Multistep Shell Model in the Complex Energy Plane

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Abstract

In this thesis the properties of unbound nuclei like $^{12,13}$Li are studied by extending the multistep shell model to the complex energy plane. The nuclei $^{12}$Li and $^{13}$Li are described starting from the one-particle states in $^{10}$Li and two-particle states in $^{11}$Li. The ground state of $^{12}$Li is found to be an antibound state. No bound or antibound state is found in $^{13}$Li. It is also shown that the odd proton plays a minor role in these nuclei.

This framework is also applied to study the recently proposed spin-aligned proton-neutron pair coupling scheme. For this the MSM is extended to the proton-neutron space as well as the isospin space. In the model, a non-orthogonal basis is introduced, which allows us to identify simultaneously the roles played by all configurations. The four-particle, six-particle and eight-particle nuclei in the heaviest $N = Z$ region are evaluated using the MSM basis within the space spanned by the single $0g_{9/2}$ hole shell.

A novel Monte Carlo representation in the complex energy plane is also developed for studying nuclear excitations in the continuum. The calculations on realistic potentials show a stable performance and high accuracy in the one-particle and two-particle cases. This will provide a convenient tool to study open systems with many nucleons in the continuum.
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List of Publications

This thesis is mainly based on the first three papers. Other papers listed below are related to the thesis.

I. Z.X. Xu, R. J. Liotta, C. Qi, T. Roger, P. Roussel-Chomaz, H. Savajols, R. Wyss, *Analysis of the unbound spectrum of $^{12}$Li*, Nucl. Phys. A 850 (2011) 53-68.

II. Z.X. Xu, C. Qi, J. Blomqvist, R. J. Liotta, R. Wyss, *Multistep shell model description of spin-aligned neutron-proton pair coupling*, Nucl. Phys. A 877 (2012) 51-58.

III. Z.X. Xu, C. Qi, *Novel Monte Carlo representation for shell model in the complex energy plane*, manuscript to be submitted.

IV. Zhen-Xiang Xu and Chong Qi, *Shell evolution and its indication on the isospin dependence of the spin-orbit splitting*, submitted for publication.

V. Chong Qi, X.B. Wang, Z.X. Xu, R. J. Liotta, R. Wyss, and F.R. Xu, *Alternate proof of the Rowe-Rosensteel proposition and seniority conservation*, Phys. Rev. C 82, 014304 (2010).

VI. Z.X. Xu, C. Qi, R. J. Liotta, R. Wyss, *Multistep shell model in the complex energy plane*, J. Phys. : Conf. Ser. 338, 012029 (2012).

VII. Chong Qi, Z.X. Xu, R. J. Liotta, *Analytic proof of partial conservation of seniority in $j = 9/2$ shells*, Nucl. Phys. A 884-885 (2012) 21-35.

VIII. Chong Qi, Z.X. Xu, *The structure of tin isotopes with a global optimized effective interaction*, Phys. Rev. C 86, 044323 (2012).
# Contents

List of Publications \hspace{1cm} vii  
Contents \hspace{1cm} viii  
1 Introduction \hspace{1cm} 1  
2 Gamow states and the Berggren representation \hspace{1cm} 3  
\hspace{1cm} 2.1 Gamow states \hspace{1cm} 3  
\hspace{1cm} 2.2 Berggren completeness relation \hspace{1cm} 5  
\hspace{1cm} 2.3 Separable interaction \hspace{1cm} 6  
3 Multistep shell model method \hspace{1cm} 9  
\hspace{1cm} 3.1 The MSM basis \hspace{1cm} 10  
\hspace{1cm} 3.2 Dynamical matrix \hspace{1cm} 12  
\hspace{1cm} 3.3 Overlap matrix \hspace{1cm} 15  
\hspace{1cm} 3.4 Hermitian matrix \hspace{1cm} 17  
\hspace{1cm} 3.5 The MSM with proton-neutron pair \hspace{1cm} 18  
\hspace{1cm} 3.6 The MSM with isospin symmetry \hspace{1cm} 27  
4 Multistep shell model method in the complex energy plane \hspace{1cm} 29  
\hspace{1cm} 4.1 Extension to the complex energy plane \hspace{1cm} 29  
\hspace{1cm} 4.2 Berggren single-particle representation \hspace{1cm} 30  
\hspace{1cm} 4.3 Two-particle states: The nucleus $^{11}\text{Li}$ \hspace{1cm} 33  
\hspace{1cm} 4.4 Three-particle states: The nucleus $^{12}\text{Li}$ \hspace{1cm} 34  
\hspace{1cm} 4.5 Four-particle states: The nucleus $^{13}\text{Li}$ \hspace{1cm} 39  
5 Multistep shell model description of spin-aligned proton-neutron pair coupling \hspace{1cm} 41  
\hspace{1cm} 5.1 Normal pair and proton-neutron pair couplings \hspace{1cm} 41  
\hspace{1cm} 5.2 Isospin symmetry \hspace{1cm} 47  
\hspace{1cm} 5.3 Spectra \hspace{1cm} 52  
6 Monte Carlo representation in the complex energy plane \hspace{1cm} 55
## CONTENTS

6.1 Monte Carlo method ........................................ 55  
6.2 Discretized Berggren representation ......................... 56  
6.3 MC method for one-particle system ......................... 59  
6.4 MC method for two-particle system ......................... 60  

7 Summary .................................................. 63

A Appendix .................................................. 67  
A.1 Coupling of angular momenta ............................. 67  
A.2 The MSM equations ...................................... 68  
A.3 The MSM with proton-neutron pair ........................ 69  
A.4 The MSM with isospin symmetry .......................... 75  

Bibliography ............................................... 79
Chapter 1

Introduction

The study of halo nuclei is one of the main subjects of research in nuclear physics at present. The first halo nucleus discovered was $^{11}\text{Li}$ with two halo neutrons [1]. It is a very interesting and challenging case because the nuclear force is not strong enough to bind a neutron to $^9\text{Li}$. However, the adding of two neutrons to $^9\text{Li}$ leads to a bound halo nucleus $^{11}\text{Li}$. In recent years, a number of experiments have been performed to explore the halo structure of heavier Li isotopes. In particular the spectrum of $^{12}\text{Li}$ was measured and $^{13}\text{Li}$ was found to be unbound [2–4].

Different theoretical models have been proposed to describe the halo phenomenon [5–8]. A general feature which was found is that a necessary condition for a nucleus to develop a halo is that the outmost nucleons move in shells which extend far in space. That is, only a weak barrier keep the system within the nuclear volume. These shells may be resonances, antibound states (also called virtual states), or even low-spin bound states which lie very close to the continuum threshold. These conditions are fulfilled by the nucleus $^{11}\text{Li}$ and also heavier Li isotopes.

To study the structure of these unstable nuclei, one has to consider the effects of the continuum [9]. A successful attempt has been done by introducing the continuum into shell model calculations (CSM) [10]. However the real-energy CSM calculations become unfeasible in general because the dimensions of the shell model basis is extremely large. In order to reduce the dimensions one can restrict the calculations by using only the continuum configurations which contain mostly the resonant states, which have the most important contribution of the continuum coupling. These resonant states can only been described properly in the complex energy plane as Gamow functions [11]. A complete representation, the so called Berggren representation, is formed in the complex energy plane by the Gamow states and a set of scattering states on a contour [12]. Based on this representation a shell model in the complex energy plane (CXSM) was recently presented [13–16]. Yet the dimension problem remains when the number of active particles is large.

Our aim is to study the nuclear excitations in the continuum on the complex energy plane. In this thesis, the multistep shell model method (MSM) [17–19] in
the complex energy plane will be applied to analyze the structure of the unbound nuclei $^{12}$Li and $^{13}$Li. An extended MSM method will also be applied to study the recently proposed spin-aligned proton-neutron pair coupling scheme. Moreover, our new development on introducing the Monte Carlo method to the complex shell model will be presented.
Chapter 2

Gamow states and the Berggren representation

One of the main difficulties when studying processes occurring in the continuum is that the relevant physical processes are time-dependent. The system is sensitive to the initial conditions and can easily fall into chaos. The complex shell model method (CXSM) [13–16] presents a way to study the continuum by time-independent formalisms in the complex energy plane. The physical reason behind this is that, when the system is trapped by a high enough barrier, it can remain in a localized region of space for a considerable long time. In this case the system can be treated as quasistationary. In the following we will present these time-independent formalisms for the evolution of the system in the complex energy plane.

2.1 Gamow states

The wave function of a resonance with a peak at energy $E_0$ and a width $\Gamma$ can be factorized as [20]

$$\Phi(E, r) = \sqrt{\frac{\Gamma/2}{\pi [(E - E_0)^2 + (\Gamma/2)^2]}} \Psi(r),$$

(2.1)

where $\Psi(r) = \sqrt{\pi \Gamma/2} \Phi(E_0, r)$. Through the Fourier transform, we obtain the time evolution of the resonance

$$\Phi(t, r) = \int_{-\infty}^{\infty} \Phi(E, r)e^{-iEt/h}dE = \Psi(r)e^{-i\tilde{E}t/h},$$

(2.2)

which gives us the resonance in the form of a stationary state, but with a complex energy

$$\tilde{E} = E_0 - i\frac{\Gamma}{2}.$$  

(2.3)
The probability of measuring the system at \( t \) is given by
\[
|\Phi(t, r)|^2 = |\Psi(r)|^2 e^{-\Gamma t/\hbar}.
\] (2.4)

The half-life of the resonance can be obtained from
\[
T_{1/2} = \frac{\hbar \ln 2}{\Gamma}.
\] (2.5)

Therefore a time-dependent process has now been transformed into a stationary problem by going to the complex energy plane. The complex solutions to the corresponding stationary Schrödinger equation are called Gamow states [11]. The wave numbers \( k_n \) are a discrete set of complex values, which satisfy
\[
\tilde{E}_n = \frac{\hbar^2}{2\mu} k_n^2.
\] (2.6)

They can be written as
\[
k_n = \kappa_n + i\gamma_n.
\] (2.7)

The states can be classified into four classes, namely:

1. bound states, for which \( \kappa_n = 0 \) and \( \gamma_n > 0 \);
2. antibound states with \( \kappa_n = 0 \) and \( \gamma_n < 0 \);
3. decay resonant states with \( \kappa_n > 0 \) and \( \gamma_n < 0 \);
4. capture resonant states with \( \kappa_n < 0 \) and \( \gamma_n < 0 \).

Since the radial wave function has the form of \( w(E_n, r) \sim e^{i k_n r} \), one can see that the wave function of the resonant states will diverge at infinity. However a narrow resonance can still be treated stationary since the wave function does not diverge at small distance. As shown in Fig. 2.1, the narrow resonance has the same wave function as a bound state inside of the nucleus, but at a large radius far out from the nuclear surface it starts to oscillate and diverge. Since we are interested in the processes occurring at the scale of nuclear distances, we can eventually consider the narrow resonance as a bound state and solve the time-independent Schrödinger equation approximately.

The antibound state has a pure negative imaginary wave number \( k_n = -i|\gamma_n| \), which gives the corresponding energy real and negative, as the bound state. However unlike the bound state, whose wave function diminishes exponentially at large distances, the antibound state diverges exponentially. As a result, the antibound state can be physically meaningful only if it is sufficiently close to the threshold. Therefore it may have a great influence on low-energy cross sections and nuclear spectroscopy.
2.2 Berggren completeness relation

The eigenvectors of a Hamiltonian provide a representation projector which allows one to write

\[ \delta(r - r') = \sum_n w_n(r) w_n(r') + \int_0^\infty dE u(r, E) u(r', E), \]  

(2.8)

where \( w_n(r) \) are the wave functions of the bound states and \( u(r, E) \) are the scattering states. The integration contour is along the real energy axis, and all the energies and radial wave functions are real, or more precisely, can be chosen to be real. Notice that only bound states and scattering states enter in Eq. (2.8).

In order to include other Gamow states, Berggren extended the integration contour to the complex energy plane [12]. By using Cauchy theorem, one gets

\[ \delta(r - r') = \sum_n \tilde{w}_n^*(r) w_n(r') + \int_{L^+} dE \tilde{u}^*(r, E) u(r', E), \]  

(2.9)

where \( \tilde{w}_n(r) \) are now the wave functions for all the bound and antibound states plus the resonances lying between the real energy axis and the integration contour \( L^+ \), as shown in Fig. 2.2. In principle the contour should start at the origin \((0, 0)\), and end at infinity \((\infty, 0)\). However, one usually cuts the basis at a certain maximum energy as in any shell model, within which only a limited number of shells are included.

The tilde over the wave function \( \tilde{w}_n(r) \) denotes the mirror state of \( w_n(r) \), namely \( \tilde{k}_n = -k_n^* \). With this one can prove that \( \tilde{w}_n^*(r) = w_n(r) \), and the same for the
scattering state \( u(r, E) \). Therefore the internal product in Eq. (2.9) is the wave function times itself, and not its complex conjugate. This internal product is called the Berg gren metric.

To make the representation useful in real calculations, one has to discretize the contour integral, i.e.

\[
\int_{L^+} dE \, u(r, E) u(r', E) = \sum_p h_p u(r, E_p) u(r', E_p),
\]

where the quantities \( E_p \) are usually selected by the Gaussian method on the contour and \( h_p \) are the corresponding weights. Therefore the complete set of orthonormal vectors \( |\varphi_j\rangle \) now includes all the bound states, antibound states and resonances inside the contour, i.e., \( \langle r | \varphi_n \rangle = w_n(r, E_n) \), and also the discretized scattering states on the contour, i.e., \( \langle r | \varphi_p \rangle = \sqrt{h_p} u_p(r, E_p) \). This is the Berggren representation used in the CXSM calculations. In Ref. [22] it was found that few discretized scattering states in the basis are enough to obtain convergency.

