n, together with the HO parameter α are chosen such that they minimize the expectation value of the Hamiltonian.

Although alternative approaches have been carried out in order to obtain an optimal functional representation for the correlation functions [45], the particular choice of a gaussian expansion has been proven to be the best. This is mainly due to the fact that such an expansion is much simpler to implement and produces essentially the same wave function and energy levels as other methods. The correlation functions $\hat{C}(\{r_{ij}\})$ discussed earlier can now easily be described by a more general extension of equation (2.33). This can be done by expressing the cluster functions of equation (2.10) using gaussians of many variables. For example the two-body cluster function containing the linear and quadratic terms, appropriate for a four-particle wave-function can be fully described by [45, 44]

$$\hat{C}_2(r_1, r_2) = \sum_{m \le n}^{m_{max}, n_{max}} A_{mn}\, S\left(e^{(b_m r_1^2 + b_n r_2^2)}\right) . \tag{2.34}$$

The constant and linear term may be recovered by setting either one or both of the parameters (b_m and b_n) to zero. The symbol S indicates that symmetrization with respect to particle indices must be performed.

2.1.6 Linear approximation of TICC wavefunctions

The non-linearity of the TICC wavefunction does not provide an easily accessible framework for examining light nuclei with the use of semi-realistic nucleon-nucleon interactions. However, it is possible to further approximate the expansion for the ground-state wavefunction by considering the removal of the non-linear terms, thus yielding a linear variational problem, similar to the configuration interaction method.

The inclusion of cluster functions containing terms of higher order than the linear

terms can be sometimes excluded, giving rise to a linear approximation of the TICC wave function. This is referred to as TICI (*Translationally invariant Configuration interaction*). The TICI avoids the complications of the full cluster expansion and was found to provide a very reasonable staring point for the calculation of binding energies of light-to-medium nuclei [47, 48, 49]. The wave function of both TICC and TICI can be used to solve the CCM equations (2.15) and (2.16). A variational approach for the binding energy is also possible, giving an upper bound to the estimated energy.

Therefore the simplest linear approximation for a many body wavefunction, that preserves translational invariance is given in the framework of TICI(2) by

$$\Psi(r_1, ..., r_N) \approx (1 + \sum_{i<j} f(r_{ij}))\Phi_0(\{r_{ij}\})\Phi_0(\mathbf{R}), \tag{2.35}$$

provided that the reference state Φ_0 can be factor into the product of intrinsic and center of mass part.

2.2 Jastrow variational wavefunction

In order to obtain a variational wavefunction using CCM we have to greatly approximate the full wavefunction as illustrated in equation (2.35). This can result in the lose of structure, according to the physical problem in question. One way of significantly improving the structure of a many body wavefunction in the case of extended strongly interacting systems is that of Jastrow [18]. The method has been adapted for finite systems and applied to a number of light nuclei [36, 50].

2.2.1 The general approach

In a system of finite size the wavefunction localizes the particles around the center of mass. If the interaction is strongly repulsive at short distances the wavefunction should be very small or even null when any of the relative particle-particle distances, r_{ij}, vanishes for any pair (ij). Further more when any one of the particles moves away from the rest the independent particle motion should be preserved. These requirements can be fulfilled by putting for each pair of particles a Jastrow correlation factor $f_J(ij)$ which is small when $r_{ij} \to 0$ and goes to a constant when $r_{ij} \to \infty$. Therefore the Jastrow variational function

has the form

$$\Psi_J = \prod_{i<j} f_J(ij)\Phi_0, \tag{2.36}$$

where Φ_0 is a starting function that incorporates all of the single particle characteristics. Furthermore Φ_0 can contain correlations that deal with the long range effects of the nuclear force. The only requirement is that it preserves the symmetries of the Hamiltonian.

2.2.2 Functional form

The choice for the factors $f_J(ij)$ will depend on the problem in question. The simplest choice is to assume some functional form for the f_J which depend on several parameters. The optimal choice for these parameters is the one that minimizes the expectation value of the Hamiltonian. However, according to the problem in question the f_J can incorporate state dependence in terms of operators. A discussion for the inclusion of state dependence is given in [37]. The most general form for the f_J is

$$f_J(ij) = 1 + \sum_{m,p} a_{m,p} g_m(r_{ij}) \hat{O}_p(ij). \tag{2.37}$$

where the $g_m(r_{ij})$ are suitable functions of the relative coordinates, while the $\hat{O}_p(ij)$ are operators acting on the pair (ij). A very common choice for the g_m is in terms of gaussians

$$g_m(r_{ij}) = \exp(-\beta_m r_{ij}^2). \tag{2.38}$$

This way the set of coefficients $a_{m,p}$ and g_m are to be determined by the variational problem. The major problem of this *ansatz* is that the variational parameters cannot be varied independently of each other since they are strongly correlated.

The operators $\hat{O}_p(ij)$ are, apart from the identity operator, can be chosen to be the exchange operators of spin, isospin and spin-isospin labels. This choice is suitable for a scalar state-dependent potential, since the same operators appear in the potential (this is discussed in chapter 3). In general more type of operators can be added, such as tensor operators. The form of equation (2.36) leads to complications when state-dependence is included, since the different operators do not commute with each other and with the hamiltonian, thus leading to a complicated evaluation for the matrix elements, particularly

when antisymmetrization is considered.

2.2.3 Jastrow-TICI variational wavefunction

The coupled cluster method can serve as a general way of unfolding the full wavefunction structure in terms of additive correlation operators. The fact that we are interested in an approximate form for the wavefunction suitable for the linear variational problem can lead to significant decrease in the included structure. This can be enhanced by combining TICC with a Jastrow variational function. This way short range correlations are accounted for by the Jastrow factors, while the TICC correlation operators take abound of the medium to long range effects. The easiest scheme is that where Jastrow and TICI(2) are combined [49], referred to as the J-TICI2 scheme. Such a formalism is similar to that of the correlated basis functions [19, 20, 21, 22], where we have a combination of linear and non-linear correlation operators acting on the wavefunction. In the J-TICI(2) formalism the wavefunction is given by the product of a linear TICI(2) operator (F_L) with the non-linear Jastrow factors (F_J) as

$$\Psi_{J-TICI2} = F_J F_L \Phi_0, \tag{2.39}$$

$$= \prod_{i<j} f_J(ij) \left(1 + \sum_{ij} f_{TICI2}(ij)\right) \Phi_{HO}, \tag{2.40}$$

where the latter equation is the specific form we shall mostly make use of in which a harmonic oscillator reference function, Φ_{HO}, takes care of translational invariance.

We shall examine this formalism in greater detail later in this chapter since it will be one of the methods we shall use.

2.3 The alpha particle

The alpha particle wavefunction is the most important ingredient of the calculation scheme and is important that an adequate structure is provided. The fact that this wavefunction can be obtained in a separate calculation is extremely convenient. One of the main assumptions in our model is that the alpha particle will be described by a spin-isospin saturated state i.e by a 0^+ ground state.

The alpha particle has been one of the starting points for the discussion and testing of

Table 2.1: This table shows the results taken form [42] for the g.s energy in MeV of ^{4}He in the TICC(2) and TICI(2) calculation using the S3 (Wigner part) and MT-V potentials. The correlation functions were expanded in terms of the oscillator basis and n_{max} is the maximum principal oscillator number at which the expansion of the correlation function was truncated.

	S3		MT-V	
n_{max}	TICI(2)	TICC(2)	TICI(2)	TICC(2)
1	-5.357	-5.379	-3.347	-3.640
10	-17.695	-17.818	-17.181	-17.657
20	-24.462	-24.634	-24.445	-24.783
29	-25.294	-25.473	-26.769	-27.062

various microscopic methods and in particular the CCM, Jastrow method and J-TICI. In this section a comparison of this methods as applied to the alpha particle is made. This will serve as an illustration of the previous discussion. Results from a number of authors will be used as well as our own.

2.3.1 TICC and TICI methods

One of the major concerns in the description of light nuclei is the center of mass motion. The TICC provides a unique way of dealing with this problem by employing harmonic oscillator reference states that are separable into relative and center of mass parts. The bosonic 0^+ state of ^{4}He was extensively described in [42] in the TICC(2) approximation and its linear version TICI(2), where the general expression (2.30) for the wavefunction was derived. The calculations were performed in the HO basis in view of what they imply for standard shell-model calculations. A sample of the results is shown in table 2.1.

A remarkable result is that for such a finite system as ^{4}He the relatively simple linear version (TICI) of CCM can provide good results, even at the lowest level of approximation. Although it was found that the TICC(2) calculation is more efficient than its related shell-model ones the final conclusion was that pursuing such calculations in the oscillator representation is not efficient due to convergence problems.

The work of [42] highlighted the fact that in order to make such calculations efficient it is necessary to concentrate on the coordinate representation of the cluster function. In the case of the linear TICI(2) the optimal form of the correlation function of (2.35) was obtained via an Euler-Lagrange approach [51], a rather cumbersome process. Instead, by making the simpler choice of expanding the correlation functions in terms of Gaussian

functions, identical results can be obtained in much more efficient way and certainly less computationally demanding [44].

Furthermore the idea of the Gaussian basis can be extended to give a variational TICC calculation beyond TICI(2) by employing double Gaussian expansion and so on [43, 45, 44]. For example the TICC(2) wavefunction has the general form

$$\Psi_{TICI(2)} = \left(1 + \sum_{i<j} f(ij) + \sum_{i<j}\sum_{k<l} f(ij)f(kl)\right), \tag{2.41}$$

$$f(ij) = \sum_{\nu=1}^{\nu_{max}} A_\nu \exp(-\beta_\nu r_{ij}^2). \tag{2.42}$$

This can be combined in a single expansion giving a wavefunction of the form

$$\Psi = \sum_{\mu<\nu}^{\mu_{max}\nu_{max}} \mathcal{S} A_{\mu\nu} \sum_{i<j} \exp(-\beta_\nu r_{ij}^2 - \beta_\mu r_{kl}^2), \tag{2.43}$$

that includes both the identity and the first order correlation function by allowing 0 in the set of coefficients β. The operator S is a symmetrizer that acts on all particle labels and is essential so that the correlation function preserves the symmetries of the reference function Φ_0. The set of coefficients $\{\beta\}$ are variational parameters, while the $\mu_{max} \times \nu_{max}$ linear components $\{A_{\mu\nu}\}$ are obtained through a generalized linear eigenvalue problem. For convenience this kind of method will be referred to as VTICC(2) in order to emphasize the variational nature of this calculation.

The above can be extended to VTICC(3) where a triple expansion can be used and so on. Instead of using a triple expansion which can be computationally demanding the alternative can be used of combining VTICC(2) with a single Gaussian function depending on the hyperspherical radius $r = (r_{12}^2 + r_{13}^2 + r_{23}^2)^{\frac{1}{2}}$. This is referred to as VTIC$(C(2)+C(3)^S)$, in contrast to the full triple expansion VTICC(3). An outline of the results obtained through Gaussian expansions of this type is given in table 2.2. The results obtained are impressive. The inclusion of higher order correlations greatly improves the results in a very efficient way.

In the description of ^{4}He up to now the cluster operators were state independent. A natural extension is to include state dependence in the cluster operators. This was done

Table 2.2: The ground-state energy of ^{4}He nucleus (expressed in MeV), taken from [45]. Various translationally invariant cluster approximations were used. In the last line we quote the statistically exact result of the Diffusion Monte Carlo (DMC) method [24]

Method	Potential		
	B1	S3 (Wigner part)	MT-V
TICI(2)	-37.82	-25.37	-29.41
VTICC(2)	-37.90	-25.56	-29.59
TICI(2)+VTICC(3)^S	-38.08	-26.67	-30.71
VTICC(3)	-38.26	-27.05	-31.04
VTIC(C(2)+C(3)^S)	-38.17	-26.83	-30.91
VTIC(C(2)+C(3))	-38.30	-27.21	-31.24
DMC	-38.32$\pm$0.01	-27.35$\pm$0.02	-31.32$\pm$0.02

Table 2.3: These results for the ground-state energy of ^{4}He nucleus (expressed in MeV) were taken from [48]. The TICI(2) approximation was used performed both with state independent cluster operators (SI) and state dependent ones (SD).

Method	Potential			
	B1	S3	MS3	MT-V
TICI(2) SI	-37.86	-25.41	-25.41	-29.45
TICI(2) SD	-37.86	-28.19	-27.99	-29.45

for the TICI(2) method [48] where the correlation operator had the form

$$f(ij) = f_c(r_{ij}) + f_\sigma(r_{ij})(\vec{\sigma}_i.\vec{\sigma}_j) + f_\tau(r_{ij})(\vec{\tau}_i.\vec{\tau}_j) + f_{\sigma\tau}(r_{ij})(\vec{\sigma}_i.\vec{\sigma}_j)(\vec{\tau}_i.\vec{\tau}_j), \qquad (2.44)$$

where $\boldsymbol{\sigma}$ and $\boldsymbol{\tau}$ are the spin and isospin matrices respectively. The results given by the authors are displayed in table 2.3, where there is a significant increase in the binding energy for the case of the S3 and MS3 potentials. This is due to the fact that these potentials contain different spin-isospin terms unlike the B1 and MT-V potentials that contain only purely radial (Wigner) and space-exchange (Majorana) terms.

The inclusion of state dependence on cluster operators can be arbitrarily extended in principle so as to include any type of operators including non central ones. However, the calculations become greatly complicated and particular in going beyond a spin-isospin saturated system. The inclusion of a tensor term in the state dependence of the correlation operator was achieved by [49], but this takes us beyond V4 interactions.

2.3.2 Jastrow and Jastrow-TICI methods

We have seen that the application of cluster operators directly in coordinate representation can be very powerful for the description of ^{4}He. There is a close relation between these correlations and the Jastrow factors. If we consider the state independent case where the Jastrow wavefunction Ψ_J is parameterized by a single gaussian, this can be expanded as

$$\Psi_J = \prod_{i<j}(1 - a\exp(-br_{ij}^2)\Phi_0 \tag{2.45}$$

$$= (1 + a\sum_{i<j} e^{-br_{ij}^2} + a^2 \sum_{i<j}\sum_{k<l}{}' e^{-br_{ij}^2} e^{-br_{kl}^2} + ... + a^6 e^{-(br_{12}^2+...+br_{34}^2)})\Phi_0, \tag{2.46}$$

where the prime indicates that the labels k and l are distinct from i and j. If we then consider the case of VTICC(4) where the wavefunction has the form

$$\Psi_{VTICC(4)} = \sum_{n_1\leq...\leq n_6} \mathcal{S}[A_{n_1...n_6} e^{-(b_{n_1} r_{12}^2+...+b_{n_6} r_{34}^2)}]\Phi_0, \tag{2.47}$$

$$= \sum_{n_1\leq...\leq n_6} [A_{n_1...0}\sum_{i<j} e^{-b_{n_1} r_{ij}^2} + A_{n_1 n_2...0}\sum_{i<j}\sum_{k<l}{}' e^{-b_{n_1} r_{ij}^2} e^{-b_{n_1} r_k^2} \tag{2.48}$$

$$+... + A_{n_1...n_6} e^{-(b_{n_1} r_{12}^2+...+b_{n_6} r_{34}^2)}]\Phi_0, \tag{2.49}$$

we can see that the Jastrow wavefunction is similar to the VTICC(4) form. The difference lies in the fact that each term of the VTICC form is given by a linear expansion in terms of gaussians of different widths, while the terms of the Jastrow factor are restricted to a single gaussian. Furthermore, the coefficients $\{a, a^2, ..., a^6\}$ in the case of Jastrow wavefunction are non-linear, something that makes there determination much harder, especially if we want to go beyond a simple gaussian expansion. This due to the fact that the linear $A_{n_1...,n_6}$ coefficients can be determined as the eigenvector of an eigenvalue problem, by pre-assigning the set of non-linear widths $\{b_1, ..., b_6\}$.

Despite the restrictions in the coefficients the Jastrow variational wavefunction can achieve better results than the state dependent TICI(2) or the higher order state independent cluster expansions. This was done in [37], where an expansion up to two gaussians was used, examining both state dependent and state independent cases for the ground state of ^{4}He. The same spin-isospin operators as in (2.44) were used. These results are shown

Table 2.4: Results (form [37]) for the ground-state energy of ^{4}He using the Jastrow variational wavefunction. The SD stands for state dependent correlations, while the SI for state independent ones.

Potential	Correlation	No. of gaussians	Energy(MeV)
S3/MS3	SI	1	-24.4042
S3	SD	1	-25.3598
MS3	SD	1	-25.3119
S3/MS3	SI	2	-27.2136
S3	SD	2	-29.9378
MS3	SD	2	-29.7034
MT-I/III, MT-V	SI	1	-29.0604
MT-I/III	SD	1	-29.3460
MT-I/III, MT-V	SI	2	-30.8752
MT-I/III	SD	2	-32.0107

in table 2.4. The resulting form for the Jastrow factors of equation (2.37) becomes

$$f_J(ij) = 1 + \sum_{m=1}^{N_\beta} e^{-\beta_m r_{ij}^2}[a_{m,c} + a_{m,\sigma}\hat{P}_\sigma(ij)], \tag{2.50}$$

as a result of the spin-isospin saturated state. The sets of coefficients, $\{a_{m,c}\}$, $\{a_{m,\sigma}\}$ and $\{\beta_m\}$ were determined variationally.

Up to now we have seen how the TICI and Jastrow methods individually behave in the case of the alpha particle. The calculation for the ground-state of the alpha particle is a lot easier to perform than for a non-saturated spin-isospin state and particularly when state dependence is considered in the correlations. In order to go beyond the closed shell structure of the alpha particle we require an efficient and at the same time economic approach. As long as central state-independent correlations are concerned the TICI and Jastrow methods provide similar results. When state-dependence is included in either the Jastrow or TICI(2) methods there is a considerable improvement in the calculation of the binding energy. Although the results obtained with the Jastrow method are by a small amount better the inclusion of state dependence is much harder to implement due to the non-linear form of the Jastrow factor, particularly for more complicated systems. However, the central state-independent Jastrow factor can provide valuable short range correlations and should be included.

Therefore we would like a formalism that would avoid the complexity of non linear

Table 2.5: The TICI(2) and J-TICI(2) methods were applied for for the binding energy of ^{4}He (in MeV) [49]. The results obtained by [52] using the Variational Monte Carlo (VMC) and an improved Jastrow factor are also listed and are indicated by (VMC). When applicable SD refers to state-dependence and SI to state-independence.

	TICI(2)		J-TICI(2)		J-TICI(2)(VMC)
Potential	SI	SD	SI	SD	SD
S3	25.41	28.19	27.20	30.16	-
MS3	-	27.99	-	29.97	30.41$\pm$0.02
B1	37.86	-	38.28	-	-
MT-V	29.45	-	31.21	-	-
MT-I/III	-	30.81	-	32.70	32.74$\pm$0.03

state dependent operators and at the same time not exclude state dependence. The simplest way of doing this is by combining central state-independent Jastrow and the state dependent TICI(2) methods. The alpha-particle can be used as a model to examine the effectiveness of such an approach. These calculations were performed in [49] using a Jastrow correlation, parameterised by a single gaussian. Later on Buendia et al [52] improved and extended the application of this method, using the Variational Monte Carlo to calculate the matrix elements, going beyond ^{4}He to the closed shell nuclei of ^{8}Be, ^{12}C and ^{16}O. The results are shown in table 2.5.

It can be clearly seen that the results obtained though this linear approximation are not worst from the state-dependent Jastrow method and that evaluation of the matrix elements with the variational Monte-Carlo (VMC) method can do as well as the analytic evaluation.

2.4 Details of the linear eigenvalue problem

2.4.1 Matrix elements

The key ingredient of the J-TICI(2) approximation is the linear dependence on the spin and isospin operators, something that gives a very similar formalism to that of state-independent approximation. For completeness we give a description of the linear eigenvalue problem that arises since it will be used al over this thesis. This description is valid for an arbitrary system and is not confined to closed shell nuclei. For simplicity we restrict ourselves to central scalar correlations and to local scalar interactions (to be discussed in detail later on).

In the linear J-TICI(2) approximation the wavefunction is given as

$$\Psi = \hat{F}_L \Phi, \tag{2.51}$$

where Φ is the part wavefunction that carries all the required quantum numbers, while $\hat{F}_L$ is the linear operator of the TICI(2) approximation. For compactness we have absorbed the state independent Jastrow factor (same as in (2.37) but without the state dependence) in the function Φ, giving

$$\Phi = F_J \Phi_0, \tag{2.52}$$

$$F_J = \prod_{i<j} \left(1 + f_J(r_{ij})\right). \tag{2.53}$$

Φ_0 is the model function which will depend on the system in question. For the alpha particle this is the 0^+ harmonic oscillator ground state parametrized by a single non-linear parameter α.

The Hamiltonian has the form

$$\hat{H} = -\frac{\hbar^2}{2m_0} \sum_{i=1}^{4} \nabla_i^2 + V, \tag{2.54}$$

where the interaction V can be written as

$$V = V_0 + V_\sigma + V_\tau + V_{\sigma\tau}. \tag{2.55}$$

Apart from V_0 the potential terms depend on the spin (σ) and isospin (τ) variables. The particular form of an individual term such as V_σ is

$$V_\sigma = \sum_{i<j} v_\sigma(r_{ij}) P_{ij}^\sigma, \tag{2.56}$$

with r_{ij} representing the radial distance between particles i and j, while P_{ij}^σ is an operator that exchanges the spin labels of particles i and j. In accordance with the interaction the correlation operator $\hat{F}$ takes the form

$$\hat{F}_L = \hat{F}_0 + \hat{F}_\sigma + \hat{F}_\tau + \hat{F}_{\sigma\tau}. \tag{2.57}$$

As a result of the TICI(2) formalism the individual terms are parametrized as

$$\hat{F}_k = \sum_{i<j} f_k(r_{ij}) P^k_{ij}, \tag{2.58}$$

where $k = 0$ stands for the identity operator (for the state-independent correlations), while $k = 1, 2, 3$ represent the spin, isospin and spin-isospin labels. The functions $f_k(r)$ and $g_J(r)$ are parametrized as a linear combination of gaussians,

$$f_k(r) = \sum_{m=1}^{M} c_m^{(k)} e^{-b_m r^2}, \tag{2.59}$$

$$g_J(r) = \sum_{n=1}^{N} a_n^{(k)} e^{-d_n r^2} \tag{2.60}$$

Therefore, we have $4M$ linear parameters ($c_m^{(k)}$), $M + 2N$ nonlinear ones (b_m, a_n, d_n) and any non-linear parameters entering the model state. The wavefunction is given explicitly in relative coordinates, since the center of mass term is separable and appears on both sides of the eigenvalue problem

$$\hat{H}\Psi = E_0 \Psi \tag{2.61}$$

and can thus be removed. The above eigenvalue problem can be solved by linear variations of the expectation values on the expansion components $\{c_m^{(k)}\}$, with the additional constraint that the wavefunction has a finite norm :

$$\frac{\partial}{\partial c_m^{(k)}} \Big(\langle \Psi | \hat{H} | \Psi \rangle - E_0 \langle \Psi | \Psi \rangle \Big) = 0 \ \ \forall m, k. \tag{2.62}$$

Following [52], the expectation value can be written as

$$\langle \Psi | \hat{H} | \Psi \rangle = \int d\mathcal{R} \Psi^* \hat{H} \Psi, \tag{2.63}$$

$$= \sum_{\chi} \int d\mathcal{R} \langle \Phi_0 | (\hat{F}_L F_J)^\dagger | \mathcal{R}\chi \rangle \langle \mathcal{R}\chi | \hat{H} \hat{F}_L F_J | \Phi_0 \rangle, \tag{2.64}$$

where the $|\mathcal{R}\chi\rangle \equiv |r_1\chi_1\rangle ... |r_n\chi_n\rangle$ is a complete set of states for the n-body system, with $\mathcal{R}$ and χ representing the spatial and spin-isospin degrees of freedom. $|\Phi_0\rangle$ is a state that carries the total angular momentum J and isospin T quantum numbers.

In matrix form we have to solve a $4M \times 4M$ dimensional generalized eigenvalue

problem of the form

$$\begin{pmatrix} \mathbf{H}_0^0 & \mathbf{H}_\sigma^0 & \mathbf{H}_\tau^0 & \mathbf{H}_{\sigma\tau}^0 \\ \mathbf{H}_0^\sigma & \mathbf{H}_\sigma^\sigma & \mathbf{H}_\tau^\sigma & \mathbf{H}_{\sigma\tau}^\sigma \\ \mathbf{H}_0^\tau & \mathbf{H}_\sigma^\tau & \mathbf{H}_\tau^\tau & \mathbf{H}_{\sigma\tau}^\tau \\ \mathbf{H}_0^{\sigma\tau} & \mathbf{H}_\sigma^{\sigma\tau} & \mathbf{H}_\tau^{\sigma\tau} & \mathbf{H}_{\sigma\tau}^{\sigma\tau} \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \\ \mathbf{c}_\tau \\ \mathbf{c}_{\sigma\tau} \end{pmatrix} = E_0 \begin{pmatrix} \mathcal{N}_0^0 & \mathcal{N}_\sigma^0 & \mathcal{N}_\tau^0 & \mathcal{N}_{\sigma\tau}^0 \\ \mathcal{N}_0^\sigma & \mathcal{N}_\sigma^\sigma & \mathcal{N}_\tau^\sigma & \mathcal{N}_{\sigma\tau}^\sigma \\ \mathcal{N}_0^\tau & \mathcal{N}_\sigma^\tau & \mathcal{N}_\tau^\tau & \mathcal{N}_{\sigma\tau}^\tau \\ \mathcal{N}_0^{\sigma\tau} & \mathcal{N}_\sigma^{\sigma\tau} & \mathcal{N}_\tau^{\sigma\tau} & \mathcal{N}_{\sigma\tau}^{\sigma\tau} \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \\ \mathbf{c}_\tau \\ \mathbf{c}_{\sigma\tau} \end{pmatrix}, \tag{2.65}$$

where the block matrices are given as

$$\mathbf{O}_{k'}^k = \langle\Psi|(\hat{F}_k)^\dagger O \hat{F}_{k'}|\Psi\rangle \tag{2.66}$$

$$(\mathbf{H}_p^k)_{lm} = \langle\Phi|(F_k^l)^\dagger \hat{H} F_p^m|\Phi\rangle, \quad (\mathcal{N}_p^k)_{lm} = \langle\Psi|(F_k^l)^\dagger F_p^m|\Phi\rangle, \tag{2.67}$$

$$F_k^l = \sum_{i<j} e^{-b_l r_{ij}} P_{ij}^k, \tag{2.68}$$

while the $\mathbf{c}_k$ are column vectors of dimensions M each. Apart from the integration involved the matrix elements require the expectation values of the exchange operators. These will depend on the quantum numbers of the model state and will be discussed in detail in the next chapter. As long as the spatial integrals are involved we shall make use of the variational Monte Carlo method (discussed in detail in chapter 4)

2.4.2 The alpha particle

If we only consider the spin-isospin saturated state corresponding to the ^{4}He the calculation greatly simplifies. As a result of the spatial symmetry of the ^{4}He ground state and the antisymmetry of the total wavefunction, the identity

$$P_{ij}^\sigma P_{ij}^\tau P_{ij}^{\sigma\tau} = -1, \tag{2.69}$$

reduces the exchange operators to a single one:

$$P_{ij}^\sigma = -P_{ij}^\tau, \quad P_{ij}^{\sigma\tau} = -P_{ij}^x = -1. \tag{2.70}$$

Therefore, the nucleon-nucleon interaction has the form

$$V = V_0 + V_\sigma$$

and thus the alpha particle wavefunction has the similar form

$$|\Psi\rangle = (\hat{F}_0 + \hat{F}_\sigma)|\Phi\rangle|\chi_{\sigma\tau}\rangle, \tag{2.71}$$

where $|\chi_{\sigma\tau}\rangle$ is just a slater determinant of the spin and isospin variables. The fact that we don't have spin-orbit terms in our interaction allows the spatial and spin-isospin parts to be separated from each other and apart from the spatial integrals we have expectation values of the form

$$\langle\chi_{\sigma\tau}|(\hat{F}_k)^\dagger V_{k'}\hat{F}_{k''}|\chi_{\sigma\tau}\rangle, \quad \langle\chi_{\sigma\tau}|(\hat{F}_k)^\dagger\hat{F}_{k''}|\chi_{\sigma\tau}\rangle, \tag{2.72}$$

that contain the structure provided by the state dependence in the correlation functions. An equivalent way to that of expansion (2.63) is by making use of the hermiticity of the antisymmetrization operator: The spin-isospin saturated slater determinant can be expressed by the action of a normalized antisymmetrization operator on a single state,

$$|\chi_{\sigma\tau}\rangle = \mathcal{A}|++,+-,-+,--\rangle, \tag{2.73}$$

$$\equiv \mathcal{A}|0\rangle, \tag{2.74}$$

where $(\pm,\pm)$ refers to the state of the isospin and spin variables of a particular nucleon (up or down). Both operators $\hat{F}_0$ and $\hat{F}_\sigma$ commute with $\mathcal{A}$ and as a result of the hermiticity and idempotence of $\mathcal{A}$ we have that

$$\langle\chi_{\sigma\tau}|(\hat{F}_k)^\dagger V_{k'}\hat{F}_{k''}|\chi_{\sigma\tau}\rangle = 4!\langle\chi_{\sigma\tau}|(\hat{F}_k)^\dagger V_{k'}\hat{F}_{k''}|0\rangle \tag{2.75}$$

As a result of the above the required expectation values of the spin exchange operators are:

$$\langle\chi_{\sigma\tau}|P^\sigma_{ij}|0\rangle, \quad \langle\chi_{\sigma\tau}|P^\sigma_{ij}P^\sigma_{kl}|0\rangle, \quad \langle\chi_{\sigma\tau}|P^\sigma_{ij}P^\sigma_{kj}P^\sigma_{mn}|0\rangle. \tag{2.76}$$

The key point in the above expectation values is that the action of the exchange operators on the ket state $|0\rangle$ will give zero unless the resultant ket state is different from $|0\rangle$ only by a permutation in which case the expectation value is the parity of that permutation. A sample of such expectation values is shown in table 2.6.

Although the above way provides a systematic method of obtaining the expectation

Table 2.6: Some of the expectation values for the spin exchange operators of ^{4}He. $\langle P\rangle$ denotes $\langle\chi_{\sigma\tau}|P|0\rangle$ with $|0\rangle = |++,+-,-+,--\rangle$, where for each pair $(\pm,\pm)$ the first symbol denotes the isospin and the second the spin.

ij	$\langle P^\sigma_{ij}\rangle$	$ij\ kl$	$\langle P^\sigma_{ij}P^\sigma_{kl}\rangle$	$ij\ kl\ mn$	$\langle P^\sigma_{ij}P^\sigma_{kl}P^\sigma_{mn}\rangle$
12	-1	12 12	1	12 12 12	-1
13	1	12 13	-1	12 12 13	1
14	0	12 14	0	12 12 14	0
23	0	12 23	0	12 23 34	1
24	1	12 24	-1	14 24 34	1
34	-1	12 34	1	12 24 34	0

values for the exchange operators the cost of missing some important simplifications. Furthermore, one has to devise an efficient algorithm to perform such a counting process since the number of terms to be considered will rabidly increase with the number of particles. One major simplification that arises as a result of the saturated spin-isospin structure of the alpha particle is the fact that

$$\langle\chi_{\sigma\tau}|P^\sigma_{ij}|\chi_{\sigma\tau}\rangle = \langle\chi_{\sigma\tau}|P^\sigma_{ij}P^\sigma_{kl}P^\sigma_{mn}|\chi_{\sigma\tau}\rangle = 0, \tag{2.77}$$

something not immediately obvious from the solution of equations (2.76). These results will be derived in detail in a later chapter and are of central importance to the extension of this method to more complicated systems where the complexity that can be avoided is of crucial importance. The key concept is the decomposition of the total wavefunction into states of conjugate permutation symmetry and the further decomposition of these states into spin/isospin states belonging to SU(2) symmetry.

As a result of the mentioned simplification the matrices of the generalized eigenvalue problem reduce to

$$\begin{pmatrix} (\hat{\mathbf{K}}+\mathbf{V}_0)^0_0 & (\mathbf{V}_\sigma)^0_\sigma \\ (\mathbf{V}_\sigma)^\sigma_0 & (\hat{\mathbf{K}}+\mathbf{V}_0)^\sigma_\sigma \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \end{pmatrix} = E_0 \begin{pmatrix} \mathcal{N}^0_0 & \mathbf{0} \\ \mathbf{0} & \mathcal{N}^\sigma_\sigma \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \end{pmatrix}, \tag{2.78}$$

where $\hat{\mathbf{K}}$ and $\mathbf{V}_k$ represent kinetic and potential block matrices.