### 2.3 Separable interaction

In the CXSM calculation, the basis states are constructed by the single-particle states in the Berggren representation. The standard two-particle shell model equation has the form

\[
(\omega - \epsilon_i - \epsilon_j) X(ij; \alpha) = \sum_{k \leq l} \langle kl; \alpha | V | ij; \alpha \rangle X(kl; \alpha),
\]

Figure 2.2: Integration contour \( L^+ \) in the complex energy plane from Ref. [21]. The open circles denote the resonances included in the sum of Eq. (2.9), while the solid circles are those excluded. The vertex \((c, 0)\) corresponds to the energy cutoff point \( c \).
2.3. SEPARABLE INTERACTION

where \(i,j,k,l\) label the single-particle states and \(\alpha\) denotes the two-particle states. \(\epsilon_i, \epsilon_j\) and \(\omega_\alpha\) are the energy of the states respectively. A convenient way of solving this equation is by using a separable two-body interaction. The matrix can thus be written as

\[
\langle \tilde{kl}; \alpha | V | ij; \alpha \rangle = -G_\alpha f_\alpha (kl) f_\alpha (ij),
\]

(2.12)

where \(G_\alpha\) is the interaction strength and \(f_\alpha (ij)\) is the matrix element of the field defining the interaction. The shell model equation becomes

\[
-\frac{X (ij; \alpha)}{G_\alpha} = \sum_{k \leq l} f_\alpha (kl) f_\alpha (ij) X (kl; \alpha)

\frac{\omega_\alpha - \epsilon_i - \epsilon_j}{(\omega_\alpha - \epsilon_i - \epsilon_j)}.
\]

(2.13)

Multiplying by \(\sum_{i \leq j} f_\alpha (ij)\) on both sides of Eq. (2.13), one obtains the dispersion relation

\[
-\frac{1}{G_\alpha} = \sum_{i \leq j} \frac{f^2_\alpha(ij)}{\omega_\alpha - \epsilon_i - \epsilon_j}.
\]

(2.14)

The two-particle wave function amplitudes are given by

\[
X (ij; \alpha) = N_\alpha \frac{f_\alpha (ij)}{\omega_\alpha - \epsilon_i - \epsilon_j},
\]

(2.15)

where \(N_\alpha\) is the normalization constant determined by

\[
\sum_{i \leq j} X^2 (ij; \alpha) = 1.
\]

(2.16)
Chapter 3

Multistep shell model method

The Shell Model is one of the most powerful tools to solve the many-body problem in nuclear physics [6,23–28]. It solves the nuclear many-body Schrödinger equation exactly within the corresponding shell model subspace, which means that the Pauli principle is automatically included. However, when the number of active particles is big enough, the dimensions of the shell model matrices will become so large that no calculation can reasonably be performed. To handle this problem, in 1961, de-Shalit proposed to use correlated states in the shell model basis [29]. Since then many models and methods that include correlated states in the basis set of elements have been introduced [17,30,31].

The idea of the multistep shell model method (MSM) [17–19] is the following: In the first step a single-particle representation is chosen, which defines the shell model space. Then one evaluates the interaction matrix elements or takes them from experiment and calculate the two-particle system. With the two-particle energies and wave functions calculated, one calculates the three-particle system in a basis which consists of the one- and two-particle vector-coupled states previously evaluated. The calculations of the four-particle system and so on can be performed in the same way. Of course it is not necessary to calculate nucleus one by one until the end. For instance one can calculate the four-particle system from the two-particle states directly. If no truncation is made, the MSM can reproduce the same results as the shell model. However, in this case, the MSM basis is overcomplete and the dimension will be much larger than the shell model dimension.

One great advantage of the MSM method is that we can carry out drastic truncations of the MSM basis which was built on the intermediate states. In fact most of the high-lying intermediate states have almost no effect on the result of low-lying states. Very few important intermediate states are selected for the following calculations, therefore the dimensions of the MSM matrices are greatly reduced. Moreover, one can also be able to check the calculated results in each given steps against the corresponding experimental data.

The price for this advantages is that the basis elements may violate the Pauli
principle. It means that the basis elements are not orthogonal to each other and that the dimension could be much larger than the corresponding physical dimension. To overcome this problem one must first evaluate the overlap (or metric) matrix among all the basis elements. By means of the overlap matrix one can restore the Pauli principle, and convert the overcomplete MSM matrix into a Hermitian matrix with the correct dimension.

In this chapter we will introduce the procedure to evaluate and solve the multistep shell model equations. Brief derivations will be given on three-particle system, two-proton two-neutron system and three-proton three-neutron system as examples. A summary of the dynamical and overlap equations in various MSM systems is given in the Appendix.

3.1 The MSM basis

We assume a $s$-particle system ($s > 2$) divided into two subsystems, which consist of $m$ particles and $n$ particles respectively, such that $s = m + n$. The corresponding MSM basis vector can be written as

$$
|\alpha_m \beta_n; \alpha_s\rangle = (P^\dagger(\alpha_m)P^\dagger(\beta_n))_{\alpha_s} |0\rangle,
$$

(3.1)

where $\alpha_m$, $\beta_n$ and $\alpha_s$ label the states of the corresponding system and $|0\rangle$ is the core wave function. The indexes denote the particle number of the system. In this thesis, we adopt the notation $c^\dagger$ for the one-particle creation operator and $P^\dagger$ for the many-particle creation operator. Therefore, in our formulism the wave function of a $s$-particle state can be defined as

$$
|\alpha_s\rangle = P^\dagger(\alpha_s) |0\rangle,
$$

(3.2)

where the symbol in parentheses in the summation indicates that the ordering is only valid for $m = n$. From Eq. (3.2) one obtains

$$
\delta_{\alpha_s \beta_s} = \sum_{\alpha_m(\leq) \beta_n} X(\alpha_m \beta_n; \alpha_s) (P^\dagger(\alpha_m)P^\dagger(\beta_n))_{\alpha_s} |0\rangle.
$$

(3.3)

Since the MSM basis is usually overcomplete, the wave function amplitudes $X$ are not unique. Instead, the physically meaningful quantities are the projections of the MSM basis vectors upon the physical vector, which we denotes as

$$
F(\alpha_m \beta_n; \alpha_s) = \langle \alpha_s |(P^\dagger(\alpha_m)P^\dagger(\beta_n))_{\alpha_s} |0\rangle.
$$

(3.4)

The projection $F$, which does not depend on the basis we choose, is closely related to the form factor of $m$- (or $n$-)particle transfer reactions [17]. Equation (3.3) now becomes

$$
\delta_{\alpha_s \beta_s} = \sum_{\alpha_m(\leq) \beta_n} X(\alpha_m \beta_n; \alpha_s) F(\alpha_m \beta_n; \beta_s).
$$

(3.5)
3.1. THE MSM BASIS

The norm of a MSM basis vector \( |\alpha_m\beta_n;\alpha_s\rangle \) in the \( s \)-particle system, i.e.,

\[
N(\alpha_m\beta_n;\alpha_s) = \sqrt{\langle \alpha_m\beta_n;\alpha_s|\alpha_m\beta_n;\alpha_s \rangle} \tag{3.6}
\]

may not be unity. Therefore for studying the importance of the MSM configuration in a certain state, the interesting quantity is not the projection \( F \) but rather the cosine of the angle between the basis vector and the physical vector, i.e., \( \cos(\phi) = x \) where

\[
x(\alpha_m\beta_n;\alpha_s) = F(\alpha_m\beta_n;\alpha_s)/N(\alpha_m\beta_n;\alpha_s). \tag{3.7}
\]

And for each single MSM basis element \( |\alpha_m\beta_n;\alpha_s\rangle \), one has

\[
\sum_{\alpha_s} x^2(\alpha_m\beta_n;\alpha_s) = 1. \tag{3.8}
\]

This is because the vectors \( |\alpha_s\rangle \), which are eigenvectors of the \( s \)-particle shell model Hamiltonian, form an orthonormal complete set. Therefore the value \( x^2(\alpha_m\beta_n;\alpha_s) \) indicates the probability of the state \( |\alpha_s\rangle \) occupying the basis state \( |\alpha_m\beta_n;\alpha_s\rangle \).

It is worthwhile to point out that if we would have taken the basis elements as a complete set of orthonormal states, such as a standard shell model basis, one would have obtained the wave function amplitude

\[
X(\alpha_m\beta_n;\alpha_s) = x^\ast(\alpha_m\beta_n;\alpha_s), \tag{3.9}
\]

as it follows from Eq. (3.5). One thus sees that the advantage of the MSM basis is that one can extract the physical structure of the calculated states just by examining the quantity \( x \).

**Amplitude \( Y \)**

The amplitude \( Y \) is defined by

\[
P^\dagger(\alpha_{2m}) = \frac{1}{2} \sum_{\alpha_m\beta_m} Y(\alpha_m\beta_m;\alpha_{2m})(P^\dagger(\alpha_m)P^\dagger(\beta_m))_{\alpha_{2m}}. \tag{3.10}
\]

By exchanging \( \alpha_m \) and \( \beta_m \), one gets the relation

\[
Y(\beta_m\alpha_m;\alpha_{2m}) = (-1)^{m+J_{\alpha_m}+J_{\beta_m}+J_{\alpha_{2m}}} Y(\alpha_m\beta_m;\alpha_{2m}) \tag{3.11}
\]

where \( J_{\alpha_m} \) in the exponent means the angular momentum of the corresponding state. When \( m > 1 \), by comparing with Eq. (3.10), one can easily obtain

\[
Y(\alpha_m\beta_m;\alpha_{2m}) = (1 + \delta_{\alpha_m\beta_m})X(\alpha_m\beta_m;\alpha_{2m}). \tag{3.12}
\]

However for \( m = 1 \), which means in a two-particle system, one needs to be more careful. In this case, the wave function amplitude \( X \) is well defined because the
basis is orthonormal. That is, the basis is constructed for the vectors \((c^\dagger_i c^\dagger_j)_{\alpha_2}|0\rangle\), which satisfy
\[
\langle 0 | (c^\dagger_i c^\dagger_j)_{\alpha_2} (c^\dagger_i c^\dagger_j)_{\alpha_2} |0\rangle = \sum_{m_i,m_j} \langle j_i m_i j_j m_j j_{\alpha_2} m_{\alpha_2} \rangle^2 \langle 0 | c_j c_i c_j^\dagger c_i^\dagger |0\rangle = 1 + \delta_{ij}. \tag{3.13}
\]
Therefore the normalized two-particle basis vector is defined as
\[
\frac{|(c^\dagger_i c^\dagger_j)_{\alpha_2}|0\rangle}{\sqrt{1 + \delta_{ij}}}, \tag{3.14}
\]
and the two particle creation operator can now be written as
\[
P^\dagger(\alpha_2) = \sum_{i\leq j} \frac{1}{\sqrt{1 + \delta_{ij}}} X(ij; \alpha_2)(c^\dagger_i c^\dagger_j)_{\alpha_2} = \sum_{ij} \sqrt{1 + \delta_{ij}} X(ij; \alpha_2)(c^\dagger_i c^\dagger_j)_{\alpha_2}. \tag{3.15}
\]
Comparing with the definition of \(Y\), one gets
\[
Y(ij; \alpha_2) = \sqrt{1 + \delta_{ij}} X(ij; \alpha_2). \tag{3.16}
\]
This relation can sometimes be easily confused with Eq. (3.12).

From Eq. (3.15) one can also obtain
\[
\sum_{i\leq j} \frac{1}{\sqrt{1 + \delta_{ij}}} X(ij; \alpha_2)(c^\dagger_i c^\dagger_j)_{\alpha_2} |0\rangle = 1. \tag{3.17}
\]
Since it is
\[
\sum_{i\leq j} X^2(ij; \alpha_2) = 1, \tag{3.18}
\]
one gets
\[
\langle \alpha_2 | (c^\dagger_i c^\dagger_j)_{\alpha_2} |0\rangle = \sqrt{1 + \delta_{ij}} X(ij; \alpha_2) = Y(ij; \alpha_2), \tag{3.19}
\]
and also
\[
\frac{1}{2} \sum_{ij} Y^2(ij; \alpha_2) = 1. \tag{3.20}
\]
These relations between \(X\), \(Y\) and \(F\), are quite useful when simplifying the MSM equations.

### 3.2 Dynamical matrix

The dynamical equations can be obtained by using the Tamm-Dancoff approximation (TDA). In general, one writes the commutation operator \([H, P^\dagger(\alpha_m)P^\dagger(\alpha_n)]\) in a normal form, where the hamiltonian is given by
\[
H = H_0 + V = \sum_i \varepsilon_i c_i^\dagger c_i + \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle c_i^\dagger c_j^\dagger c_k c_l. \tag{3.21}
\]
However for our procedure it is more convenient to define the quantity

$$\Lambda(\alpha_m\beta_n;\alpha_s) = \langle \alpha_s \left| \left[ [H, P^\dagger(\alpha_m)], P^\dagger(\beta_n) \right] \right| 0 \rangle, \quad (3.22)$$

where the plus sign in the subscription only applies when \(m\) and \(n\) are both odd. This means that when \(m\) and \(n\) are both odd, the square brackets is an anti-commutation operation, otherwise it is a commutation operation as usual. Since it is easy to prove that

$$\langle \alpha_s \left| \left[ [H_0, P^\dagger(\alpha_m)], P^\dagger(\alpha_n) \right] \right| 0 \rangle = 0, \quad (3.23)$$

one can thus write

$$\Lambda(\alpha_m\alpha_n;\alpha_s) = \langle \alpha_s \left| \left[ [V, P^\dagger(\alpha_m)], P^\dagger(\alpha_n) \right] \right| 0 \rangle. \quad (3.24)$$

On the other hand, from Eq. (3.22) one can obtain

$$\Lambda(\alpha_m\alpha_n;\alpha_s) = (W(\alpha_s) - W(\alpha_m) - W(\alpha_n))\langle \alpha_s | P^\dagger(\alpha_m)P^\dagger(\alpha_n) | 0 \rangle, \quad (3.25)$$

where \(W(\alpha_s)\) denotes the energy of the \(s\)-particle states referring to the core. Besides, we will adopt the notation \(\epsilon_i\) for the one-particle energy. The plus-minus sign in the subscription is canceled when exchanging \(P^\dagger(\alpha_m)\) and \(P^\dagger(\alpha_n)\) in the derivation.

The two-particle dynamical equation can be derived from Eq. (3.24) and (3.25)

$$\Lambda(pq;\alpha_2) = (W(\alpha_2) - \epsilon_p - \epsilon_q)\langle \alpha_2 | c_p^\dagger c_q^\dagger | 0 \rangle = \langle \alpha_2 | [V, c_p^\dagger c_q^\dagger] | 0 \rangle, \quad (3.26)$$

where

$$[V, c_p^\dagger, c_q^\dagger] = \frac{1}{2} \sum_{ijl} \langle ij | V | kl \rangle [c_i^\dagger c_j^\dagger c_k c_l, c_p^\dagger c_q^\dagger]$$

$$= \frac{1}{2} \sum_{ijkl} \langle ij | V | kl \rangle [c_i^\dagger c_j^\dagger c_k c_l] - \frac{1}{2} \sum_{ijk} \langle ij | V | kp \rangle [c_i^\dagger c_j c_k, c_p^\dagger c_q^\dagger]$$

$$= \frac{1}{2} \sum_{ij} \langle ij | V | pq \rangle c_i^\dagger c_j^\dagger. \quad (3.27)$$

Therefore we have

$$(W(\alpha_2) - \epsilon_p - \epsilon_q)\langle \alpha_2 | c_p^\dagger c_q^\dagger | 0 \rangle = \frac{1}{2} \sum_{ij} \langle ij | V | pq \rangle \langle \alpha_2 | c_i^\dagger c_j^\dagger | 0 \rangle. \quad (3.28)$$

And one can obtain the two-particle wave function

$$(W(\alpha_2) - \epsilon_p - \epsilon_q)X(pq;\alpha_2) = \sum_{i<j} \langle ij | \alpha_2 | pq | \alpha_2 \rangle X(ij;\alpha_2), \quad (3.29)$$
One can use the relations in which Eq. (3.24) and (3.25) one gets $\langle \text{Herewe use} \rangle$

vectors are experimentally known. Special cases, the two-particle states whose energies and wave function amplitudes of this is not only to simplify the derivation, but also one can be able use, in some special cases, the two-particle states whose energies and wave function amplitudes are experimentally known.

The three-particle system is calculated in the following way. The MSM basis vectors are

$$|\alpha_2; \alpha_3 \rangle = (c^\dagger Y \alpha_2) |0\rangle.$$

(3.30)

The two-particle creation operator in uncoupled form is

$$P^t(\alpha_2) = \frac{1}{2} \sum_{qr} Y(qr; \alpha_2)(c^\dagger \alpha_2 c^\dagger \alpha_3)_{\alpha_2} = \frac{1}{2} \sum_{qr} Y(qr; \alpha_2)(\alpha_2) c^\dagger P^t(\alpha_2) c^\dagger.$$

(3.31)

Here we use $\langle qr; \alpha_2 \rangle$ to denote the $3j$-coefficient $\langle j_0 m_0 j_1 m_1 j_2 m_2 \rangle$ for short. From Eq. (3.24) and (3.25) one gets

$$(W(\alpha_3) - \epsilon_p - W(\alpha_2)) (\alpha_3 | c^\dagger P^t(\alpha_2) | 0) = (\alpha_3 | [[V, c^\dagger], P^t(\alpha_2)] | 0),$$

(3.32)

in which

$$[[V, c^\dagger], P^t(\alpha_2)] = \frac{1}{2} \sum_{ijl} (ij|V|pl)_{\alpha_2} [c^\dagger c^\dagger, c^\dagger, P^t(\alpha_2)]$$

$$= \frac{1}{4} \sum_{ij} \sum_{qr} Y(qr; \alpha_2)(\alpha_2)$$

$$\times \left[ (ij|V|pq)_{\alpha_2} c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger - (ij|V|pr)_{\alpha_2} c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger \right].$$

(3.33)

One can use the relations

$$Y(qr; \alpha_2) = (-1)^{1+j_0+j_1+j_2} Y(qr; \alpha_2),$$

(3.34)

$$\langle qr; \alpha_2 \rangle = (-1)^{1+j_0+j_1+j_2} (qr; \alpha_2),$$

(3.35)

to obtain

$$[[V, c^\dagger], P^t(\alpha_2)] = \frac{1}{2} \sum_{ijqr} (ij|V|pr)_{\alpha_2} Y(qr; \alpha_2)(\alpha_2) c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger.$$

(3.36)

By introducing the identity matrix $\sum_{\beta_2} |\beta_2 \rangle \langle \beta_2|$, Eq. (3.32) becomes

$$(W(\alpha_3) - \epsilon_p - W(\alpha_2)) (\alpha_3 | c^\dagger P^t(\alpha_2) | 0)$$

$$= \frac{1}{2} \sum_{ijqr} (ij|V|pr)_{\alpha_2} Y(qr; \alpha_2)(\alpha_2) c^\dagger P^t(\alpha_2)(\alpha_2) c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger c^\dagger.$$

(3.37)
3.3. OVERLAP MATRIX

Replacing the two-body interaction matrices by using Eq. (3.28), and putting the coupling coefficients on the MSM basis vectors, one gets

\[
(W(\alpha_3) - \epsilon_p - W(\alpha_2)) \langle \alpha_3 | (c_{p,P}^\dagger(\alpha_2))_{\alpha_3} | 0 \rangle = \sum_{qr} \sum_{\beta_2} (W(\beta_2) - \epsilon_p - \epsilon_r) \langle \alpha_3 | (c_{q,P}^\dagger(\beta_2))_{\alpha_3} | 0 \rangle \times Y(rq;\alpha_2)Y(pr;\beta_2)Y(pr;\beta_2)(p\alpha_2;\alpha_3)(q\beta_2;\alpha_3). \tag{3.38}
\]

By using the relation between 6j-symbol and 3j-symbols in Eq. (A.1) and the sum rules of c-g coefficients, one finally obtains the three-particle dynamical equation as

\[
(W(\alpha_3) - \epsilon_p - W(\alpha_2)) \langle \alpha_3 | (c_{p,P}^\dagger(\alpha_2))_{\alpha_3} | 0 \rangle = \sum_{qr} \sum_{\beta_2} (W(\beta_2) - \epsilon_p - \epsilon_r) A(p\alpha_2,q\beta_2;\alpha_3) \langle \alpha_3 | (c_{q,P}^\dagger(\beta_2))_{\alpha_3} | 0 \rangle, \tag{3.39}
\]

where

\[
A(p\alpha_2,q\beta_2;\alpha_3) = \hat{\alpha}_2 \hat{\beta}_2 \left\{ \begin{array}{ccc} p & r & \beta_2 \\ q & \alpha_3 & \alpha_2 \end{array} \right\} Y(rq;\alpha_2)Y(rp;\beta_2),
\]

and \(\hat{\alpha}_2 = \sqrt{2J_{\alpha_2} + 1}\).

The four-particle states can be described as the two-particle correlated states coupling with themselves

\[
|\alpha_2\beta_2\alpha_4\rangle = (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4}|0\rangle, \tag{3.40}
\]

where \(\alpha_2 \leq \beta_2\). The corresponding dynamical equation can be obtained in the same way as in the three-particle system. The formulas are shown in detail in Appendix A.2.

3.3 Overlap matrix

As we mentioned before, the MSM basis is overcomplete and may also violate the Pauli principle. To correct these deficiencies, one must evaluate the overlap matrix, which is given by

\[
\langle 0 | (P^\dagger(\gamma_m)P^\dagger(\delta_n))_{\alpha_s}^{-1} (P^\dagger(\alpha_m)P^\dagger(\beta_n))_{\alpha_s} | 0 \rangle. \tag{3.41}
\]

The overlap matrix is calculated by writing all the \(P^\dagger\) operators in terms of their single-particle components, and then making all the possible contractions. This process may spoil the simplicity of the MSM if the overlap matrix is difficult to calculate. However, it happens that the overlap matrix and the dynamical matrix are usually very similar to each other not only in the procedure, but also in the formalism.
The most convenient way to evaluate the overlap matrix is to write it as

\[
\langle 0 | (P^T(\gamma_m)P^T(\delta_n))^{\dagger}_{\alpha_3} (P^T(\alpha_m)P^T(\beta_n))_{\alpha_3} | 0 \rangle = \delta_{\alpha_m \gamma_m} \delta_{\beta_n \delta_n} + \Delta(\gamma_m \delta_n, \alpha_m \beta_n; \alpha_s) + \Omega(\gamma_m \delta_n, \alpha_m \beta_n; \alpha_s), \tag{3.42}
\]

with

\[
\Delta(\gamma_m \delta_n, \alpha_m \beta_n; \alpha_s) = \pm \langle \delta_n | P^T(\alpha_m)P(\gamma_m) | \beta_n \rangle \langle \alpha_m | \beta_n; \alpha_s \rangle \langle \gamma_m | \delta_n; \alpha_s \rangle,
\]

\[
\Omega(\gamma_m \delta_n, \alpha_m \beta_n; \alpha_s) = \langle \delta_n \left[ [P(\gamma_m), P^T(\alpha_m)]_{\downarrow}, P^T(\beta_n) \right] | 0 \rangle \langle \alpha_m | \beta_n; \alpha_s \rangle \langle \gamma_m | \delta_n; \alpha_s \rangle. \tag{3.43}
\]

Note that the minus sign in front of \( \langle \delta_n | P^T(\alpha_m)P(\gamma_m) | \beta_n \rangle \) and the subscript plus sign outside the square bracket of \([P(\gamma_m), P^T(\alpha_m)]_{\downarrow}\) only apply when \( m = n \) is an odd number. One may notice that the \( \Delta \) term has a very simple expression when \( m = n \)

\[
\Delta(\gamma_m \delta_n, \alpha_m \beta_n; \alpha_{2n}) = \pm (-1)^{\alpha_m + \beta_n - \alpha_{2n}} \delta_{\alpha_m \gamma_m} \delta_{\beta_n \delta_n}. \tag{3.44}
\]

Let us take the three-particle system as an example, the overlap matrix can be written as

\[
\langle 0 | (c^\dagger_q P^T(\beta_2))^{\dagger}_{\alpha_3} (c^\dagger_p P^T(\alpha_2))_{\alpha_3} | 0 \rangle = \delta_{pq} \delta_{\alpha_2 \beta_2} + \Omega(q \beta_2, p \alpha_2; \alpha_3) + \Delta(q \beta_2, p \alpha_2; \alpha_3). \tag{3.45}
\]

In this case, since

\[
\langle \beta_2 | [c^\dagger_q, c^\dagger_p]_{\downarrow}, P^T(\alpha_2) \rangle | 0 \rangle = 0, \tag{3.46}
\]

the \( \Omega \) term is quite straightforward to obtain. For the \( \Delta \) term, one has

\[
\Delta(q \beta_2, p \alpha_2; \alpha_3) = - \langle \beta_2 | c^\dagger_p c^\dagger_q | 0 \rangle \langle 0 | c_p c_q | \alpha_2 \rangle \langle \alpha_2 | \beta_2; \alpha_3 \rangle \langle \beta_2 | q \beta_2; \alpha_3 \rangle
\]

\[
= - \sum_r \langle \beta_2 | c^\dagger_p c^\dagger_q | 0 \rangle \langle 0 | c_p c_q | \alpha_2 \rangle \langle \alpha_2 | \beta_2; \alpha_3 \rangle \langle \beta_2 | Y(qr; \beta_2)Y(qr; \alpha_2) \langle qr; \beta_2 | \alpha_3 \rangle \langle q \beta_2; \alpha_3 \rangle \rangle.
\]

\[
\tag{3.47}
\]

Comparing with the Eq. (3.38), one finds

\[
\Delta(q \beta_2, p \alpha_2; \alpha_3) = \sum_r A(p \alpha_2, q \beta_2; \alpha_3). \tag{3.48}
\]

Therefore the overlap equation for three particle has the final form

\[
\langle 0 | (c^\dagger_q P^T(\beta_2))^{\dagger}_{\alpha_3} (c^\dagger_p P^T(\alpha_2))_{\alpha_3} | 0 \rangle = \delta_{pq} \delta_{\alpha_2 \beta_2} + \sum_r A(p \alpha_2, q \beta_2; \alpha_3). \tag{3.49}
\]
3.4 Hermitian matrix

To restore the Pauli principle, one can use the Schmidt procedure to produce a set of orthonormal basis \( \{|u_m\}\) from the overlap matrix, which has the right dimension \( \mathcal{D} \). It means that the overlap matrix is thus transformed into an identity matrix

\[
\langle u_m | u_n \rangle = I_{mn} = \sum_{ij} \xi_m(i)O(i,j)\xi_n(j),
\]

(3.50)

where \( O(i,j) = \langle j|i \rangle \) denotes the overlap matrix (3.41). The vector \( |i\rangle \) is the element in the overcomplete MSM basis which has the dimension \( \mathcal{N} \). The amplitudes \( \xi_m(i) \) of the Schmidt orthonormal vectors are obtained from

\[
|u_m\rangle = \sum_i \xi_m(i)|i\rangle.
\]

(3.51)

Making use of the Schmidt basis one can transform the dynamical matrix into a hermitian matrix \( T \) with the right dimension if all possible basis states are included. The dynamical matrix \( M(i,j) \) in the MSM basis can be written as

\[
W(\alpha)\langle \alpha |i \rangle = \sum_j M(i,j)\langle \alpha |j \rangle.
\]

(3.52)

To transform it into the orthonormal Schmidt basis, one can use Eq. (3.51) and the identity equation to obtain

\[
W(\alpha)\langle \alpha |\sum_i \xi_m(i)|i\rangle = \sum_i \xi_m(i) \sum_j M(i,j)\sum_n |u_m\rangle\langle u_n |j \rangle
\]

\[
W(\alpha)\langle \alpha |u_m \rangle = \sum_n \left\{ \sum_{ij} \xi_m(i)M(i,j)\sum_k \xi_n(k)\langle k |j \rangle \right\} \langle \alpha |u_n \rangle.
\]

(3.53)

The expression in the braces is therefore the hermitian matrix \( T \), which can be written as

\[
T(m,n) = \sum_{ijk} \xi_m(i)M(i,j)O(k,j)\xi_n(k).
\]

(3.54)

Through diagonalizing the \( T \) matrix, one calculates the energy \( W \), the wave function \( X \), the projection \( F \), the cosine \( x \) and all the other information about the system.