We carried out the above calculation using the VMC method for the spatial integrals. The results obtained for the ground state energy is given in table 2.7 for a number of local scalar interactions. The calculation is the same as the one performed by [52]. When

Table 2.7: The J-TICI(2) method was applied for the ground state energy of ^{4}He (in MeV). A central state independent Jastrow factor was used together with a state-depended TICI(2) part. The variational Monte Carlo method was used.

Potential	TICI(2)		J-TICI(2)	
	SI	SD	SI	SD
S3	-25.42±0.02	-28.74±0.02	-27.20±0.01	-31.38±0.01
MS3	-	-28.76±0.02	-	-31.36±0.01
B1	-37.93±0.02	-	-38.400±0.003	-
MT-V	-29.44±0.05	-	-30.91±0.03	-
MT-I/III	-29.46±0.05	-31.10±0.05	-33.10±0.02	-33.19±0.03

compared with table 2.5 our results are slightly improved. This is due to the fact that we made use of a better approximation for the Jastrow factor, containing two gaussian components rather than a single one. Furthermore, we used a different set of variational parameters.

In the case of the nonlinear coefficients entering the expansion of the linear correlation operator we made the choice of a geometric series i.e

$$\beta_i = k\beta_{i-1}, \tag{2.79}$$

as a result of the convergence properties. The behaviour of the ground state energy with the number of components used to expand the linear correlation function is shown in figure 2.1 (for the S3 interaction). The same set of coefficients was used both for the state-independent and the state-dependent correlations. The state-dependent components were added to the state-independent ones. In both cases the value for the contribution to the ground-state energy converges with a relatively small number of components. However, when the Jastrow correlations are considered the convergence of the calculation becomes smoother. The effect of the Jastrow factor can be viewed as a better reference state for the correlation operator to act on, since there is a difference of about 20 MeV between the result obtained with just a single component (only Jastrow).

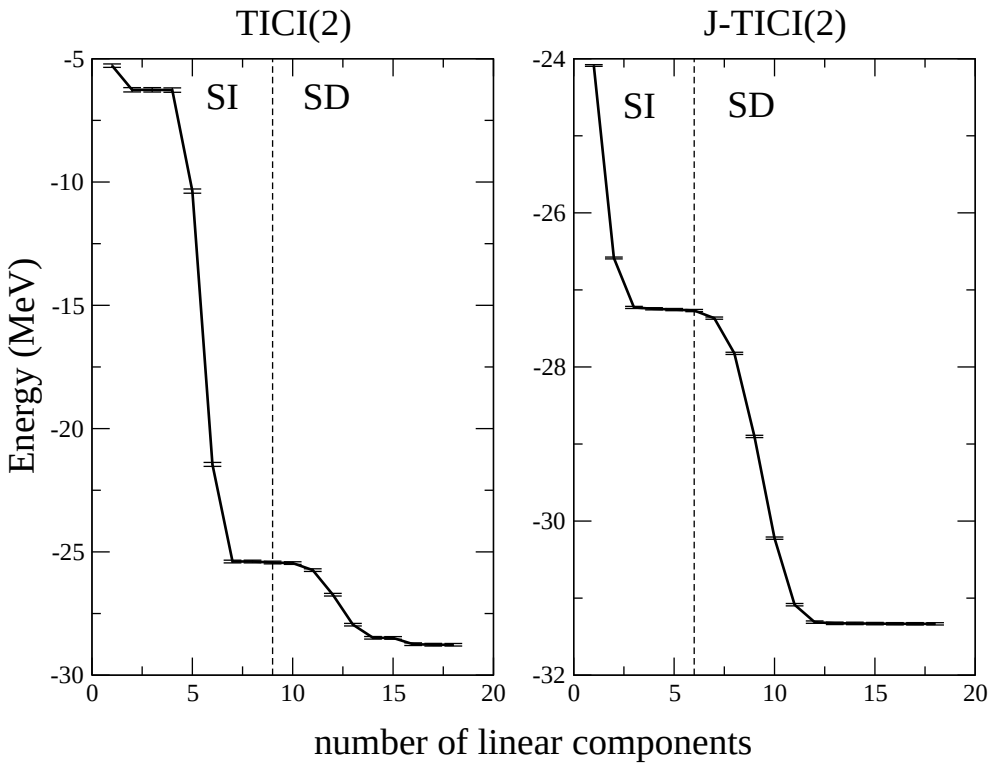


Figure 2.1: The behaviour of the ground state energy with the total number of components used to expand the correlation function was plotted for the TICI(2) and J-TICI(2) calculations for the S3 interaction. SI corresponds to the state-independent part while SD to the state-dependent one. The linear SD components (right part of broken line) were added to the linear SI components (left part of broken line).

2.4.3 Density Matrices

Although a wavefunction can be obtained either through some analytical method or with the aid of a numerical technique such as the variational Monte Carlo, this wavefunction is usually too complicated to provide a simple physical picture of the system. It is possible to define a series of density matrices, [53], which have a simpler and more direct physical meaning. Once the wavefunction is known these can be obtained and in the case of Monte Carlo sampling the task is relatively straight forward and can be applied to wavefunctions of arbitrary forms.

If the wavefunction, Ψ, is normalized and fulfills the antisymmetry condition appropriate for fermions a series of density matrices of various orders can be defined as

$$\begin{aligned}
\gamma(x_1'|x_1) &= N\int \Psi^*(1'23...N)\Psi(123...N)dx_2dx_3...dx_N \qquad (2.80)\\
\Gamma(x_1'x_2'|x_1x_2) &= \binom{N}{2}\int \Psi^*(1'2'3...N)\Psi(123...N)dx_3dx_4...dx_N.\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
\Gamma^{(p)}(x_1'x_2'...x_p'|x_1x_2...x_p) &= \binom{N}{p}\int \Psi^*(1'2'3'...p'...N)\Psi(123...p...N)dx_{p+1}dx_{p+2}...dx_N.\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\
\gamma^{(N)}(x_1'x_2'...x_N'|x_1x_2...x_N) &= \Psi^*(1'2'3...N')\Psi(123...N)
\end{aligned}$$

In the above equations x_i represents all coordinates assigned to the ith particle including spatial ($\vec{r}_i$), spin (s_i) and isospin (t_i) degrees of freedom, while dx_i represents both the volume element for the ith particle and any finite summations. The density matrices are antisymmetric for each pair of indices, thus they are symmetric for each pair of particle labels.

We are only interested in the diagonal elements defined as

$$\begin{aligned}
\gamma(x_1) &= \gamma(x_1|x_1) \qquad (2.81)\\
\Gamma(x_1,x_2) &= \Gamma(x_1x_2|x_1x_2) \qquad (2.82)\\
&\ldots\ldots..
\end{aligned}$$

These are positive definite and have direct physical interpretations. $\gamma(x_1)dv_1 =$ number of particles $\times$ the probability for finding a particle within the volume dv_1 around the point

r_1 having the spin s_1, etc., when all other particles have arbitrary positions and spins. $\Gamma(x_1, x_2)dv_1dv_2$ =number of pairs $\times$ the probability for finding one particle within the volume dv_1 and another within the volume dv_2 at positions x_1 and x_2 respectively.

From the diagonal second and first-order density matrices we can define the pair correlation function as

$$g(x_1, x_2) = \frac{\Gamma(x_1, x_2) - \gamma(x_1)\gamma(x_2)}{\gamma(x_1)\gamma(x_2)}. \tag{2.83}$$

$g(x_1, x_2)dv_1dv_2$ is the difference between the conditional probability of finding a particle around x_1 provided that another particle is at x_2 with the probability of finding the particles at x_1 and x_2 independent of each other. The denominator acts as a weight. This difference can be interpreted as the correlation between the positions of particle pairs.

It would be nice if we could associate a pair of observables with the pair correlation function. In the general case the correlation between two observables A and B is given as

$$g(A, B) = \frac{\langle AB\rangle - \langle A\rangle\langle B\rangle}{\langle A\rangle\langle B\rangle}. \tag{2.84}$$

In the case of the pair correlation function the the operators in the place of A and B are $\delta(\vec{r}_1 - \vec{r}_1')\delta_{s_1s_1'}$ and $\delta(\vec{r}_2 - \vec{r}_2')\delta_{s_2s_2'}$ since the diagonal elements of the one and two body density matrices can be given as

$$\gamma(x_1) = \int \Psi^*(1'2'...N')\delta(\vec{r}_1 - \vec{r}_1')\delta_{s_1s_1'}\Psi(1'2'...N')dx_1'...dx_N' \tag{2.85}$$

$$\Gamma(x_1, x_2) = \int \Psi^*(1'2'...N')\delta(\vec{r}_1 - \vec{r}_1')\delta_{s_1s_1'}\delta(\vec{r}_2 - \vec{r}_2')\delta_{s_2s_2'}\Psi(1'2'...N')dx_1'...dx_N' \tag{2.86}$$

The use of the pair correlation function in our case is to provide qualitative information about the wavefunction and we want to avoid any complications for its calculation. Therefore ,we can make use of a related quantities that can be very easily obtained through Monte Carlo sampling. Instead of the pair correlation function we can make use of the spherically averaged one- and two-body densities, normalized to unity, defined for an N body system as

$$\rho_1(r) = \left\langle \frac{1}{N}\sum_{i=1}^{N}\frac{1}{r^2}\delta(r - |\vec{r}_i - \vec{R}|\right\rangle, \quad \vec{R} = \frac{1}{N}\sum_{i=1}^{N}\vec{r}_i, \tag{2.87}$$

$$\rho_2(r) = \left\langle \frac{2}{N(N-1)}\sum_{i<j}\frac{1}{r^2}\delta(r - |\vec{r}_i - \vec{r}_j|)\right\rangle. \tag{2.88}$$

Both ρ_1 and ρ_2 are translationally invariant quantities that can be used in order to provide qualitative information about a physical system and in general it is not easy to obtain these quantities analytically starting from correlated wavefunctions. Figure 2.2 shows the difference in the density distributions between the state-independent TICI(2) and the J-TICI(2) formalism, while figure 2.3 shows the difference between state-dependent and state-independent correlations in both the J-TICI(2) and TICI(2) methods.The presence of the Jastrow factor reduces the probability of finding a pair of particles close to each other by introducing short-range correlations, particularly in the presence of state dependent correlations. In the presence of a Jastrow factor there is not any significant difference between the density distributions both in the state-dependent and state-independent cases. Although the difference in binding energy between the state-dependent J-TICI(2) and TICI(2) methods is relatively small there is a significant difference in the short range effects of the two-body density distribution, something that emphasizes th importance of the Jastrow correlations.

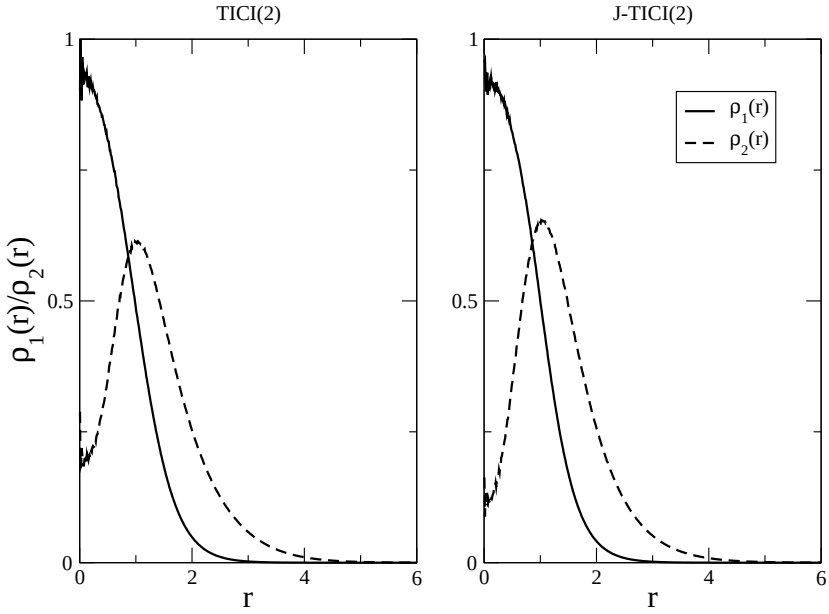


Figure 2.2: The alpha-particle spherically averaged one-body and two-body density distribution for the TICI(2) and J-TICI(2) methods. The continuous line is for the one-body distribution while the broken line is for the two-body one. The purpose of this graph is to show the difference between having and not having the Jastrow factor

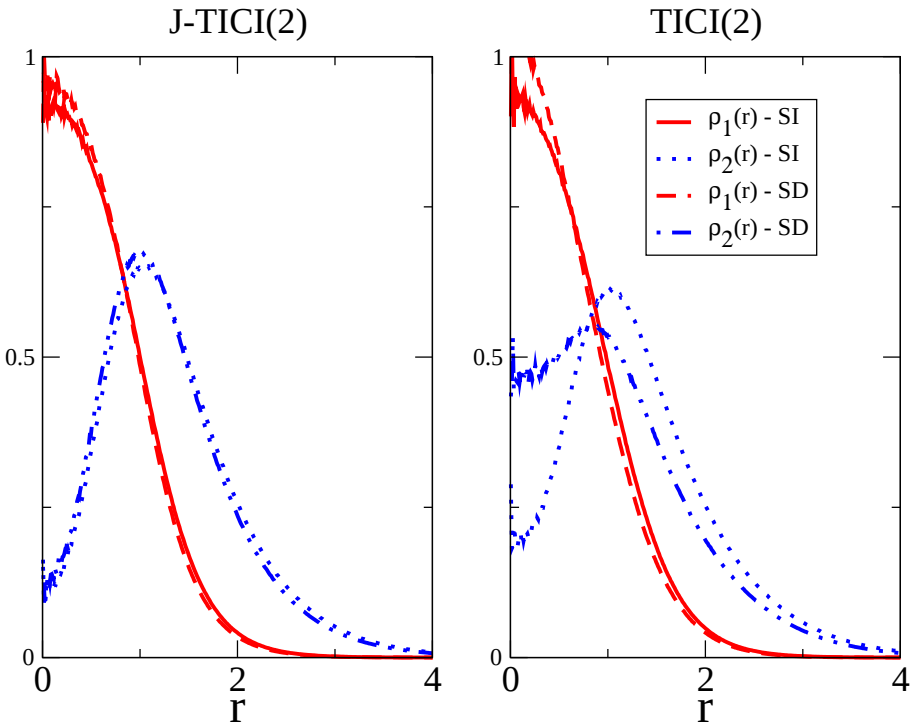


Figure 2.3: The alpha-particle spherically averaged one-body and two-body density distribution for the TICI(2) and J-TICI(2) methods with (SI) and without (SD) state dependence. The continuous and dotted lines are for ρ_1 and ρ_2 without state-dependence, while the broken and chain lines correspond to the state depended cases.The purpose of this graph is to show the difference between state-dependent and state-independent correlations, with or without the Jastrow factor.

2.5 Conclusion and general remarks

The basic principle of the CCM is that the exact wavefunction can be obtained by correlating a starting reference function. This correlation operator can be given directly in coordinate representation. The translationally invariant coupled cluster method provides a parametrization of the correlation operator in terms of functions depending on the relative distances. We can obtain several truncated forms for the correlation operator that can be used in a variational calculation. The most general variational wavefunction consists of a multilinear expansion of the correlation operator.

We are particularly interested in an economic method in terms of effort that does not lack substantial accuracy. The simplest choice would be to consider a linear form for the correlation operator containing only pair correlations. When compared with higher order approximations this choice is rather poor. However, a further improvement is to enrich the structure of the reference function. One of the requirements for translational invariance is that the reference function is separable into relative and center-of-mass parts and any choice for the reference factor should respect this. The Jastrow correlation factor is such a choice. Combining the simplest approximation of the CCM, namely the TICI(2), with the Jastrow correlation factor leads to a variational calculation that is easily accessible both analytically and numerically, termed as the J-TICI(2) scheme.

The alpha-particle has provided a reliable method for testing the accuracy of both the method to be used and the numerical calculation. When compared with the statistically exact GFM and DMC methods the results obtained are in close agreement. Despite the complexity of such methods both in implementation and computer time, the J-TICI(2) scheme was relatively easy and straight forward to apply. We managed to slightly improve the previously obtained results at no expense, provided a numerical solution of the equations is performed.

It must be noted that the closed shell structure of the alpha-particle ground state provided an easy ground for the calculations. However, our objective is not the alpha particle but the cluster description of light halo nuclei in terms of an alpha particle accompanied by a number of neutrons. Although the J-TICI(2) scheme can be applied beyond the alpha particle it is by no means implied that an extension of this method to the open shell structure of halo nuclei will lead to any positive results.

Chapter 3

Cluster-like model for light nuclei

The linearized variational wavefunction developed for the alpha-particle can be extended to include a number of additional nucleons, especially neutrons, as well as additional alpha-particles. This involves changing the reference state into one compatible with the system in question. The change should be such that the required permutation symmetry can be imposed. Furthermore, the additional particles should be introduced without violating translational invariance.

Since there is adequate experimental proof (see chapter1) that halo nuclei are weakly bound systems we can impose a cluster-like structure without removing any of the microscopic nature of our model, but by restricting the wavefunction to a particular subspace of the full many-body Hilbert space. This can be achieved by assuming specific symmetry configurations for the variational wavefunction. Furthermore, such an approach is convenient as a starting point, since it follows the previous development for the alpha-particle naturally.

We shall make use of both the J-TICI(2) formalism and an RGM-like method. This chapter is composed of a description of the structure of the cluster wavefunction, the type of interactions used and a rather extensive discussion for the symmetry of the states. The inclusion of the right permutation symmetry is of particular importance and an appendix is devoted that provides the general tools required for our cluster-like description of light nuclei.

3.1 The extended J-TICI(2) formalism

The alpha particle wavefunction describing the 0^+ ground state can be constructed in a very efficient way by the J-TICI(2) method. We can extend this formalism beyond that of the alpha-particle. This has already been done for a number of spin-isospin saturated nuclei [48, 52]. Apart from the increase in the number of particles the main difference is in the reference function. In the case of the alpha-particle the reference function for the ground-state is simply a harmonic oscillator ground state, saturated in spin-isospin. The approach of [48, 52] in the case of ^{8}Be was to introduce translationally invariant p-shell states in order to describe the additional particles. This was done by introducing a product of ($L = 1, M_L = 0$) solid-harmonic (i.e. z-component) for the nucleons of one of the alpha-particles relative to other. This way the wavefunction was not an eigenstate of total angular momentum J (L in the case of spin-orbit force absence) but was a superposition of several J states. We shall adopt a formalism that preserves the right quantum numbers.

We can firstly consider the case of a single alpha-particle accompanied by a number (k) of nucleons, that could be weakly bound. One possibility is to assign to the particles outside the alpha-particle spatial coordinates relative to the alpha-particle center-of-mass. This method explicitly imposes translational invariance at the cost of having to antisymmetrize the reference state by hand. The reference function $\Phi_{J,T}$ in the case of an alpha-particle accompanied by r neutrons can be written as

$$\Phi_{J,T} = \mathcal{A}\{\Phi_\alpha \Phi^{\rm rel}_{J,T}\}, \tag{3.1}$$

$$\Phi^{\rm rel}_{J,T} = \Phi^{\rm rel}_{J,T}(r_{\alpha 1}, ..., r_{\alpha k}, r_{12}, ..., r_{ij}, ..., r_{k-1\ k}), \tag{3.2}$$

where $\Phi^{\rm rel}_{J,T}$ is a function that contains information about the additional nucleons with $r_{\alpha i}$ referring to the set of coordinates assigned to the ith weakly bound neutron relative to the alpha-particle center-of-mass, while r_{ij} are the relative coordinates between the additional nucleons. $\mathcal{A}$ is an antisymmetrizer and Φ_α is the four-particle harmonic oscillator ground state or the alpha-particle wavefunction (that can be obtained from a separate calculation). J and T are the total angular momentum and isospin. Translational invariance is preserved in a rather artificial way, since relative coordinates are explicitly included, rather than obtained through some separation process (such as Jacobi coordinates).

There are several possibilities for the wavefunction $\Phi^{\rm rel}_{J,T}$ and the choices we are going

to make are more intuitive than anything else. As described earlier the total wavefunction is described by a correlation operator acting on a reference state. The correlation operator (state-dependent or not) is a scalar and commutes with all symmetry operators of the Hamiltonian. All quantum numbers are carried by the reference function and despite the intuitive choice for $\Phi^{\rm rel}_{J,T}$ we shall explicitly impose the right quantum numbers.

One choice for the wavefunction $\Phi^{\rm rel}_{J,T}$ could be as follows: the ith additional nucleon can be assigned a wavefunction relative to the alpha-particle that will in general be the product of a radial and an angular part described by an angular momentum J_i. In order to preserve rotational invariance we have to couple the angular momenta of the additional nucleons to a total angular momentum J. However, the additional nucleons will be correlated with each other, something that can be imposed with the presence of a function depending on the relative distances r_{ij}. This way $\Phi^{\rm rel}_{J,T}$ is composed of the product of angular and radial parts and can have the general form

$$\Phi^{\rm rel}_{J,T} = \sum_{j_1,..,j_r} A^{JM_J}_{j_1,..,j_r} \left[\bigotimes_{i=1}^{r} \Phi_{j_i}(\vec{r}_{\alpha i}) \right]^{J}_{M_J} R(r_{12},..,r_{ij},..,r_{k-1,k}) \times \left[\bigotimes_{i=1}^{r} \chi_{\tau_i} \right]^{T}_{M_T} . \quad (3.3)$$

The $A^{JM}_{j_1,..,j_r}$ is a set of coefficients that must be truncated for practical purposes. $R(r_{12},..,r_{ij},..,r_{k-1,k})$ is the wavefunction that correlates the additional neutrons with each other. The functions Φ_{j_i}, which represent the extra neutrons, are composed of a product of angular, radial and spin-isospin parts, for example

$$\Phi_{j_i}(\vec{r}_{\alpha i}) = \prod_{i=1}^{k} \phi(r_{\alpha i}) \left[Y^{l_i}(\theta_i,\phi_i) \otimes \chi(\sigma_i) \right]^{J_i}_{M_i} . \quad (3.4)$$

The angular brackets,

$$\left[Y^{l_i}(\theta_i,\phi_i) \otimes \chi(\sigma i) \right]^{J_i}_{M_i} = \sum_{m_i s_i} C^{J_i M_i}_{l_i m_i, 1/2 m_{s_i}} Y^{l_i}_{m_i} \chi_{s_i}(\sigma_i), \quad (3.5)$$

denote spin-orbit coupling and $C^{J_i M_i}_{l_i m_i, 1/2 m_{s_i}}$ are the Glebsch Gordan coefficients for SU(2). It must be emphasized that the coordinates $r_{\alpha i}$ as well as the angles θ_i and ϕ_i represent the coordinates and angles of the ith neutron relative to the alpha particle's center of mass. The importance of this choice is that we preserve the translational invariance of the reference state, in a relatively simple manner.

As indicated in equation (3.3) the relative wavefunctions must be written in the j-j coupling scheme, where the undetermined coefficients will in general depend on the value of the total angular momentum assigned to the ith particle. However, when the spin-orbit term is not included in the interaction the relative wavefunction takes the simpler form

$$\Phi^{\rm rel}_{L,S,T} = \sum_{l_1,\ldots,l_r} A^{LM_L}_{l_1,\ldots,l_r} \left[\bigotimes_i \Phi_{l_i}(\vec{r}_{\alpha i})\right]^L_{M_L} R(\{r_{ij}\}) \times \left[\bigotimes_{i=1}^r \chi_{\sigma_i}\right]^S_{M_S} \times \left[\bigotimes_{i=1}^r \chi_{\tau_i}\right]^T_{M_T} \quad (3.6)$$

$$\equiv \phi^{\rm rel}_L(\{\vec{r}_i\})\chi_{\sigma\tau}(S,T), \quad \chi_{\sigma\tau}(S,T) = \left[\bigotimes_{i=1}^r \chi_{\sigma_i}\right]^S_{M_S} \times \left[\bigotimes_{i=1}^r \chi_{\tau_i}\right]^T_{M_T}, \quad (3.7)$$

where the relative wavefunctions are coupled to a total orbital momentum L, while S is the total spin. In the L-S coupling scheme the wave-function can be described as the 'inner product' of a spatial with a spin-isospin part, something that will be described in detail later.

The next step is to consider more than one alpha-particle. For z alpha-particles and k additional nucleons the wavefunction of (3.1) changes to

$$\Phi_{L,S,T} = \mathcal{A}\{\Phi_{\alpha_1}\Phi_{\alpha_2}\ldots\Phi_{\alpha_k}\Phi^{\rm rel}_{L,S,T}\}, \quad (3.8)$$

where $\Phi^{\rm rel}_{L,S,T}$ must be extended to include the correlations between different alpha-particles apart from the ones between alpha-particles and weakly-bound nucleons and between weakly-bound nucleons. Contrary to the case above where we have only one alpha-particle, this case is much harder to generalize and we only consider the situation of two alpha-particles alone (corresponding to ^{8}Be) and two alpha-particles with one additional nucleon (^{9}Be).

In the case of two alpha particles the spatial part $\phi^{\rm rel}_{L,S,T}$ of the wavefunction $\Phi^{\rm rel}_{L,S,T}$ becomes

$$\phi^{\rm rel}_{L,S,T} = \Phi_L(\vec{r}_{\alpha_1\alpha_2})R(r_{\alpha_1\alpha_2}), \quad (3.9)$$

where $\vec{r}_{\alpha_1\alpha_2}$ is the coordinated vector between the two alpha particles. This will be the type of correlation that will be used between alpha particles. When we add one more nucleon e.g. ^{9}Be then one possibility for $\phi^{\rm rel}_{L,S,T}$ is

$$\phi^{\rm rel}_{L,S,T} = \Phi^L(\vec{r}_9)R_1(r_{\alpha_1\alpha_2})R_2(r_{\alpha_1 9}, r_{\alpha_2 9}), \quad (3.10)$$

where $\vec{r}_9$ is the coordinate of the additional nucleon with respect to the system center-of-mass, while $\vec{r}_{\alpha_1 9}$ and $\vec{r}_{\alpha_2 9}$ are it's coordinates with respect to the two alpha particles.

Increasing the number of weakly bound neutrons greatly complicates the structure of $\Phi^{\rm rel}_{L,S,T}$ as well as the required coupling. However, we will only deal with three cluster systems where the number of weakly bound neutrons is restricted to two. Furthermore, working with an alpha particle not confined in the scalar 0^+ state would involve further implications.

3.1.1 RGM-like wavefunction

As mentioned in the introductory chapter, a method that is fully microscopic and at the same time provides a decomposition of the wavefunction in terms of clusters, is that of the resonating group method (RGM) [12]. In the RGM, the wavefunction is given as a superposition of the different cluster structures and depends only in the internal coordinates of the clusters. For practical purposes the RGM wavefunction can be approximated by retaining only a particular decomposition. Our situation shares similarities with the RGM, since our reference function is equivalent to maintaining a particular cluster decomposition that correspond to leaving an alpha-particle 0^+ part. The difference lies in the fact that the RGM method provides an expansion for the individual cluster structures, while in the J-TICI(2) we correlate the reference function.

An alternative to the J-TICI method that in a way resembles the RGM formalism is the technique developed in [54]. In this method the wavefunction is described by a similar reference state as in the J-TICI(2) model, but instead of using a linear correlation operator the reference function is described by a linear expansion, where each amplitude corresponds to a different set of the variational parameters used to describe the separation between individual clusters. In our formalism this corresponds in expanding the function $\Phi^{\rm rel}$ of equation (3.2) in terms of a set of variational parameters. We shall describe this in more detail in chapter 5, when we consider individual cases.

Both the extended J-TICI(2) and RGM-like methods will be applied in a later chapter. The extended J-TICI(2) is a more natural consequence of our previous work on the alpha-particle. There is an advantage of the J-TICI(2) method over the RGM-like model in terms of practicality that is discussed in chapter 5.

3.2 Nucleon-nucleon interactions

In the case of the alpha-particle a number of realistic nucleon-nucleon were used. Although the description of the nuclear force problem is beyond our purpose, a general discussion of the basic characteristics of the most common realistic interactions used is given below. The term 'realistic interactions' refers to interactions depending on all particle labels but obtained from an incomplete theory in order to reproduce some experimental results.

At first approximation realistic interactions are given as two-nucleon potential terms. These potentials are builded by fitting deuteron properties and nucleon-nucleon scattering data. An example of a realistic type of potentials is the Argonne V14 [55] and its extended version Argonne V18 [56]. The potential V14 is written as a sum of 14 operator components

$$V(ij) = \sum_{p=1}^{14} v^p(r_{ij}) O^p(ij), \tag{3.11}$$

where $v^p(r_{ij})$ are terms depending only on the relative distance and the $O^p(ij)$ are operators. These are given as

$$O^{p=1,14}(ij) = [1, \vec{\sigma}_i.\vec{\sigma}_j, S_{ij}, (\vec{L}.\vec{S})_{ij}, L^2, L^2(\vec{\sigma}_i.\vec{\sigma}_j), (\vec{L}.\vec{S})^2_{ij}] \otimes [1, \vec{\tau}_i, \vec{\tau}_j], \tag{3.12}$$

where

$$S_{ij} = 3(\vec{\sigma}_i.\hat{r}_{ij})(\vec{\sigma}_j.\hat{r}_{ij}) - \vec{\sigma}_i.\vec{\sigma}_j \tag{3.13}$$

is the tensor operator. The non-local terms arise because of the inclusion of the non-local spin orbit term $(\vec{L}.\vec{S})_{ij}$, where $\vec{L}$ is the relative orbital angular momentum and $\vec{S}$ is the total spin of the pair. In our calculations we shall only consider local interactions, that is interactions independent of the nucleon velocities. Because of translational invariance, the interaction involves only the relative distance $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$. Furthermore, it can be separated into interactions depending only on the magnitude of $\vec{r}_{ij}$, termed central forces, and forces that dependent also on the direction, non-central forces such as the tensor force. For simplicity we shall further restrict ourselves to the case of central forces.

The structure of the V18 potential is an extension of the V14. These type of potentials are most realistic ones currently present as result of their rich operator structure. Although a calculation should include as many potential terms as possible, approximations

are usually taken and a subset of the operators is taken. However, this will require to use a different type of realistic interactions than the Argonne ones, which are adapted for a smaller set of operators.

The simplest type of realistic interactions are the local-scalar ones, usually termed V4 interactions (due to the four terms), which have the form

$$V_4(i,j) = V_0(r_{ij}) + V_\sigma(r_{ij})\vec{\sigma}_i.\vec{\sigma}_j + V_\tau(r_{ij})\vec{\tau}_i.\vec{\tau}_j + V_{\sigma\tau}(r_{ij})\vec{\sigma}_i.\vec{\sigma}_j\vec{\tau}_i.\vec{\tau}_j. \tag{3.14}$$

A very useful representation of the V4 interactions is in terms of exchange operators that interchange the spin/isospin of a pair of particles. These are defined as

$$P^\sigma_{ij} = \frac{1}{2}(1 + \vec{\sigma}_i.\vec{\sigma}_j), \tag{3.15}$$

for the spin exchange and

$$P^\tau_{ij} = \frac{1}{2}(1 + \vec{\tau}_i.\vec{\tau}_j) \tag{3.16}$$

for isospin exchange. The central potential can be written in terms of the Wigner, Majorana, Barlett and Heisenberg components (denoted by their initials), giving the form

$$V(i,j) = V_W(r_{ij}) + V_M(r_{ij})P^\sigma_{ij}P^\tau_{ij} + V_B(r_{ij})P^\sigma_{ij} + V_H(r_{ij})P^\tau_{ij}. \tag{3.17}$$

In the case of projection operators, the potential is defined in term of singlet or triplet spin-isospin channels and even or odd spatial parts.

One type of V4 potentials are those of Volkov [57] and Brink and Boeker [58], consisting of radial and Majorana components. These two types use a sum of two Gaussians for the radial part, giving

$$V(r) = S_1(1 - m_1 + m_1P^x)e^{-r^2/\mu_1^2} + S_2(1 - m_2 + m_2P^x)e^{-r^2/\mu_2^2}, \tag{3.18}$$

where $P^x = -P^\sigma\tau$ is the Majorana exchange operator of spatial coordinates. The parameters $\{\mu\}$, $\{m\}$ and $\{S\}$ were fitted to reproduce experimental results. The V4 interaction of Malfliet and Tjon [59], describes the radial part in terms of a superposition of two

Yukawa potentials one of which is repulsive, giving

$$V(r) = -\lambda_A \frac{e^{-\mu_A r}}{r} + \lambda_R \frac{e^{-\mu_R r}}{r}, \tag{3.19}$$

where again fit parameters are used. Different cases of the Malfiet and Tjon potential are the MT I/III which correspond to the singlet (S=0, T=1) and triplet (S=1,T=0) spin channels respectively, with even parity.

The Afnan and Tang [60] potential (S3) and its modified version [61] (MS3), are other examples of V4 potentials, where a sum of three Gaussians is used for each channel. The channels used for the S3 potential are the same as the previous cases, while the MS3 potential is adjusted to include channels of total odd parity, i.e. with (S=0, T=0) and (S=1, T=1). These are the two interactions that we will mostly use.

V6 interactions are composed of a V4 part, together with the additional terms of the tensor force. In term of exchange operators the general form of a V6 potential is

$$V(ij) = V_c(r_{ij}) + V_\tau(r_{ij})P_\tau^{ij} + V_\sigma(r_{ij})P_\sigma^{ij} + V_{\sigma\tau}(r_{ij})P_\sigma^{ij}P_\tau^{ij} + V_{T_0}(r_{ij})S_{ij} + V_{T_\tau}(r_{ij})P_{ij}^\tau. \tag{3.20}$$

The above equation describes a local interaction, which can be extended to include non-local terms of spin-orbit coupling. The Gogny [62] potential is composed of a V6 part and a spin orbit coupling part, containing both first and second order terms (V8). It is given by

$$V(ij) = V_{V6}(ij) + V_{LS}(r_{ij})\vec{L}.\vec{S} + V_{LL}(r_{ij})L_{ij}, \tag{3.21}$$

with

$$L_{ij} = (\hat{\sigma}_i.\hat{\sigma}_j)\vec{L}^2 - \frac{1}{2}[(\hat{\sigma}_i.\vec{L}).(\hat{\sigma}_j.\vec{L}) + (\hat{\sigma}_j.\vec{L})(\hat{\sigma}_i.\vec{L})], \tag{3.22}$$

being a second order spin orbit interaction. The radial parts of the Gogny potential are expressed as summation of Gaussians.

In general there is a large number of realistic nucleon-nucleon interactions. We shall mainly make use of the S3 and MS3 V4-type interactions. These provide an easy ground for a first approximation and can be referred to as semi-realistic interactions since they are composed of gaussians and are finite at zero nucleon separation (usually termed 'super-soft core' interactions). The nice analytic properties of these interactions do not impose any immediate problems for the numerical evaluation of the hamiltonian expectation

value.

3.3 Symmetry of states

One important part of any quantum mechanical calculation is the inclusion of the correct symmetry, since it will effect the expectation value of any observable. In most cases the Hamiltonian of a system commutes with a number of operators. The set of operators with which the hamiltonian commutes can be the elements of finite groups (such as permutations) or the generators of continuous groups (e.g. SO(3), SU(2)) which are the elements of Lie algebras. According to the symmetry of the hamiltonian each space of degenerate eigenstates (eigenspace) belonging to some eigenvalue of the hamiltonian can be labelled by a distinct set of quantum numbers, which correspond to conserved quantities. The properties of the states in a particular eigenspace are important for the evaluation of expectation values of different operators.

In the case of the nuclear many-body problem and particularly when the nuclear forces do not depend strongly on the spin we can write the wavefunction as the product of an orbital function and a function of the spin and isospin variables. This is the case corresponding to the local-scalar (V4) realistic interactions described earlier. The spatial part will obey rotational invariance and will thus belong to the SO(3) group. The spin-isospin has overall SU(4) symmetry that is described by Wigner multiplets [63]. We shall discuss this in more detail later on in section 3.3.2.

In addition to the individual symmetries of the spatial and spin-isospin parts we require that the full wavefunction is antisymmetric in the exchange of particle labels (simultaneous exchange of spatial, spin and isospin coordinates). This implies that the wavefunction belongs to a one-dimensional representation of the permutation group. This condition requires the orbital and spin-isospin parts to belong to conjugate representations of the permutation group instead of being confined to the antisymmetric one-dimensional irreps. This is a subject that requires special attention when exchange operators are involved and we examine it in the next section.

A brief discussion of the representations of the symmetric group and of some general results that will become useful later, is given in the first section of appendix A.

3.3.1 Totally antisymmetric product functions

As was already stated, in the absence of spin-orbit coupling the total wavefunction is constructed in a product space of the spatial and spin-isospin parts. We demand the full wavefunction to be totally antisymmetric which in turn implies that each space is invariant under the permutation group and the full wavefunction is given by the Clebsch-Gordan coefficients of the permutation group. Since each state is also described by other continues symmetries there must be a connection between functions belonging to the irreps of these groups and the irreps of the permutation group. This is indeed the case [64] and is discussed later on.

For the moment we can describe in simple terms the process by which we can construct a totally antisymmetric product function. By S_n we denote the permutation group of order n. The basis functions for irrep μ of S_n for the spatial part are the Φ_i^μ while those of the spin-isospin part (belonging to the irrep ν) are the χ_i^ν. The 'inner-product' between the spatial and spin-isospin part is the linear combination of product of wavefunctions with definite permutation symmetry in each degree of freedom into a wavefunction with a definite symmetry in the overall degrees of freedom. Thus a function Ψ^ν belonging to the inner product space of the irreps α and β can be written as

$$\Psi_i^\nu = \sum_{j,k}^{\eta_\alpha,\eta_\beta} C_{\alpha j,\beta k}^{\nu,i} \Phi_j^\alpha \chi_k^\beta, \tag{3.23}$$

where $C_{\alpha j,\beta k}^{\nu,i}$ are the Clebsch-Gordan coefficients. There is usually one additional multiplicity label associated with ν that we can ignore (the number of times the irrep ν appears in $\alpha \times \beta$) because it does not appear in the spin-isospin states we shall consider. η_α and η_β are the dimensions of α and β.

In order for the full wavefunction to be totally antisymmetric we want Ψ_i^ν to be invariant with respect to permutations P apart from a phase factor $(-)^P$. This means that Ψ_i^ν belongs to the one-dimensional irrep of S_n denoted as $\Psi^{[1^n]}$, where $[1^n]$ is the tableau consisting of a column of n boxes (see appendix). For this case the Clebsch-Gordan coefficients take the simple form

$$C_{\alpha j,\beta k}^{[1^n],1} = \frac{1}{\sqrt{\eta_\alpha}} \Lambda_j^\alpha \delta_{\beta\tilde{\alpha}} \delta_{jk}, \tag{3.24}$$

where Λ_j^α is a phase factor that can be either ± 1, while $\tilde{\alpha}$ denotes the irrep conjugate to α. The action of a permutation P on Ψ gives

$$P\Psi = \sum_i \Lambda_i^\alpha (P\Phi_i^\alpha)(P\chi_i^{\tilde{\alpha}}), \tag{3.25}$$

$$= \sum_{k,l} \left(\sum_i \Lambda_i^\alpha U^\alpha(P)_{ki} U^{\tilde{\alpha}}(P)_{li} \right) \Phi_k^\nu \chi_l^\mu, \tag{3.26}$$

where $U^\mu(P)_{ki}$ is a matrix element of the μth irreducible representation of P, which can be assumed to be real and orthogonal. The demand that Ψ is antisymmetric with respect to P requires the condition

$$\sum_i \Lambda_i^\alpha U^\alpha(P)_{ki} U^{\tilde{\alpha}}(P)_{li} = (-)^P \delta_{kl}, \tag{3.27}$$

which in turn requires that

$$\Lambda_i^\alpha U^{\tilde{\alpha}}(P)_{ki} = (-)^P U^\alpha(P)_{ki}. \tag{3.28}$$

Therefore, having a totally antisymmetric wavefunction implies having a linear combination of products with the form

$$\Psi = \sum_i \Phi_i^\alpha \chi_i^{\tilde{\alpha}}, \tag{3.29}$$

where the transformation of the sets Φ_i^α and $\chi_i^{\tilde{\alpha}}$ under a permutation is given as

$$P\Phi_i^\alpha = \sum_j U^\alpha(P)_{ji} \Phi_j^\alpha, \qquad P\chi_i^{\tilde{\alpha}} = (-)^P \sum_j U^\alpha(P)_{ji} \chi_j^\alpha. \tag{3.30}$$

3.3.2 SU(4) quantum numbers

An antisymmetric wavefunction that is a linear superposition of spatial and spin-isospin functions can be labelled by several quantum numbers that are related to the transformation of the spatial and spin-isospin parts under rotations in coordinate, spin and isospin space. These are the orbital momentum quantum number L, the total spin S and total isospin T. Furthermore, additional 'quantum numbers' or labels are required to uniquely specify the state of the system as a result of permutation symmetry. The fact that we

require the spin-isospin functions to be of conjugate permutation symmetry to the spatial one implies some restrictions on the possible sets of quantum numbers. We provide an analysis of the decomposition of the wavefunction since its important for the expectation value of the hamiltonian.

In the case of total angular momentum, L, the requirement is that the spatial part, Φ_i^ν, belonging to the ν irrep of $\mathcal{S}_N$ is restricted to representations compatible with the group SO(3). In our case the situation is simple since we shall only couple a pair of particles. This can be applied by the usual way of coupling two integer representations of the SU(2) algebra, with l_1 and l_2 quantum numbers, into an irrep with $L = l_1 + l_2$ and definite parity $(-1)^{L-l1-l2}$. Therefore the labels for the spatial part are the irrep of S_n , the quantum number L and its 'z-axis' projection M_L. In general more labels are needed to uniquely specify the spatial symmetry since for some L with the same irrep label of S_n we can find several linear combinations of coordinate tensor-product functions. This way the spatial functions of expansion (3.29) can be written as

$$\Phi_i^\nu \;\rightarrow\; \Phi_{L,i}^\nu, \tag{3.31}$$

where we drop M_L since it will not effect the expectation value.

Apart from conjugate permutation symmetry to the spatial part, the spin-isospin part belongs to SU(4) symmetry. This is a result of the fact that the hamiltonian is invariant under rotations in spin as well as in isospin space. The invariance is expressed by the following commutation relations:

$$\left[\hat{H}, \sum_{i=1}^{n} s_k(i)\right] = \left[\hat{H}, \sum_{i=1}^{n} t_k(i)\right] = \left[\hat{H}, \sum_{i=1}^{n} s_k(i) s_l(i)\right] = 0, \;\; k, l = 1, 2, 3. \tag{3.32}$$

Here $s_k(i)$ and $t_k(i)$ are the kth spin and isospin components, respectively, for nucleon i. The 15 operators appearing in (3.32) are the generators of the SU(4) Lie algebra. The first two commutators imply that the states can also be labeled by the total spin S and isospin T of SU(2). Apart from S and T the basis states have one additional label, resulting from the third commutation relation (3.32). This additional label classifies the permutation symmetry to which the spin-isospin state belongs, that has to be conjugate to that of the spatial part.

The symmetry of the spin-isospin state leads to the general problem of the direct product SU(m)×SU(n) of two unitary groups in a subgroup of SU(mn) [65]. Therefore, we need the SU(mn)⊃ SU(m)×SU(n) irreducible basis. This is equivalent to the inner products of two irreps of the permutation group $\mathcal{S}_n$ (one for the spin and one for the isospin degrees of freedom) into an irrep of $\mathcal{S}_n$ [64]. The spin-isospin function is given as

$$\chi_i^\nu \equiv \left| {}^{[\nu]\ i}_{S\ M_S,T\ M_T} \right\rangle = \sum_{j,k} C^{[\nu],i}_{[\nu_1]j,[\nu_2]k} \left| {}^{[\nu_1]\ j}_{S\ M_S} \right\rangle \left| {}^{[\nu_2]\ k}_{T\ M_T} \right\rangle, \tag{3.33}$$

where $C^{[\nu],i}_{[\nu_1]j,[\nu_2]k}$ are the Clebsch-Gordan coefficients of $\mathcal{S}_n$ for the coupling to the irreducible basis $[\nu]$ of $[\nu_1] \times [\nu_2]$. The spin-isospin functions are completely labelled : each of the spin or isospin functions has a label that specifies the irrep of $\mathcal{S}_n$ that is equivalent to the total spin S or isospin T, as well as the labels M_S or M_T that specify the z-axis component of the spin/isospin and is equivalent to the Weyl tableau (see appendix). Therefore, the complete labelling for spin-isospin functions of (3.29) is

$$\chi_i^\nu \rightarrow \left| {}^{[\nu]\ i}_{S\ M_S,T\ M_T} \right\rangle. \tag{3.34}$$

The above classification arises as a result of the fact that the invariant operators (Casimirs) that label the basis functions of the tensor-product SU algebra(group) are functions of the invariant operators (class operators) of the permutation group, i.e. operators that commute with all elements of the group algebra. In the case of the V4 interaction this is evident from the fact that the exchange operators P^σ_{ij}, P^τ_{ij} and $P^{\sigma\tau}_{ij}$ can be used in the place of the terms $\vec{\sigma}_i.\vec{\sigma}_j$, $\vec{\tau}_i.\vec{\tau}_j$ and $(\vec{\sigma}_i.\vec{\sigma}_j)(\vec{\tau}_i.\vec{\tau}_j)$. The total spin and total isospin operators, $\hat{S}^2 = (\sum_{i=1}^N \hat{S}_i)^2$ and $\hat{T}^2 = (\sum_{i=1}^N \hat{T}_i)^2$ can be decomposed as

$$\hat{S}^2 = \sum_{i,j=1}^N \hat{S}_i.\hat{S}_j = \frac{N}{4}(4-N) + \sum_{i<j} P^\sigma_{ij} = \frac{N}{4}(4-N) + P^\sigma, \tag{3.35}$$

$$\hat{T}^2 = \sum_{i,j=1}^N \hat{T}_i.\hat{T}_j = \frac{N}{4}(4-N) + \sum_{i<j} P^\tau_{ij} = \frac{N}{4}(4-N) + P^\tau. \tag{3.36}$$

The operators P^σ and P^τ are class operators of $\mathcal{S}_n$ in spin and isospin space, respectively (the class operators composed of the product of all transpositions). These operator commute with the spin and isospin exchange operators appearing in the interaction and their

eigenvalues are the total spin and isospin quantum numbers apart from a constant term. Furthermore, the class operator $P^{\sigma\tau} = \sum_{i<j} P^{\sigma}_{ij} P^{\tau}_{ij}$ commutes with all exchange terms of spin and isospin coordinates simultaneously and thus provides an additional eigenvalue describing the permutation symmetry in the spin-isospin tensor-product space.

Correct permutation symmetry in the many-body wavefunction is equivalent to having the right quantum numbers. The eigenfunctions Ψ for the SU(4) hamiltonian can be written as

$$\Psi \equiv |[\nu], L, S, T\rangle = \sum_{i} \left| {}^{[\nu]\ i}_{L,M_L} \right\rangle \left| {}^{[\tilde{\nu}]\ i}_{S\ M_S,T\ M_T} \right\rangle, \tag{3.37}$$

where the eigenvalues depend on the set of labels $\{[\nu], L, S, T\}$. The structure provided by the permutation symmetry is important for the evaluation of expectation values. This is described in the next section.

3.4 Expectation values

We have to deal with the expectation value of an operator $\hat{O}$ in the totally antisymmetric wavefunction. Apart from state dependence in $\hat{O}$ in general we have to consider the state dependence in the wavefunction resulting from the correlation operator. As it was previously shown the state dependence will appear in terms of exchange operators. We can rewrite the full wavefunction as

$$|\Psi\rangle = \hat{F}|[\nu], L, S, T\rangle, \tag{3.38}$$

where $|[\nu];, L, S, T\rangle$ is given in (3.37), while

$$\hat{F} = \hat{F}_0 + \hat{F}_\sigma + \hat{F}_\tau + \hat{F}_{\sigma\tau}, \tag{3.39}$$

is a state-dependent scalar correlation operator.

3.4.1 Exchange operators

For the matrix elements of the hamiltonian and normal matrices we require the matrix elements of a single or a number of pairwise spin-exchange operators with respect to the

wavefunction of equation (3.37):

$$\langle [\nu], L, S, T | f(i,j) P^{\sigma}_{ij} | [\nu], L, S, T \rangle, \quad \langle [\nu], L, S, T | f(ij) P^{\sigma}_{ij} g(k,l) P^{\sigma}_{kl} | [\nu], L, S, T \rangle, \ldots \quad ,$$

where $f(i,j)$ and $g(k,l)$ are functions of the particle pairs (i,j) and (k,l), that are independent of the spin or isospin coordinates. The above expectation values require knowledge evaluation of the matrix elements for the spin-exchange operators in the irrep of $\mathcal{S}_n$ provided by the spin-isospin states:

$$\langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P^{\sigma}_{ij} | {}^{[\tilde{\nu}]i}_{SM_S,TM_T} \rangle, \quad \langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P^{\sigma}_{ij} P^{\sigma}_{kl} | {}^{[\tilde{\nu}]i}_{SM_S,TM_T} \rangle, \ldots \quad . \tag{3.40}$$

In order to avoid explicitly dealing with the different particle pairs we shall represent the above exchanges as a general permutation of the spin labels that will be denoted as P_σ and the associated function as F_σ. These matrix elements are

$$\begin{aligned} \langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P_\sigma | {}^{[\tilde{\nu}]i'}_{SM_S,TM_T} \rangle &= \sum_{jkl} C^{[\nu],i}_{[\nu_1]j,[\nu_2]k} U^{[\nu_1]}_{jl}(P) C^{[\nu],i'}_{[\nu_1]l,[\nu_2]k}, & (3.41) \\ &\equiv M^{\nu,i,i'}_{S,T}(P_\sigma), & (3.42) \end{aligned}$$

where knowledge of the Clebsch-Gordan coefficients and of the irreps of $\mathcal{S}_n$ are required. Similarly for isospin exchanges we have

$$\begin{aligned} \langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P_\tau | {}^{[\tilde{\nu}]i'}_{SM_S,TM_T} \rangle &= \sum_{jkm} C^{[\nu],i}_{[\nu_1]j,[\nu_2]k} U^{[\nu_2]}_{km}(P) C^{[\nu],i'}_{[\nu_1]j,[\nu_2]m}, & (3.43) \\ &\equiv M^{\nu,i,i'}_{S,T}(P_\tau). & (3.44) \end{aligned}$$

The notation $M^{\nu,i,i'}_{S,T}(P)$ is introduced for later convenience.

Apart from purely spin or isospin exchanges we will have to deal with mixed exchanges, such as

$$\langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P^{\sigma\tau}_{ij} | {}^{[\tilde{\nu}]i'}_{SM_S,TM_T} \rangle, \quad \langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T} | P^{\sigma}_{ij} P^{\tau}_{kl} | {}^{[\tilde{\nu}]i'}_{SM_S,TM_T} \rangle, \ldots \quad .$$

In general this will result in the product of two permutations, one in spin space (P_σ), and one in isospin space (P'_τ). The prime is important since apart from acting in different spaces the two permutations will in general be different. For this mixed case the matrix

elements become

$$\langle {}^{[\tilde{\nu}]i}_{SM_S,TM_T}|P_\sigma P'_\tau|{}^{[\tilde{\nu}]i'}_{SM_S,TM_T}\rangle = \sum_{jj'kk'} C^{[\nu]i}_{[\nu_1]j,[\nu_2]k} U^{[\nu_1]}_{jj'}(P) U^{[\nu_2]}_{kk'}(P') C^{[\nu]i}_{[\nu_1]j',[\nu_2]k'}, \quad (3.45)$$

$$\equiv M^{\nu,i,i'}_{S,T}(P_\sigma P'_\tau). \quad (3.46)$$

Therefore, the Clebsch-Gordan coefficients and the representation matrices of the symmetric group carry the action of the spin, isospin and spin-isospin permutations on the fully antisymmetric wavefunction. It must be noted that the above formalism is also valid for $J-J$ coupling apart from some relabelling (the isospin part described by the $j=1/2$ irrep of the SU(2) algebra, must belong to the conjugate irrep of the spatial-spin part, the latter being a Clebsch-Gordan series of integer and half integer ($j=1/2$) irreps of SU(2) algebras).

3.4.2 Spatial integrals

As described in chapter 2, the variational principle for the ground state energy leads to a $4M \times 4M$ dimensional generalized eigenvalue problem (where M is the number of components used to expand the correlation functions) of the form

$$\begin{pmatrix} \mathbf{H}^0_0 & \mathbf{H}^0_\sigma & \mathbf{H}^0_\tau & \mathbf{H}^0_{\sigma\tau} \\ \mathbf{H}^\sigma_0 & \mathbf{H}^\sigma_\sigma & \mathbf{H}^\sigma_\tau & \mathbf{H}^\sigma_{\sigma\tau} \\ \mathbf{H}^\tau_0 & \mathbf{H}^\tau_\sigma & \mathbf{H}^\tau_\tau & \mathbf{H}^\tau_{\sigma\tau} \\ \mathbf{H}^{\sigma\tau}_0 & \mathbf{H}^{\sigma\tau}_\sigma & \mathbf{H}^{\sigma\tau}_\tau & \mathbf{H}^{\sigma\tau}_{\sigma\tau} \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \\ \mathbf{c}_\tau \\ \mathbf{c}_{\sigma\tau} \end{pmatrix} = E_0 \begin{pmatrix} \mathcal{N}^0_0 & \mathcal{N}^0_\sigma & \mathcal{N}^0_\tau & \mathcal{N}^0_{\sigma\tau} \\ \mathcal{N}^\sigma_0 & \mathcal{N}^\sigma_\sigma & \mathcal{N}^\sigma_\tau & \mathcal{N}^\sigma_{\sigma\tau} \\ \mathcal{N}^\tau_0 & \mathcal{N}^\tau_\sigma & \mathcal{N}^\tau_\tau & \mathcal{N}^\tau_{\sigma\tau} \\ \mathcal{N}^{\sigma\tau}_0 & \mathcal{N}^{\sigma\tau}_\sigma & \mathcal{N}^{\sigma\tau}_\tau & \mathcal{N}^{\sigma\tau}_{\sigma\tau} \end{pmatrix} \begin{pmatrix} \mathbf{c}_0 \\ \mathbf{c}_\sigma \\ \mathbf{c}_\tau \\ \mathbf{c}_{\sigma\tau} \end{pmatrix}, \quad (3.47)$$

where the block matrices are given as

$$\mathbf{O}^k_{k'} = \langle [\nu], L, S, T|(\hat{F}_k)^\dagger O \hat{F}_{k'}|[\nu], L, S, T\rangle \quad (3.48)$$

$$(\mathbf{H}^k_{k'})_{lm} = \langle [\nu], L, S, T|(F^l_k)^\dagger \hat{H} F^m_{k'}|[\nu], L, S, T\rangle, \quad (3.49)$$

$$(\mathcal{N}^k_{k'})_{lm} = \langle [\nu], L, S, T|(F^l_k)^\dagger F^m_{k'}|[\nu], L, S, T\rangle, \quad (3.50)$$

$$F^l_k = \sum_{i<j} f^l_k(ij) P^k_{ij}, \quad (3.51)$$

while the $\mathbf{c}_k$ are column vectors of dimensions M each. The above equations were already given in chapter 1 but we quote them again for convenience. Furthermore, the hamiltonian

has the decomposition:

$$\hat{H} = \hat{K} + V_0 + V_\sigma + V_\tau + V_{\sigma\tau}; \quad V_k = \sum_{i<j} v_k(r_{ij}) P^k_{ij}. \tag{3.52}$$

The kinetic energy operator and the wigner-part of the potential, V_0, are the only state-independent terms entering the hamiltonian. If we denote the different particle pairs by r and r' ($r \equiv (r_1, r_2)$), the matrix elements of the kinetic energy matrix become

$$\begin{aligned} (\mathbf{K}^k_{k'})_l m &= \langle [\nu], L, S, T | F^l_k \hat{K} F^m_{k'} | [\nu], L, S, T \rangle, & (3.53)\\ &= \sum_{i,i'} \sum_{r,r'} M^{\nu,i,i'}_{S,T} (P^k_r P^{k'}_{r'}) \left\langle {}^{[\nu]i}_{L,M_L} \right| f^l_k(r) \hat{K} f^m_k(r') \left| {}^{[\nu]i}_{L,M_L} \right\rangle, & (3.54) \end{aligned}$$

with

$$\left\langle {}^{[\nu]i}_{L,M_L} \right| f^l_k(r) \hat{K} f^m_k(r') \left| {}^{[\nu]i}_{L,M_L} \right\rangle = \int \Phi^{[\nu]i}_{L,M_L}(r_1, ..., r_n) f^l_k(r) \hat{K} f^m_k(r') \Phi^{[\nu]i}_{L,M_L}(r_1, ..., r_n) d\Omega. \tag{3.55}$$

The result is the same for the overlap and potential (Wigner part) matrices, where in the former $\hat{K}$ is replaced by 1 while in the latter by V_0. In the case of state-dependent operators, such as the spin-dependent part of the interaction the situation is similar :

$$((\mathbf{V}_\sigma)^k_{k'})_{lm} = \sum_{i,i'} \sum_{r,r'} M^{\nu,i,i'}_{S,T} (P^k_r P^\sigma_{r'} P^{k'}_{r''}) \left\langle {}^{[\nu]i}_{L,M_L} \right| f^l_k(r) v_\sigma(r') f^m_k(r'') \left| {}^{[\nu]i}_{L,M_L} \right\rangle. \tag{3.56}$$

The number of required integrals can be further reduced by considering an alternative form of expansion 3.37 for the ket state:

$$\Psi \equiv |[\nu], L, S, T\rangle = \sum_i \left| {}^{[\nu]i}_{L,M_L} \right\rangle \left| {}^{[\tilde{\nu}]i}_{SM_S,TM_T} \right\rangle = \mathcal{A} |[\nu]1\rangle |[\tilde{\nu}]1\rangle, \tag{3.57}$$

where $\mathcal{A}$ is an antisymmetrizer (proved in the appendix) and for simplicity the quantum numbers are ignored. Because $\mathcal{A}$ is hermitian and idempotent the expectation value of an operator $\hat{O} \equiv \hat{F}_k \hat{O}' \hat{F}_{k'}$ becomes

$$\begin{aligned} \langle \hat{O} \rangle &= \{ \mathcal{A} \langle [\nu]1 | \langle [\tilde{\nu}]1 | \} \, \hat{O} \mathcal{A} | [\nu]1 \rangle | [\tilde{\nu}]1 \rangle, & (3.58)\\ &= \frac{N!}{n_\nu} \{ \mathcal{A} \langle [\nu]1 | \langle [\tilde{\nu}]1 | \} \, \hat{O} | [\nu]1 \rangle | [\tilde{\nu}]1 \rangle. & (3.59) \end{aligned}$$

In all cases the presence of state-dependent correlations increases the number of the required integrals for a particular matrix element. The number of required integral is proportional to the number of relative coordinates ($(\frac{n(n-1)}{2})^3$). This can be a serious drawback for large systems. The above display of the integrals for the matrix elements are in the most general form. According to the system under examination there can be simplifications, such as the case of the alpha-particle. This, with the cases of ^{5}He, ^{6}He, ^{8}Be and ^{9}Be are examined in the nest section.

3.4.3 Alpha-particle

In our approximation the correct permutation symmetry for the alpha particle ground-state is straight forward. Since the spatial part is totally symmetric the only possibility to obtain an antisymmetric wavefunction is by considering a totally antisymmetric spin-isospin state. The wavefunction is given as

$$\Psi \equiv |[4], L=0, S=0, T=0\rangle = \left|{}^{[4]1}_{0,0}\right\rangle \left|{}^{[1^4]1}_{S=0,T=0}\right\rangle, \tag{3.60}$$

$$= \left|{}^{[4]1}_{L=0}\right\rangle \sum_{i=1}^{4} |{}^{[2^2]i}_{S=0}\rangle |{}^{[2^2]i}_{T=0}\rangle, \tag{3.61}$$

where the spin-isospin part belongs in the inner-product space of a self-conjugate irrep of $\mathcal{S}_4$:

$$\left|{}^{[1^4]1}_{S=0,T=0}\right\rangle \in \begin{array}{|c|c|}\hline \ & \ \\ \hline \ & \ \\ \hline \end{array} \times \begin{array}{|c|c|}\hline \ & \ \\ \hline \ & \ \\ \hline \end{array} \quad . \tag{3.62}$$

The only state dependence in the alpha-particle appears in terms of spin (or isospin) exchange operators. The expectation value of spin exchange operators becomes

$$\langle {}^{[1^4]1}_{S=0,T=0}|P_\sigma|{}^{[1^4]1}_{S=0,T=0}\rangle = \sum_{i,i'} \langle {}^{[2^2]i}_{S=0}|\langle {}^{[2^2]i}_{T=0}|P_\sigma|{}^{[2^2]i'}_{S=0}\rangle |{}^{[2^2]i'}_{T=0}\rangle, \tag{3.63}$$

$$= \sum_i U^{[2^2]}_{ii}(P) = \mathrm{Tr}^{[2^2]}(P), \tag{3.64}$$

where the effect of a spin-permutation is the trace of the permutation in the irrep of the spin-space. The result of this simplification was already used in chapter 2, where the trace of the permutations depends on the cycle structure. The non-zero traces of interest are those of the products of two transpositions that can belong to either of two classes : the first one is when the transpositions do not commute and give a cycle structure of

order 3 (e.g. $P_{12}P_{13} = P_{123}$) that has a trace equal to -1 and the second one is when the transpositions commute (e.g. $P_{12}P_{34}$) that gives a trace equal to 2.

The above result for the alpha-particle could have been generalized to an arbitrary spin-isospin state $|^{[\nu]i}_{S,T}\rangle$ of an n-particle system, provided that is given by the inner product of spin and isospin parts belonging to a self-conjugate irrep of $\mathcal{S}_n$ i.e

$$|^{[\nu]i}_{S,T}\rangle = \sum_j |[\alpha]j;S\rangle|[\tilde{\alpha}]j;T\rangle. \tag{3.65}$$

However, this kind of simplification does not appear beyond $\mathcal{S}_4$ for the SU(4)⊂SU(2)×SU(2) classification.

Because of the above simplification the alpha-particle wavefunction in the $SU(4)$ approximation shares no resemblance with any other wavefunction of more than 4 particles. The calculation of the matrix elements is straight forward.

3.4.4 ^{5}He

The first case where we have an alpha particle accompanied by a number of neutrons is that of ^{5}He. In our approximation there is only one possibility for the tableau describing the permutation symmetry of the spatial part :

$$[4,1] \equiv \begin{array}{|c|c|c|c|}\hline \multicolumn{1}{|c}{} & \multicolumn{1}{c|}{} & \multicolumn{1}{c|}{} & \multicolumn{1}{c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \end{array}. \tag{3.66}$$

The tableau describing the conjugate permutation symmetry for the spin-isospin part is

$$[2,1^3] \equiv \begin{array}{|c|c|}\hline \multicolumn{1}{|c}{} & \multicolumn{1}{c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \end{array}. \tag{3.67}$$

There is only one possible decomposition of the spin-isospin states compatible with SU(2)×SU(2) (see [65]):

$$|[2,1^3]i\rangle \in \begin{array}{|c|c|c|}\hline \multicolumn{1}{|c}{} & \multicolumn{1}{c|}{} & \multicolumn{1}{c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \end{array} \times \begin{array}{|c|c|c|}\hline \multicolumn{1}{|c}{} & \multicolumn{1}{c|}{} & \multicolumn{1}{c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \end{array} \quad (S=\frac{1}{2}, T=\frac{1}{2}) \tag{3.68}$$

This corresponds to an alpha-particle accompanied by a single neutron (or proton with charge independent interaction) since this is the only configuration that can be reduced to that of the alpha particle by removing a neutron (or proton). The simplification of

Table 3.1: The content in terms of SU(2)×SU(2) irreps of the (2^2,1^2) and (3,1^3) partitions of $\mathcal{S}_6$

SU(2)×SU(2)	[2^2,1^2]	[3,1^3]	(S,T)/(T,S)
[4,2]×[4,2]	-	1	(1,1)
[4,2]×[3^2]	1	-	(1,0)
[3^2]×[3^2]	-	1	(0,0)

exchange operators in term of traces cannot be applied, but since the irreps describing the spin and isospin states are identical the matrix elements of spin and isospin exchange operators coincide. This means that we can either use spin or isospin exchange operators and not both. The potential and correlation operators reduce to

$$V = V_0 + V_\sigma + V_\tau + V_{\sigma\tau} = V_0' + V_\sigma' + V_{\sigma\tau}', \tag{3.69}$$

$$\hat{F} = \hat{F}_0 + \hat{F}_\sigma + \hat{F}_\tau + \hat{F}_{\sigma\tau} \rightarrow \hat{F}_0 + \hat{F}_\sigma + \hat{F}_{\sigma\tau}. \tag{3.70}$$

3.4.5 ^{6}He

The next case is that of ^{6}He. There are two possible spatial states associated with the following partitions.

$$[4,2] \equiv \begin{array}{|c|c|c|c|}\hline \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} \\ \cline{1-2} \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} \\ \cline{1-2} \end{array}, \quad [4,1,1] \equiv \begin{array}{|c|c|c|c|}\hline \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} & \multicolumn{1}{|c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \multicolumn{1}{|c|}{} \\ \cline{1-1} \end{array}. \tag{3.71}$$

The associated conjugate spin-isospin states are $|[2^2,1]i\rangle$ and $|[3,,1^3]i\rangle$ respectively. Unlike the case of ^{5}He only one of these spin-isospin states has a unique SU(2)×SU(2) decomposition in terms of spin and isospin states. The different possibilities are displayed in table 3.1, where each irrep is denoted by its partition.