In most of the cases, our MSM basis is overcomplete, which means the dimensions of the dynamical and overlap matrix \( \mathcal{N} \) are usually much larger than the dimension of the system \( \mathcal{D} \). However, to generate the hermitian matrix \( T \), it is unnecessary to evaluate the whole \( \mathcal{N} \times \mathcal{N} \) dynamical and overlap matrix. Through the Schmidt procedure, we will be able to select the necessary \( \mathcal{D} \) vectors within the MSM basis, which are enough to reproduce the orthonormal Schmidt basis

\[
|u_m\rangle = \sum_{i=1,\mathcal{D}} \xi_m(i)|i\rangle.
\]

(3.55)
The Equation (3.54) now becomes

\[ T(m,n) = \sum_{i=1}^{D} \sum_{j=1}^{N'} \sum_{k=1}^{D} \xi_m(i)M(i,j)O(k,j)\xi_n(k). \] (3.56)

If the MSM vectors are well arranged, only the first \( D \times N \) matrix elements are required to generate the hermitian matrix \( T \). Using this property one can greatly reduce the calculation time and also the memory space of the program.

In order to obtain the complete hermitian matrix \( T \) we need to have all the possible correlated vectors in the MSM basis. However, in many cases, we need to neglect the high-lying states in the middle steps and only select few important states for the following calculations. An excessive truncation of the basis will cause the matrix \( T \) to loose its hermiticity and lead to inaccurate results. An inspection on how well the hermiticity was preserved in the \( T \) matrix may tell us how far we have gone with the truncation.

3.5 The MSM with proton-neutron pair

One of the great advantage of the MSM method is that we are able to solve the system within a non-orthogonal overcomplete basis. For instance, we can study a two-proton two-neutron system in terms of the \((\pi\pi) \otimes (\nu\nu)\) excitations and \((\pi\nu) \otimes (\pi\nu)\) ones at the same time. In this section, we will present the MSM for \( N = Z \) nuclei, which allow us to study the role of both proton-neutron pairing and normal pairing. A summary of all the dynamical matrices and overlap matrices in two-proton two-neutron, three-proton three-neutron and four-proton four-neutron systems are given in Appendix A.3

In the proton-neutron representation, the hamiltonian can be written as

\[
H = \sum_{p_i} \varepsilon_{p_i} c_{p_i}^\dagger c_{p_i} + \sum_{n_i} \varepsilon_{n_i} c_{n_i}^\dagger c_{n_i} + \sum_{p_i p_j p_k n_l} \langle p_i p_j | V_{pp} | p_k n_l \rangle c_{p_i}^\dagger c_{p_j} c_{n_l} c_{p_k} \\
+ \frac{1}{2} \sum_{p_i p_j p_k n_l} \langle p_i p_j | V_{pp}^* | p_k n_l \rangle c_{p_i}^\dagger c_{p_j} c_{n_l} c_{p_k} \\
+ \frac{1}{2} \sum_{n_i n_j n_k n_l} \langle n_i n_j | V_{nn} | n_k n_l \rangle c_{n_i}^\dagger c_{n_j} c_{n_k} c_{n_l},
\] (3.57)

where \( c_{p_i}^\dagger \) and \( c_{n_i}^\dagger \) denote the single proton and neutron creation operators respectively. We will use the notation \( P^\dagger \) for the many-particle creation operator as before. The creation and annihilation operators of single proton and neutron excitations follow the following commutation relations

\[
[c_{p_i}, c_{p_j}^\dagger]_+ = \delta_{p_i, p_j}, \quad [c_{n_i}, c_{n_j}^\dagger]_+ = \delta_{n_i, n_j}, \\
[c_{p_i}^\dagger, c_{p_j}]_+ = [c_{p_i}, c_{p_j}]_+ = [c_{n_i}^\dagger, c_{n_j}]_+ = [c_{n_i}, c_{n_j}]_+ = 0, \\
[c_{p_i}^\dagger, c_{n_j}]_- = [c_{p_i}, c_{n_j}]_- = [c_{n_i}^\dagger, c_{n_j}]_- = [c_{n_i}, c_{n_j}]_- = 0.
\] (3.58)
3.5. THE MSM WITH PROTON-NEUTRON PAIR

One needs to be especially careful on counting the minus signs when exchanging operators between protons and neutrons, since the commutators and anticommutators are mixed.

As usual, the two-particle interaction matrices in the MSM equations are conveniently replaced by the corresponding correlated two-particle energies and wave functions. The relations can be obtained straightforwardly by calculating the quantity $\Lambda(ij; \alpha_2)$ with the new hamiltonian

$$
(W(\alpha_2) - \varepsilon_p - \varepsilon_n) |\alpha_2p, \alpha_2n\rangle = 1 \sum_{p_i, p_j} \langle p_i p_j | V_{pp} | p_i p_j \alpha_2 n \rangle |\alpha_2p, \alpha_2n\rangle ,
$$

$$
(W(\alpha_2n) - \varepsilon_p - \varepsilon_n) |\alpha_2n, \alpha_2n\rangle = 1 \sum_{n_i, n_j} \langle n_i n_j | V_{nn} | n_i n_j \alpha_2 n \rangle |\alpha_2n, \alpha_2n\rangle,
$$

$$
(W(\alpha_2) - \varepsilon_p - \varepsilon_n) |\alpha_2p, \alpha_2n\rangle = 1 \sum_{p_i, n_j} \langle p_i n_j | V_{pn} | p_i n_j \alpha_2 n \rangle |\alpha_2p, \alpha_2n\rangle.
$$

(3.59)

Here we use $\alpha_s$ to label the $s/2$-proton $s/2$-neutron states. In which case the system has the same proton and neutron numbers, and $s$ should be an even number. The label $p$ or $n$ in the subscript of $\alpha_{sp}$ and $\alpha_{sn}$ denotes a $s$-proton or $s$-neutron state respectively.

Since we are considering both normal pairing and proton-neutron pairing, the corresponding equation contains three terms. After adding the angular momentum coupling coefficients, one gets the standard two-particle shell model equation

$$
(W(\alpha_2) - \varepsilon_p - \varepsilon_n) X(n_i, n_j; \alpha_2) = 1 \sum_{n_i, n_j} \langle n_i n_j | V_{nn} | n_i n_j \alpha_2 n \rangle |\alpha_2n, \alpha_2n\rangle X(n_i, n_j; \alpha_2),
$$

$$
(W(\alpha_2) - \varepsilon_p - \varepsilon_n) X(p_i, n_j; \alpha_2) = 1 \sum_{p_i, n_j} \langle p_i n_j | V_{pn} | p_i n_j \alpha_2 n \rangle |\alpha_2p, \alpha_2n\rangle X(p_i, n_j; \alpha_2),
$$

(3.60)

through which we can calculate the energies and wave functions of all the two-particle states.

**Two-proton two-neutron system**

In the proton-neutron representation, we can expand the two-proton two-neutron state $|\alpha_4\rangle = P^\dagger(\alpha_4)|0\rangle$ in an overcomplete basis as

$$
P^\dagger(\alpha_4)|0\rangle = \sum_{\alpha_2, \beta_2} X(\alpha_2, \beta_2; \alpha_4) \langle P^\dagger(\alpha_2) P^\dagger(\beta_2) \rangle_{\alpha_4} |0\rangle
$$

$$
+ \sum_{\alpha_2, \alpha_2} X(\alpha_2, \alpha_2; \alpha_4) \langle P^\dagger(\alpha_2) P^\dagger(\beta_2) \rangle_{\alpha_4} |0\rangle.
$$

(3.61)
In this case, the basis vectors \((P^l(\alpha_{2p})P^l(\beta_{2n}))\alpha_4 \rangle_0\) and \((P^l(\alpha_{2p})P^l(\beta_{2n}))\alpha_4 \rangle_0\) describe the same shell model space, and therefore the MSM basis is overcomplete. The orthonormality condition now reads

\[
\delta_{\alpha_4'\alpha_4} = \sum_{\alpha_{2p}\beta_{2n}} X(\alpha_{2p}\beta_{2n}; \alpha_4) F(\alpha_{2p}\beta_{2n}; \alpha_4') + \sum_{\alpha_{2p}\beta_{2n}} X(\alpha_{2p}\beta_{2n}; \alpha_4') F(\alpha_{2p}\beta_{2n}; \alpha_4),
\]

where the wave function amplitudes \(X\) are not well defined, while the projections \(F\) are the physically meaningful quantities, which are denoted as

\[
F(\alpha_{2p}\beta_{2n}; \alpha_4) = \langle \alpha_4 | (P^l(\alpha_{2p})P^l(\beta_{2n})) \rangle_0, \\
F(\alpha_{2p}\beta_{2n}; \alpha_4') = \langle \alpha_4' | (P^l(\alpha_{2p})P^l(\beta_{2n})) \rangle_0. 
\]

The dynamical equation of the system contains two parts, which can be derived by calculating the quantities \(\Lambda(\alpha_{2p}\beta_{2n}; \alpha_4)\) and \(\Lambda(\alpha_{2p}\beta_{2n}; \alpha_4')\) respectively

\[
\Lambda(\alpha_{2p}\beta_{2n}; \alpha_4) = (W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | P^l(\alpha_{2p})P^l(\beta_{2n}) \rangle_0 \\
= \langle \alpha_4 | [V, P^l(\alpha_{2p})P^l(\beta_{2n})] \rangle_0, \\
\Lambda(\alpha_{2p}\beta_{2n}; \alpha_4') = (W(\alpha_4) - W(\alpha_{2p}) - W(\beta_{2n})) \langle \alpha_4' | P^l(\alpha_{2p})P^l(\beta_{2n}) \rangle_0 \\
= \langle \alpha_4' | [V, P^l(\alpha_{2p})P^l(\beta_{2n})] \rangle_0. 
\]

After expanding the commutation operators one can rewrite the formula in the form of single-particle operators

\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | P^l(\alpha_{2p})P^l(\beta_{2n}) \rangle_0 \\
= \sum_{p_1p_2n_1n_2} X(p_1n_1; \alpha_2)(p_1n_1; \alpha_2) X(p_2n_2; \beta_2)(p_2n_2; \beta_2) \\
\times \left\{ - \sum_{p, n_j} \langle p, n_j | V_{pn} | p_1n_2 \rangle \langle \alpha_4 | c_{p_1}^\dagger c_{n_1}^\dagger c_{p_2}^\dagger c_{n_2}^\dagger \rangle_0 \\
- \sum_{p, n_j} \langle p, n_j | V_{pn} | p_1n_2 \rangle \langle \alpha_4 | c_{p_1}^\dagger c_{n_1}^\dagger c_{p_2}^\dagger c_{n_2}^\dagger \rangle_0 \\
+ \frac{1}{2} \sum_{p, p_j} \langle p, p_j | V_{pp} | p_1p_2 \rangle \langle \alpha_4 | c_{p_1}^\dagger c_{p_2}^\dagger c_{n_1}^\dagger c_{n_2}^\dagger \rangle_0 \\
+ \frac{1}{2} \sum_{n_1n_2} \langle n_1n_2 | V_{nn} | n_1n_2 \rangle \langle \alpha_4 | c_{n_1}^\dagger c_{n_2}^\dagger c_{p_1}^\dagger c_{p_2}^\dagger \rangle_0 \right\}. 
\]
3.5. THE MSM WITH PROTON-NEUTRON PAIR

\[
(W(\alpha_4) - W(\alpha_{2p}) - W(\beta_{2n}))\langle \alpha_4|P^I(\alpha_{2p})P^I(\beta_{2n})|0\rangle = \sum_{p_1p_2n_1n_2} Y(p_1p_2; \alpha_{2p}) Y(n_1n_2; \beta_{2n}) \langle n_1n_2; \beta_{2n}|p_1p_2; \alpha_{2p}\rangle \times \sum_{p_i, n_j} \langle p_i n_j|V_{pn}|p_1 n_1\rangle \langle \alpha_4|c_{p_1}^+ c_{n_1}^+ c_{p_2}^+ c_{n_2}^+|0\rangle, \tag{3.66}
\]

These two formulas can be very useful during further derivations. Just as we used two-particle energies and wave functions to replace the two-body interaction matrices before, we can also use the energies and wave functions of four-particle system to replace (part of) the interaction matrices in further steps. This can not only immensely simplify the equations and derivation, but also greatly reduce the calculating works of the computing code. Since many coupling constants and coefficients are already calculated and absorbed in the energies and wave functions, one should use these resources and make the calculation easier.