3.4.6 ^{8}Be and ^{9}Be

After introducing additional neutrons to an alpha-particle we can consider the case of two alpha-particles and that of two-alpha-particles accompanied by a neutron. These two cases correspond to the nuclei ^{8}Be and ^{9}Be respectively.

In our approximation there is only one possibility for the tableau describing the per-

mutation symmetry of the ^{8}Be spatial part :

$$[4,4] \equiv \begin{array}{|c|c|c|c|}\hline & & & \\ \hline & & & \\ \hline \end{array} . \tag{3.72}$$

The tableau describing the conjugate permutation symmetry for the spin-isospin part is

$$[2^4] \equiv \begin{array}{|c|c|}\hline & \\ \hline & \\ \hline & \\ \hline & \\ \hline \end{array} . \tag{3.73}$$

There is only one possible decomposition of the spin-isospin states compatible with SU(2)×SU(2):

$$|[2^4]i\rangle \in \begin{array}{|c|c|c|c|}\hline & & & \\ \hline & & & \\ \hline \end{array} \times \begin{array}{|c|c|c|c|}\hline & & & \\ \hline & & & \\ \hline \end{array} \quad (S=0, T=0). \tag{3.74}$$

The case of ^{9}Be is very similar to ^{5}He. By adding one more neutron to the above configuration of ^{8}Be there is only one possibility for the permutation symmetry of the spatial part:

$$[4,4,1] \equiv \begin{array}{|c|c|c|c|}\hline & & & \\ \hline & & & \\ \hline \\ \cline{1-1} \end{array} . \tag{3.75}$$

The tableau describing the conjugate permutation symmetry for the spin-isospin part is

$$[3,2^3] \equiv \begin{array}{|c|c|c|}\hline & & \\ \hline & \\ \cline{1-2} & \\ \cline{1-2} & \\ \cline{1-2} \end{array} . \tag{3.76}$$

There is only one possible decomposition of the spin-isospin states compatible with SU(2)×SU(2) with quantum numbers $(S = 1/2, T = 1/2)$.

3.5 Conclusions and general remarks

The cluster-like variational model we wish to examine preserves the full microscopic nature of the nuclear many-body problem. The approximations imposed are of two types: one concerning the actual wavefunction and the other concerning the type of interaction used. In the latter approximation we restrict ourselves in the study of central local interactions. The main reason is due to the difficulty that can arise because of the required matrix elements of tensor operators and spin-orbit terms. Although such terms have been

examined for the closed shell alpha-particle, we do not wish to pursue them at this stage for the lightly bound systems to be examined. In principle is always possible to include such terms.

The approximations chosen for the wavefunction are such that lead to a linear variational problem where the solution is well known. The J-TICI(2) method has the advantage over the RGM-like method that it can incorporate state-dependent correlations. The fact that we are allowed to have a spin-isospin saturated structure is due to the exclusion of spin-orbit coupling. This results in SU(4) symmetry for the spin-isospin part of the wavefunction. The spin-isospin part of the wavefunction should have a decomposition into SU(2) irreps for the spin and isospin labels respectively, something related with the permutation symmetry.

The incorporation of the antisymmetry condition, appropriate for fermions, has been given special attention. It was shown that the complexity greatly increases in going from the alpha- particle to ^{5}He, ^{6}He, ^{8}Be and ^{9}Be. Some simple group-theoretical results can simplify the expectation values. In general the antisymmetry condition can be applied without any difficulty to the alpha-particle, where only either spin or isospin exchanges are required. Beyond that there are no radical simplifications.

In any-case the present model is as an extension of previous related work concerning the closed shell alpha-particle into the area of halo nuclei. A major drawback can be the closed shell alpha-particle structure since it restricts the possible configurations of the reference function. In practice the bound system might require a superposition of different reference function having the alpha particle ‘broken’.

Chapter 4

Monte Carlo evaluation of expectation values

As described in the previous chapters we will approximately solve the many-body Schrödinger equation through a linear variational principle. Although the theoretical background is fairly simple, a numerical evaluation of the matrix elements is usually required, due to the complexity of the many-body expectation values. In this chapter we examine the application of the well known variational Monte Carlo (VMC) [66].

The most important task of the analysis provided in this chapter is to ensure the validity of the error estimate and in particular as applied to the linear eigenvalue problem. We shall make use of a number of statistical concepts, most of which can easily be found in the literature such as [67].

We also describe the application of a method that is used to improve the performance of VMC.

4.1 The variational problem

We are going to make use of the time-independent Schrödinger equation,

$$H(x)\Psi(x) = E\Psi(x), \tag{4.1}$$

where in general we approximate $\Psi(x)$ as

$$\Psi(x) = \sum_n C_n f^n(x). \tag{4.2}$$

The wavefunction is expanded in terms of a set of normalizable trial functions linear in the coefficients $\{C_n\}$ and H is the hamiltonian. In general, x denotes the set of coordinates appropriate for the many-body hamiltonian. However, for simplicity spin-isospin degrees of freedom are ignored here. Multiplying equation (4.1) on the left by the complex conjugate wavefunction and integrating over the appropriate variable, the equation takes the form

$$\sum_n C_k^* \left(\int f_k^* \hat{H} f_n d\Omega \right) C_n = E \sum_n C_k^* \left(\int f_k^* f_n d\Omega \right) C_n \tag{4.3}$$

where $d\Omega$ is the volume element. The above equation can now be written as

$$E = \frac{\sum_n C_k^* \mathcal{H}_{kn} C_n}{\sum_n C_k^* \mathcal{N}_{kn} C_n}, \tag{4.4}$$

where $\mathcal{H}_{kn}$ and $\mathcal{N}_{kn}$ represent the Hamiltonian and overlap matrix elements with

$$\mathcal{H}_{kn} = \int f_k^* H f_n d\Omega, \tag{4.5}$$

$$\mathcal{N}_{kn} = \int f_k^* f_n d\Omega. \tag{4.6}$$

The variational principle states that if E_0 represents the exact lowest eigenvalue of the particular Hamiltonian then any estimate, E, for E_0 obtained from (4.4) will be an upper bound of E_0. Using this fact a particular form for $\Psi(x)$ may be optimized by varying the adjustable parameters to minimize the expectation value of (4.4). The best approximation to the true lowest eigenvalue is obtained by the variation of the coefficients C_n. This leads to a set of coupled equations of the form

$$\sum_n \mathcal{H}_{kn} C_n - E \sum_n \mathcal{N}_{kn} C_n = 0, \tag{4.7}$$

that constitute a generalized eigenvalue problem. Once the matrix elements are known, solution of the eigenvalue problem is straightforward.

4.1.1 Error estimate

The matrix elements entering the eigenvalue problem might well be evaluated numerically (as discussed in the next section), leading to an error in the estimated eigenvalue. In case where an error estimate for individual matrix elements exists, the total error for the eigenvalue problem of (4.7) can be obtain from the linear perturbation of the eigenvalue problem

$$\sum_n (\mathcal{H}_{kn} + \delta\mathcal{H}_{kn})(C_n + \delta C_n) = (E + \delta E)\sum_n (\mathcal{N}_{kn} + \delta\mathcal{N}_{kn})(C_n + \delta C_n), \qquad (4.8)$$

where δE is the unknown error. Multiplying on the right by the same eigenvector and keeping only first order terms leads to

$$\delta E = \frac{1}{C_k\mathcal{N}_{kn}C_n}\left(C_k\delta\mathcal{H}_{kn}C_n - EC_k\delta\mathcal{N}_{kn}C_n\right), \qquad (4.9)$$

with summation convention implied. If the Hamiltonian and overlap matrix errors were independent of each other the right hand side of the above equation could have been taken in quadrature giving value for the maximum possible error, ΔE, that is the required error for the numerical calculation :

$$\Delta E = \frac{1}{C_k\mathcal{N}_{kn}C_n}\sqrt{(C_k\Delta\mathcal{H}_{kn}C_n)^2 + (EC_k\Delta\mathcal{N}_{kn}C_n)^2}. \qquad (4.10)$$

However, the above equation can lead to a wrong error estimate since in reality the errors in the hamiltonian and overlap matrix elements are likely to be correlated (depending on the method used for their evaluation). A way of dealing with this problem is through the covariance matrix, which can be used to define a set of uncorrelated (independent) observables whose errors can be added in quadrature. The elements of the covariance matrix are cov$(B_z B_{z'})$, defined as

$$\text{cov}(B_z B_{z'}) = \langle B_z B_{z'}\rangle - \langle B_z\rangle\langle B_{z'}\rangle, \qquad (4.11)$$

with $B_z \in \{\{H_z\}, \{N_z\}\}$, while the angular brackets denote an expectation value. This gives a real symmetric matrix of the form

$$\mathbf{C} = \begin{pmatrix} \sigma^2(H_{11}) & \dots & \text{cov}(H_{11}H_{nn}) & \text{cov}(H_{11}N_{11}) & \dots & \text{cov}(H_{11}N_{nn}) \\ \vdots & \ddots & & & & \vdots \\ \text{cov}(H_{nn}H_{11}) & \dots & \sigma^2(H_{nn}) & \text{cov}(H_{nn}N_{11}) & \dots & \text{cov}(O_{nn}N_{nn}) \\ \text{cov}(N_{11}H_{11}) & \dots & \text{cov}(N_{11}H_{nn}) & \sigma^2(N_{11}) & \dots & \text{cov}(N_{11}N_{nn}) \\ \vdots & & & & \ddots & \vdots \\ \text{cov}(N_{nn}H_{11}) & \dots & \text{cov}(N_{nn}H_{nn}) & \text{cov}(N_{nn}N_{11}) & \dots & \sigma^2(N_{nn}) \end{pmatrix} \tag{4.12}$$

with dimensions $(2n^2) \times (2n^2)$, where $n \times n$ is the dimension of the hamiltonian and overlap matrices. The diagonal elements correspond to the variance of the hamiltonian and overlap matrix elements σ^2 that is discussed later. Diagonalizing the covariance matrix is equivalent to obtaining a new set of uncorrelated observables that each is a linear combination of the old ones. This new set of uncorrelated observables, $\{Q_z\}$, can then be defined from the eigenvectors of $\mathbf{C}$ as

$$B_z = \sum_k R_{zk} Q_k, \tag{4.13}$$

$$\sum_k \mathbf{C}_{zk}\mathbf{R}_{kz} = \lambda_z \mathbf{R}_{zz}, \tag{4.14}$$

$$\mathbf{C} = \mathbf{R}\mathbf{\Lambda}\mathbf{R}^T. \tag{4.15}$$

Here R_{kz} is the zth eigenvector of $\mathbf{C}$, while $\mathbf{\Lambda} \equiv \text{diag}(\lambda_1, ..., \lambda_{2n^2})$. The new observables independent satisfy the condition

$$\text{cov}(Q_k Q_z) = \delta_{kz}\lambda_z, \tag{4.16}$$

i.e. their covariance vanishes and their variance is equal to the eigenvalues of $\mathbf{C}$. The error associated with the new observables is their standard deviation, which according to the above equation can be found as

$$(\Delta Q_k)^2 = \frac{\lambda_k}{N-1}, \tag{4.17}$$

with N denoting the number of samples taken for the observable. This way equation (4.10) can be written as

$$\Delta E = \frac{1}{C_k \mathcal{N}_{kn} C_n} \sqrt{\sum_k \left(\sum_{ij} C_i (\mathbf{R}_{H_{ijk}} - E\mathbf{R}_{N_{ijk}}) C_j \right)^2 (\Delta Q_k)^2}, \tag{4.18}$$

where the errors corresponding to the independent set of observables, $\{Q_k\}$, can be added in quadrature.

4.2 Monte Carlo Integration

The generalized eigenvalue problem of equation (4.7) requires the computation of the Hamiltonian and overlap matrix elements which in general are complicated integrals and one may wish to choose Monte Carlo sampling to perform the integration. The matrix elements of equations (4.5) and (4.6) can be written as

$$\mathcal{H}_{kn} = \int dx\, w(x) \left(\frac{f_k(x) H(x) f_n(x)}{w(x)} \right), \tag{4.19}$$

$$\mathcal{N}_{kn} = \int dx\, w(x) \left(\frac{f_k(x) f_n(x)}{w(x)} \right), \tag{4.20}$$

where $w(x)$ plays the role of the probability density function provided that is definite positive and shares the same symmetries as the full wave function. The eigenvalue problem leads to

$$\begin{aligned} \sum_n C_n \int dx\, w(x) H_{kn}(x) &= E \sum_n C_n \int dx\, w(x) N_{kn}(x,) \\ \sum_n \langle H_{kn} \rangle C_n &= E \sum_n \langle N_{kn} \rangle C_n, \end{aligned} \tag{4.21}$$

which can be viewed as the expectation value of two distinct arbitrary functions of a random variable (H_{kn} and N_{kn}) taken from the same probability distribution.

Because of the parametrization of the wavefunction in terms of the unknown coefficients C_n a single probability distribution function appropriate for each individual matrix element cannot be extracted. Although in principle is possible to sample each matrix element based on its own distribution leading to n^2 distinct Monte Carlo algorithms (or $\frac{n(n+1)}{2}$ for a symmetric matrix), time requirements make such a calculation impractical. A

way around this difficulty is to sample all of the matrix elements based on a single probability distribution. Although, this approach reduces the number of required simulations, it can lead to a large variance for individual matrix elements and special care is required.

4.2.1 Statistical sampling

In Monte Carlo methods, $\langle H_{kn} \rangle$ or $\langle N_{kn} \rangle$ are estimated using a large but finite set of values for x (a finite set of configurations $\{x_i\}$ for the multi-dimensional case) distributed according to w. In order to avoid referring to individual matrix elements we consider the expectation value of a general operator O which is denoted by $\langle O \rangle$.

One practical well known method of obtaining the required distribution is the Metropolis algorithm and this is the one we shall use. In order to generate values of the variable x having the required distribution the Metropolis algorithm makes use of a random walk: An initial point (set of coordinates), x_0, is chosen and subsequent points are generated in steps by moving in a random direction, but each time within a prescribed radius from each individual coordinate. Not all points, however, are kept but an 'accept or reject' method is used. This means that every point x_l in the random walk belonging to the l_{th} step, is weighted against the previous point, x_{l-1}, and is either chosen or rejected. The decision process is given by the Metropolis algorithm which generates a Markov chain. In order to fulfill the criteria for a Markov chain it is essential for each step that the decision process governing the evolution of the random walk should not have any dependence on configurations belonging to previous steps. This means that the decision of keeping or rejecting point x_l should only depend on the value of the point x_{l-1} and not on any previous points. An equivalent statement would be to say that the set of values, $\{O(x_i)\}$, chosen to form the average should be uncorrelated with each other.

The random walk provides as with a statistical average that is different from the exact expectation value, but can be used as an approximation. The expectation value $\langle O \rangle$ corresponds to the average of the quantity O over an infinite ensemble of statistically independent trials. This average can in principle be obtained exactly if integrals similar to (4.19) and (4.20) can be evaluated analytically. The random walk that is actually performed in simulations provides an average over a finite sequence of measurements. This sample average or mean will be denoted by $\bar{O}$. In the case of N samples taken from a

distribution, the expectation value is approximated as

$$\langle O \rangle \approx \bar{O}, \tag{4.22}$$

$$= \frac{1}{N} \sum_{i=1}^{N} O(x_i), \tag{4.23}$$

where the x_i represents the set of appropriate coordinates that are distributed according to a probability density w(x).

4.2.2 Error estimate and correlations

Provided we have a statistical average composed of N uncorrelated samples taken from an arbitrary probability distribution, the central limit theorem states that in the limit of large N, the above average follows a normal distribution with mean $\langle O \rangle$ and variance

$$\sigma^2 = \frac{1}{N} \sigma_0^2, \tag{4.24}$$

with

$$\sigma_0^2 = \langle O^2 \rangle - \langle O \rangle^2. \tag{4.25}$$

However, in a Monte Carlo sampling we are limited to a finite average and the actual error deviates from the limiting case provided by the central limit theorem. We would like to know how to estimate the error of such an average which is the deviation from $\langle O \rangle$. The theoretical value of this error can be obtained by considering an ensemble of independent random walks, where we can introduce the notion of the expected value of a sample average, $\langle \bar{O} \rangle$, as well as that of the expected value of any single measurement ($O_i \equiv O(x_i)$) corresponding to a particular step i of the random walks, denoted by $\langle O_i \rangle$. The demand that the individual measurements belong to a Markov chain is then expressible as

$$\langle O_i \rangle = \langle O_j \rangle = \langle \bar{O} \rangle = \langle O \rangle, \tag{4.26}$$

meaning that all samples or measurements in the random walk are independent of their position relative to the others. The fact that there is a correlation between individual

measurements corresponds to the case where

$$\langle O_i O_j \rangle \neq \langle O_i \rangle \langle O_j \rangle \tag{4.27}$$

When the above is taken into consideration the variance of the mean becomes

$$\begin{aligned}
\sigma^2(\bar{O}) &= \langle (\bar{O} - \langle O \rangle)^2 \rangle & (4.28)\\
&= \langle (\bar{O} - \langle \bar{O} \rangle)^2 \rangle & (4.29)\\
&= \langle \bar{O}^2 \rangle - \langle \bar{O} \rangle^2, & (4.30)\\
&= \frac{1}{N^2} \sum_{ij} \left(\langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle \right). & (4.31)
\end{aligned}$$

This describes the deviation of the calculated mean from the theoretical expectation value.

However, in practise is impossible to have an algorithm which can generate samples that are completely uncorrelated. Such is the case of the Metropolis algorithm. By the nature of the algorithms used the individual measurements are not statistically independent. Such correlations between statistical measurements have in general two effects. First, they reduce the number of independent measurements from the total number of performed measurements, hence the calculation converges more slowly. Second, the estimation for the statistical error will have to incorporate the effect of such correlations otherwise any error estimate will be an underestimate. As for any numerical method a correct error estimate is of crucial importance for the validity of the results. The rest of this section is devoted to the analysis of the error estimates on averages of correlated data. Most of the results are taken from [68] and [69].

In case that (4.27) does not hold the equation for the variance of $\bar{O}$ reduces to that of equation (4.24). However, when (4.27) holds the true variance for the mean can be written as [68]

$$\sigma^2(\bar{O}) = \frac{1}{N} \left[\sigma_0 + 2 \sum_{t=1}^{N-1} \left(1 - \frac{t}{N} \right) \rho_t \right], \tag{4.32}$$

where

$$\begin{aligned}
\rho_t &\equiv \langle O_i O_j \rangle - \langle O_i \rangle \langle O_j \rangle \quad t = |i - j|,\\
&= \langle O_i O_{i+t} \rangle - \langle O_i \rangle \langle O_{i+t} \rangle. & (4.33)
\end{aligned}$$

Furthermore, the presence of correlations also influences the value of the covariance between the means of two different quantities, O and $O^{'}$, since

$$\begin{aligned} \text{cov}(\bar{O}\bar{O}^{'}) &= \langle \bar{O}\bar{O}^{'} \rangle - \langle \bar{O} \rangle \langle \bar{O}^{'} \rangle & (4.34) \\ &= \frac{1}{N^2} \sum_{ij} \left(\langle O_i O_j^{'} \rangle - \langle O_i \rangle \langle O_j^{'} \rangle \right) & (4.35) \\ &= \frac{1}{N} \left[\gamma_0 + 2 \sum_{t=1}^{N-1} \left(1 - \frac{t}{N} \right) \gamma_t \right], & (4.36) \end{aligned}$$

where similarly to equation (4.33) we define

$$\gamma_t \equiv \langle O_i O_j^{'} \rangle - \langle O_i \rangle \langle O_j^{'} \rangle \quad t = |i - j| \, . \tag{4.37}$$

An essential assumption for both ρ_t and γ_t is the invariance under 'time translations', meaning that only the separation between the measurements is of importance and not their place in the random walk (something also included in (4.26)), i.e.

$$\langle O_i O_j \rangle = \langle O_j O_i \rangle, \tag{4.38}$$

$$\langle O_i^{'} O_j \rangle = \langle O_i O_j^{'} \rangle \, . \tag{4.39}$$

As we have seen earlier a reliable error estimate requires two quantities. Firstly, an estimate of the error for each individual matrix element, something provided by the variance of the mean for the particular matrix element. Secondly, an estimate for the covariance between different matrix elements, so that a set of uncorrelated observables can be obtained. In theory both of these objects are provided by ρ_t and γ_t. However, in a practical simulation only approximate measurements can be made.

4.2.3 Estimation of variance and covariance

An estimate for ρ_t and γ_t can be obtained through the auto- and cross-correlation coefficients. The auto-correlation coefficient, C_t is defined in the case of N samples as

$$C_t(O) = \frac{1}{N-1} \sum_{i=1}^{N-t} (O_i - \bar{O})(O_{i+t} - \bar{O}), \tag{4.40}$$

while the cross-correlation coefficient as

$$\mathbb{C}_t(O,O^{'}) = \frac{1}{N-1}\sum_{i=1}^{N-t}(O_i-\bar{O})(O^{'}_{i+t}-\bar{O}^{'}). \tag{4.41}$$

The variable t will be refereed to as the correlation time. These two coefficients provide biased estimators for ρ_t and γ_t, in the sense that they underestimate the actual values. This is expressed as

$$\begin{aligned}\langle C_t(O)\rangle &= \rho_t - \sigma^2(O) + \Delta_t, &(4.42)\\ \langle \mathbb{C}_t(O,O^{'})\rangle &= \rho_t - \sigma^2(O) + \Delta^{'}_t, &(4.43)\end{aligned}$$

where the terms Δ_t and $\Delta^{'}_t$ are given as

$$\Delta_t = 2\left(\sigma^2(\bar{O}) - \frac{1}{N(N-t)}\sum_{i=1}^{N-t}\sum_{j=1}^{N}\gamma_{ij}\right), \tag{4.44}$$

$$\Delta^{'}_t = 2\left(\mathrm{cov}(\bar{O}\bar{O}^{'}) - \frac{1}{N(N-t)}\sum_{i=1}^{N-t}\sum_{j=1}^{N}\gamma^{'}_{ij}\right), \tag{4.45}$$

with

$$\begin{aligned}\gamma_{ij} &= \langle O_iO_j\rangle - \langle O_i\rangle\langle O_j\rangle,\\ \gamma^{'}_{ij} &= \langle O_iO^{'}_j\rangle - \langle O_i\rangle\langle O^{'}_j\rangle.\end{aligned}$$

However, in most applications the largest correlation time in ρ_t and γ_t is finite, meaning that equations (4.32) and (4.36) can be approximated by

$$\begin{aligned}\sigma^2(\bar{O}) &\approx \frac{1}{N}\left[\sigma_0^2 + 2\sum_{t=1}^{T}\left(1-\frac{t}{N}\right)\rho_t\right], &(4.46)\\ \mathrm{cov}(\bar{O},\bar{O}^{'}) &\approx \frac{1}{N}\left[\mathrm{cov}(O,O^{'}) + 2\sum_{t=1}^{T}2\left(1-\frac{t}{N}\right)\gamma_t\right]. &(4.47)\end{aligned}$$

The meaning of the above approximation for a random walk is that the correlation between different samples is of finite range in the sense that $\langle O_iO_j\rangle - \langle O_i\rangle\langle O_j\rangle$ and $\langle O_iO^{'}_j\rangle - \langle O_i\rangle\langle O^{'}_j\rangle$ become zero for large enough correlation time $t = |i-j|$. The parameter T in the above equations represents a cutoff parameter and is the maximum correlation

time that will be taken into account. The significance of a finite correlation time is that the biases Δ_t and $\Delta_t^{'}$ in equations (4.42) and (4.43) will become arbitrarily small for sufficiently large number of samples n.

Provided that $\frac{T}{N}$ is sufficiently small, the variance and covariance can be approximated by

$$\begin{aligned} \sigma^2(0) &\approx \frac{\sigma_0^2 + 2\sum_{t=1}^{T} C_t}{N} \\ &= \left(1 + 2\frac{\sum C_t}{\sigma_0^2}\right)\frac{\sigma_0^2}{N} \qquad (4.48) \\ \text{cov}(O, O^{'}) &\approx \frac{\mathbb{C}_0 + 2\sum_{t=1}^{T} \mathbb{C}_t}{N} \\ &= \left(1 + 2\frac{\sum \mathbb{C}_t}{\mathbb{C}_0}\right)\frac{\mathbb{C}_0^2}{N}. \qquad (4.49) \end{aligned}$$

The above equations provide as with a way of measuring the strength of correlations in a particular simulation through the 'normalized' correlation coefficients, C_t/σ_0^2 and $\mathbb{C}_t/\mathbb{C}_0$. These can be obtained for a particular simulation as a function of the correlation time t.

In order to get an idea about the correlation coefficient we can consider the case of the alpha-particle. The probability density function w was taken to be the square of one of the components in the expansion of the state-independent wavefunction i.e

$$w = (\hat{F}_0^l \Phi_0)^2. \qquad (4.50)$$

The variance of equation (4.48) and the normalized auto and cross-correlation coefficients of (4.40) and (4.41) were sampled as functions of correlation-time. This was done for the matrix elements of both the hamiltonian and overlap matrices. The result is shown in figure 4.1. We can see in the upper part of the figure that the variance strongly depends on the correlation coefficient, starting from a minimum and finally converging. According to the previous analysis this indicates that despite the fact that the variance depends on the correlation time, there is a cutoff in the correlation coefficient, which implies that the dependence on the correlation coefficient will be over a restricted range of the correlation time (approximately about the cutoff). This is backed up by sampling the correlation coefficient (lower graphs of figure 4.1), where we can see that the value of the normalized correlation coefficient rapidly decays as the correlation time increases. According to the

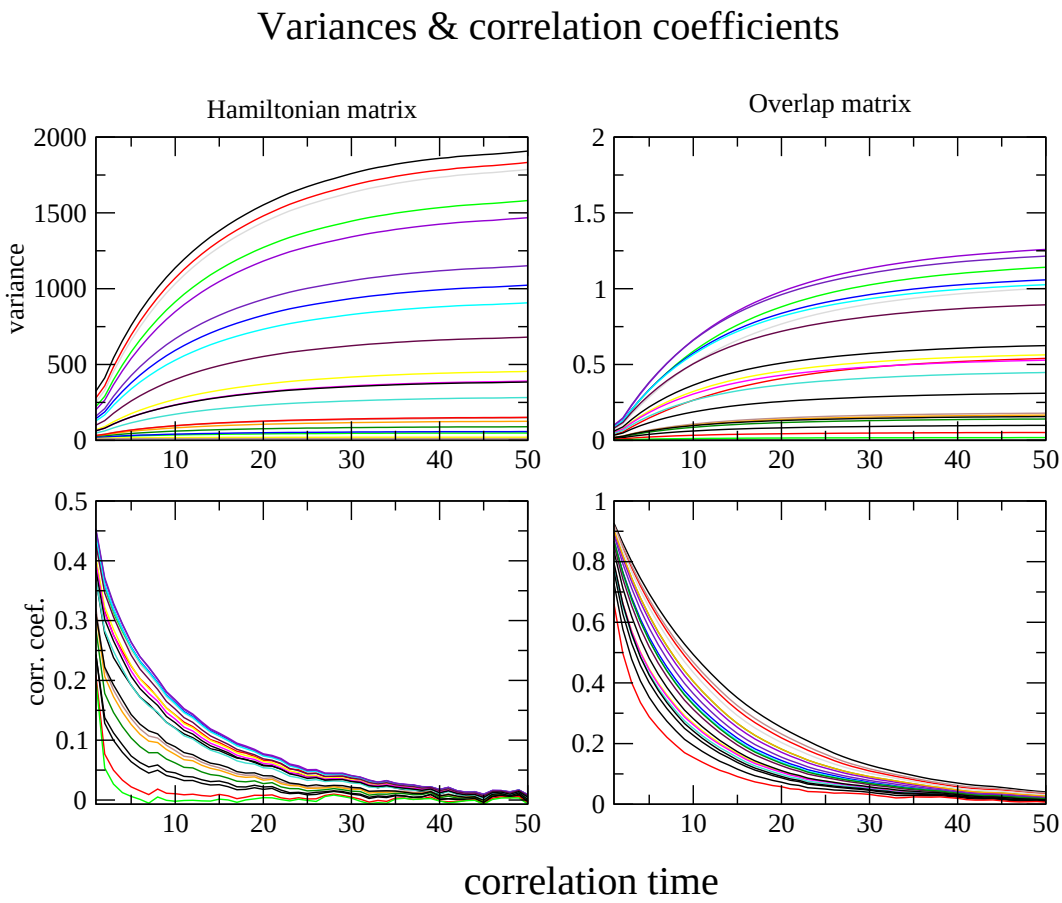


Figure 4.1: The variance (upper part) and the normalized auto- and cross-correlation coeffi cients (lower part) as a function of correlation time. These results are for the hamiltonian and overlap matrices of the alpha-particle J-TICI(2) calculation.

figure we can safely assume 50 samples as the value of the cutoff.

4.2.4 Application

In the alpha-particle calculation we do not have knowledge of the exact simulation variance, since this would require the expectation value of the sample average. We assume that the value obtained through the approximate equations (4.48) and (4.40) is sufficiently accurate. This assumption is backed up by the results illustrated in figure 4.1. In order to examine the accuracy of the variance estimate a simple one dimensional problem was considered. A hamiltonian of the form

$$H(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{\cosh^2 x} \tag{4.51}$$

was used, where the exact value of the lowest eigenvalue is known and is equal to $-\frac{1}{2}$. We can approximate this value through a variational problem in terms of the eigenvalue equation (4.7). A Gaussian non-orthogonal expansion of the form

$$f_n = e^{-\mu_n x^2}. \tag{4.52}$$

was used to approximate the wave function with the $\{\mu_n\}$ belonging to a geometric series. Since a numerically exact result can obtained for this approximation, we can also use Monte Carlo sampling in order to verify the error estimate. The probability density function was taken to be the square of the first Gaussian. Since we can obtain the numerically exact values for $\mathcal{H}_{kn}$ and $\mathcal{N}_{kn}$ we can use this to construct an unbiased estimator for the variance and thus to obtain an uncorrelated estimate for the variance of each matrix element. For example the variance for the Hamiltonian matrix elements is given as

$$\begin{aligned} \frac{\sigma^2(\mathcal{H}_{kn})}{N} &= \langle(\bar{\mathcal{H}}_{kn} - E_{kn})^2\rangle \\ &\approx \sum_{i=1}^{n}(\bar{\mathcal{H}}^i_{kn} - E_{kn})^2, \end{aligned} \tag{4.53}$$

where E_{kn} corresponds to the exact value while the summation is over a number of distinct random walks with $\bar{\mathcal{H}}^i_{kn}$ denoting the distinct average obtained in the i_{th} walk consisting of N samples. The approximation symbol becomes an equality in the limit of large n. For

our simple one dimensional model the convergence is relatively fast and the results obtained can be referred to as statistically exact. Simultaneously we can obtain the value of the variance through the biased estimator of (4.48) for any one of the performed averages.

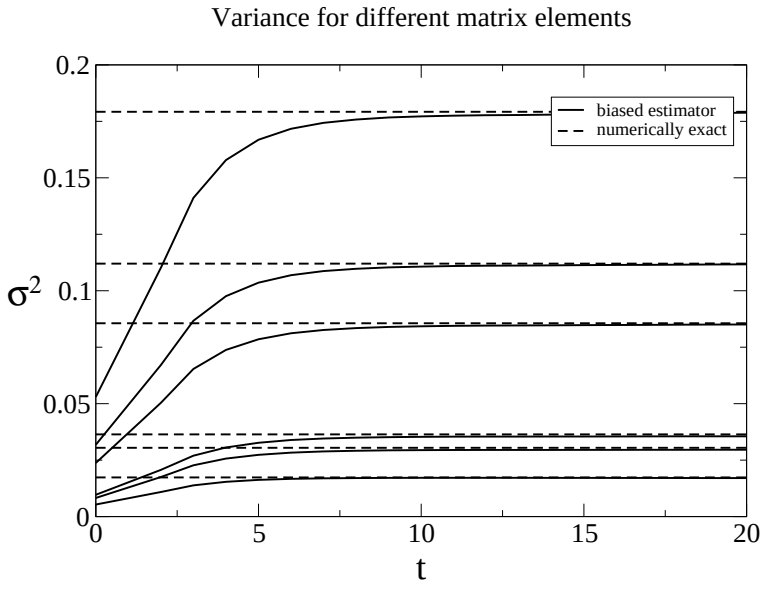


Figure 4.2: The (biased) variance estimate for different matrix elements of the Hamiltonian matrix as a function of the correlation time t, for a simple one-dimensional model. The fact that the biased estimate approaches a constant value with respect to t indicates that there is a cutoff in the correlation coeffi cients (as shown previously). The dotted lines represent the value for the variance obtained through an unbiased measurement.

The statistically exact value of the variance and that of the biased estimator depending on the correlation time are shown in figure 4.2, which is a demonstration for the accuracy of the variance estimate. Provided that the correlation time is large enough the value for the variance obtained as a result of (4.48) agrees with that of the statistically exact value of (4.53). Although, the statistically exact value cannot be obtained directly for practical calculations (it requires the analytical results), the estimation through the biased estimator of (4.48) becomes statistically exact provided there is a cutoff in the correlation coefficient.

When the maximum correlation time is relatively small an unbiased error estimate can be obtained without having to consider the correlation coefficient. The samples taken from the random walk are consecutively obtained from each other and thus the separation from each other in simulation time is exactly equivalent to the correlation time. If we call the maximum correlation time T, then each sample is correlated with samples separated

from it by at most T steps. Therefore, if from the total number of samples obtained only the ones separated by T steps (or random walk moves) are considered, this new set of samples will be uncorrelated. In the literature these intermediate moves are usually referred to as 'thermalisations' [67], where is expected that a relatively small number is adequate. However, for more complicated models, the maximum correlation time might be too large for either completely removing the correlations or estimating the effect of the correlation coefficient without any intermediate moves.

It must be noted that the more samples are discarded or the largest the correlation time is, the more time consuming the simulation becomes. Therefore, in general the most efficient approach that can guarantee a correct variance estimate is to make use both of intermediate moves and the correlation coefficient.

4.2.5 Variance reduction

Although correlations can be taken into account or even removed from the sampling of a particular observable, this can only provide an algorithm with a reliable error estimate. In order to get an adequate error a large number of samples are required, the number depending on the particular observable. The so called 'zero-variance principle' is a way of increasing the efficiency of a Monte Carlo algorithm by reducing the variance. In general the principle is to use in the place of each observable to be computed an improved estimator which has the same mean but a different variance. The method is described in [70] where applications of the zero-variance principle were shown to be very powerful. This variance reduction technique is examined in order to establish its application for the case of many-body cluster models.

Method

We consider the expectation value of an observable O_{kn} given as

$$\langle O_{kn} \rangle = \int w(x) O_{kn}(x) dx, \tag{4.54}$$

where as usual $w(x)$ represents a normalized probability density function (pdf). In our case $\langle O_{kn} \rangle$ corresponds to a particular matrix element of either the Hamiltonian or overlap matrices, where for practical purposes all expectation values are over the same single pdf.

This implies that we can optimize $w(x)$ for at most one of the matrix elements.

We introduce the 'renormalized' observable $\tilde{O}_{kn}$ where

$$\tilde{O}_{kn} = O_{kn} + \frac{\hat{h}\psi_{kn}}{\sqrt{w}}, \tag{4.55}$$

$$= O_{kn} + \bar{O}_{kn} \tag{4.56}$$

with $\hat{h}$ and ψ_{kn} representing a trial operator and a trial function appropriate for the expectation of each individual matrix element. In order for the expectation value of $\tilde{O}_{kn}$ to be the same as that of the original observable the operator $\hat{h}$ must satisfy the condition

$$\hat{h}\sqrt{w} = 0 \tag{4.57}$$

This leads to the equation

$$\hat{h}\psi_{kn} = (\langle O_{kn}\rangle - O_{kn})\sqrt{w}, \tag{4.58}$$

which has the consequence that the error of the calculation, $\sigma(\tilde{O}_{kn})$, vanishes. Although in principle equation (4.58) should be satisfied, in practise an approximate solution can be searched that minimizes the variance of the calculation. The variance for the expectation value of the new operator of equation (4.56) now becomes

$$\sigma^2(\tilde{O}_{kn}) = \sigma^2(O_{kn}) + \sigma^2(\bar{O}_{kn}) + 2(\langle O_{kn}\bar{O}_{kn}\rangle - \langle O_{kn}\rangle\langle\bar{O}_{kn}\rangle). \tag{4.59}$$

A possible way to approximate the function ψ_{kn} would be to consider a finite expansion linear in some coefficients like in the case of the wavefunction Ψ (equation (4.2)). This means that ψ_{kn} can be given as

$$\psi_{kn} = \sum_i A_i^{kn} g_i, \tag{4.60}$$

where the functions $\{g_i\}$ are taken to be common for all matrix elements, while the coefficients $\{A_i^{kn}\}$ are determined by minimizing the variance of a particular matrix element, in this case the observables $\langle\tilde{O}_{kn}\rangle$. The condition that the variance is minimized can be imposed by demanding that upon variation of the coefficients A_i^{kn} the value of the variance

reaches a minimum :

$$\delta\sigma^2(\tilde{O}_{kn}) = 0 \tag{4.61}$$

$$\Rightarrow \quad \frac{\partial\tilde{O}_{kn}}{\partial A_i^{kn}} = 0, \quad \forall A_i^{kn}. \tag{4.62}$$

This leads for each matrix element to an equation of the form

$$\sum_j A_j^{kn}\Delta_{ij} + K_i^{kn} = 0, \tag{4.63}$$

where

$$\Delta_{ij} = \left\langle \frac{\hat{h}g_i\hat{h}g_j}{w} \right\rangle - \left\langle \frac{\hat{h}g_i}{\sqrt{w}} \right\rangle \left\langle \frac{\hat{h}g_j}{\sqrt{w}} \right\rangle, \tag{4.64}$$

$$K_i^{kn} = \left\langle O_{kn}\frac{\hat{h}g_i}{\sqrt{w}} \right\rangle - \langle O_{kn}\rangle \left\langle \frac{\hat{h}g_i}{\sqrt{w}} \right\rangle. \tag{4.65}$$

Therefore, for a particular set of functions $\{g_i\}$, the coefficients $\{A_i^{kn}\}$ can then be obtained as

$$A_j^{kn} = -\sum_i (\Delta)_{ji}^{-1} K_i^{kn}. \tag{4.66}$$

One difficulty that might arise is when one or more of the eigenvalues of $\mathbf{\Delta}$ is near zero (zero for all practical purposes), in which case solving equations (4.63) by inverting $\mathbf{\Delta}$ will lead to numerical instabilities. Diagonalizing $\mathbf{\Delta}$ is equivalent to obtaining linear superpositions of the functions $\{g_i\}$ that are uncorrelated with respect to the operator $\frac{h}{\sqrt{w}}$. However, this might not be possible for the entire set $\{g_i\}$. This problem can be bypassed by solving (4.63) with singular value decomposition, which is equivalent to considering a reduced set of functions $\{g_i\}$.

By substituting the coefficients back to equation (4.59) the variance of each particular matrix element becomes

$$\sigma^2(\tilde{O}_{kn}) = \sigma^2(O_{kn}) + \sum_{ij} K_i^{kn}A_i^{kn}, \tag{4.67}$$

$$= \sigma^2(O_{kn}) - \sum_{ij} A_i^{kn}\Delta_{ij}A_j^{kn}, \tag{4.68}$$

which is always bound to be less than $\sigma^2(O_{kn})$, whatever the choice for the g_i's due to the

fact that the eigenvalues of $\mathbf{\Delta}$ are always positive.

An efficient method of obtaining an appropriate set of functions g_i is to run a number of short Monte Carlo algorithms until a set that reduces the variance of the calculation efficiently is found. The set of coefficients $\{A_i\}$ can be obtained from a short sampling and used as input for a larger computation.

Note: The error for the zero variance calculation can also be obtained from a set of uncorrelated errors giving an equation similar to (4.18). The only difference is in the covariance matrix to be calculated. The new matrix elements are

$$\begin{aligned} C_{ij} &= \text{cov}(\tilde{B}_i\tilde{B}_j), \\ &= \text{cov}([B_i + \bar{B}_i][B_j + \bar{B}_j]), \\ &= \text{cov}(B_iB_j) + \sum_n A_n^j K_n^i + \sum_n A_n^i K_n^j + \sum_{nm} A_n^i A_m^j \Delta_{nm}, \end{aligned} \tag{4.69}$$

where i is a collective index representing a particular matrix element of either the Hamiltonian or overlap matrix ($\{O_{nm}, N_{nm}\} \equiv \{B_i\}$), while $\mathbf{\Delta}$ and $\mathbf{K}$ are defined in equations (4.64) and (4.65).

Applications

Although the variance reduction technique in principle can reduce the variance of an observable, for practical calculations we are confined within the effectiveness of the linear approximation of equation (4.60). For a complicated many-body problem the choice of the functions $\{g_i\}$ entering (4.60) is not obvious. For our calculations we shall make use the same set as the one used for the linear eigenvalue problem. This is the simplest available choice. We can examine the applicability of this approach through the same one dimensional problem as before before going to the many-body case. In this case the integrals of equation (4.67) can be solved in a numerically exact manner without having to make use of Monte Carlo sampling. The numerically exact results for the variance of the one-body problem are shown in figure (4.3). In this case the variance reduction greatly reduces the variance of the matrix elements and can lead to a zero variance (within the numerical accuracy of the machine used).

We can then proceed and apply the same method to the case of the alpha-particle in

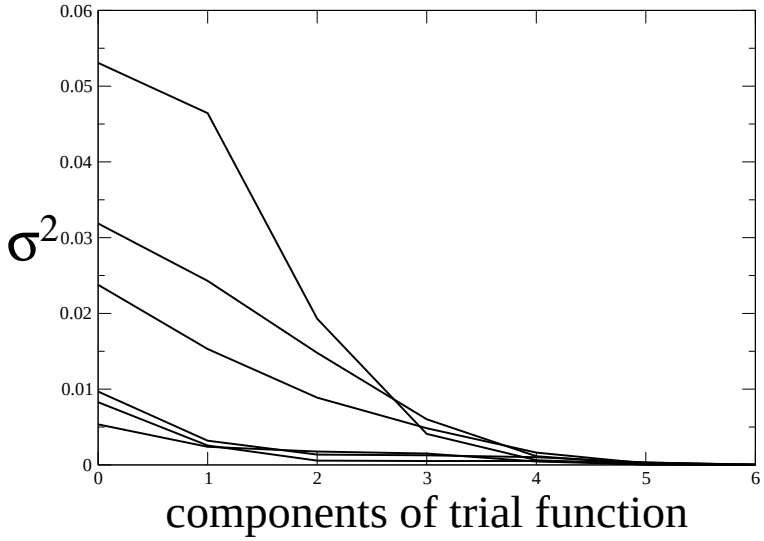


Figure 4.3: The variance of the various matrix elements of the hamiltonian matrix for the one-dimensional problem as a result of applying the zero variance principle. The variance was plotted against the number of components used to approximate the trial function.

the J-TICI(2) approximation, this time using Monte Carlo sampling. Figure 4.4 is the variance of a few of the hamiltonian matrix elements as functions of the number of linear components used in equation (4.60). Although there is a substantial reduction in the variance, the effect is not as strong as in the one-dimensional case (not a zero-variance principle any more)

Although there is a substantial reduction in the variance of the alpha-particle calculation (about 80%), this is not a reduction that can be of practical help. Having in mind that the error is given by the standard deviation (that is the square root of the variance) we have that its value changes with the number of samples as $\frac{1}{\sqrt{N}}$. An 80% reduction is (approximately) equivalent to an error dependence of the form $\frac{1}{2\sqrt{N}}$. This is not much of an error reduction, particularly when compare with the simple one-dimensional case. For the 'zero variance' principle to be valuable we require a radical variance reduction. Therefore, the variance reduction for the alpha particle is not sufficient for aiding the numerical calculation.

Furthermore, we attempted to apply the variance reduction technique beyond the alpha-particle e.g the for ^{5}He and ^{6}He. In these case the wavefunction is no longer given by a 0^+ but by a more complicated antisymmetrized product of spatial and spin-isospin parts. The more complicated structure of the wavefunction seems to require a more complicated approximation of (4.58) than a simple linear one, for any effective reduction of

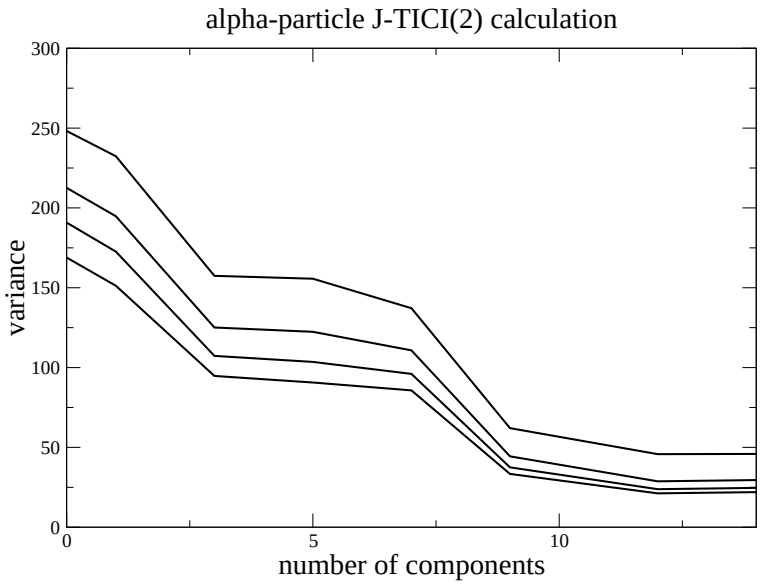


Figure 4.4: The variance of the various matrix elements of the hamiltonian matrix for the alpha-particle in the J-TICI(2) approximation as a result of applying the 'zero-variance' principle. The variance was plotted against the number of components used to approximate the trial function.

the variance.

4.3 Conclusions and general remarks

The variational Monte Carlo method is an important ingredient of our model since it allow as to investigate different structures in the cluster model without having to worry about the analytical solution of many-body integrals. This requires the numerical method to be both accurate and precise in the error estimate.

In terms of accuracy we are interested in obtaining results that are accurate within 0.1% ($\sim$10-50KeV). Although, the linear approximation of the 'zero-variance' principle seems not to be of any substantial help for systems more complicated than the alpha-particle, we can always obtain the required accuracy within reasonable time-limits. In principle we could have looked for a more complicate approximation than the one at hand, but this is beyond our purpose since it over-complicates an already complicate problem.

The error provided by the Monte Carlo method is of statistical nature (variance). This was analyzed in detail in the main body of this chapter. As indicated by a number of results we can obtain a reliable error estimate. For this purpose special attention is required in the presence of correlations between the different random walk samples.

The work provided by this chapter ensures a reliable numerical method and we are

confident that the results obtained are within the error bounds.

Chapter 5

Neutron halo nuclei

In the previous chapters we discussed the structure of our cluster-like model as well as the technical requirements such as the inclusion of SU(4) symmetry and the evaluation of expectation values by Monte Carlo sampling. In this chapter we apply the cluster model in the simplest cases where halo phenomena are observed. Apart from the case of ^{5}He we shall not make use of state-dependent correlations, due to the complexity of the calculation. As we have illustrated in the case of the alpha-particle (both through our work and the work of others) the role of state-dependent correlations is to lower the binding structure but does not seem to effect any of the structure of the system.

One important issue in our model is the absence of the spin-orbit components from the nucleon force. For this reason a preliminary discussion of experimental results is provided for the cases of interest, that will highlight the importance of this issue and help to justify the obtained results.

5.1 Experimental results for ^{5}He, ^{6}He, ^{8}Be and ^{9}Be

Apart from ^{4}He the nuclei that we will use as an example are ^{5}He, ^{6}He, ^{8}Be and ^{9}Be. Therefore, it is useful to include some of the experimental results for these nuclei focusing at the ground state properties. These are summarized in table 5.1, and are taken from [71] and [72].

The nucleus of ^{4}He is bound by about -28 MeV with a difference of about 20 MeV between the 0^+ ground and first excited state (0^+ again). ^{5}He is unbound by -0.798 MeV and is observed as a $J^\pi = \frac{3}{2}^-; T = \frac{1}{2}$ resonance in the neutron scattering on ^{4}He. There

Table 5.1: Some simple ground state properties of the nuclei ^{5}He, ^{6}He, ^{8}Be and ^{9}Be. We indicate the ground or resonance states in the J^π form. For the lowest lying resonances we give the difference in MeV from threshold, while in the cases where the nucleus is unbound the decay channel is indicated.

Nucleus	Ground state J^π	Lowest resonances	Isospin (T)	Decay channel
^{5}He	$\frac{3}{2}^-$ (0.798 MeV)	$\frac{1}{2}^-$ (1.27 MeV)	$\frac{1}{2}$	^{4}He + n
^{6}He	0^+	2^+ (1.797 MeV)	1	bound
^{8}Be	0^+ (0.09 MeV)	2^+ (3.06 MeV)	0	^{4}He + ^{4}He
^{9}Be	$\frac{3}{2}^-$	$\frac{1}{2}^+$ (1.68 MeV)	$\frac{1}{2}$	bound

is also a $\frac{1}{2}^-$ resonance that lies 1.27 MeV above the $\frac{3}{2}^-$ one. In the two-body picture this illustrates that spin-orbit coupling is required in order to produce the observed resonances, since both can result from the coupling of an $S = \frac{1}{2}$ with an $L = 1$ state giving a valence neutron in the $0p1/2$ and $0p3/2$ shell-model levels. The next resonance state for ^{5}He is a $\frac{3}{2}^+$ and occurs at 16.84 MeV.

In the case of ^{6}He we have a Borromean structure as a result of the fact that ^{5}He is unbound, while the ^{6}He ground state is a stable 0^+ bound state. This state lies only 0.973 MeV below the threshold for decay into an alpha-particle and two neutrons (^{4}He + $2n$) and thus ^{6}He is weakly bound. The first resonance of ^{6}He ($J^\pi = 2^+$) lies 1.797 MeV above the ground state and has a strong decay to the ^{4}He + $2n$ channel. The next resonance state for ^{6}He occurs at 5.6 MeV and has uncertain spin assignment (2^+,1^-,0^+). Therefore it seems reasonable to consider ^{6}He as a weakly bound three-body system where a 0^+ alpha-particle ground state is accompanied by two weakly bound neutrons. Then the total spin of the two valance neutrons has only two possible values $S = 0, 1$ and thus the total orbital momentum is confined to the positive parity states $L = 0$ and $L = 1$, both with positive parity.

The nucleus ^{8}Be is also unbound and is observed as a resonance in the scattering of two alpha-particles, just 0.09 MeV above the ^{4}He+^{4}He threshold. The resonance can be described by a 0^+ deformed closed shell structure. There is only another low-lying resonance that occurs at 3.06 MeV, $J^\pi = 2^+$, and is part of the deformed band. These are strong indications that these states can be described by the relative motion of two alpha-particles with even orbital momentum, so that we find positive parity. We analyze this later on within the framework of our cluster model.

^{9}Be is another interesting nucleus with a stable $\frac{3}{2}^-$ ground state and with total isospin $T = \frac{1}{2}$. Since ^{8}Be and ^{5}He are unbound ^{9}Be is again a Borromean nucleus, made from two alpha-particles and a neutron. There is a number of known resonance states, the lowest of which is a $\frac{1}{2}^+$ at 1.68 MeV and lies just above the ^{8}Be + n threshold by a few keV. The next resonances are $\frac{5}{2}^-$ (2.429 MeV), $\frac{1}{2}^-$ (2.8 MeV) and $\frac{1}{2}^+$ (3.05 MeV). These resonances decay to the ^{8}Be + n configuration, which indicates that the ^{9}Be ground state is not far from the three-body picture ($\alpha + \alpha + n$) with $S = \frac{1}{2}$. The ground state orbital momentum is then $L = 1$ assigned to the neutron relative to the two alpha-particles, which explains the negative parity.

The experimental results provide strong evidence for the importance of spin-orbit coupling in binding the light halo nuclei of ^{6}He and ^{9}Be. For example the splitting of the $L = 1$ level into $\frac{3}{2}^-$ and $\frac{1}{2}^-$ occurs both in ^{5}He and ^{9}Be. As mentioned earlier we are going to confine ourselves in the absence of spin-orbit terms from the interaction. This does not undermine the importance of the calculations to be performed since they provide the first step of extending previous work in the field of open-shell systems and an important task is the incorporation of full antisymmetry. However, we will need (and do) to justify the implications of the absence of a spin-orbit force.

5.2 Application and discussion of results

5.2.1 ^{5}He

Although experimentally ^{5}He is not a bound system we can use it as a starting point to test our cluster model. In the J-TICI(2) method the wavefunction is given by (3.37):

$$\Psi = \sum_i \left| \begin{matrix} [4,1]i \\ L,M_L \end{matrix} \right\rangle \left| \begin{matrix} [2,1^3]i \\ S{=}1/2\ M_s, T{=}1/2\ M_t \end{matrix} \right\rangle , \tag{5.1}$$

where the two necessary ingredients are the reference state and the correlation operator entering the wavefunction that will take the form

$$\left| \begin{matrix} [4,1]i \\ L,M_L \end{matrix} \right\rangle = \hat{F} Y_i^{[4,1]} \Phi^{\text{ref}}_{L,M_L}, \tag{5.2}$$

where $\Phi^{\rm ref}_{L,M_L}$ is the reference function, while $Y^{[4,1]}_i$ is an operator projecting it to the ith basis state of the $Y^{[4,1]}$ irrep of $\mathcal{S}_5$. There is a number of options for the reference state, while the correlation operator is the same like in the case of the alpha-particle.

The choice we make for the reference state is to extend the reference state, Φ_α, of the alpha particle by adding a part representing the weakly bound neutron. One way to do this that preserves translational invariance is to assign coordinates to the extra particle relative to the alpha particle center-of-mass. Therefore, the reference state for ^{5}He can look like

$$\Phi^{\rm ref}_L = \Phi_\alpha f(r_{\alpha 5}) \mathcal{Y}^L_M(\vec{r}_{\alpha 5}), \tag{5.3}$$

where

$$\vec{r}_{\alpha 5} = \frac{1}{4}(\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4)-\vec{r}_5, \tag{5.4}$$

$$r_{\alpha 5} = |\vec{r}_{\alpha 5}|. \tag{5.5}$$

The purpose of the function $f(r_{\alpha 5})$ is to localize the additional neutron with respect to the alpha-particle center-of-mass, while $\mathcal{Y}^L_M(\vec{r}_{\alpha 5})$ is a solid harmonic,

$$\mathcal{Y}^L_M(\vec{r}_{\alpha 5}) = r^L_{\alpha 5} Y^L_M(\theta,\phi), \tag{5.6}$$

that assigns angular dependence to the same neutron with respect to the alpha-particle center-of-mass.

A possible choice for $f(r_{\alpha 5})$ is in terms of spherical shells

$$f(r_{\alpha 5}, d, w) = \exp\left(-\alpha^2 \frac{(r_{\alpha 5}-d)^2}{w^2}\right), \tag{5.7}$$

where α is the harmonic oscillator parameter appearing in the reference state of the alpha-particle. The parameter d represents the 'distance' of the shell from the center-of-mass of the alpha-particle, while w stands for the 'width' of the shell. This is a structure that has been used before in [11, 54]. The parameters d, w and the set of parameters entering the Jastrow factor of the correlation operator are variational parameters. The correlation operator is given as in the case of the alpha-particle, where the linear coefficients used for the expansion are minimized by a linear eigenvalue problem.

In the RGM-like formalism the correlation operator is just a Jastrow-part, while the functions f entering the reference function are given as

$$f(r_{\alpha 5}, d, w) = \sum_i c_i \exp\left(-\beta_i \frac{(r_{\alpha 5} - d)^2}{w^2}\right). \tag{5.8}$$

Instead of expanding the linear correlation operators we expand the spherical-shell functions in a way corresponding to a linear superposition of spherical shells of different width, at a distance d from the alpha-particle center-of-mass. The set of non-linear coefficients β is chosen beforehand. In principle the expansion should involve both the distance and width of the spherical shells.

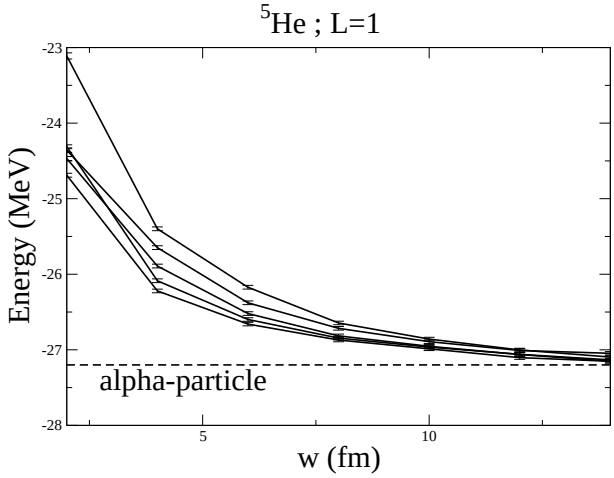


Figure 5.1: The ground-state energy for the state-independent J-TICI(2) calculation of ^{5}He for $L = 1$ using the S3 interaction. The broken line corresponds to the alpha-particle ground-state energy for the same type of calculation. The error bars is due to the Monte Carlo evaluation of the integrals. The value of w is in relative units (i.e. scaled fm) since is multiplied by the harmonic oscillator parameter α. The different number of plots correspond to different values of the separation parameter d.

A selection of the results obtained using the J-TICI(2) method and the S3 interaction are displayed in figure 5.1. The value of the energy was obtained for variations of d and w for the $L = 1$ state. In the case of spin and isospin quantum numbers there is only the possibility of ($S = 1/2$,$T = 1/2$), as is illustrated in chapter 4. It can be clearly seen that for a particular value of the 'distance' parameter d, there is no variational stationary point but as the 'width' w of the relative function $f(r_{\alpha 5})$ increases, the value for the ground-state energy approaches that of the alpha-particle. Furthermore, the dependence on d becomes negligible for large enough w and despite the value of d the energy approaches the same

value, i.e. the driving parameter is the 'width' w. When we move from $L = 1$ to some other value of L there is no change in the overall behaviour of the ground state-energy and the same asymptotic behaviour is observed for large w as is illustrated in figure 5.2. The only difference between the different values of L is for relatively small values of the parameters d and w.

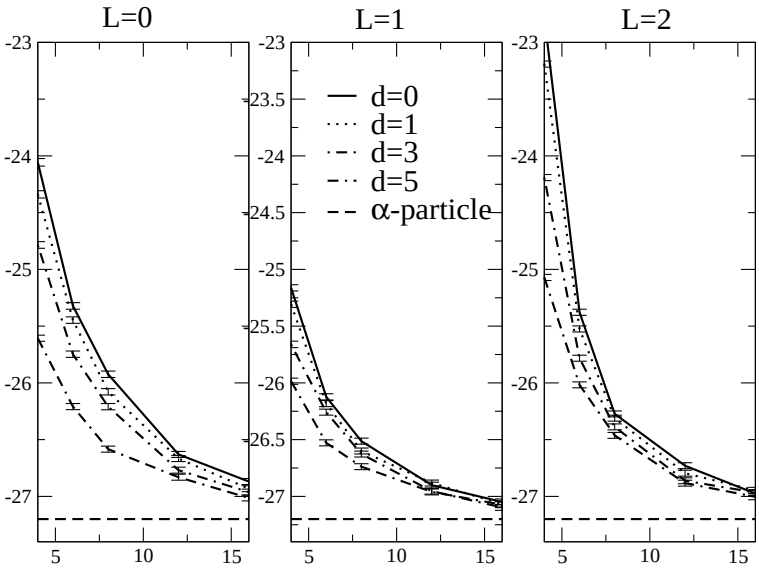


Figure 5.2: The ground-state energy for the state-independent J-TICI(2) calculation of ^{5}He for different values of L using the S3 interaction. The broken line corresponds to the alpha-particle ground-state energy for the same type of calculation. The error bars are a result of the Monte Carlo evaluation of the integrals. The value of w is in relative units (i.e. scaled fm) since is multiplied by the harmonic oscillator parameter α.

Although, we can always use a number of different interactions, S3 provides a starting for examining such cluster-like models. Furthermore, it is not expected that the nature of the results will change for different types of V4 interactions. This is illustrated in figure 5.3, where a selection of the S3 interaction results was recalculated for a number of V4 interactions.

The fact that there is no variational minimum implies that no bound state exists for ^{5}He within our approximation. We would like to get some inside in the structure provided by the wavefunction. For this purpose we can make use of the spherically averaged one- and two- body density distribution introduced for the alpha-particle (equations 2.87 and 2.88). The results obtained for the density matrices with the S3 interaction are shown in figures 5.4, 5.5 and 5.6.

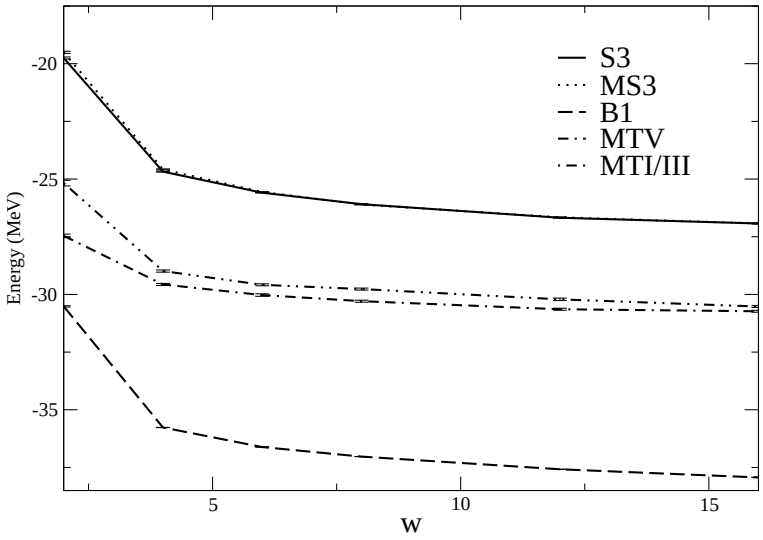


Figure 5.3: The ground-state energy for the state-independent J-TICI(2) calculation of ^{5}He for different types of V4 interactions. The results indicate the similarity between calculations done with different type of potentials.

We expect that the parameters d and w will be associated with the separation of the additional neutron from the alpha-particle. Intuitively the value of w is associated with the 'freedom' that we assign to the additional neutron in the model state, that is centred at d. When this is acted upon by the correlation operator the resulting picture can be different. The spherically averaged one-body density distribution $\rho_1(r)$ measures the probability of finding a nucleon a distance r from the center-of-mass. We expect that when the additional neutron is moved away from the center-of-mass (in terms of d and w), that the overall one-body probability distribution will be effected. The effect of changing w and d is displayed on the the right hand graph of 5.4 and in figure 5.6, respectively. Figure 5.4 clearly shows that increasing the value of w broadens the distribution and shifts the maximum away from the origin, indicating that overall the system becomes less localized. A similar behaviour is illustrated in figure 5.6 for the case of the parameter d but the influence of d on the one-body density distribution is less strong than that of w. Figure 5.6 also illustrates the effect of adding orbital momentum to the additional nucleon relative to the alpha-particle, where by adding orbital momentum we get less distribution close to the center-of-mass.

The effect of the variational parameters on the two-body density distribution is more subtle. The separation of the additional neutron from the alpha-particle (effected by increasing d and w) on the two-body density appears as a small change in the behaviour of

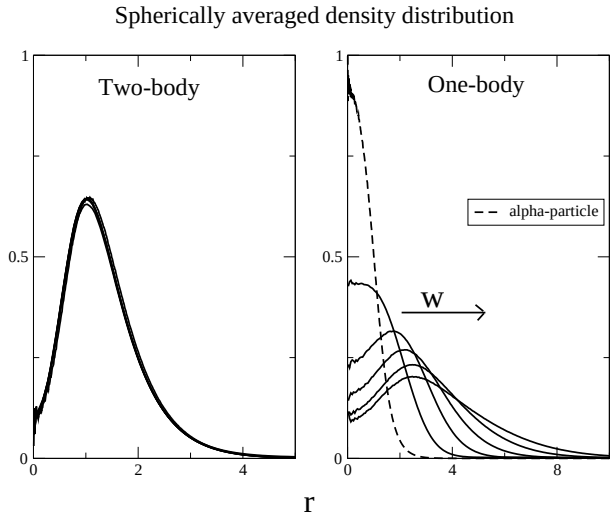


Figure 5.4: The one-body (right) and two-body (left) density distribution for ^{5}He (using the S3 interaction) for a number of values of the width parameter w. The two-body density distribution has only a trivial difference overall from the alpha particle one and does not depend on w. In the case of the one-body density the curve with the broken line is for the alpha particle, while the arrow indicates an increase in the value of w.