By introducing the identity matrix such as \(\sum_\gamma |\gamma_2\rangle\langle \gamma_2|\), one can convert the single-particle operators into the MSM basis. However, it is a bit tricky when dealing with the \(V_{pn}\) terms. In order to avoid double counting, we have \(\alpha_2 \leq \beta_2\) for each basis vector \(|\alpha_2\beta_2\alpha_4\rangle\). In this case, we should split the formula into two halves. For instance, we can rewrite the \(V_{pn}\) terms in Eq. (3.65) into

\[
\sum_{p_i, n_j} \left\{ \langle p_i n_j|V_{pn}|p_1 n_1\rangle \langle \alpha_4|c_{p_1}^+ c_{n_1}^+ c_{p_2}^+ c_{n_2}^+|0\rangle + \langle p_i n_j|V_{pn}|p_2 n_2\rangle \langle \alpha_4|c_{p_2}^+ c_{n_2}^+ c_{p_1}^+ c_{n_1}^+|0\rangle \right\}
\]

\[
= \frac{1}{2} \sum_{p_i, n_j} \sum_{\gamma_2} \left\{ \langle p_i n_j|V_{pn}|p_1 n_1\rangle \langle \alpha_4|c_{p_2}^+ c_{n_1}^+|\gamma_2\rangle \langle \gamma_2|c_{p_1}^+ c_{n_2}^+|0\rangle + \langle p_i n_j|V_{pn}|p_2 n_2\rangle \langle \alpha_4|c_{p_1}^+ c_{n_2}^+|\gamma_2\rangle \langle \gamma_2|c_{p_2}^+ c_{n_1}^+|0\rangle \right\} + \frac{1}{2} \sum_{p_i, n_j} \sum_{\delta_2} \left\{ \langle p_i n_j|V_{pn}|p_1 n_1\rangle \langle \alpha_4|c_{p_2}^+ c_{n_1}^+|\delta_2\rangle \langle \delta_2|c_{p_1}^+ c_{n_2}^+|0\rangle + \langle p_i n_j|V_{pn}|p_2 n_2\rangle \langle \alpha_4|c_{p_1}^+ c_{n_2}^+|\delta_2\rangle \langle \delta_2|c_{p_2}^+ c_{n_1}^+|0\rangle \right\}, \tag{3.67}
\]

and replace the two-body interaction matrices by using Eq. (3.59)

\[
\sum_{p_i, n_j} \left\{ \langle p_i n_j|V_{pn}|p_1 n_1\rangle \langle \alpha_4|c_{p_1}^+ c_{n_1}^+ c_{p_2}^+ c_{n_2}^+|0\rangle + \langle p_i n_j|V_{pn}|p_2 n_2\rangle \langle \alpha_4|c_{p_2}^+ c_{n_2}^+ c_{p_1}^+ c_{n_1}^+|0\rangle \right\}
\]

\[
= \frac{1}{2} \sum_{\gamma_2\delta_2} (W(\gamma_2) + W(\delta_2) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{n_1} - \varepsilon_{n_2}) \langle \alpha_4|P^I(\gamma_2)P^I(\delta_2)|0\rangle \times \left\{ \langle \gamma_2|c_{p_1}^+ c_{n_1}^+|0\rangle \langle \delta_2|c_{p_2}^+ c_{n_2}^+|0\rangle + \langle \gamma_2|c_{p_2}^+ c_{n_2}^+|0\rangle \langle \delta_2|c_{p_1}^+ c_{n_1}^+|0\rangle \right\}. \tag{3.68}
\]

From here we can correct the order in the basis by using

\[
\frac{1}{2} \sum_{\gamma_2\delta_2} = \sum_{\gamma_2 \leq \delta_2} \frac{1}{1 + \delta_2 \gamma_2}. \tag{3.69}
\]
The other parts of the equation can be calculated in a similar way. After tidying up all the coefficients and including the proper phase factors, the dynamical matrix for the two-proton two-neutron system can be obtained as

\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle
\]

\[
= \sum_{\gamma_2 \leq \delta_2} \left\{ \sum_{p_1p_2n_1n_2} (-1)^{\gamma_2} \frac{(W(\gamma_2) + W(\delta_2) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{n_1} - \varepsilon_{n_2})}{1 + \delta_{\gamma_2\delta_2}} \times (A_1 + A_2) \right\} \langle \alpha_4 | (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} | 0 \rangle
\]

\[
+ \sum_{\gamma_2 \leq \delta_2} \left\{ \sum_{p_1p_2n_1n_2} (W(\gamma_{2p}) + W(\delta_{2n}) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{n_1} - \varepsilon_{n_2}) \times B_1 \right\} \langle \alpha_4 | (P^\dagger(\gamma_{2p})P^\dagger(\delta_{2n}))_{\alpha_4} | 0 \rangle,
\]

where

\[
A_1 = (-1)^{2p_1 + n_1 + n_2 + p_2 + \delta_2} \begin{pmatrix} p_1 & n_1 & \alpha_2 \\ n_2 & p_2 & \beta_2 \\ \gamma_2 & \delta_2 & \alpha_4 \end{pmatrix} \times X(p_1n_1; \alpha_2)X(p_2n_2; \beta_2)X(p_1n_2; \gamma_2)X(p_2n_1; \delta_2),
\]

\[
A_2 = (-1)^{2p_1 + n_1 + n_2 + p_2 + \delta_2 + \alpha_4} \begin{pmatrix} p_1 & n_1 & \alpha_2 \\ n_2 & p_2 & \beta_2 \\ \delta_2 & \gamma_2 & \alpha_4 \end{pmatrix} \times X(p_1n_1; \alpha_2)X(p_2n_2; \beta_2)X(p_1n_2; \gamma_2)X(p_2n_1; \delta_2),
\]

\[
B_1 = \begin{pmatrix} p_1 & n_1 & \alpha_2 \\ p_2 & n_2 & \beta_2 \\ \gamma_{2p} & \delta_{2n} & \alpha_4 \end{pmatrix} \times X(p_1n_1; \alpha_2)X(p_2n_2; \beta_2)Y(p_1p_2; \gamma_{2p})Y(n_1n_2; \delta_{2n}),
\]
3.5. THE MSM WITH PROTON-NEUTRON PAIR

The only term remaining is

\[ \mathbb{B}_2 = \delta_2 \beta_2 \gamma_2 \delta_2 \left\{ \begin{array}{c} p_1 \ p_2 \ \alpha_{2p} \\ n_1 \ n_2 \ \beta_{2n} \\ \gamma_1 \ \delta_2 \ \alpha_4 \end{array} \right\} \times Y(p_1p_2; \alpha_{2p})Y(n_1n_2; \beta_{2n})X(p_1n_1; \gamma_2)X(p_2n_2; \delta_2). \]

The overlap matrix of the two-proton two-neutron system can be written in terms of three parts, by

\[
\begin{align*}
\langle 0| & (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} |0 \rangle, \\
\langle 0| & (P^\dagger(\gamma_2)P^\dagger(\beta_{2n}))_{\alpha_4} (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} |0 \rangle, \\
\langle 0| & (P^\dagger(\gamma_2)P^\dagger(\delta_{2n}))_{\alpha_4} (P^\dagger(\alpha_{2p})P^\dagger(\beta_2))_{\alpha_4} |0 \rangle.
\end{align*}
\] (3.71)

Let us take the first matrix as example. As we have discussed in Section 3.3, it is more convenient to rewrite the overlap in three terms

\[
\langle 0| (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} |0 \rangle = \delta_{\alpha_2\gamma_2} \delta_{\beta_2\delta_2} + \Delta(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4) + \Omega(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4),
\] (3.72)

in which, according to Eq. (3.44), one has

\[
\Delta(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4) = (-1)^{\alpha_2+\beta_2-\alpha_4} \delta_{\alpha_2 \gamma_2} \delta_{\beta_2 \delta_2}.
\] (3.73)

The only term remaining is

\[
\Omega(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4) = \Delta(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4). \]
(3.74)

One can uncouple the two-particle operators and expand the commutation operator

\[
\begin{align*}
\Omega(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4) &= - \sum_{p_1p_2n_1n_2} X(p_1n_1; \alpha_2)X(p_2n_2; \beta_2) \\
& \quad \times \left\{ X(p_1n_2; \gamma_2)\langle p_1n_2; \gamma_2 \rangle X(p_2n_1; \delta_2)\langle p_2n_1; \delta_2 \rangle \right. \\
& \quad + X(p_2n_1; \gamma_2)\langle p_2n_1; \gamma_2 \rangle X(p_1n_2; \delta_2)\langle p_1n_2; \delta_2 \rangle \} \\
& \quad \times (p_1n_1; \alpha_2)\langle p_2n_2; \beta_2 \rangle (\alpha_2 \beta_2; \alpha_4)\langle \gamma_2 \delta_2; \alpha_4 \rangle.
\end{align*}
\] (3.75)

After recouping the coefficients, one gets

\[
\Omega(\gamma_2 \delta_2, \alpha_2 \beta_2; \alpha_4) = - \sum_{p_1p_2n_1n_2} (A_1 + A_2).
\] (3.76)
The other two parts of the overlap matrix can be derived similarly. Another major term in the overlap matrix is

\[
\Omega(\gamma_2\delta_2, \alpha_2\beta_2; \alpha_4) = \langle \delta_2n | [P(\gamma_2), P^\dagger(\alpha_2)] | P^\dagger(\beta_2) | 0 \rangle \langle \alpha_2\beta_2; \alpha_4 | \gamma_2\delta_2n; \alpha_4 \rangle
\]

\[
= \sum_{p_1p_2n_1n_2} X(p_1n_1; \alpha_2) X(p_2n_2; \beta_2) Y(p_1p_2; \gamma_2p) Y(n_1n_2; \delta_2n) \\
\times \langle \delta_2n | P(\gamma_2) | \gamma_2p \rangle \langle \alpha_2 \beta_2; \alpha_4 | \gamma_2p \delta_2n; \alpha_4 \rangle
\]

\[
= \sum_{p_1p_2n_1n_2} B_1. \tag{3.77}
\]

The rest of terms are trivial, such like

\[
\Delta(\gamma_2\delta_2, \alpha_2\beta_2; \alpha_4) = \langle \delta_2n | P^\dagger(\alpha_2) P(\gamma_2p) | \beta_2 \rangle = 0, \tag{3.78}
\]

and

\[
\Omega(\gamma_2\delta_2, \alpha_2\beta_2; \alpha_4) = \langle \delta_2n | [P(\gamma_2), P^\dagger(\alpha_2)], P^\dagger(\beta_2n) | 0 \rangle = 0. \tag{3.79}
\]

Thus the complete overlap matrix of the two-neutron two-proton system is given as follows

\[
\langle 0 | (P^\dagger(\gamma_2) P^\dagger(\delta_2))_{\alpha_4} (P^\dagger(\alpha_2) P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle = \delta_{\alpha_2\gamma_2} \delta_{\beta_2\gamma_2} + (-1)^{\alpha_2+\beta_2+\alpha_4} \delta_{\alpha_2\delta_2} \delta_{\beta_2\gamma_2} - \sum_{p_1p_2n_1n_2} (\mathbb{A}_1 + \mathbb{A}_2),
\]

\[
\langle 0 | (P^\dagger(\gamma_2) P^\dagger(\delta_2n))_{\alpha_4} (P^\dagger(\alpha_2) P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle = \sum_{p_1p_2n_1n_2} B_1,
\]

\[
\langle 0 | (P^\dagger(\gamma_2p) P^\dagger(\delta_2n))_{\alpha_4} (P^\dagger(\alpha_2p) P^\dagger(\beta_2n))_{\alpha_4} | 0 \rangle = \delta_{\alpha_2\gamma_2p} \delta_{\beta_2n}. \tag{3.80}
\]

**Three-proton three-neutron system**

Starting with the quantity \( A(\alpha_2 \alpha_4; \alpha_6) \) in the three-proton three-neutron system, we will have

\[
(W(\alpha_6) - W(\alpha_2) - W(\alpha_4)) \langle \alpha_6 | P^\dagger(\alpha_2) P^\dagger(\alpha_4) | 0 \rangle = \langle \alpha_6 | [V, P^\dagger(\alpha_2)], P^\dagger(\alpha_4) | 0 \rangle, \tag{3.81}
\]

in which the two-proton two-neutron creation operator \( P^\dagger(\alpha_4) \) should be uncoupled under the full overcomplete basis

\[
P^\dagger(\alpha_4) = \frac{1}{2} \sum_{A_2B_2} Y(A_2B_2; \alpha_4) \langle P^\dagger(A_2) P^\dagger(B_2) \rangle_{\alpha_4} + \sum_{A_2B_2n_2} X(A_2pB_2n; \alpha_4) \langle P^\dagger(A_2p) P^\dagger(B_2n) \rangle_{\alpha_4}. \tag{3.82}
\]
3.5. THE MSM WITH PROTON-NEUTRON PAIR

The quantity $\Lambda(\alpha_2 \alpha_4; \alpha_6)$ can be written as the sum of two terms, which consist of $(\pi \nu) \otimes (\pi \nu) \otimes (\pi \nu)$ term and $(\pi \nu) \otimes (\pi \pi) \otimes (\nu \nu)$ term. Let us take the first term as an example. By uncoupling the creation operators and expanding the commutation operators, the term can be written in the form of single particle operators as

$$
\sum_{A_2 B_2} Y(A_2 B_2; \alpha_4) \langle A_2 B_2; \alpha_4 \rangle \sum_{\beta_4} \langle \alpha_6 | P^\dagger (B_2) P^\dagger (\beta_4) | 0 \rangle \\
\times \sum_{p_1 n_1 p_2 n_2} X(p_1 n_1; \alpha_2) (p_1 n_1; \alpha_2) X(p_2 n_2; A_2) (p_2 n_2; A_2) \\
\times \left\{ - \sum_{p_1 n_j} (p_1 n_j | V_{p n} | p_1 n_2) \langle \beta_4 | c_{p_1}^\dagger c_{n_j}^\dagger c_{p_2}^\dagger c_{n_1}^\dagger | 0 \rangle \\
- \sum_{p_1 n_j} (p_1 n_j | V_{p n} | p_2 n_1) \langle \beta_4 | c_{p_1}^\dagger c_{n_j}^\dagger c_{p_2}^\dagger c_{n_2}^\dagger | 0 \rangle \\
+ \frac{1}{2} \sum_{p_1 p_j} (p_1 p_j | V_{p p} | p_1 p_2) \langle \beta_4 | c_{p_1}^\dagger c_{p_j}^\dagger c_{p_2}^\dagger c_{n_2}^\dagger | 0 \rangle \\
+ \frac{1}{2} \sum_{n_1 n_j} (n_1 n_j | V_{n n} | n_1 n_2) \langle \beta_4 | c_{n_1}^\dagger c_{n_j}^\dagger c_{n_2}^\dagger c_{n_1}^\dagger | 0 \rangle \right\}. 
$$

(3.83)