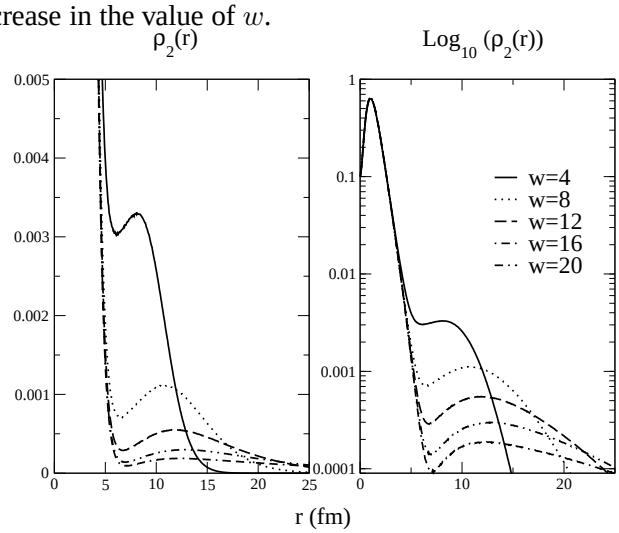


Figure 5.5: The tail of the two-body density distribution for ^{5}He (using the S3 interaction) for a number of values of the width parameter w (left hand graph) and the entire graph plotted on a logarithmic scale (right hand graph)

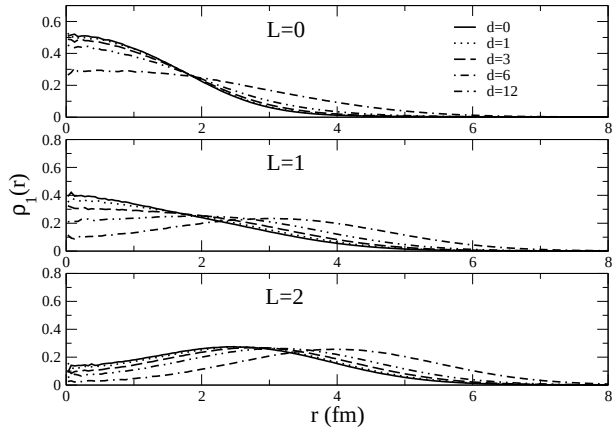


Figure 5.6: The one-body spherically averaged density distribution for ^{5}He (using the S3 interaction) for a number of values of the distance parameter d and orbital momentum L. The value of w was kept constant.

the tail as shown in the left-hand side graph of figure 5.5. We can illustrate this effect on the whole density-distribution by using a logarithmic plot of the density as is illustrated on the right-hand graph of figure 5.5. Overall the two-body density, it is almost identical with that of the alpha-particle, as is illustrated in the left graph of figure 5.4 apart from a small fraction that is distributed as a halo over a relatively long distance. This is not an unexpected result, since such a structure is provided by the reference function.

In the J-TICI(2) formalism the wavefunction of equation (5.2.1) has the property that the correlation operator $\hat{F}$ is invariant under the exchange of particles, thus the antisymmetrized reference function is the same for all the required integrals of the hamiltonian and overlap matrix elements (as a result of the linear expansion of the correlation operator). This can be an advantage over the RGM-like method where the reference function is approximated by a linear expansion and each matrix element requires it own antisymmetrization, particularly when a numerical method like Monte-Carlo integration is used. The results obtained for the S3 interaction are equivalent to the ones obtained for the J-TICI(2) method. However, we shall abandon this method since carrying out the antisymmetrization for every matrix element is an unnecessary complexity that can reduce the efficiency of our numerical algorithm.

Despite the fact that ^{5}He provides a non bound structure the calculation has provided as with the important lesson that the variation of the energy with respect to the variational parameters and L is different between a well localized reference function (i.e. close to

Table 5.2: The lowest allowed configurations for ^{6}He with $T = 1$ in $L - S$ coupling.

T	S	Lowest L	J^π
1	0	0	0^+
1	0	1	1^+
1	1	1	0^-, 1^-, 2^-

the alpha-particle) and one with a less-localized structure (as indicated by the density distribution). In the former case all of the variational parameters as well as the orbital momentum L contribute in the value of the energy, while in the later case of a less-localized structure the only parameter that matters is that of w.

5.2.2 ^{6}He

Contrary to the case of ^{5}He, where there is only a single choice for the permutation symmetry, ^{6}He has two options for the wavefunction of (3.37) resulting in two distinct spin-isospin configurations (described in chapter 4) with $T = 1$. The two wavefunctions can be represented as

$$\Psi^{(0,1)} = \sum_i \left| \begin{matrix}[4,2]i \\ L,M_L \end{matrix} \right\rangle \left| \begin{matrix}[2^2,1^2]i \\ S=0,T=1M_t \end{matrix} \right\rangle , \tag{5.9}$$

$$\Psi^{(1,1)} = \sum_i \left| \begin{matrix}[4,1^2]i \\ L,M_L \end{matrix} \right\rangle \left| \begin{matrix}[3,1^3]i \\ S=1M_s,T=1M_t \end{matrix} \right\rangle . \tag{5.10}$$

The above wavefunctions can be assigned several values for the total orbital momentum L The different configurations that we are allowed to use in the $L - S$ coupling scheme and can correspond to the ground state (lowest L) are given in table 5.2. Only when $S = 0$ is possible to obtain a $J^\pi = 0^+$ state. When $S = 1$ the two valence neutron are in a symmetric state and the only way to obtain a totally antisymmetric wavefunction is to have an antisymmetric di-neutron spatial part (as is explained in chapter 3), something that gives a negative parity state.

We can construct a reference state for ^{6}He similar to that of ^{5}He, that looks like

$$\Phi_L^{\text{ref}} = \Phi_\alpha f(r_{\alpha 5}) f(r_{\alpha 6}) f(r_{56}) \mathcal{Y}_M^L(\vec{r}_{56}), \tag{5.11}$$

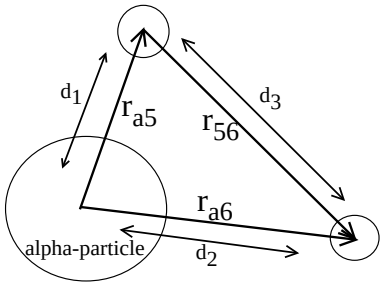


Figure 5.7: Artists impression of ^{6}He

where

$$\vec{r}_{\alpha 5} = \frac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_5, \tag{5.12}$$

$$\vec{r}_{\alpha 6} = \frac{1}{4}(\vec{r}_1 + \vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \vec{r}_6, \tag{5.13}$$

$$r_{\alpha 5} = |\vec{r}_{\alpha 5}|, \quad r_{\alpha 6} = |\vec{r}_{\alpha 6}|, \tag{5.14}$$

$$\vec{r}_{56} = \vec{r}_5 - \vec{r}_6, \quad r_{56} = |\vec{r}_5 - \vec{r}_6| \, . \tag{5.15}$$

The purpose of the functions $f(r_{\alpha 5})$ and $f(r_{\alpha 6})$ is to localize the additional neutrons with respect to the alpha-particle center-of-mass. $\mathcal{Y}^L_M(\vec{r}_{56})$ is a solid harmonic that couples the orbital momenta of the two-weakly bound neutrons relative to the alpha-particle in a translationally invariant way:

$$\mathcal{Y}^L_M(\vec{r}_{56}) = \sum_{l_1,l_2} a^L_{l_1,l_2} \left(\sum_{m_1,m_2} C^{L0}_{l_1 m_1, l_2 m_2} \mathcal{Y}^{l_1}_{m_1}(\vec{r}_{\alpha 5}) \mathcal{Y}^{l_2}_{m_2}(\vec{r}_{\alpha 6}) \right), \tag{5.16}$$

where $C^{L0}_{l_1 m_1, l_2 m_2}$ are the Clebsch-Gordan coefficients (we make the choice of M_L=0 since the expectation value does not depend on M_L), while the $a^L_{l_1,l_2}$ are linear variational coefficients. The function $f(r_{56})$ describes the relative motion of the two neutrons with respect to each other.

As in the case of ^{5}He a possible choice for the $f(r_{\alpha 5})$ and $f(r_{\alpha 6})$ is in terms of spher-

ical shells

$$f(r_{\alpha 5}, d_1, w_1) = \exp\left(-\alpha^2 \frac{(r_{\alpha 5} - d_1)^2}{w_1^2}\right), \tag{5.17}$$

$$f(r_{\alpha 6}, d_2, w_2) = \exp\left(-\alpha^2 \frac{(r_{\alpha 5} - d_2)^2}{w_2^2}\right), \tag{5.18}$$

$$\tag{5.19}$$

where α is the harmonic oscillator parameter appearing in the reference state of the alpha-particle. The 'distance' parameters d_1, d_2 and the 'width' parameters w_1 and w_2 localize each particle individually. In the case of $f(r_{56})$ we choose the similar parametrization

$$f(r_{56}, d_3, w_3) = \exp\left(-\alpha^2 \frac{(r_{56} - d_3)^2}{w_3^2}\right). \tag{5.20}$$

The intuitive picture of the structure provided by the reference function is relatively straight forward as is illustrated in figure 5.7.

When compared with ^{5}He the calculation for ^{6}He is substantially more complicated. The variational non-linear parameters entering the reference function increase from just d and w to $\{d_1, d_2, d_3\}$ and $\{w_1, w_2, w_3\}$. Furthermore, the linear expansion used to approximate the correlation operator becomes bilinear in order to accommodate the coefficients $a^L_{l_1,l_2}$ that superimpose different coupled configurations of orbital momenta (l_1, l_2) into a total L. It is therefore, useful to analyze the structure provided by the reference function before proceeding into the full calculation.

The number of linear coefficients $a^L_{l_1,l_2}$ required for the expansion of the angular part can be examined independent of the rest of the calculation. It would be useful to know the minimum number of the $a^L_{l_1,l_2}$ required for a reasonable convergence (at least within the numerical error) of the energy. The behaviour of the energy with respect to the number of coefficients $a^L_{l_1,l_2}$ is displayed in 5.8, for a restricted number of the variational parameters. The distance parameter d_1 d_2 and d_3 were set to zero, while one single width parameter w was used. A small value of w corresponds to a well localized system. The number of linear coefficients $a^L_{l_1,l_2}$ required is very small and the contribution of different coefficients diminishes as the system becomes less localized (increase in w). For example the $L = 0$, that would correspond to the ground-state for our approximation, just two coefficients are enough i.e using ($l_1 = 0, l_2 = 0$) and ($l_1 = 1, l_2 = 1$). The situation is similar for $L = 1$.

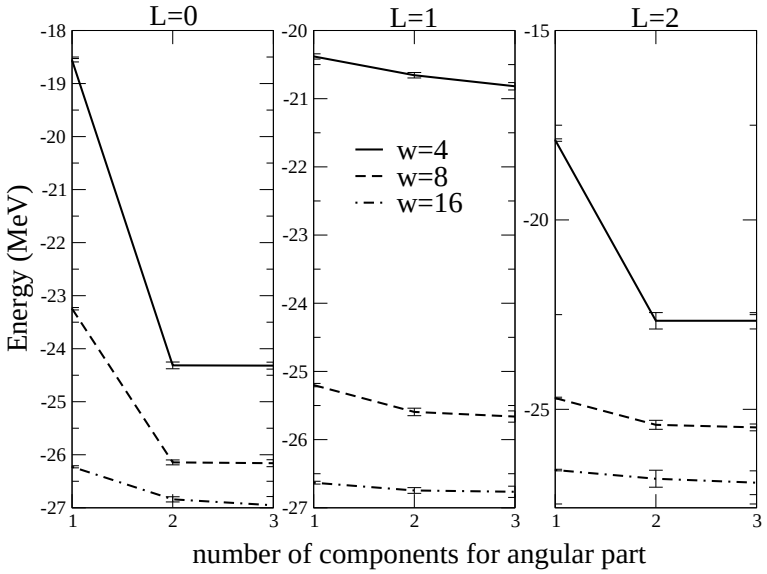


Figure 5.8: The dependence of the ground -state energy of ^{6}He with respect to the number of linear coeffi cients $a^L_{l_1,l_2}$. The results were taken using the S3 interaction. The coeffi cients d_1 d_2 and d_3 were set to zero, while $w = w_1 = w_2 = w_3$

We carried out the calculation for ^{6}He with state-independent correlations for various sets of quantum numbers L, S and T. The general pattern observed is similar to that of ^{5}He. Although there exists a dependence of the energy on the various configurations (variational parameters and quantum numbers), this happens at small values of the width parameters w_1 w_2 and w_3 where the value for the energy is well above that of the alpha-particle. As the width parameters become larger the energy approaches that of the alpha-particle, without passing through a stationary point or going below the alpha-particle limit. Since the number of parameters is too many for the entire set to be displayed in an eligible plot we demonstrate the general behaviour of the ^{6}He calculation through some selected configurations, that nevertheless are conclusive.

Instead of using the reference function of equation (5.11) we can use a related form that corresponds to an alpha particles correlated with a di-neutron structure

$$\Phi^{\rm ref}_L = \Phi_\alpha f(r_{\alpha 56}, d_1, w_1) f(r_{56}, d_2, w_2) \mathcal{Y}^L_M(\vec{r}_{56}), \tag{5.21}$$

$$\vec{r}_{\alpha 56} = \vec{r}_\alpha - \frac{1}{2}(\vec{r}_5 + \vec{r}_6), \tag{5.22}$$

where the function $f(r_{56})\mathcal{Y}^L_M(\vec{r}_{56})$ can be thought of as the di-neutron. The functions $f(r_{\alpha 56})$ and $f(r_{56})$ have the same structure as before, but instead of correlating each indi-

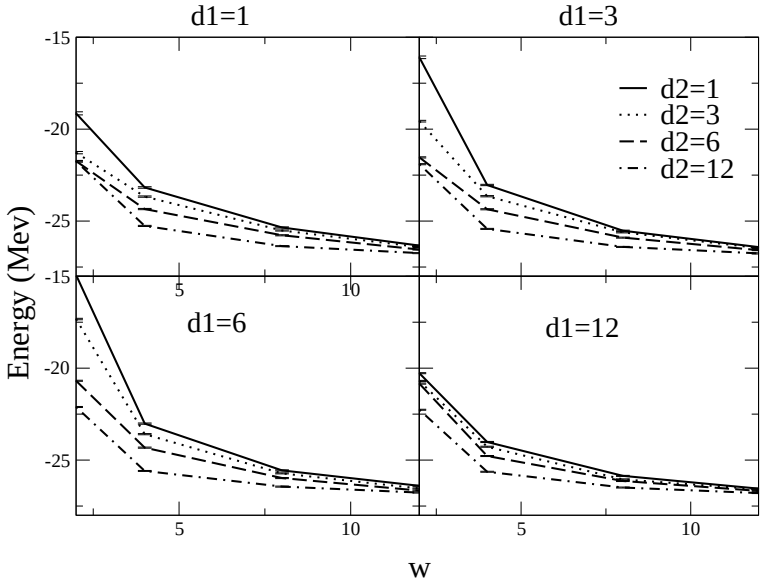


Figure 5.9: The ground state energy of ^{6}He for the reference function of (5.21). The S3 interaction was used, while$S = 0$, $T = 1$ and $L = 0$. The parameter d_1 is related to the separation of the di-neutron from the alpha-particle, while d_2 is the separation between the two neutrons of the di-neutron. The width parameter w is in relative units since is multiplied by the harmonic oscillator parameter.

vidual neutron with the alpha-particle independently we correlate the di-neutron with the alpha-particle. This description of the model state is compatible with all the spin/isopsin configurations as long as the required permutation symmetry is included in the di-neutron part, i.e. for the ($S = 0, T = 1$) we require the di-neutron wave-function to be symmetric with respect to the two neutron labels, while for all others it has to be anti-symmetric. We use the above structure to illustrate the behaviour of ^{6}He since it provides a restricted configuration, where the key variational parameters are $d_1,\ d_2$ and $w_1,\ w_2$. The results for the ground-state energy for the $S = 0, T = 1$ and $L = 0$ configuration using the S3 interaction are shown in figure 5.9. A number of configurations were used were d_1 is the distance between the alpha-particle center-of-mass and the di-neutron, while d_2 is the average separation between the two neutrons. For the widths we used $w = w_1 = w_2$. Increasing w corresponds to allowing the system to be less localized around the average separation indicated by d_1 and d_2. Figure 5.9 indicates that the system is not bound but the energy tends to a minimum when the system becomes less localized. This is valid both when the di-neutron is moved away from the alpha-particle while keeping the two-neutron at a fixed distance from each other, and in the opposite situation where the di-neutron is

kept at a fixed distance from the alpha-particle, but the two neutrons are separated from each other.

Very similar results are obtained when instead we use the reference function of (5.11) while selecting configurations that give a similar picture to that of the reference function (5.21). In figure 5.10 we display the results for the $(S = 0, T = 1)$ spin-isospin configuration and for $L = 0$, using the S3 interaction. The choice made for the distance and width parameters is that where $d_1 = d_2$, while d_3 and $w = w_1 = w_2 = w_3$ are varied. Although, this is one of the simplest possible configurations it is conclusive for the case of $(S = 0, T = 1)$ spin and isospin quantum numbers. Again the variational behaviour is similar to that of ^{5}He, where for large enough w the dependence on the distance parameters becomes negligible, while the value for the ground state energy approaches that of the alpha-particle as the value of w increases. Furthermore, when we move to the $(S = 1, T = 1)$ spin-isospin configuration a very similar behaviour is observed as illustrated in figure 5.11. The set of quantum numbers $(S = 0, T = 1)$ and $(S = 1, T = 1)$ are the only ones in our approximation that correspond to two-neutrons (or two-proton because of charge independence) added to an alpha-particle.

We can again refer to the spherically averaged one- and two-body density distributions to get an idea of the structure provided by the wavefunction. These are displayed in figures 5.12 and 5.13 ,where the two-body density is displayed with a logarithmic scale in order to emphasise the tail effect. For the one-body density we can clearly see that the effect of either moving the dineutron away from the alpha-particle or the two neutrons away from each other or both shifts the average probability away from the center-of-mass (the origin) and furthermore broadens the distribution. This is again a similar behaviour to ^{5}He. In the case of the two-body density, the logarithmic graphs of figure 5.13 clearly demonstrate the tail effect on the alpha-particle probability distribution. The tail effects for 6He are more profound that those of figure 5.5 for ^{5}He, particularly for more localized configurations.

The non-existence of a variational minimum suggests an unbound structure. Furthermore, this is supported by the fact that the value for the ground-state energy never goes below that of the alpha-particle. Despite the fact that we have a rich configuration space, the importance of the variational parameters is only significant for a well localized system (characterized by small values of the w_1, w_2 and w_3). The value obtained for the binding

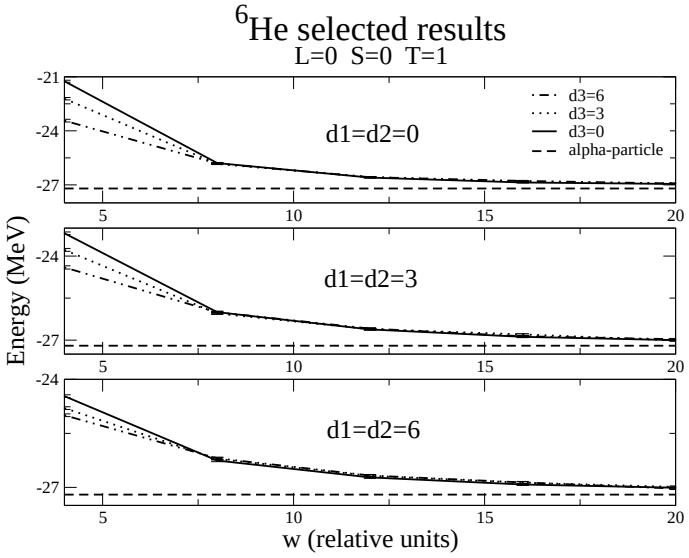


Figure 5.10: The ground-state energy for the state-independent J-TICI(2) calculation of ^{6}He as function of w for $L = 0$, $S = 0$, $T = 1$ using the S3 interaction. $d1$ and $d2$ correspond to the value of the 'distance' parameter for each of the two weakly bound neutrons (corresponding to the instance between them and the alpha-particle). $d3$ corresponds to the 'distance' parameter describing the separation between the two weakly-bound neutrons. In this confi guration $d1 = d2$ and a single 'width' parameter is used for each point. The broken line corresponds to the alpha-particle ground-state energy for the same type of calculation. The error bars is due to the Monte Carlo evaluation of the integrals. This can lead to a 0^+ state when spin-orbit coupling is used.

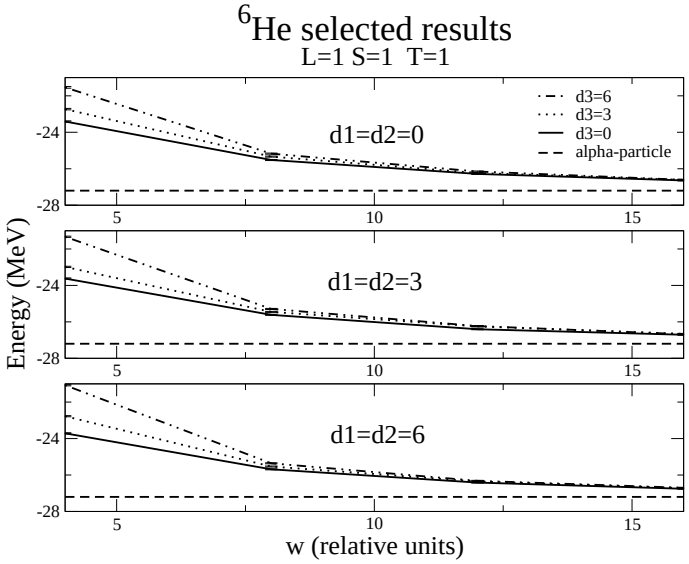


Figure 5.11: The ground-state energy for the state-independent J-TICI(2) calculation of ^{6}He as function of w for $L = 1$; $(l_1 = l_2)$, $S = 1$, $T = 1$ using the S3 interaction. $d1$ and $d2$ correspond to the value of the 'distance' parameter for each of the two weakly bound neutrons (corresponding to the instance between them and the alpha-particle). $d3$ corresponds to the 'distance' parameter describing the separation between the two weakly-bound neutrons. In this confi guration $d1 = d2$ and a single 'width' parameter is used for each point. This can lead to a 0^- state when spin-orbit coupling is used, rather than to a 0^+.

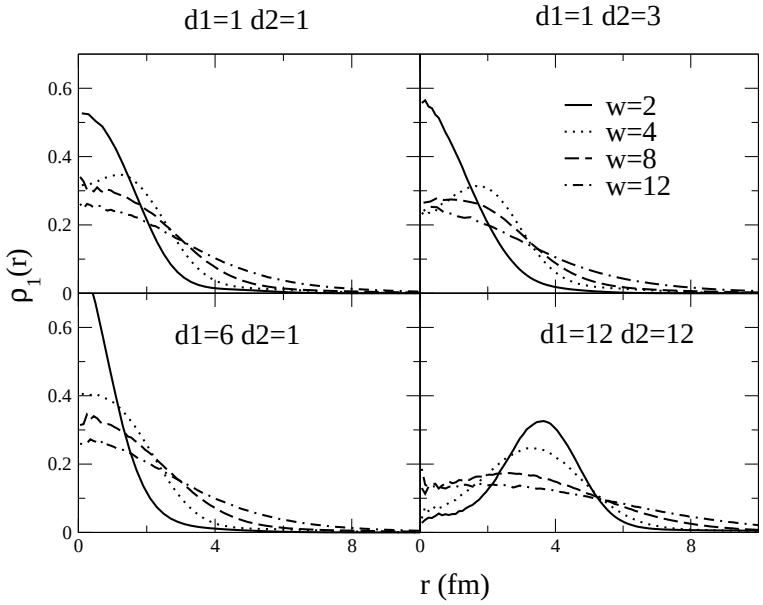


Figure 5.12: The one-body density distribution for ^{6}He. The wavefunction was obtained for the S3 interaction, while $S = 0$, $T = 1$ and $L = 0$. The parameters d_1 and d_2 are the ones of equation (5.21): d_1 is related to the distance of the di-neutron from the alpha-particle, while d_2 to distance between the two neutrons. w is the width parameter.

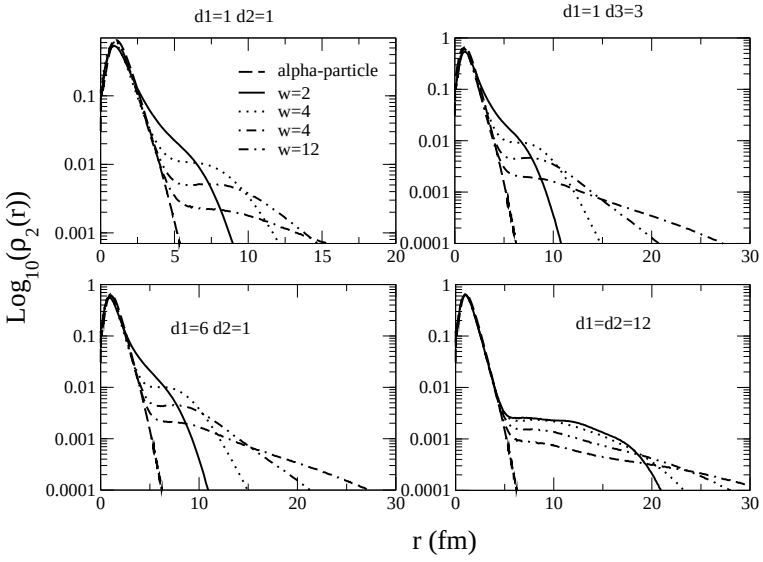


Figure 5.13: The two-body density distribution for ^{6}He. The wavefunction was obtained for the S3 interaction, while $S = 0$, $T = 1$ and $L = 0$. The configuration is the same as that of figure 5.12.

energy of a well localized wavefunction is well above that of the alpha-particle. Thus our approximation of ^{6}He as an α+n+n (alpha-particle + neutron + neutron) system is not adequate to construct the Borromean system in the absence of a spin-orbit force.

5.2.3 Force modification

We expect that the failure of the method to reproduce the experimental results for ^{6}He can at least be partially due to the absence of spin-orbit coupling. However, this does not undermine the capability of our method as an evaluation technique for the nuclear many-body problem. Therefore, we would like to demonstrate the capability of the current model to produce bound states beyond that of the closed-shell structure such as the alpha-particle. We shall do this by modifying the form of the potential function, as long as the over-binding for the alpha-particle which is irrelevant in such a modification is relatively small. For this reason we modify the Wigner part of the S3 potential function by adding a long-range tail effect, while keeping the short-range behaviour unaltered. Since the S3 force is a sum of gaussians it does not have the exponential tail expected from a meson exchange picture, and such long-range modifications are thus quite sensible.

The Wigner part of the original potential function is given as

$$\begin{aligned} V_w(r) &= 500\exp(-3r^2) - 81.675\exp(-1.05r^2) - 10.75\exp(-0.6r^2) \\ &\quad -41.5\exp(-0.8r^2) - 5.75\exp(-0.4r^2) \end{aligned} \tag{5.23}$$

The choice we make changes the potential function $V_w(r)$ to $V'_w(r) + \lambda\exp(-0.03r^2)$, where $V'_w(r)$ is given by

$$\begin{aligned} V'_w(r) &= 485\exp(-3r^2) - 61.675\exp(-1.05r^2) - 10.75\exp(-0.6r^2) \\ &\quad -41.5\exp(-0.8r^2) - 5.75\exp(-0.4r^2) \end{aligned} \tag{5.24}$$

and was chosen so that the short range behaviour remains approximately unchanged for reasonable values of λ centered around 2. The change in the shape of the potential is illustrated in figure 5.14, where the value of λ used is 2.2, which, as described later, can produce bound states for the $L = 0$ and $L = 1$ configurations of ^{6}He, as well as for $L = 1$ in ^{5}He.

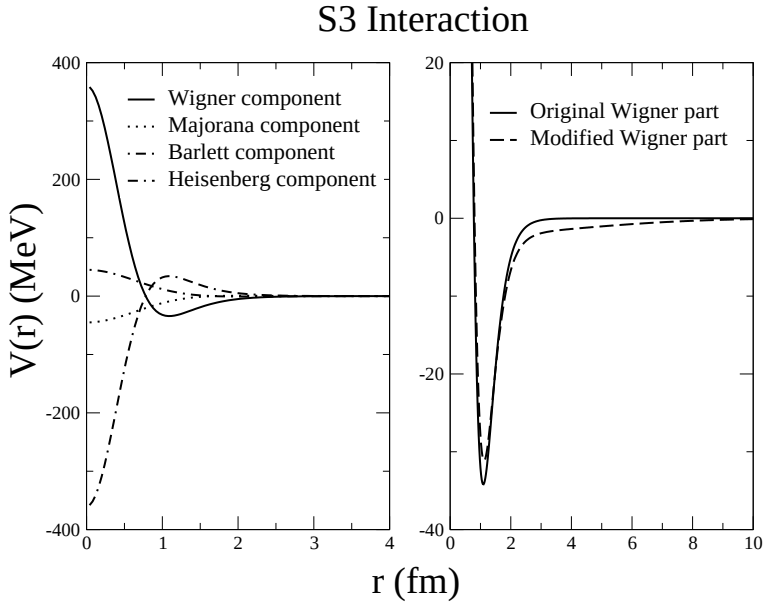


Figure 5.14: The S3 potential (left part) and the modifi ed Wigner part (right part) that binds ^{6}He by just 0.1 MeV. The modifi cation is obtained by adding the term -2.2$\exp(-0.03r^2)$.

We can first adjust λ so that we just obtain a stationary point in the variational calculation. In the case of ^{6}He the result is illustrated in figure 5.15, were the variational parameters where optimised to a single width parameter w. It is possible to obtain a variational stationary point above the ground state of the alpha-particle. For $L = 0$ this is harder to obtain and requires a larger λ than for $L = 1$. Furthermore, the energy becomes more or less constant, something that may indicate a resonance-like behaviour. The same modification that just binds ^{6}He also produces an $L = 1$ bound state in ^{5}He while the $L = 0$ state remains unbound. This in agreement with experiment since the $L = 1$ state can lead to the observed low-energy resonances. Furthermore, at small values of the parameter λ the $L = 1$ states for ^{5}He and ^{6}He are below the alpha-particle ground state energy by almost the same amount as is illustrated in figure 5.16 and is not clear whether ^{6}He is bound. Later on we shall see that this changes and ^{6}He becomes more bound, provided that λ is further increased.

We are guaranteed a bound state when the variational result has a stationary point below the ground state of the alpha-particle, since for large w we always obtain the alpha-particle ground state energy. The above changes in the potential function provides us with the minimum change required to produce a stationary point for ^{6}He in the $L = 1$, $S = 0$, $T = 1$ configuration. Further increase of λ also leads to a bound state for both

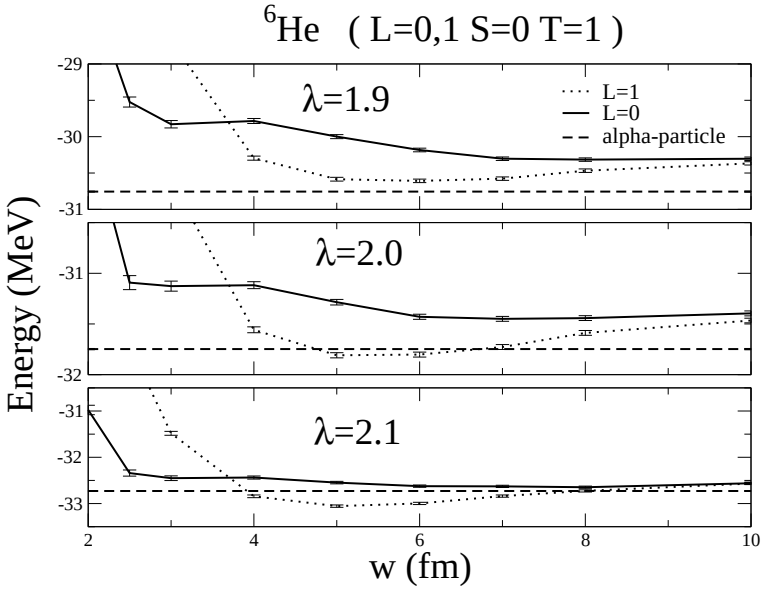


Figure 5.15: The variational results for ^{6}He after modifying the Wigner part of the S3 interaction for $S = 0$ and $T = 1$. The results for three different values of λ are shown for both $L = 0$ and $L = 1$.