Comparing with Eq. (3.65), one can simplify these terms by replacing all the interaction matrices with the two-particle and four-particle energies and projections. The first term now simply becomes

$$
\sum_{A_2 B_2} Y(A_2 B_2; \alpha_4) \langle A_2 B_2; \alpha_4 \rangle \sum_{\beta_4} \langle \alpha_6 | P^\dagger (B_2) P^\dagger (\beta_4) | 0 \rangle \\
\times (W(\beta_4) - W(\alpha_2) - W(A_2)) \langle \beta_4 | P^\dagger (\alpha_2) P^\dagger (A_2) | 0 \rangle. 
$$

(3.84)

Through the same procedure in the other term, and omitting numerous calculations of the coefficients and phases, finally we get the full dynamic matrix in the three-proton-three-neutron system

$$
(W(\alpha_6) - W(\alpha_2) - W(\alpha_4)) \langle \alpha_6 | (P^\dagger (\alpha_2) P^\dagger (\alpha_4)) | \alpha_6 \rangle \\
= \sum_{\beta_2 \beta_4} \langle \alpha_6 | (P^\dagger (\beta_2) P^\dagger (\beta_4)) | \alpha_6 \rangle \left\{ A_2 (W(\beta_4) - W(\alpha_2) - W(A_2)) \times \Lambda \\
+ \sum_{p_1 p_2 p_3 n_1 A_2 B_2 c_{2p}} (W(\beta_2) + W(C_{2p}) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{p_3} - \varepsilon_{n_1}) \times \mathbb{B}_1 \\
+ \sum_{p_1 n_1 n_2 n_3 A_2 B_2 d_{2n}} (W(\beta_2) + W(D_{2n}) - \varepsilon_{p_1} - \varepsilon_{n_1} - \varepsilon_{n_2} - \varepsilon_{n_3}) \times \mathbb{B}_2 \right\}. 
$$

(3.85)
CHAPTER 3. MULTISTEP SHELL MODEL METHOD

with

\[ A = \hat{\alpha}_4 \hat{\beta}_4 \left\{ \frac{\alpha_2}{\beta_2} \frac{A_2}{\alpha_6} \frac{\beta_4}{\alpha_4} \right\} Y(A_2 \beta_2; \alpha_4) F(A_2 \alpha_2; \beta_4), \]

\[ B_1 = \sum_{X_4} (-1)^{p_1+n_1+\alpha_2+\beta_2+A_2p+x_4} \hat{\alpha}_2 \hat{\beta}_2 \hat{A}_2 \hat{B}_2 \hat{C}_2 \hat{D}_2 \hat{X}_4 \]

\[ \times \left\{ \frac{p_1}{n_1} \frac{n_1}{\alpha_2} \frac{A_2p}{B_2n} \frac{X_4}{\alpha_4} \right\} \left\{ \frac{\beta_2}{B_2n} \frac{C_2p}{\alpha_6} \frac{X_4}{\beta_4} \right\} \]

\[ \times X(p_1 n_1; \alpha_2) X(p_1 n_2; \beta_2) Y(p_2 n_3; A_2p) Y(n_1 n_2; C_2p) \]

\[ \times X(A_2p B_2n; \alpha_4) F(C_2p B_2n; \beta_4), \]

\[ B_2 = \sum_{X_4} (-1)^{n_2+n_3+\alpha_2+\beta_2+B_2n+\alpha_4+\beta_4} \hat{\alpha}_2 \hat{\beta}_2 \hat{B}_2n \hat{D}_2n \hat{X}_4 \]

\[ \times \left\{ \frac{p_1}{n_3} \frac{n_2}{B_2n} \frac{X_4}{A_2p} \frac{X_4}{\alpha_4} \right\} \left\{ \frac{\beta_2}{B_2n} \frac{D_2n}{\alpha_6} \frac{X_4}{\beta_4} \right\} \]

\[ \times X(p_1 n_1; \alpha_2) X(p_1 n_3; \beta_2) Y(n_2 n_3; B_2n) Y(n_1 n_2; D_2n) \]

\[ \times X(A_2p B_2n; \alpha_4) F(A_2p D_2n; \beta_4). \]

Note that here \( X_4 \) is just an integer number which runs through all the possible angular momentum in the 9j-coefficients. Since \( X_4 \) is not a real physical state, it could be possible to reach a higher value than the maximum allowed angular momenta of a physical state.

The overlap matrix of the three-proton three-neutron system can be written as

\[ (0) (P^\dagger(\beta_2) P^\dagger(\beta_4))_{\alpha_6} (P^\dagger(\alpha_2) P^\dagger(\alpha_4))_{\alpha_6} |0\rangle = \delta_{\alpha_2 \beta_2} \delta_{\alpha_4 \beta_4} + \sum_{A_2} \mathcal{A}' \]

\[ + \sum_{p_1 p_2 p_1 n_1} \sum_{A_2p B_2n C_2p} \mathcal{B}_1 + \sum_{p_1 n_1 n_2 n_3} \sum_{A_2p B_2n D_2n} \mathcal{B}_2 + \sum_{A_2 B_2 C_2} \mathcal{C}, \quad (3.86) \]

where

\[ \mathcal{A}' = \hat{\alpha}_4 \hat{\beta}_4 \left\{ \frac{\alpha_2}{\beta_2} \frac{A_2}{\alpha_6} \frac{\beta_4}{\alpha_4} \right\} F(A_2 \beta_2; \alpha_4) F(A_2 \alpha_4; \beta_4), \]

\[ \mathcal{C} = \sum_{X_4} \hat{\alpha}_4 \hat{\beta}_4 X_4 \left\{ \frac{\alpha_2}{B_2} \frac{A_2}{\alpha_6} \frac{X_4}{\alpha_4} \right\} \left\{ \frac{\beta_2}{B_2} \frac{C_2}{\alpha_6} \frac{X_4}{\beta_4} \right\} \]

\[ \times Y(A_2 B_2; \alpha_4) F(C_2 B_2; \beta_4) \Omega(A_2 \alpha_2, C_2 \beta_2; X_4). \]
3.6. THE MSM WITH ISOSPIN SYMMETRY

By orthonormalizing the basis vectors and solving the $T$ matrix, one can obtain the projections of the basis vectors upon the physical six-particle state $F(\alpha_2\alpha_4;\alpha_6)$, and the cosine of the angle between them $x(\alpha_2\alpha_4;\alpha_6)$. In addition to these two physical quantities, we can also construct the MSM basis elements as the direct tensorial product of three pairs. This is a unique feature of the MSM method. The projection of such MSM basis upon the physical vector is

$$F(\alpha_2\beta_2\gamma_2;\alpha_6) = \langle \alpha_6|\left( P^\dagger(\alpha_2)P^\dagger(\beta_2)P^\dagger(\gamma_2)\right)_{\alpha_6}|0\rangle$$

$$= \sum_{\alpha_4} F(\alpha_2\alpha_4;\alpha_6)F(\beta_2\gamma_2;\alpha_4). \quad (3.87)$$

The norm of three-pair basis vector can be calculated from

$$N^2(\alpha_2\beta_2\gamma_2;\alpha_6) = \langle 0|\left( P^\dagger(\alpha_2)P^\dagger(\beta_2)P^\dagger(\gamma_2)\right)_{\alpha_6}\right)^\dagger \left( P^\dagger(\alpha_2)P^\dagger(\beta_2)P^\dagger(\gamma_2)\right)_{\alpha_6}|0\rangle$$

$$= \sum_{\alpha_4,\beta_4} F(\beta_2\gamma_2;\alpha_2)\langle \alpha_2\alpha_4;\alpha_6|\alpha_2\beta_4;\alpha_6\rangle F(\beta_2\gamma_2;\beta_4), \quad (3.88)$$

where $\langle \alpha_2\alpha_4;\alpha_6|\alpha_2\beta_4;\alpha_6\rangle$ is the corresponding overlap element. The cosine of the angle between a three-pair basis vector and the physical state is

$$x(\alpha_2\beta_2\gamma_2;\alpha_6) = F(\alpha_2\beta_2\gamma_2;\alpha_6)/N(\alpha_2\beta_2\gamma_2;\alpha_6). \quad (3.89)$$

In the former two-proton two-neutron calculation, our MSM basis contains two sets of complete vectors. When we use the Schmidt procedure to build the orthonormal basis $|u_m\rangle$, it is enough to use only one of the complete sets. For instance, we may use only $\{ |\alpha_2p^2\beta_2n^2;\alpha_4\rangle \}$ to produce the orthonormal basis. In this case all the wave function amplitude on the other set of vectors $X(\alpha_2\beta_2;\alpha_4) = 0$. Yet we are still able to produce all the correct projections $F$ and $x$ on both sets of vectors.

This property is very useful in the subsequent calculations. In the three-proton three-neutron system, if we have $X(\alpha_2\beta_2;\alpha_4) = 0$, we can simply neglect the $A$ and $\mathbb{C}$ terms in the MSM and overlap matrices, which will significantly reduce the computing work. Anyway it is still worthwhile to have the full dynamical and overlap matrix, even though we may only use part of the equations in the real calculations.

3.6 The MSM with isospin symmetry

In nuclear physics, the isospin symmetry is reflected in the identical behavior between the proton and the neutron, except their charge difference. It is significant for the study of nuclei near the $N = Z$ line [32].

By considering the isospin symmetry, the MSM can be more efficient for the calculation of nuclei near the $N = Z$ line. The procedure of evaluating the MSM equations with isospin symmetry are the same as before. The only difference is that we have to evaluate two sets of angular momentum coupling coefficients which
correspond to angular momentum as well as isospin. For instance, the uncoupling of two group of particles becomes

$$|\alpha_m \alpha_n; \alpha_s\rangle = \langle J_{\alpha_m} J_{\alpha_n}; T_{\alpha_m} T_{\alpha_n}; T_{\alpha_s}\rangle P^\dagger(\alpha_m) P^\dagger(\alpha_n)|0\rangle,$$

(3.90)

where $J_{\alpha_m}$ denotes the angular momentum of the state $\alpha_m$, and $T_{\alpha_m}$ its corresponding isospin. Consequently the phase of exchanging $\alpha_m$ and $\beta_m$ in $Y(\alpha_m \beta_m; \alpha_2 m)$ becomes

$$Y(\beta_m \alpha_m; \alpha_2 m) = (-1)^{m_j + J_{\alpha_m} + J_{\beta_m} + J_{\alpha_2 m} + T_{\alpha_m} + T_{\beta_m} + T_{\alpha_2 m}} Y(\alpha_m \beta_m; \alpha_2 m).$$

(3.91)

We will not present these repetitive derivations here for simplicity. The final formula of the dynamical matrix and overlap matrix with isospin symmetry for the four-particle, six-particle and eight-particle systems are given in Appendix A.4.
Chapter 4

Multistep shell model method in the complex energy plane

The complex shell model method (CXSM) has been shown to be successful to treat systems in the continuum. However, as with the standard shell model, the dimension of the shell model matrix becomes too large when the number of active particles is big. This problem becomes even worse as we include scattering states in the basis [33]. Inspired from this similarity, we attempt to combine the multistep shell model method (MSM) with the CXSM. The idea is to reduce the dimension of the matrices by selecting the necessary states in each step, and make the calculation tractable.

In this chapter we will apply the Multistep shell model method in the complex energy plane (CXMSM) to study the Li isotopes. First we will show that the MSM method can be extended to the complex energy plane (Section 4.1). Then we will apply the CXMSM on Li isotopes by considering $^9$Li as a core. We will define the Berggren single-particle representation by taking the energy levels of $^{10}$Li (Section 4.2). In Section 4.3 we will evaluate the two-particle states of $^{11}$Li by using a separable interaction fitted to experimental levels. With both the one-particle and two-particle basis thus calculated we will apply the MSM to calculate the three-particle nucleus $^{12}$Li and four-particle case $^{13}$Li in Section 4.4 and Section 4.5 respectively.

4.1 Extension to the complex energy plane

As mentioned in Chapter 3, the MSM method was originally applied to the real energy axis. To combine with the CXSM, we have to extend the formulism to the complex energy plane. Therefore before applying the CXMSM in the continuum, we must first show that this extension of the MSM method is correct and reliable.

In Section 3.4, we have discussed that the hermitsicity of the $T$ matrix can be used for examining if the MSM method was appropriately used. Within the
Berggren metric, “Hermiticity” becomes “symmetric matrix”. That is, now the matrix $T$ has to be symmetric. In this section we will also examine the symmetry of the $T$ matrix in the Berggren space when the MSM is applied in the complex energy plane.

We took a very simple three-particle case as a test. The single-particle basis is constructed only by two levels, namely a bound state $1/2^+$ at $-0.500$ MeV and a resonance $5/2^+$ at the energy of $1.000$ MeV with a width of $108$ keV. To simplify the problem, no scattering state was included in the basis. The following two-particle states are all calculated with a fixed separable interaction strength $G$ in the basis. As a result we obtained five states in total, which consist of two $0^+$ states, two $2^+$ states and one $4^+$ state. The corresponding energies are given in Table 4.1.

Table 4.1: The two-particle states (in MeV) corresponding to a fixed separable interaction strength. The single-particle basis contain a bound state $1/2^+$ at $-0.500$ MeV and a resonance $5/2^+$ at $(1.000, -0.054)$ MeV.

|       | $0^+_1$ | $0^+_2$ | $2^+_1$ | $2^+_2$ | $4^+_1$ |
|-------|---------|---------|---------|---------|---------|
| Energy | (-1.092,0.000) | (1.881,-0.089) | (0.110,-0.020) | (1.889,-0.092) | (1.895,-0.091) |

The three-particle system was calculated by using the CXMSM. Since the incompleteness of the basis elements may also affect the hermiticity, we included all the five two-particle states into the MSM basis. As a result, nine states are obtained from the three-particle calculation. There are one $1/2^+$ state, two $3/2^+$ states, three $5/2^+$ states, one $7/2^+$ state and two $9/2^+$ states, as expected. The $T$ matrix for the $5/2^+$ states is given as

$$T_{5/2} = \begin{pmatrix}
(2.644, -0.105) & (0.085, -0.007) & (-0.145, 0.018) \\
(0.085, -0.007) & (-0.389, -0.031) & (-0.206, 0.025) \\
(-0.145, 0.018) & (-0.206, 0.025) & (1.180, -0.072)
\end{pmatrix}. \quad (4.1)$$

One can see that the $T$ matrix for the $5/2^+$ states is instead a complex symmetric matrix. We checked that the remaining $T$ matrices are also symmetric.

Confirming the symmetry of the $T$ matrix in this test, we can conclude that the CXMSM is indeed applicable on the complex energy plane. Although in the following calculations we will also need to reduce the basis dimension by cutting off the unnecessary intermediate states, which will consequently lead to the incompleteness of the basis elements, the reliability of the results can always be checked by the symmetry of the $T$ matrix when needed.

4.2 Berggren single-particle representation

In our case we will take the nucleus $^9$Li as the core. This is because the three protons included in $^9$Li are deeply bound and hardly excited, therefore can be considered...
frozen [34]. The single-particle states referring to $^9$Li can be obtained by a Woods-Saxon potential with different depths for even and odd orbital angular momenta $l$. As in Ref. [35], the corresponding parameters are given by $a = 0.67$ fm, $r_0 = 1.27$ fm, $V_0 = 50(36.9)$ MeV and $V_{so} = 16.5(12.624)$ MeV for even (odd) $l$ values. With these parameters, we found two bound states $0s_{1/2}$ at $-23.280$ MeV and $0p_{3/2}$ at $-2.589$ MeV, which form the $^9$Li core. There are also two low-lying resonances $0p_{1/2}$ at $(0.195, -0.047)$ MeV and $0d_{5/2}$ at $(2.731, -0.545)$ MeV. Besides, there is a $1s_{1/2}$ state appears as an antibound state at $-0.050$ MeV. These energy levels we produced agree with the experimental single-particle energies as given in Ref. [36].

In a recent letter [2], a $0p_{1/2}$ resonance was found at around $0.540$ MeV. Since the $0p_{1/2}$ resonance is an important element of the basis, we will use both energies in our following calculation. To obtained this $0p_{1/2}$ energy at $(0.563, -0.252)$ MeV, we chose $V_0 = 34.755$ MeV for $l$ odd and kept all the other parameters unchanged.

With this set of parameters, we found a number of high-lying resonances as well. However they are either too wide to be considered as meaningful resonances, or too high that they are out of the 10 MeV limit of the basis. We found that even expanding the basis from this limit does not produce any effect upon the calculation up to a certain precision.

To complete the Berggren single-particle basis we also need to include the scattering states on contour $L^+$. Here we performed two sets of calculations with two different contours. The contour $L^+_1$ includes both the antibound state and the Gamow resonances as in Fig. 4.1. The number of Gaussian points for each segment are given in Table 4.2. The other contour $L^+_2$ in Fig. 4.2 only includes the Gamow resonances, and the number of points are given in Table 4.3. Through these two calculations with different contours, we can study the effect of the antibound state $1s_{1/2}$. Besides, since the physical quantities will not change by the contours we chose, it can help us to find the physical states by comparing the results from two different calculations.

One may notice that the number of points on each contour are not uniformly distributed. This is because for those scattering states which are close to the anti-

Table 4.2: Number of Gaussian points in the different segments of the contour $L^+_1$.

| Segment        | Number |
|----------------|--------|
| $(0, 0) - V_1$ | 30     |
| $[V_1 - V_2]$  | 30     |
| $[V_2 - V_3]$  | 30     |
| $[V_3 - V_4]$  | 30     |
| $[V_4 - V_5]$  | 30     |
| $[V_5 - V_6]$  | 16     |
| $[V_6 - V_7]$  | 6      |

Table 4.3: Number of Gaussian points in the different segments of the contour $L^+_2$.

| Segment        | Number |
|----------------|--------|
| $(0, 0) - V_1$ | 30     |
| $[V_1 - V_2]$  | 30     |
| $[V_2 - V_3]$  | 30     |
| $[V_3 - V_4]$  | 8      |
| $[V_4 - V_5]$  | 4      |
CHAPTER 4. MULTISTEP SHELL MODEL METHOD IN THE COMPLEX ENERGY PLANE

Figure 4.1: Contour $L_1^+$ which includes the antibound state and the Gamow resonances (see also, Ref. [35]). The points $B_i$ denote bound state energies while $A$ denotes the antibound state. The points $V_i$ correspond to the vertices defining the contour. They have the values $V_1=(-0.05,0.05)$ MeV, $V_2=(-0.1,0)$ MeV, $V_3=(0,-0.4)$ MeV, $V_4=(0.5,-0.4)$ MeV, $V_5=(8,-0.4)$ MeV, $V_6=(8,0)$ MeV and $V_7=(10,0)$ MeV.

Figure 4.2: Contour $L_2^+$ includes only the Gamow resonances. The vertices are $V_1=(0,-1)$ MeV, $V_2=(1,-1)$ MeV, $V_3=(8,-1)$ MeV, $V_4=(8,0)$ MeV and $V_5=(10,0)$ MeV.
bound state or to a resonance, the overlap of their wave functions are much stronger and these states are more important for the calculation. Therefore we chose more points in those segments closer to the poles.

The scattering states on the contour together with the antibound state and the Gamow resonances defined the Berggren single-particle representation. With this complete single-particle basis we continue with the calculation of the two-particle state.

4.3 Two-particle states: The nucleus $^{11}\text{Li}$

The two-particle states of $^{11}\text{Li}$ were calculated by using a separable interaction, as shown in Section 2.3. The only state experimentally measured is the bound ground state which was found to lie at an energy of $-0.295$ MeV [37]. In a recent experiment, this state was measured more precisely to be at the energy of $-0.369$ MeV [38–40]. In the following calculations, we will use both values for comparison. The corresponding spin is observed to be $3/2^-$, which comes from the single proton lying on the deeply bound $0p_{3/2}$ orbit. Since this proton is considered as frozen, the dynamics of the system is determined by the two neutrons outside the core $^9\text{Li}$. The angular momentum contain of this ground state has also been measured. The wave function has about 60\% of s-waves, 40\% of p-waves, and some small components of other angular momenta [37].

By fitting the experimental energy of $^{11}\text{Li}(gs)$ we can determine the interaction strength $G_0$ and calculate the wave functions of all the $0^+$ states. The angular momenta contains of the ground state are shown in Table 4.4. The results in each cases are both in a reasonable agreement with the experiment values. Besides the ground state, there might be other meaningful states not been found yet. Therefore we have to evaluate all the possible two-particle states and decide for each state whether it can be considered as a meaningful resonance. There is an important feature of our method which we can make use of. Since the measurable physical quantities are defined on the real axis, they will remain the same when we change the contour. However, the complex states which are part of the continuum background do not have any counterpart on the real energy axis, and they will mainly rely

Table 4.4: Angular momentum contain of $^{11}\text{Li}(gs)$ corresponding to the energies $\epsilon_{p_{1/2}}$ discussed in the text.

| $\epsilon_{p_{1/2}}$ (MeV) | component(%) |   |   |
|--------------------------|--------------|---|---|
|                          | s-waves | p-waves | d-waves |
| (0.195,-0.047) | 46.8   | 49.1   | 4.2   |
| (0.563,-0.252) | 72.6   | 20.9   | 6.4   |
on the scattering states we choose on the contour. Therefore these states have
different values for different contours we choose [21]. We use this property and find
that there is no meaningful $0^+$ resonances.

We also calculated states with other angular momenta. In our calculations,
only normal parity states are considered, which means the states have the angular
momentum $\lambda$ and parity $(-1)^\lambda$. Since there is no experimental data for them, we
have to set the strength $G$ in a reasonable range to see if it is possible to get any
physically meaningful state. For instance we found the state $1^-$ at $(0.084, -0.002)$
MeV which is built by the pole configuration $(0s_{1/2}0p_{1/2})_{1^-}$ and therefore may be
physically meaningful. The state $2^+_1$ we found is at an energy around $(2.300, -0.372)$
MeV, and practically built by the pole configuration $(0s_{1/2}0d_{5/2})_{2^+}$. Checking the
corresponding radial wave function $\Psi_{2^+_1}(r)$ in Fig. 4.3 one can see that the wave
function is rather localized and the imaginary part is relatively small compared
with the corresponding real part. This state is about at the limit of which can be
considered as a physically meaningful resonance. Yet it can influence significantly
the spectrum of $^{12}\text{Li}$. Therefore the only meaningful two-particle states we found
for the following calculations are $^{11}\text{Li}$(gs), $^{11}\text{Li}(1^-$) and $^{11}\text{Li}(2^+_1)$.

One can understand why there are so few physically meaningful two-particle
states in $^{11}\text{Li}$ by looking at the radial wave functions of the single-particle states. In Fig. 4.4 we show the wave function of the antibound state $1s_{1/2}$. One can see
that it increases rapidly out from the nuclear surface, as expected for an antibound
state. The wave function of the resonance $0p_{1/2}$ and $0d_{5/2}$ are shown in Fig. 4.5 and
4.6 respectively. We found that these single-particle wave functions have a relatively
large imaginary part and start to diverge at a very short radius. This means that
these states live such a short time that they cannot produce any meaningful two-
particle resonances.

By using the physically meaningful two-particle states $0^+_1$, $1^-_1$ and $2^+_1$ and the
single-particle representation obtained in last section, we can now proceed to cal-
culate the three-particle and four-particle systems.

### 4.4 Three-particle states: The nucleus $^{12}\text{Li}$

The three-particle states of $^{12}\text{Li}$ are calculated by using the MSM method in the
complex energy plane. With the single-particle states from $^{10}\text{Li}$ and the two-particle
states $^{11}\text{Li}$(gs), $^{11}\text{Li}(1^-)$ and $^{11}\text{Li}(2^+_1)$, we can get all the possible three-particle
states. Since in the single-particle representation we have included a large number
of scattering states, the number of the possible three-particle states is still large. To
pick out the physical states among them we will use the same feature as discussed in
the two-particle case, which is that the measurable physical states will remain the
same when we change the contour. Furthermore there is another feature that we
can also use. Unlike the complex states which mainly rely on the scattering states,
the physically meaningful states mainly depend on the discrete states (which we will
call "poles"), such as antibound states or resonances. Therefore, the wave function
4.4. THREE-PARTICLE STATES: THE NUCLEUS $^{12}$Li

Figure 4.3: Radial function $\Psi(r)$ corresponding to the two-particle state $^{11}$Li$(2^+_1)$ at an energy of $(2.300, -0.372)\text{MeV}$. The dashed line is the imaginary part of the wave function.

Figure 4.4: Radial function $\phi(r)$ corresponding to the single-particle neutron anti-bound state $0s_{1/2}$ at an energy of $-0.050 \text{MeV}$. 
CHAPTER 4. MULTISTEP SHELL MODEL METHOD IN THE COMPLEX ENERGY PLANE

Figure 4.5: Same as Fig. 4.4 but for the Gamow resonance $0p_{1/2}$ at an energy of $(0.563, -0.252)$ MeV. The dashed line is the imaginary part of the wave function.

Figure 4.6: Same as Fig. 4.4 but for the Gamow resonance $0d_{5/2}$ at an energy of $(2.731, -0.545)$ MeV. The dashed line is the imaginary part of the wave function.
4.4. THREE-PARTICLE STATES: THE NUCLEUS $^{12}\text{Li}$

Table 4.5: Calculated three-particle states in $^{12}\text{Li}$ (in MeV) corresponding to the two energies $\epsilon_{p_{1/2}}$ of Table 4.4 and the two-particle energies taken to be $W(0^+_1) = -0.295\text{MeV}$, $W(1^-_1) = (0.084, -0.002)\text{MeV}$ and $W(2^+_1) = (2.300, -0.372)\text{MeV}$.

| $\epsilon_{p_{1/2}}$ | $1/2^+$ | $1/2^-$ | $5/2^+$ |
|---------------------|---------|---------|---------|
| (0.195, -0.047)     | (-0.294, 0.016) | (-0.171, 0.010) | (2.054, -0.377) |
| (0.563, -0.252)     | (-0.237, -0.041) | (-0.161, 0.007) | (1.953, -0.352) |

Table 4.6: Same as Table 4.5 but for $W(0^+_1) = -0.369\text{MeV}$.

| $\epsilon_{p_{1/2}}$ | $1/2^+$ | $1/2^-$ | $5/2^+$ |
|---------------------|---------|---------|---------|
| (0.195, -0.047)     | (-0.381, 0.023) | (-0.205, 0.010) | (1.999, -0.380) |
| (0.563, -0.252)     | (-0.468, -0.014) | (-0.041, 0.003) | (1.902, -0.353) |

components of the physically relevant states will be dominated only by the poles, while the scattering states will contribute little.

By using these properties we can now obtain the physically meaningful three-particle states. We will see that the corresponding spins and parities of these states are $1/2^+$, $1/2^-$ and $5/2^+$. We found that these states are mainly determined by the antibound state $^{11}\text{Li}(\text{gs})$. There is state such as $3/2^+$, with only the configuration $|1s_{1/2} \otimes 2^+_1; 3/2^+\rangle$, which is not a meaningful state. In Table 4.5 and 4.6 we listed the energies of the calculated three-particle states. Comparing the different energies, one can find that these states in fact do not depend much on the energy of $^{11}\text{Li}(\text{gs})$ or $\epsilon_{p_{1/2}}$.

An important feature we found is that the lowest state $1/2^+$ in these tables has a real and negative energy, which means it could be an antibound state, as the single-particle $1s_{1/2}$ state itself. This property agrees with Ref. [2], where the ground state of $^{12}\text{Li}$ was found to be an antibound (or virtual) state.

Taking the experimental energy values for the $0p_{1/2}$ and $^{11}\text{Li}(\text{gs})$ states as in the first line of Table 4.6, we find an antibound ground state $1/2^+$, with two resonances as well, which are $1/2^-$ at $0.176\text{ MeV}$ and $5/2^+$ at $(2.380, -0.380)\text{ MeV}$ above the threshold. In Ref. [3] a state was found at $1.5\text{ MeV}$ which probably has spin and parity $5/2^+$. The theoretical results are in a reasonable agreement with experiment.