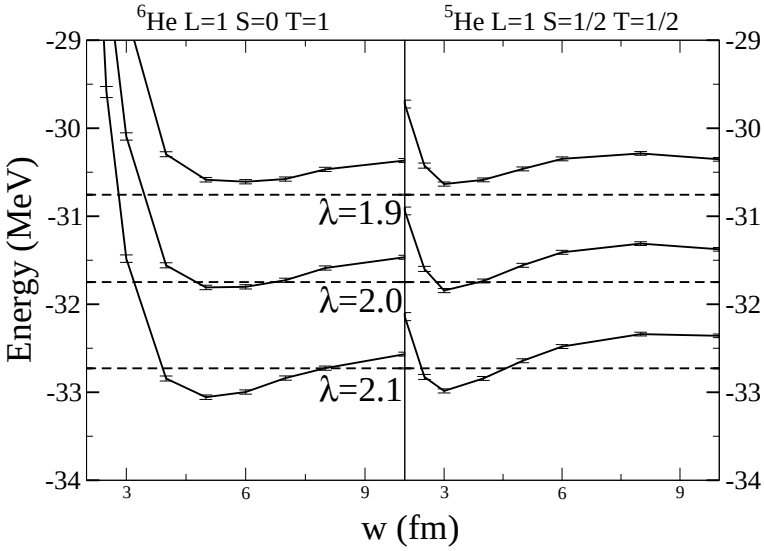


Figure 5.16: The variational results for the $L = 1$ state of ^{6}He and ^{5}He after modifying the Wigner part of the S3 interaction. The results for three different values of λ for both nuclei are shown.

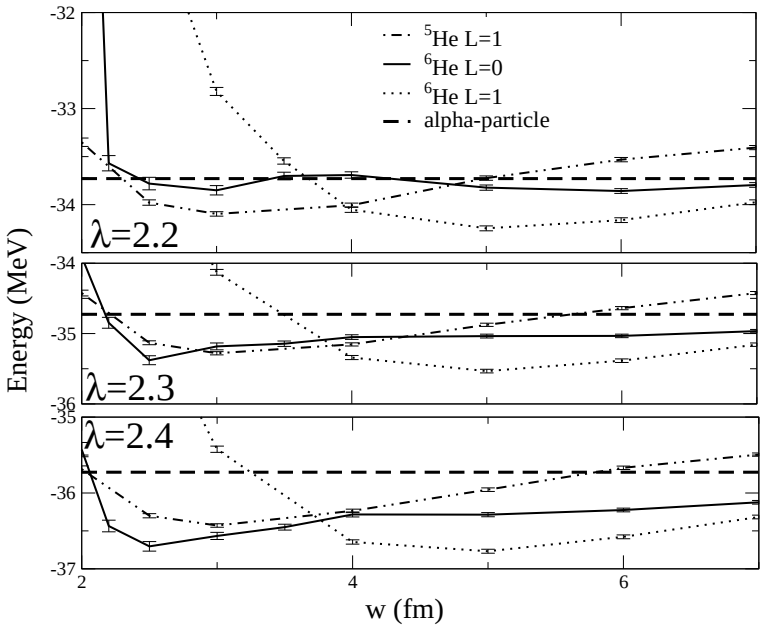


Figure 5.17: The variational results for ^{6}He after modifying the Wigner part of the S3 interaction for $S = 0$ and $T = 1$. The binding energy for for both $L = 0$ and $L = 1$ states of ^{6}He and for the $L = 1$ state of ^{5}He when λ is further increased. We can see that for large enough λ both the $L = 0$ and $L = 1$ states of ^{6}He become more bound from the $L = 1$ state of ^{5}He.

the $L = 0$ and $L = 1$ configurations as is illustrated in figure 5.17 for the configurations ($L = 0,\ S = 0,\ T = 1$) and ($L = 1,\ S = 0,\ T = 1$) of ^{6}He as well as for $L = 1$ of ^{5}He. Therefore, a bound structure emerges for both configurations of ^{6}He. This is in agreement with experiment since the $L = 0$ state gives $J^\pi = 0^+$. Another point illustrated by figure 5.17 is the fact that the binding energy for both $L = 0$ and $L = 1$ states of ^{6}He becomes greater than the $L = 1$ state in ^{5}He, provided that λ is further increased. This is also important since it is an indication that is possible to obtain a bound state for ^{6}He but not one for ^{5}He. However, this will require a more careful fine-tunning of the interaction and at this stage we are only interested in verifying the capability of our model in producing bound states. In the calculation for $\lambda = 2.4$ of figure 5.17 the $L = 1$ energy level for ^{5}He is about 500 keV below the alpha particle ground state energy. For ^{6}He both the $L = 0$ and $L = 1$ lie about 700 keV lower than alpha-particle ground state and the calculation indicates that ^{6}He is weakly bound by just 200 keV.

As before we can plot the one- and two-body density distributions. Figure 5.18 shows the density distributions for the variational minimum of the $L = 0$ and $L = 1$ states of ^{6}He as well as for the $L = 1$ state of ^{5}He. In the same figure the distribution for a variational

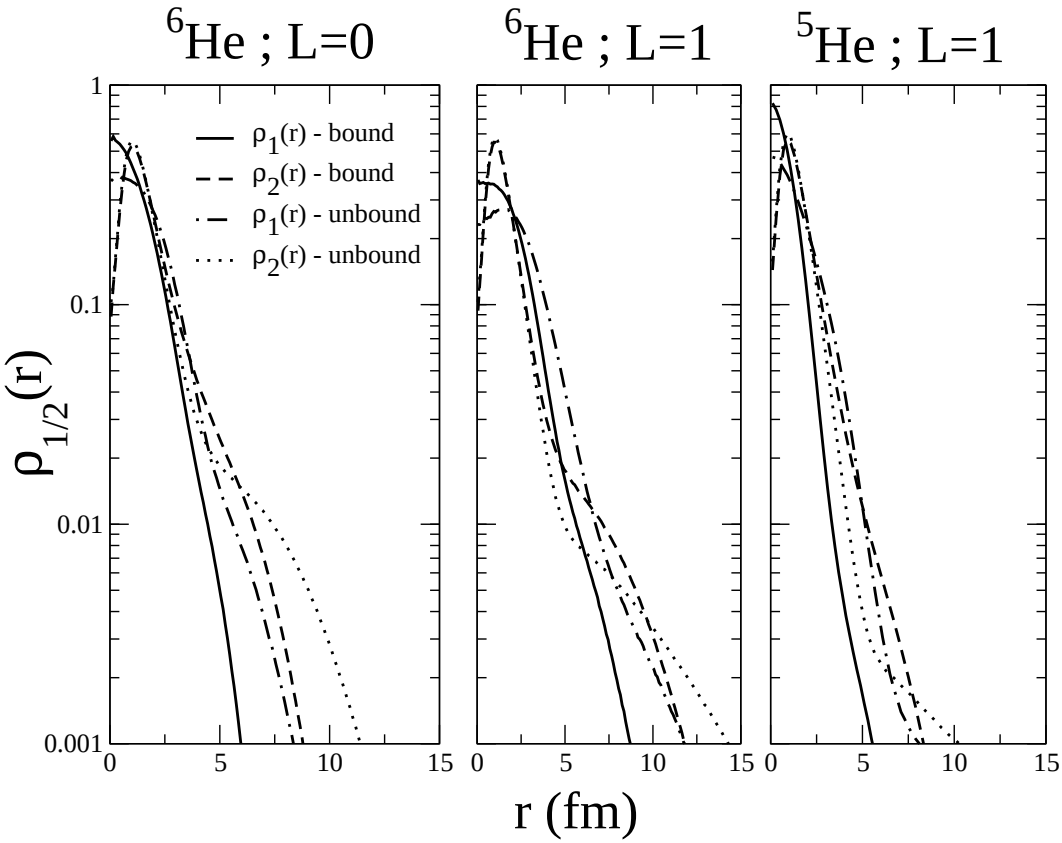


Figure 5.18: The one- and two-body spherically averaged density distributions of ^{6}He and ^{5}He for the bound and unbound states with λ=2.3.

point corresponding to an unbound state close to the alpha-particle limit is also shown. These density distributions were taken for $\lambda = 2.2$. We can see that the bound states are more localized than the unbound ones. As stated in the previous sections these density distributions provide us with a qualitative picture and we see that the ^{6}He bound states have a longer tale effect than the one of ^{5}He with the ^{6}He $L = 1$ bound state showing the largest tale effect, something that is expected.

We can clearly see that by artificially increasing the strength of the attractive part of the Wigner component in the inter-nucleon interaction we can get a bound state of the ^{6}He nucleus. This result illustrates that our model is capable of producing positive results for light halo nuclei and indeed provides an extension from closed- to open-shell systems in a way consistent with experiment. Furthermore, the fact that an $L = 1$ bound state for ^{5}He is consistent with the presence of $\frac{3}{2}^-$ and $\frac{1}{2}^-$ resonances when spin-orbit coupling is considered.

5.2.4 ^{8}Be

Within our approximation the case of two alpha-particles, corresponds to the nucleus of ^{8}Be. Although, ^{8}Be is not a bound system we wish to examine it since by adding one more neutron we have ^{9}Be that is a bound halo nucleus. This will be examined later on. The choice we make for the reference state of ^{8}Be is to add together two translationally invariant alpha-particle wavefunctions correlated by a function depending on the relative distance between the two alpha-particles centers-of-mass. The reference function can have the form

$$\Phi_L^{\text{ref}} = \Phi_{\alpha_1}\Phi_{\alpha_2} f(r_{\alpha_{12}})\mathcal{Y}_M^L(\vec{r}_{\alpha_{12}}), \tag{5.25}$$

where

$$\vec{r}_{\alpha_1} = \frac{1}{4}\left(\vec{r}_1+\vec{r}_2+\vec{r}_3+\vec{r}_4\right), \tag{5.26}$$

$$\vec{r}_{\alpha_2} = \frac{1}{4}\left(\vec{r}_5+\vec{r}_6+\vec{r}_7+\vec{r}_8\right), \tag{5.27}$$

$$r_{\alpha_{12}} = |\vec{r}_{\alpha_1}-\vec{r}_{\alpha_2}|. \tag{5.28}$$

The purpose of the function $f(r_{\alpha_{12}})$ is to correlate the two alpha-particle with each other while $\mathcal{Y}_M^L(\vec{r}_{\alpha_{12}})$ is a solid harmonic,

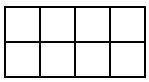
$$\mathcal{Y}_M^L(\vec{r}_{\alpha_{12}}) = r_{\alpha_{12}}^L Y_M^L(\theta,\phi), \tag{5.29}$$

that assigns angular dependence to one alpha-particle with respect to the other. Thus the reference function for ^{8}Be is the same as that of ^{5}He with the only difference that r_5 is replaced by r_{α_2}. The choice we make for $f(r_{\alpha 5})$ is again in terms of spherical shells, where

$$f(r_{\alpha_{12}},d,w) = \exp\left(-\alpha^2\frac{(r_{\alpha_{12}}-d)^2}{w^2}\right). \tag{5.30}$$

The presence of $\mathcal{Y}_M^L(\vec{r}_{\alpha_{12}})$ arranges the two alpha-particles along a common axis of symmetry. The value of $L=0$ corresponds to the spherical distribution of both alpha-particles around the system centre-of-mass, in terms of spherical shells separated by a distance d. The presence of orbital momentum breaks this spherical shape. However, there is a restriction on the allowed values of L, as a result of the required permutation

symmetry: the permutation symmetry of the spatial part is described by the tableau



that is required to be symmetric with respect to the two alpha-particles. In our approximation the orbital momentum is given by homogeneous polynomials in the components of the relative coordinate $\vec{r}_{\alpha_{12}} = \vec{r}_{\alpha_1} - \vec{r}_{\alpha_2}$, hence polynomials of odd orders of $\vec{r}_{\alpha_1\alpha_2}$ (odd value of L) are antisymmetric in the exchange of alpha-particles and cannot be included. Such an antisymmetry cannot be counter-measured by the radial part of the wavefunction (by also being antisymmetric with respect to the exchange of alpha particles), since by our approximation it is bound to be symmetric with respect to the two alpha-particles.

A selection of the results that can be obtained for the ground-state energy as a function of d and w are displayed in figure 5.19. Two different values for the orbital momentum were used ($L = 0$ and $L = 2$). Again we made use of the S3 interaction. The pattern appearing is similar to that of ^{5}He. For small values of the width w the energy depends on the values of d and L. However, as w becomes large enough the dependence on the other parameters vanishes. Furthermore, there is not a stationary value but the energy approaches the limit corresponding two non-interacting alpha-particles (that is twice the value for the ground-state energy obtained for the alpha-particle with the same calculation). Therefore, we can conclude that in the J-TICI(2) approximation ^{8}Be is not a bound system.

Again we can make use of the one- and two-body density distributions to get an idea of the structure provided by the different variational parameters. The results for the spherically averaged one- and two-body density distributions are displayed in figures 5.20 and 5.21, for orbital momentum values of $L = 0$ and $L = 2$. The density distributions were taken for a fixed value of the distance parameter d. Although d does effect the density distribution, as in the case of the energy the width w is the driving parameter. We can clearly see that the one-body density distribution becomes less localized as w increases, with the maximum moving away from the centre-of-mass. This is an indication that the two alpha particles prefer to be separated from each other. When orbital momentum is present the one-body density distribution becomes broader, something that further indicates the breaking of the ^{8}Be nucleus into two-alpha particles. This is not unexpected since the

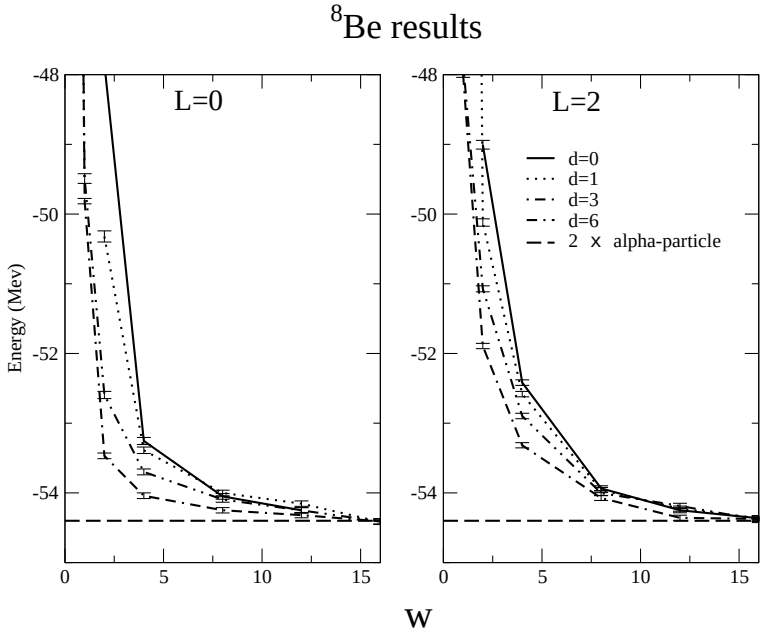


Figure 5.19: The ground-state energy for the state-independent J-TICI(2) calculation of ^{8}He for $L = 0$ and $L = 2$ using the S3 interaction. The broken line corresponds to twice the alpha-particle ground-state energy for the same type of calculation. The error bars is due to the Monte Carlo evaluation of the integrals. The value of w is in relative units (i.e. scaled fm) since is multiplied by the harmonic oscillator parameter α.

presence of orbital momentum provides a distribution around the axis of symmetry and thus reducing the probability of finding a nucleon at the center-of-mass.

In the case of the two-body distribution we get a more pronounced tail effect effect than the previous cases of ^{5}He and ^{6}He. This is indicated in figure 5.21. Furthermore, the presence of orbital momentum provides secondary maxima to the distribution indicating that the system tend to break into two distinct structures, as is illustrated in the right-hand graph of figure 5.21

As in the case of ^{5}He the calculation indicates that ^{8}Be composed by two correlated alpha-particles is not a bound structure, at least within our approximation, since the variational value for the ground-state energy does not have a stationary value. Although, the results displayed are based on the S3 V4-type interaction the same situation holds for a number of similar V4-type interactions such as MS3, B1, MTI/III and MTV. By observing the spherically averaged one- and two-body density distributions we get a clear picture that the value for the ground state energy approaches that of two uncorrelated alpha-particles.

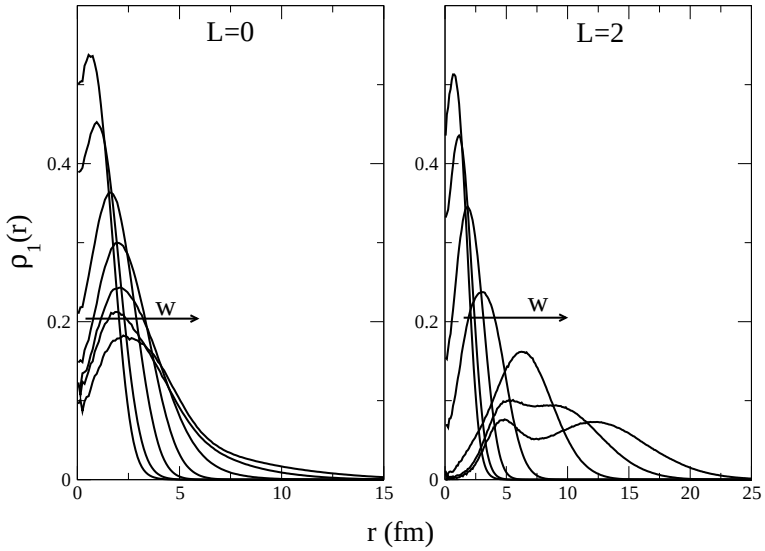


Figure 5.20: The one-body spherically-averaged density distribution of ^{8}Be. The wavefunction was obtained using the S3 interaction for the $L = 0$ and $L = 2$ state. The density distributions were obtained for several values of w for a fi xed valued of d. The arrow indicates increasing values of w.

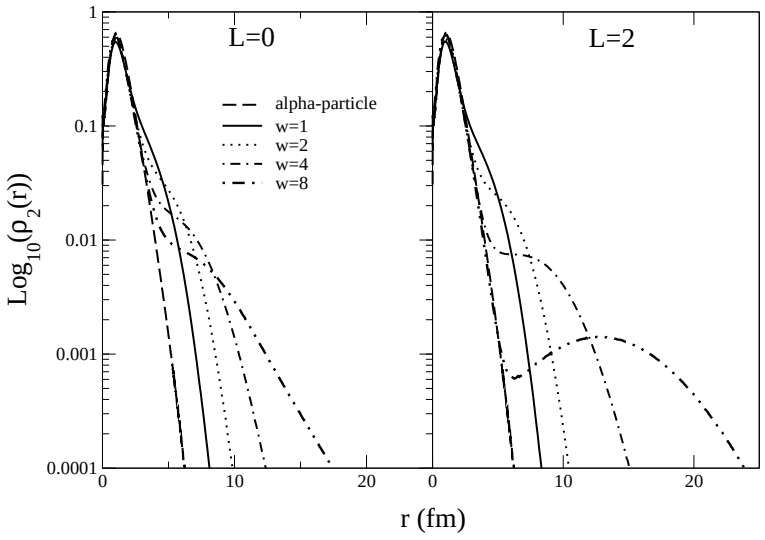


Figure 5.21: The logarithmic spherically averaged two-body density distribution of ^{8}Be for the $L = 0$ and $L = 2$ states. The wavefunction was obtained for the S3 interaction.

5.2.5 ^{9}Be

We can obtain the nucleus of ^{9}Be by adding one neutron to the configuration of ^{8}Be. This case is very similar to that of ^{6}He where instead of an alpha-particle and two neutrons we have two alpha-particles and one neutron. The reference function can be composed from that of (5.25) for ^{8}Be by adding a term correlating the additional neutron with the two alpha-particles :

$$\Phi_L^{\text{ref}} = \left(\Phi_{\alpha_1}\Phi_{\alpha_2} f_1(r_{\alpha_{12}})\right) f_2(r_{\alpha_{19}}) f_3(r_{\alpha_{29}}) \mathcal{Y}_M^L(\vec{r}_{\alpha 1}, \vec{r}_{\alpha 2}, \vec{r}_9), \tag{5.31}$$

where

$$\vec{r}_{\alpha_{19}} = \vec{r}_{\alpha_1} - \vec{r}_9, \tag{5.32}$$

$$\vec{r}_{\alpha_{29}} = \vec{r}_{\alpha_2} - \vec{r}_9. \tag{5.33}$$

The functions f_1, f_2 and f_3 are of identical form and like before are given in terms of spherical shells, each characterized by a different set of variational parameters. f_2 and f_3 adjust the position of the weakly-bound neutron with respect to each of the alpha-particles, while f_1 adjusts the separation between the two alpha-particles. The inclusion of orbital momentum is more complicated than before. The function $\mathcal{Y}_M^L(\vec{r}_{\alpha 1}, \vec{r}_{\alpha 2}, \vec{r}_9)$ describes the angular dependence of the wavefunction and in general depends on the coordinates of the two alpha-particles and that of the additional neutron in a translationally invariant way.

There are two possible schemes for the inclusion of angular dependence corresponding to two distinct physical situations. One possibility is where we have the orbital momentum of the additional neutron with respect to the center-of-mass of the ^{8}Be subsystem (^{9}Be$\sim$ ^{8}Be+n). In this case

$$\mathcal{Y}_M^L(\vec{r}_{\alpha 1}, \vec{r}_{\alpha 2}, \vec{r}_9) = \mathcal{Y}_M^L(\vec{r}_9'), \tag{5.34}$$

$$\vec{r}_9' = \vec{r}_9 - \frac{1}{2}(\vec{r}_{\alpha_1} + \vec{r}_{\alpha_2}). \tag{5.35}$$

There is no restriction as a result of permutation symmetry in the possible values of L arising from this coupling.

On the other hand we can have the orbital momentum of the additional neutron with

respect to one of the alpha-particles and then couple this to the orbital momentum of the other alpha-particle, i.e.

$$\mathcal{Y}^L_M(\vec{r}_{\alpha 1}, \vec{r}_{\alpha 2}, \vec{r}_9) = \left[\mathcal{Y}^{l_1}_{m_1}(\vec{r}_{\alpha_{19}}) \otimes \mathcal{Y}^{l_2}_{m_2}(\vec{r}'_{\alpha_2})\right]^L_M , \tag{5.36}$$

$$= \vec{r}'_{\alpha_2} = \vec{r}_{\alpha_2} - \frac{1}{9}\sum_{i=1}^{9} \vec{r}_i. \tag{5.37}$$

In general the orbital momentum is a linear expansion over different combinations of l_1 and l_2 that can be coupled to L. This coupling must be symmetric with respect to the two alpha-particles.

The calculation for ^{9}Be did not show any different behaviour from the previous cases. Again there is not a variational stationary point and at the limit of large separation between the two alpha-particles and the additional neutron the energy approaches its minimum (that of two uncorrelated alpha-particles). In figures 5.22 and 5.23 we illustrate the results for the ground-state energy and the spherically averaged density distributions respectively. Again we made a selection for the variation parameters that is conclusive for the behaviour. We used the S3 interaction and set $L = 0$. The error bars of figure 5.22 are considerably bigger than any of the previous cases, since we restricted the number of Monte-Carlo samples due to the rapid increase in computation time. Nevertheless, the restricted sampling did not effect the clarity of the results, although in principle we could always allow for more computer time.

5.2.6 Three-body correlations

As we have seen the trial form of our wavefunction was not adequate to bind the nuclei of ^{6}He and ^{9}Be, unless we artificially changed the potential function. We expect that the major reason for this is the absence of spin-orbit coupling in our hamiltonian. However, there exist further improvements in the correlation mechanism and the reference state, that might also influence the results. The reference function is confined to include an alpha-particle 0^+ state in our calculation and it would be interesting to examine the effect of improving the correlation mechanism.

The linear TICI(2) part of the correlation operator consists of pair correlations between all particles, while the non-linear Jastrow part consists of products of pair correlation functions. We can enrich the correlation mechanism by adding linear three-body

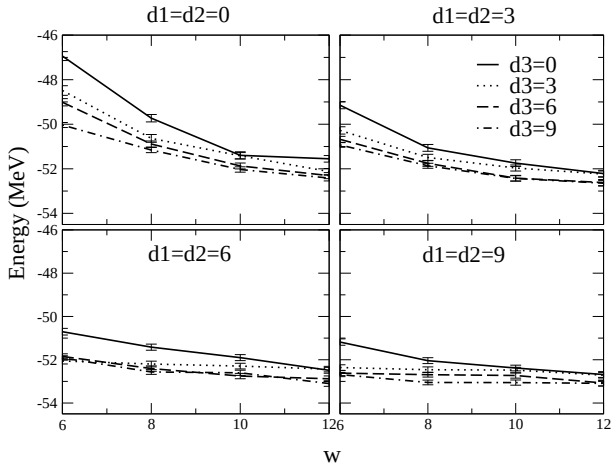


Figure 5.22: The ground state energy of ^{9}Be using the S3 interaction for $L = 0$. The parameters d_1 and d_2 are related to the separation of the additional neutron from each of the two alpha-particle, while d_3 is the separation between the two alpha-particles. The width parameter w is in relative units since is multiplied by the harmonic oscillator parameter.

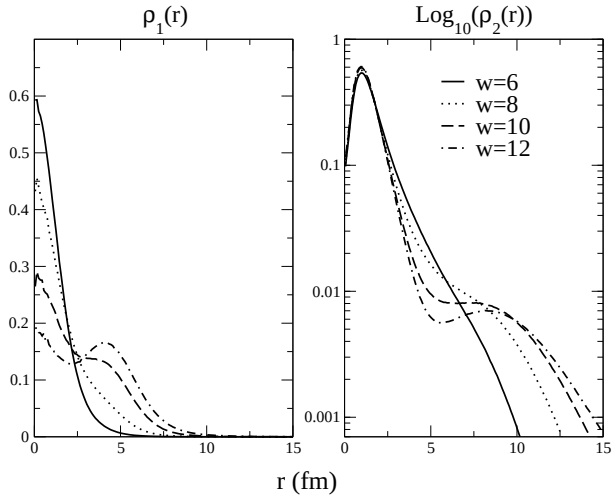


Figure 5.23: The one- and two-body spherically-averaged density distribution of ^{9}Be. The wave-function was obtained using the S3 interaction for the $L = 0$ The density distributions were obtained for several values of w.

correlations. We will refer to this as the J-TICI(2)+J-TICI(3) method. Three-body correlations were considered in [43, 45, 44]. As shown in table 2.2 the inclusion of linear correlations higher than second-order can improve the value for the binding energy when only linear correlations are used. However, the same contribution to linear pairwise correlations is provided by the non-linear Jastrow factor (table 2.5). As discussed in chapter 2 the J-TICI(2) method is sufficient for the alpha-particle. Nevertheless we examine the inclusion of three-body correlations in our cluster-like model since it can provide further evidence of what might be necessary for a successful calculation.

The functional form used for the two-body correlations in terms of gaussians, can be extended to three-body correlations via the triple gaussian expansion [45]

$$C_3^{\rm F} = \sum_{m\le n\le p} A_{mnp}\mathcal{S}\left(\sum_{i<j<k} e^{-(b_m r_{ij}^2 + b_m r_{ik}^2 + b_m r_{jk}^2)}\right), \tag{5.38}$$

where $C_3^{\rm F}$ replaces the linear correlation operator $\hat{F}$ that acts on the reference function. The operator $C_3^{\rm F}$ can include both two- and three-body correlations with the appropriate choice of parameters. The form of $C_3^{\rm F}$ is the most natural extension of what we have for the two-body terms. In order to avoid the complexity provided by the triple expansion we can use either of the simpler forms

$$C_3^{\rm S1} = \sum_m A_m\mathcal{S}\left(\sum_{i<j<k} e^{-b_m(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)}\right), \tag{5.39}$$

$$C_3^{\rm S2} = \sum_m A_m\mathcal{S}\left(\sum_{i<j<k} e^{-b_m(\rho_{ijk}^2)}\right) \;\; ; \;\; \vec{\rho}_{ijk} = \vec{r}_i - \frac{1}{2}(\vec{r}_j + \vec{r}_k), \tag{5.40}$$

that incorporate only a single expansion. The form $C_3^{\rm S1}$ has been used before in [43, 44], where $(r_{ij}^2 + r_{ik}^2 + r_{jk}^2)$ is the hyperspherical radius. The form $C_3^{\rm S2}$ is intuitively easier to understand, since $\vec{\rho}_{ijk}$ is the coordinate of the ith particle with respect to the center-of-mass of particles j and k. This is an extension on the sum over particle pairs without having to incorporate a multilinear expansion.

At his stage we are only interested in a preliminary examination of three-body correlations, while a more detail analysis is one of the possibilities for future research. We apply three-body correlations through the operator $C_3^{\rm S2}$ for the case of ^{6}He using the S3 interaction. The purpose is to examine whether the inclusion of linear three-body terms

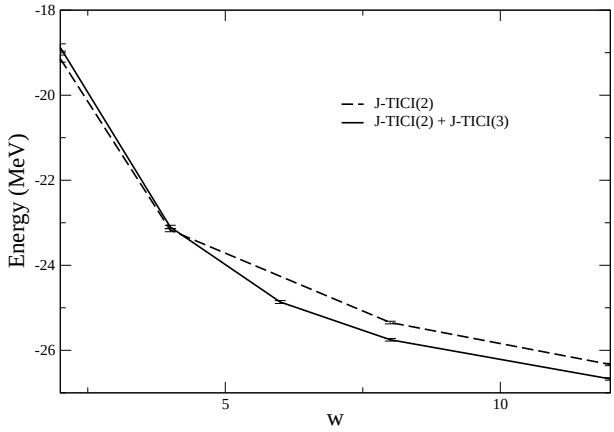


Figure 5.24: The ^{6}He ground-state energy in the J-TICI(2) calculation and the J-TICI(2) with added three-body correlations (J-TICI(2)+J-TICI(3)), for different values of the width parameter w. The results were obtained for the S3 interaction.

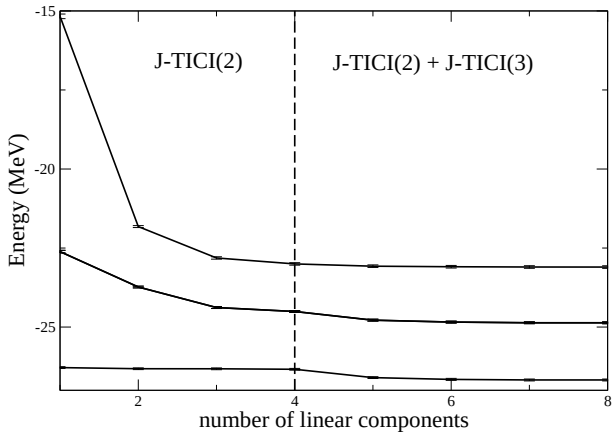


Figure 5.25: The ground-state energy for the J-TICI(2)+J-TICI(3) calculation of ^{6}He as a result of the total number of linear components used. The first four components (left-hand side of the vertical broken line) include only two-body correlations while the remaining components (right-hand side of the broken line) include the added three-body correlations. The results were obtained for the S3 interaction.

can radically change the results obtained for the J-TICI(2) method. Figure 5.24 illustrates through some selected configuration the effect that three-body correlations have on the variational behaviour of the calculation. We can clearly see that the overall behaviour is not changed, despite some local changes (with respect to the variational parameter w) in the binding energy. The effect that the inclusion of the C_3^{S2} terms had at a number of points is further illustrated in figure 5.25, where a total of 8 linear components were used, 4 for the two-body part and 4 for the three-body part. We can see that although the three-body correlations contribute to the total result, this is only by a very small amount. Both figures 5.24 and 5.25 demonstrate that the contribution of linear three-body correlation will not radically change the results, i.e. produce a bound wavefunction.

Although we restricted the application of three-body correlations to a 'naive' linear term the constancy of the results illustrates that the correlation mechanism alone cannot produce a bound state of the halo nuclei.

5.3 Conclusion and general remarks

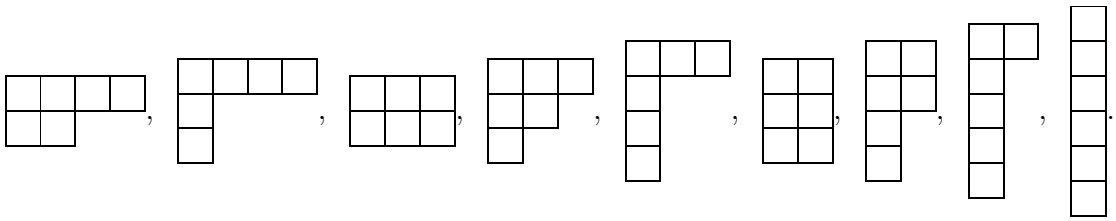
We extended the variational method discussed in chapter 3 beyond the alpha-particle. Although the number of variational parameters is in some cases considerably large, we could restrict the calculation into selected sets of these parameters. Despite the restrictions the results we obtained are conclusive (to the best of our knowledge). Furthermore, we could make use of the one- and two-body density distributions to get a qualitative picture of the wavefunction.

The general conclusion is that our simple version of a variational approach to light halo nuclei is capable of producing bound states for open-shell systems. However, this required a small modification of the potential function. In the case where direct use of available semi-realistic interactions was made we could not find any of the nuclei examined to be bound, i.e. to poses a variational stationary point. Apart from the nuclei of ^{5}He and ^{8}Be that experimentally are unbound, those of ^{6}He and ^{9}Be are known halo nuclei. It seems that the absence of spin-orbit coupling is critical for these nuclei.

In addition to the absence of spin-orbit terms in the interaction that can alter the symmetry and thus the binding energy of the ground state the form of the wavefunction employed has a number of approximations. Although, this is important for the case of light

halo nuclei and is not necessarily the major approximation for the general many-body problem. The general approximation scheme can be summarized as follows:

- One major approximation in the model is the alpha-particle that is kept in the 0^+ state. In terms of the many-body trial wavefunction it implies that a restricted configuration is available. This can be illustrated in terms of the Young tableau. If we consider the case of ^{6}He the possible Young tableau that describe the allowed permutation symmetry of the spatial part (their conjugate tableau is compatible with the SU(2)×SU(2) spin-isospin decomposition) are



  The reference state should in general be a superposition of several of the above structures. Our approximation for the alpha-particle restricts the calculation to a single structure (either of the first two). Inclusion of a multireference can be examined in the future.

- We have restricted the calculation to include only local scalar semi-realistic interactions. It is possible that a more realistic type of interaction will alter the results. This, however, will require more careful consideration. Although we examined several cases of V4 interactions it might be possible that different types will alter the results. However, inclusion of further types of interactions in the results is not a problem at all, since it only involves a small change in the numerical algorithms.

- We examined two-body and a 'naive' three-body correlation mechanism. There is still the possibility of improving the correlation mechanism. We avoided using state-dependent correlations, apart from the case of ^{5}He, where the effect is shown in figure 5.26, where we can see that state-dependence does not effect the nature of the results. Although state-dependent correlations lower the binding energy (as is also shown for the alpha-particle in chapter 2) they do not provide a linear correlation mechanism beyond that of pair correlations but rather improve the choice

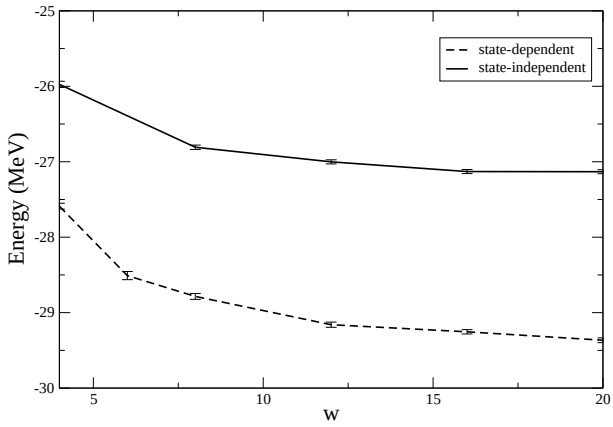


Figure 5.26: The ground state energy of ^{5}He using the S3 interaction for state-dependent and state-independent correlations. The width parameter w is in relative units since is multiplied by the harmonic oscillator parameter.

for such terms. It is likely that inclusion of state-dependence in the correlation mechanism will not provide a variational stationary point. The reason for avoiding state-dependence is due to the inefficiency of the numerical algorithm when these are present. The involved algebra can be dealt with as is illustrated in the appendix. Furthermore, it is not difficult to write a computer program that can deal with the state-dependence (as we did based on the procedure discussed in the appendix). Nevertheless no conclusive statement can be made for the correlation mechanism and it can be one of the reasons contributing to the failure of our approximation.

The complexity for this calculation arises from the required antisymmetrization. Although a simple form can be chosen for either the ket wavefunction, the expectation value of an operator will in general require different permutations of the equivalent bra state as a result of the spin and isopsin degrees of freedom. The calculation of ^{5}He is the easiest to perform numerically since the involved antisymmetrization requires a small number of permutations. The complexity depends on the number of required permutations of a relatively simple form that dramatically increases when we go from ^{5}He (10 permutations) to ^{9}Be (635 permutations). In the case of Monte-Carlo sampling these will be performed per sampling point and can reduce the efficiency of the calculation, particularly when the number of non-linear variational parameters is large.

And finally a word of caution. The antisymmetry condition is the most cumbersome part of the calculation. However, a naive cluster model in terms of permutation symmetry,

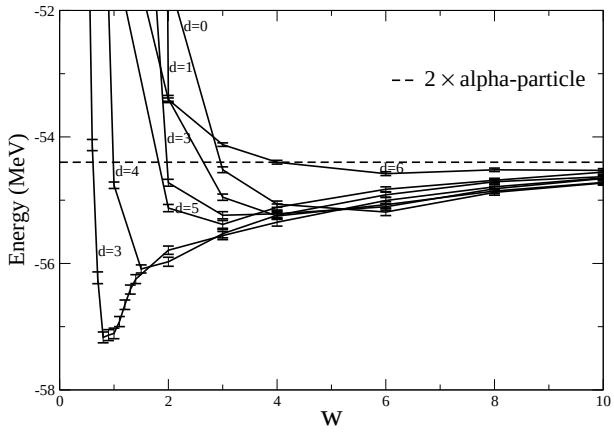


Figure 5.27: The ^{8}Be ground-state energy in the J-TICI(2) calculation when the Pauli exclusion principle is not fully effected between the two alpha-particles. The results were obtained for the S3 interaction.

can lead to completely different results results (wrong) as is illustrated in figure 5.27. In that case we did not fully antisymmetrize the reference state between the two alpha-particles. Although the remaining antisymmetry forces the wavefunction to be unbound at relatively small separations, there appears a strong minimum, indicating that ^{8}Be is bound. This is in contradiction from we we found when we correctly imposed the full antisymmetry (figure 5.19).

Chapter 6

Overview and future prospective

6.1 Overview of the research and conclusions

The subject of this thesis was the approximate solution of the few-body Schrödinger equation in terms of a linear variational problem with application to light nuclei. The most basic ingredient in such an approximation is the construction of the trial wavefunction. One way of doing this is by appropriately approximating some rather complicated parameterization, usually non-linear. One type of such a parameterization is given by the Coupled Cluster Method (CCM) and was discussed in chapter2. The basic principle of the CCM is that the exact wavefunction can be obtained by correlating a starting reference function. This correlation operator is non-linear and can be given directly in coordinate representation. Furthermore the coordinate representation of the coupled cluster method provides a parameterization of the correlation operator in terms of functions depending on the relative distances, thus preserving translational invariance (provided that the reference state is translationally invariant). We can obtain several truncated forms for the correlation operator that can be used in a variational calculation. The most general variational wavefunction consists of a multilineal expansion of the correlation operator.

Another type of non-linear parametrization of the many-body wavefunction that is variational in nature is the Jastrow method. We also provided a brief discussion of this method and ways of approximating it. Both the CCM and the Jastrow method can include state-dependent correlations. It is considerably more complicated to include state-dependence correlations in the Jastrow method than in the CCM. The final form of the wavefunction that we made use of was obtained by combining these two methods in a

way appropriate for a linear variational method. We obtained an economic wavefunction (in terms of complexity) by combining the simplest approximation of the CCM, namely the TICI(2), with the Jastrow correlation factor. This lead to a variational calculation that is easily accessible both analytically and numerically, termed as the J-TICI(2) scheme.

The effectiveness of the approximation scheme introduced was examined by considering the calculation for the ground-state of the alpha-particle. For this purpose we quoted results from a number of authors as well as our own. Apart from the ground-state energy, we also calculated the spherically averaged one- and two-body density distributions that were used to provide qualitative information about the wavefunction. The alpha-particle has provided a reliable method for testing the accuracy of both the method and the numerical calculation. When compared with statistically methods the results obtained are in close agreement. Contrary to the complexity of such methods, both in implementation and computer time, the J-TICI(2) scheme was relatively easy and straight forward to apply. We managed to slightly improve the previously obtained results for the alpha-particle at no expense.

The linearized variational wavefunction developed for the alpha-particle was then extended to include a number of additional nucleons, especially neutrons, as well as additional alpha-particles. This involved changing the reference state into one compatible with the symmetries of system in question. A number of non-linear variational parameters were introduced that described the separation between the different clusters. We worked in the $L-S$ coupling scheme and assumed that the alpha-particle remained in the 0^+ state. The incorporation of the antisymmetry condition, appropriate for fermions, has been given special attention, where it was found that the complexity greatly increases in going beyond the alpha- particle. Some simple group-theoretical results can simplify the matrix elements required for the expectation value of the hamiltonian. However, despite the case of the alpha-particle that can be greatly simplified, inclusion of state-dependent correlations leads to a considerably more complicated problem than the one with state-independent correlations. We have devoted an appendix that includes some technical details of permutation symmetry as well as the method of dealing with it in a computer code.

Apart from the wavefunction our approximation involved a semi-realistic type of interaction. We restricted ourselves in the study of central local interactions of the V4 type.

These include only spatial, spin, isospin and spin-isospin terms and are fitted in terms of gaussians (soft-core). The main reason is due to the difficulty that can arise because of the required matrix elements of tensor operators and spin-orbit terms. Although such terms have been examined for the closed shell alpha-particle, we do not wish to pursue them at this stage for the lightly bound systems to be examined. In principle is always possible to include such terms.

Although the theoretical background is fairly simple, a numerical evaluation of the matrix elements is required, due to the complexity of the many-body integrals. In chapter 4 we examined the application of the well known variational Monte Carlo (VMC). The most important task of the analysis was to ensure the validity of the error estimate and in particular as applied to the linear eigenvalue problem. We made use of a number of statistical concepts that are essential for a reliable error estimate. We found that for this purpose special attention is required in the presence of correlations between the different random walk samples. We also described the application of a method that can be used to improve the performance of VMC, known as the 'zero variance principle'. We restricted ourselves to a simple linear approximation of this method. Although, the linear approximation of the 'zero-variance' principle is not of any substantial help for systems more complicated than the alpha-particle, we could always obtain the required accuracy within reasonable time-limits. In principle we could have looked from a more complicate approximation than the one at hand, but this is beyond our purpose since it overcomplicates an already complicate problem. We expended a lot of effort in ensuring a reliable numerical method and we are confident that the results obtained are within the right error bounds.

In chapter 5 we extended the variational method discussed in chapter 2 beyond the alpha-particle. We could demonstrate the applicability of our model to open-shell systems by initially making use of the same semi-realistic interactions that bind the alpha-particle. Although this could not produce bound-states for ^{6}He and ^{9}Be our calculations demonstrated the several aspects of our model. We expect that our simple version of the nuclear interaction is not adequate to reproduce what is expected for halo nuclei from experimental evidence. This conclusion was drawn from the variational character of the results. since could not find any of the nuclei examined to be bound, i.e. to poses a variational stationary point. Apart form the nuclei of ^{5}He and ^{8}Be that experimentally are unbound, those of ^{6}He and ^{9}Be are known halo nuclei. The general behaviour obtained

was that the energy approached a minimum, as the separation between the several constituents increased. This could be monitored by observing the spherically averaged one- and two-body density distributions. We could clearly see that the energy was minimized as the one-body distribution broadened with the center shifting away from the origin. The two-body density distribution separated into two parts: a main body similar to the alpha-particle and a small tale effect. We used a logarithmic scaling in order to distinguish the two parts.

Despite the fact that our interaction is not adequate for the light halo nuclei of ^{6}He and ^{9}Be we demonstrated that our model can produce bound states for such open-shell systems by modifying the inter-nucleon force. This was done by artificially altering the Wigner part of the S3 interaction, where we could obtain bound states for both ^{5}He and ^{6}He. Therefore, the general conclusion is that we have a successful cluster-like model that can produce bound states of open-shell nuclei, despite the fact that in reality a spin-orbit term might be necessary.

6.2 Future prospective

The fact that our results using the semi-realistic V4 interactions introduced in chapter 3 did not provide a bound state for the halo nuclei of interest was expected since the experimental evidence points towards the need for spin-orbit terms. A possible future development is the inclusion of such terms in the interaction. We can both add more terms and investigate some more realistic types of nucleon-nucleon potentials. Furthermore, working with spin-orbit force will require to rethink the inclusion of permutation symmetry and will increase the allowed configuration.

Another possibility is to include more structure in the reference function. In the J-TICI(2) this can be achieved by providing a multi-linear expansion, where we expand both the linear operator and the reference function. However, such a formalism is not as straight-forward as the case of a single 0^+ alpha-particle state, since it is not clear what type of basis-functions will be used. An adequate alpha-particle 0^+ state can be obtained by correlating a harmonic oscillator ground state. Extra nucleons can then be added by assigning coordinates relative to the alpha-particle center-of-mass. It is not clear how the model will develop if we wish to go beyond the alpha-particle 0^+ state. However, this is

not the most immediate future development.

We avoided using state-dependent correlations because of simplicity. Another possibility for future work is to examine more closely the effect of these correlations, so that a more economic approach can be found for including them into our calculations. As shown in chapter 3, the number of spatial integrals required greatly increases when state-dependence is included in the correlations. This makes calculations of this type impractical when moving to heavier systems. However, the analysis performed for the alpha-particle greatly simplifies matters, by using some simple results from the theory of the symmetric group. Despite the fact that this simplification is lost when we move away from the alpha-particle, reconsidering the problem might yield further simplifications that are applicable beyond the alpha-particle.

Apart from improvements in the current model we can broaden our investigation in order to examine the continuum states provided by our formalism, such as resonance states. This can be done using the method of complex scaling [73]. This reduces the study of resonances to that of bound states by examining complex eigenvalues. The complex scaling method has been shown to be a powerful method for solving resonances of three-body systems [74], where ^{6}He and ^{11}Li were studied as three-body systems. By studying the unbound states produced by our model we can obtain further information about the structure of the wavefunction.

Appendix A

Some useful aspects of permutation symmetry

A.1 Representations and basis functions of the symmetric group

Here we review some simple concepts of group theory, relevant for the calculation of the many-body expectation value. We refere to [75, 64] for more details.

One of the standard theorems of group representation theory is that the total number of irreducible representations (irreps) for a finite group is equal to the number of conjugacy classes in the group. The group elements of the symmetric group $\mathcal{S}_N$ are the permutations of order N. Each permutation can be decomposed into a product of commuting cycles. Permutations belonging to a particular cycle structure remain unchanged under a similarity transformation and thus belong to the same conjugacy class. Therefore, the number of irreps $\mathcal{S}_N$ is equal to the number of different cycle structures. The total number of different cycle structures for $\mathcal{S}_N$ is equal to the number of partitions of the integer N,

$$N = \lambda_1 + \lambda_2 + ... + \lambda_N \; ; \; \lambda_1 \geq \lambda_2 \geq ... \geq \lambda_N. \tag{A.1}$$

A 'tableau' is a diagrammatic representation of such a partition or of a particular irrep of $\mathcal{S}_N$. For the above partition a tableau consists of λ_1 boxes in the first row, λ_2 boxes in the second row and so on. We shall denote such a tableau by the symbol $Y^{[\lambda_1,\lambda_2,...,\lambda_N]}$. As

an example the tableau corresponding to the partition $3 = 2 + 1$ is

$$Y^{[2,1]} \equiv \begin{array}{|c|c|}\hline & \\ \hline \\ \cline{1-1}\end{array}\,. \tag{A.2}$$

We are mostly interested in the construction of functions that can serve as basis functions for the irreps of $\mathcal{S}_N$. We can assume that these can be obtained from the action of some operators acting on a starting function. Whether this is possible will depend on the problem in question.

In general starting with any function Φ_0 that does not have any specific symmetry, we can obtain the basis functions belonging to the irreducible representations of a finite group G in terms of hermitian projection operators (see [75] pages 111-114). These operators can be constructed once the irreducible representations are known and require the action of all of the group elements on Φ_0. For example in the case of the symmetric group the symmetrizer S

$$S = \frac{1}{\sqrt{N!}} \sum_P P \tag{A.3}$$

and the antisymmetrizer

$$\mathcal{A} = \frac{1}{\sqrt{N!}} \sum_P (-)^P P \tag{A.4}$$

are the two most well known hermitian projection operators. In the above equation P represents any permutation belonging to $\mathcal{S}_N$, while $(-)^P$ is the parity of the permutation P. These generate the one dimensional representations of the symmetric group.

A.1.1 Standard basis for $\mathcal{S}_n$

Associated with each tableau of $\mathcal{S}_n$ is a a number of tableau with labels ranging from 1 to n in each box. When the labels are put in a standard way (all numbers increase when reading from left to right and from top to bottom along rows and columns respectively) the tableau obtained are terms 'Young tableau'. We will denote the Young tableau by using subscripts for the same symbol used to denote the tableau. As an example the standard Young tableau for $\mathcal{S}_3$ are

$$Y_1^{[1^3]} \equiv \begin{array}{|c|}\hline 1 \\ \hline 2 \\ \hline 3 \\ \hline\end{array},\; Y_1^{[3]} \equiv \begin{array}{|c|c|c|}\hline 1 & 2 & 3 \\ \hline\end{array},\; Y_1^{[2,1]} \equiv \begin{array}{|c|c|}\hline 1 & 2 \\ \hline 3 \\ \cline{1-1}\end{array},\; Y_2^{[2,1]} \equiv \begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array}. \tag{A.5}$$

A function associated with a tableau of k columns and k' rows can be brought either into a form that is symmetric in k or antisymmetric in k' of it's labels. The number of standard Young table for each tableau (irrep) is equal to the dimension of the irrep. The standard Young tableau provide a distinct way of labeling the basis functions of some irrep. This is termed as the Yamanouchi basis and a discussion for the properties of this basis can be found in almost all books that discuss group theory.

We can obtain the standard basis in a different way that is more close to physics, developed by Chen [64]. For the group $\mathcal{S}_n$ we can find a complete set of commuting operators, that can be simultaneously diagonalized, providing distinct eigenvalues and thus distinct eigenvectors for the irreps. These are the 'class operators' that are composed of a summation over all the element of a particular class. It happens that for $\mathcal{S}_n$ the sum over all transpositions, $C_2(n)$, has a distinct eigenvalue in each irreducible representation space, where

$$C_2(n) = \sum_{j>i=1}^{n} P_{ij}, \tag{A.6}$$

with P_{ij} representing transpositions of particle labels i and j e.g. for a state such as $|\alpha\alpha\beta\rangle$, this is equivalent to keeping particle labels fixed and moving the states of particle positions i and j. Therefore, diagonalizing $C_2(n)$ can provide a set of functions that belong in some particular irrep of $\mathcal{S}_n$. A complete set of operators (up to a multiplicity factor) is provided by considering the classes of transpositions for the subgroups of $\mathcal{S}_n$ i.e. for $\mathcal{S}_4$, the set of operators

$$C_2(2) = P_{12}, \quad C_2(3) = P_{12} + P_{13} + P_{23}, \quad C_2(4) = P_{12} + P_{13} + P_{14} + P_{23} + P_{24} + P_{34}\ , \tag{A.7}$$

provide a complete set of commuting operators that can be simultaneously diagonalized and distinctly label the basis states within a particular irrep of $\mathcal{S}_n$. The set of required eigenvalues can be found easily by considering the tableau: the eigenvalue for $C_2(n)$ of some tableau of n boxes is the maximum possible number of symmetric pairs minus the maximum possible number of antisymmetric pairs.

There is the possibility of an irrep occurring more than once given a particular set of functions. This multiplicity can be removed by enlarging the set of commuting operators to include class operators of the intrinsic group. For $\mathcal{S}_n$ this is the group of state permutations i.e. state labels are fixed and particle labels move. This is equivalent to associating

for a standard tableau a number of tableaux termed 'Weyl tableaux'. Details for this procedure can be found in [64]. In our work there will be no ambiguity since this is removed by considering different quantum numbers (total spin or isospin projection M_S and M_T).

A.1.2 Non-orthogonal basis functions

The symmetric group algebra can be separated into commuting subalgebras called ideals. Furthermore, when these ideals cannot be decomposed further (termed 'primitive') they provide irreducible representation spaces for the group algebra and their elements (basis vectors) can be used as projection operators. A particular set of such projection operators can be obtained by considering the decomposition of the identity element, e, into primitive idempotents (which by definition are elements of the ideals of the algebra):

$$e = e^1 + ... + e^i + ..., \quad e^i e^j = \delta_{ij} e^j. \tag{A.8}$$

The e^i of the symmetric group can be chosen to be the Young symmetrizers [65]. These are operators associated with the Young tableau by taking the product of all raw symmetrizers and column antisymmetrizers. For the above tableau of (A.5) the Young symmetrizers are

$$Y^{[1^3]} = \mathcal{A}_{123},\ Y^{[3]} = S_{123},\ Y_1^{[2,1]} = \mathcal{A}_{13} S_{12},\ Y_2^{[2,1]} = \mathcal{A}_{12} S_{13}. \tag{A.9}$$

The decomposition of the identity in this case is

$$e = Y^{[1^3]} + Y^{[3]} + Y_1^{[2,1]} + Y_2^{[2,1]}. \tag{A.10}$$

Each of the Young symmetrizers projects into an irreducible space of the group algebra with respect to the Symmetric group.

A.1.3 Expectation value of exchange operators

The properties of the basis states of $\mathcal{S}_n$ is important when one considers the expectation value of a state-dependent interaction, like the realistic ones introduced in chapter 3. As

described in chapter 3 the fully antisymmetric wavefunction can be expressed as

$$\Psi = \sum_i \Phi_L^{[\nu]i} \left| \begin{matrix} [\tilde{\nu}]i \\ S,\ T \end{matrix} \right\rangle , \tag{A.11}$$

where the spin-isospin part has the further decomposition

$$\left| \begin{matrix} [\tilde{\nu}]i \\ S\ T \end{matrix} \right\rangle = \sum_{j,k} C^{[\tilde{\nu}]i}_{[\alpha]j,[\beta]k} \left| \begin{matrix} [\alpha]j \\ S\ M_S \end{matrix} \right\rangle \left| \begin{matrix} [\beta]k \\ T\ M_T \end{matrix} \right\rangle . \tag{A.12}$$

$C^{[\tilde{\nu}]i}_{[\alpha]j,[\beta]k}$ are the Clebsch-Gordan coefficients for $\mathcal{S}_n$. The spatial states $\Phi_L^{[\nu]i}$ are in general non-orthogonal, contrary to the spin-isospin ones.

The state-dependence requires the expectation value of exchange operators with respect to the fully antisymmetric state, something that requires knowledge of the Clebsch-Gordan coefficients and the representation matrices of $\mathcal{S}_n$. Although this provides an analytic expression it can lead to a cumbersome evaluation for two reasons:

- the Clebsch-Gordan coefficients for $\mathcal{S}_n$ are not easy to obtain and in particular for relatively large n such as the case of ^{9}Be (n=9),

- even if these coefficients are available, expression (3.44) requires full knowledge of the basis functions of $\mathcal{S}_n$ and in particular of the $\Phi_L^{[\nu]i}$, something that will lead to complicated and unnecessarily large spatial integrands.

In order to avoid the above complications, we can devise a procedure for the evaluation of the expectation values that is easily applicable through a computer code and minimizes the group theoretical input.

The totally antisymmetric wavefunction can be expressed by an antisymmetrizer $\mathcal{A}$ acting on a simple product of spatial and spin-isospin parts:

$$\Psi = \mathcal{A}\{|\Phi_0\rangle|0\rangle\}. \tag{A.13}$$

A choice for the states $|\Phi_0\rangle|0\rangle$ is any of the products appearing in the expansion of the wavefunction i.e

$$|\Phi_0\rangle|0\rangle \rightarrow \Phi_L^{[\nu]i} \left| \begin{matrix} [\tilde{\nu}]i \\ S,\ T \end{matrix} \right\rangle , \tag{A.14}$$

for some i, or in general any state that will give the right quantum numbers upon antisym-

metrization. For this purpose we can make use of the Young symmetrizers. Because $\mathcal{A}$ is hermitian and idempotent the expectation value of an operator $\hat{O}$ becomes

$$\begin{aligned} \langle \hat{O} \rangle &= N! \langle \Psi | \hat{O} | \Phi_0 \rangle | 0 \rangle, & \text{(A.15)} \\ &= N! \mathcal{A} \{ \langle \Phi_0 | \langle 0 | \} \hat{O} | \Phi_0 \rangle | 0 \rangle, & \text{(A.16)} \end{aligned}$$

provided that $\hat{O}$ is invariant with respect to any permutation of the particle labels. The state $|0\rangle$ will contain internal symmetries due to the finite number of spin/isospin states such that there is a set of permutations $\mathbb{1}'$, where

$$P|0\rangle = |0\rangle, \quad P \in \mathbb{1}'. \tag{A.17}$$

The expectation value of the operator $\hat{O}$ will result in expectation values of the form

$$N! \mathcal{A} \{ \langle \Phi_0 | \langle 0 | \} P_\sigma P'_\tau | \Phi_0 \rangle | 0 \rangle, \tag{A.18}$$

where P_σ and P'_τ are permutations in spin and isospin space. The general idea is that this permutations can be easily effected on $|0\rangle$, giving a new state $|0'\rangle$. We then have to consider from the fully antisymmetric bra state the parts which have a spin-isospin state identical to $|0'\rangle$, since the spin-isospin states are by definition orthogonal. It must be noted that $|0\rangle$ is not necessarily a single state but in general is a sum of different terms.

We first consider the case where the where the permutations acting on the ket state leave it unchanged. In this case the total antisymmetrizer acting on the bra state reduces to an 'effective antisymmetrizer' $\mathcal{A}_{\text{eff}}$ defined as

$$\mathcal{A}_{\text{eff}} = \sum_{P \in \mathbb{1}'} (-)^P P. \tag{A.19}$$

In the case of a permutation $\mathcal{P}_k$ acting on the ket the antisymmetrizer on the bra state reduces to

$$\mathcal{A} \to \delta_{\mathcal{P}} \mathcal{P} \mathcal{A}_{\text{eff}}, \tag{A.20}$$

where $\mathcal{P}_k$ is a permutation in either spin or isospin space or both, while $\mathcal{P}$ is the same permutation acting simultaneously on spin,isospin and coordinate space. $\delta_{\mathcal{P}}$ is a constant and has two choices: if the action on $\mathcal{P}_k$ on $|0\rangle$ results in something more that a permutation

then $\delta_{\mathcal{P}} = 0$, otherwise is equal to the parity of that permutation $(-)^{\mathcal{P}}$.

This provides a systematic way of obtaining the expectation value of exchange operators by associating with each operator a reduced antisymmetrizer acting on the bra state. We provide the results obtained for some of the nuclei of interest.

^{5}He:

In the case of ^{5}He the choice of $|0\rangle$ can be a single ket, without any ambiguity in the spin or isospin quantum numbers, since there is only one choice. If we denote the four possible spin-isospin states available to a single particle by $\uparrow\uparrow\equiv |\alpha\rangle, \uparrow\downarrow\equiv |\beta\rangle, \downarrow\uparrow\equiv |\gamma\rangle, \downarrow\downarrow\equiv |\delta\rangle$ then the possible choises could be

$$|0\rangle = \{|\alpha\beta\gamma\delta\alpha\rangle, |\alpha\beta\gamma\delta\beta\rangle\}, \tag{A.21}$$

which are symmetric between particles 1 and 5 and 2 and 5 respectively. The full wavefunction is obtained by antisymmetrizing the product of $|0\rangle$ with an appropriate spatial part. For the case of $|\alpha\beta\gamma\delta\alpha\rangle$, the only requirement of the spatial part is that it does not have the same intrinsic symmetry like $|0\rangle$, i.e. is not symmetric between particle coordinates 1 and 5. The effective antisymmetrizer is simply

$$\mathcal{A}_{\text{eff}} = 1 - P_{15}, \tag{A.22}$$

while the action of an arbitrary spin-isospin exchange operator $\mathcal{P}$ on $|0\rangle$ reduces the antisymmetrizer for the bra state to

$$\mathcal{A} \to \delta_{\mathcal{P}} \left(\mathcal{P} - \mathcal{P}P_{15}\right). \tag{A.23}$$

Table (A.1) displays the value of $\delta_{\mathcal{P}}$ for the spin, isospin and spin-isospin transpositions of ^{5}He.

^{6}He:

The condition of total antisymmetry is more complicated in ^{6}He. The are two possible sets of quantum numbers corresponding to the addition of two neutrons to the alpha-particle

Table A.1: The value of $\delta_{\mathcal{P}}$ for the spin, isospin and spin-isospin transpositions of ^{5}He.

ij	$\delta_{\mathcal{P}^\sigma_{ij}}$	$\delta_{\mathcal{P}^\tau_{ij}}$	$\delta_{\mathcal{P}^{\sigma\tau}_{ij}}$
12	-1	1	-1
13	1	-1	-1
14	0	0	-1
15	1	1	1
23	0	0	-1
24	1	1	-1
25	0	0	-1
34	-1	1	-1
35	1	-1	-1
45	0	0	-1

((S=0,T=1) and (S=1,T=1). For both of these cases the choice of $|0\rangle$ can be a single ket:

$$|0\rangle \rightarrow |\alpha\beta\gamma\delta\alpha\beta\rangle;\ (S=0,T=1), \tag{A.24}$$

$$|0\rangle \rightarrow |\alpha\beta\gamma\delta\alpha\alpha\rangle;\ (S=1,T=1), \tag{A.25}$$

where the effective antisymmetrizers are simply

$$\mathcal{A}_{\text{eff}} = (1-P_{15})(1-P_{26}), \quad (S=0,T=1) \tag{A.26}$$

$$\mathcal{A}_{\text{eff}} = \mathcal{A}_{156} = 1 - P_{15} - P_{16} - P_{56} + P_{15}P_{16} + P_{16}P_{15}, \quad (S=1,T=1) \tag{A.27}$$

The action of an arbitrary spin-isospin exchange operator $\mathcal{P}$ on $|0\rangle$ reduces the antisymmetrizer for the bra state to

$$\mathcal{A} \rightarrow \delta_{\mathcal{P}}\mathcal{P}\mathcal{A}_{\text{eff}}. \tag{A.28}$$

Table (A.2) displays the value of $\delta_{\mathcal{P}}$ for the spin, isospin and spin-isospin transpositions of ^{6}He.

The case of $(S=0,T=0)$ is more complicated and $|0\rangle$ is not just a simple ket but four different kets:

$$|0\rangle \rightarrow |\alpha\beta\gamma\delta\alpha\gamma\rangle + |\alpha\beta\gamma\delta\gamma\alpha\rangle - |\alpha\beta\gamma\delta\beta\gamma\rangle - |\alpha\beta\gamma\delta\gamma\beta\rangle. \tag{A.29}$$

Table A.2: The value of $\delta_{\mathcal{P}}$ for the spin, isospin and spin-isospin transpositions of ^{6}He for the $(S=0,T=1)$ and $(S=1,T=1)$ quantum numbers.

	$(S=0,T=1)$			$(S=1,T=1)$		
ij	$\delta_{\mathcal{P}^{\sigma}_{ij}}$	$\delta_{\mathcal{P}^{\tau}_{ij}}$	$\delta_{\mathcal{P}^{\sigma\tau}_{ij}}$	$\delta_{\mathcal{P}^{\sigma}_{ij}}$	$\delta_{\mathcal{P}^{\tau}_{ij}}$	$\delta_{\mathcal{P}^{\sigma\tau}_{ij}}$
12	-1	1	-1	-1	1	-1
13	1	-1	-1	1	-1	-1
14	0	0	-1	0	0	-1
15	1	1	1	1	1	1
16	-1	1	-1	1	1	1
23	0	0	-1	0	0	-1
24	1	1	-1	1	1	-1
25	1	-1	-1	-1	1	-1
26	1	1	1	-1	1	-1
34	-1	1	-1	-1	1	-1
35	1	-1	-1	1	-1	-1
36	0	0	-1	1	-1	-1
45	0	0	-1	0	0	-1
46	1	-1	-1	0	0	-1
56	-1	1	-1	1	1	1

This requires the construction of four separate effective antisymmetrizers, one for each simple ket of $|0\rangle$. Despite this complexity (that will only increase the required computation time) the method is the same as before. Instead of considering only one table for the spin isospin exchanges we have to consider the sum of four such tables.

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