In a recent experiment the states of $^{12}\text{Li}$ were measured by using two-proton removal reactions [4]. It was found that there are an antibound ground state as we predicted, and also two excited resonances which were first observed at $0.250\text{ MeV}$ and $0.555\text{ MeV}$. To explain these two low-lying resonances we have to consider the $0p_{3/2}$ proton in the core and also the proton-neutron interaction. For instance through the proton excitation, the antibound ground state $1/2^+$ can provide a $1^-$ and a $2^-$
CHAPTER 4. MULTISTEP SHELL MODEL METHOD IN THE COMPLEX ENERGY PLANE

Figure 4.7: Experimental level scheme in $^{12}$Li. The three lowest levels are from [4], while the one at 1.5 MeV is from [40]. In the second column are the three-neutron CXMSM results. In the columns A-C are the shell model calculations corresponding to different truncation schemes: A) within $0-1\hbar\omega$ excitations, B) within $0-3\hbar\omega$ excitations and C) full psd space. Dashed lines indicate the widths of the resonances.

state. This is also presented in the shell model calculation of Ref. [4]. However the states in the continuum, which are important to describe the very unstable states, are not included in this shell model calculation.

To compare these two models, we took $^4$He as the core and repeated the calculation in Ref. [4]. The corresponding calculated energies are presented in Fig. 4.7. One can see that in shell model calculation, the excited states are above the experimental values. It is worthwhile to point out that in shell model the states $2^-_1$ and $1^-_1$ are mainly composed of the configuration $|\pi[0p_3/2]\nu[(0p_{1/2})^21s_{1/2}]\rangle$, whereas in our CXMSM calculation the wave function of the ground state is mainly $|1s_{1/2} \otimes ^{11}\text{Li(gs)}\rangle$. The differences between the two calculations can be seen in two ways. First the state $^{11}\text{Li(gs)}$ contains both $0p_{1/2}$ and $1s_{1/2}$ components. Second, in the CXMSM the continuum have to be important building up the ground state due to the Pauli principle. Besides, another important advantage of our CXMSM method is that the antibound character of the ground state are predicted, which cannot be found by using the standard of shell model.

In this thesis we will not attempt to evaluate the $^{12}$Li states by taking account the $0p_{3/2}$ proton. To do this, one has to include the proton-neutron interaction
which will make the system much more complicated. This will be done in a further study.

4.5 Four-particle states: The nucleus $^{13}$Li

Using the two-particle states of $^{11}$Li within the Berggren single-particle representation, we can calculate the four-particle system $^{13}$Li. The four-particle CXMSM basis is constructed by two correlated two-particle states. The two-particle states we included here are $^{11}$Li($0^+_1$), $^{11}$Li($1^-_1$) and $^{11}$Li($2^+_1$), which are the same as the three-particle case. In this basis we formed the symmetric Hamiltonian matrix by evaluated the dynamical matrix (A.6) and the overlap matrix (A.7). And after the diagonalization we obtain the four-neutron states.

The only four-particle states we got are $0^+$, $1^-$, $2^+$, $3^-$ and $4^+$. The calculations, refer to different single-particle $\epsilon_{p_{1/2}}$ and two-particle $^{11}$Li(gs) energies, are listed in Table 4.7 and Table 4.8. We found that there is no bound or antibound state in $^{13}$Li, which agrees with experiment since $^{13}$Li was found to be unbound [2]. The ground state is a resonance at around 1 MeV, however the configuration and the energy strongly depend on which single-particle energy $\epsilon_{p_{1/2}}$ we choose. For the case $\epsilon_{p_{1/2}} = 0.195$MeV, the ground state is $[^{11}\text{Li}(0^+_1) \otimes ^{11}\text{Li}(1^-_1); 2^+]$ at the energy of $(0.715, -0.114)$MeV, while for $\epsilon_{p_{1/2}} = 0.563$MeV case, the ground state is $0^+$ at an energy $(1.505, -0.041)$MeV and with the components $[^{11}\text{Li}(1^-_1) \otimes ^{11}\text{Li}(1^-_1); 0^+]$ and $[^{11}\text{Li}(0^+_1) \otimes ^{11}\text{Li}(0^+_1); 0^+]$ about half and half. Comparing between tables one can find that the four-particle states are not much affected by the energy of $^{11}$Li(gs), instead some of the these states are greatly affected by the energy $\epsilon_{p_{1/2}}$.

In our calculation we only included the resonances of $^{11}$Li which are physically meaningful for building the whole four-particle basis. However as we mentioned before, there are lots of other continuum states which belong to the background and have large pole components. Although these states are not in themselves physically meaningful resonances, they might have some influence on the spectrum of $^{13}$Li. Therefore, for a more precise calculation, one should include some of these two-particle states. This will be done in a further study.
Table 4.7: Calculated energies (in MeV) of the four-particle states in $^{13}\text{Li}$ corresponding to different single-particle $\epsilon_{p_{1/2}}$ energies. The two-particle states $W(0^+_1) = -0.295\text{MeV}$, $W(1^-_1) = (0.084, -0.002)$ and $W(2^+_1) = (2.300, -0.372)\text{MeV}$ are included in the calculation.

| $\epsilon_{p_{1/2}} = (0.195, -0.047)$ | $\epsilon_{p_{1/2}} = (0.563, -0.252)$ |
|---------------------------------|---------------------------------|
| 0$^+$                           |                                |
| (0.868,-0.059)                  | (1.505,-0.041)                |
| (5.127,-0.964)                  | (5.274,-1.009)                |
| 1$^-$                           |                                |
| (0.836,-0.117)                  | (1.722,-0.166)                |
| (3.244,-0.593)                  | (3.921,-0.721)                |
| 2$^+$                           |                                |
| (0.715,-0.114)                  | (1.802,-0.257)                |
| (2.907,-0.445)                  | (3.373,-0.478)                |
| (5.131,-0.910)                  | (5.205,-0.966)                |
| 3$^-$                           |                                |
| (2.541,-0.391)                  | (2.674,-0.413)                |
| 4$^+$                           |                                |
| (5.715,-1.119)                  | (5.715,-1.119)                |

Table 4.8: Same as Table 4.7 but for $W(0^+_1) = -0.369\text{MeV}$.

| $\epsilon_{p_{1/2}} = (0.195, -0.047)$ | $\epsilon_{p_{1/2}} = (0.563, -0.252)$ |
|---------------------------------|---------------------------------|
| 0$^+$                           |                                |
| (0.855,-0.057)                  | (1.527,-0.033)                |
| (5.142,-0.970)                  | (5.303,-1.020)                |
| 1$^-$                           |                                |
| (0.828,-0.122)                  | (1.744,-0.169)                |
| (3.244,-0.593)                  | (3.921,-0.721)                |
| 2$^+$                           |                                |
| (0.715,-0.114)                  | (1.802,-0.257)                |
| (2.903,-0.450)                  | (3.367,-0.477)                |
| (5.137,-0.916)                  | (5.213,-0.973)                |
| 3$^-$                           |                                |
| (2.541,-0.391)                  | (2.674,-0.413)                |
| 4$^+$                           |                                |
| (5.715,-1.119)                  | (5.715,-1.119)                |
Chapter 5

Multistep shell model description of spin-aligned proton-neutron pair coupling

The low-lying yrast states in the $N=Z$ nucleus $^{92}$Pd were recently measured [41]. It was found that in $^{92}$Pd and its neighboring nuclei, such as $^{96}$Cd, the single $0g_{9/2}$ shell can determine the low-lying spectra [42,43]. Moreover, to explain the structure of these states, a spin-aligned proton-neutron pair coupling scheme was proposed. That is, the ground state was not mainly constructed by the pairs of protons or neutrons coupled to zero angular momentum, but rather by isoscalar proton-neutron pairs coupled to the maximum angular momentum [41,42].

The multistep shell model method is an ideal representation to study the importance of normal pairing and proton-neutron pairing simultaneously. It is straightforward to examine the projections of any basis vectors upon a physical state in the MSM. In this chapter we will evaluate the $^{96}$Cd, $^{94}$Ag and $^{92}$Pd systems by steps, within the overcomplete MSM basis constructed by both normal pairings and proton-neutron pairings. Our calculations will be restricted to the single $0g_{9/2}$ hole shell with the interaction matrix elements taken from Ref. [42,44]. We will also evaluate the neighboring systems in this heavy $N=Z$ region by using the MSM method with the isospin symmetry. All the formulas related are given in the Appendix.

5.1 Normal pair and proton-neutron pair couplings

Four-particle system $^{96}$Cd

The calculation of the four-particle system $^{96}$Cd was based on one single $0g_{9/2}$ hole level and all the isoscalar and isovector two-particle states obtained from the two-body interactions. The basis vectors were constructed in such ways that both
CHAPTER 5. MULTISTEP SHELL MODEL DESCRIPTION OF
SPIN-ALIGNED PROTON-NEUTRON PAIR COUPLING

Figure 5.1: Coefficients \( x^2 \) corresponding to the wave function of the ground state and the first \( 2^+, 4^+, 6^+ \) states of \(^{96}\text{Cd}\) as a function of the controlling parameter \( \delta \) (see text). Upper left frame: The red line indicates \( |(\pi\nu_0)^2;0\rangle \), and the blue line indicates \( |(\pi\pi)_0(\nu\nu)_0;0\rangle \). Upper right frame: The red line indicates \( |(\pi\nu_0)^2;2\rangle \), and the blue line indicates \( |(\pi\pi)_0(\nu\nu)_2;2\rangle \). Lower left frame: The red line indicates \( |(\pi\nu_0)^2;4\rangle \), and the blue line indicates \( |(\pi\pi)_0(\nu\nu)_4;4\rangle \). Lower right frame: The red line indicates \( |(\pi\nu_0)^2;6\rangle \), and the blue line indicates \( |(\pi\pi)_0(\nu\nu)_6;6\rangle \).

\((\pi\pi) \otimes (\nu\nu)\) and \((\pi\nu) \otimes (\pi\nu)\) excitations are included in the MSM basis. After solving the dynamic and overlap matrices, one can easily assess the importance of all the possible configurations in a physical state by examining the cosine value \( x \).

In Fig. 5.1 we show the main values of the probabilities \( x^2 \) as a function of a controlling parameter \( \delta \) for the ground state and the first \( 2^+, 4^+, 6^+ \) states of \(^{96}\text{Cd}\). The parameter \( \delta \) controls the intensity of the isoscalar matrix element

\[
|(g_{9/2})^2;9\rangle \langle (g_{9/2})^2;9\rangle = V_9(\delta) = V_9(0)(1 + \delta). \tag{5.1}
\]

\( V_9(0) \) is the original matrix element which is strongly attractive due to the large sparial overlap of the particle distributions [45]. The striking feature in this figure is that the spectrum for \( \delta = 0 \) is dominated by the isoscalar configuration \( |(\pi\nu_0)^2\rangle \), instead of the normal pairing one. Moreover, as \( V_9 \) becomes more attractive \( (\delta \to 1) \) the normal pairing configuration becomes less and less relevant while the importance of the isoscalar configuration increases.
5.1. NORMAL PAIR AND PROTON-NEUTRON PAIR COUPLINGS

In Table 5.1 the largest components of the lowest-lying states are shown for different total angular momenta in $^{96}$Cd. One sees that the normal pairing configuration $|((\pi\pi)_0(\nu\nu); I)\rangle$ does not dominate other low-lying states either. On the contrary, the isoscalar aligned mode $|((\pi\nu)_9)^2; I)\rangle$ is mainly concentrated in the yrast states.

It is also interesting to point out that the overlap of the isoscalar aligned state is

$$
\langle((\pi\nu)_9)^2; 0|((\pi\nu)_9)^2; 0\rangle = 2.00001.
$$

Which means that the influence of the Pauli principle upon $|((\pi\nu)_9)^2; 0\rangle$ is negligible. Therefore we can say that it represents virtually a bosonic mode (see also Ref. [43]).

Six-particle system $^{94}$Ag

The calculated spectra of the odd-odd nucleus $^{94}$Ag at different $\delta$ are shown in Fig. 5.2. For simplicity, we have only plotted the yrast states for the $T = 0$ and $T = 1$ channels in the single $0g_{9/2}$ shell. In the figure one can find that at $\delta = -1$ (denotes a weaker isoscalar interaction $V_9$) the $T = 1$ yrast states has a seniority-like spectrum form, while at $\delta = 1$ (denotes a much stronger interaction $V_9$) it becomes a vibrational-like spectrum form. This is not unique in this region. Actually in the cases of $^{96}$Cd and $^{92}$Pd, the low-lying spectra are also greatly affected by the isoscalar matrix element $V_9$, and have the same feature as in $^{94}$Ag.

![Figure 5.2: Shell model spectra of $^{94}$Ag calculated in the $0g_{9/2}$ shell at different $\delta$.](image-url)
Table 5.1: Leading configurations in the first five states of $^{96}\text{Cd}$ for a given total angular momentum $I$.

| n | Configuration | $|x|$ | Configuration | $|x|$ | Configuration | $|x|$ | Configuration | $|x|$ |
|---|---------------|-----|---------------|-----|---------------|-----|---------------|-----|
| 1 | $(\pi\nu)_{9}(\pi\nu)_{9}$ | 0.96 | $(\pi\nu)_{9}(\pi\nu)_{9}$ | 0.99 | $(\pi\nu)_{9}(\pi\nu)_{9}$ | 0.97 | $(\pi\nu)_{9}(\pi\nu)_{9}$ | 0.84 |
| 2 | $(\pi\nu)_{5}(\pi\nu)_{5}$ | 0.88 | $(\pi\nu)_{8}(\pi\nu)_{9}$ | 0.92 | $(\pi\nu)_{8}(\pi\nu)_{9}$ | 0.93 | $(\pi\nu)_{7}(\pi\nu)_{9}$ | 0.60 |
| 3 | $(\pi\nu)_{0}(\pi\nu)_{0}$ | 0.77 | $(\pi\nu)_{7}(\pi\nu)_{9}$ | 0.94 | $(\pi\nu)_{7}(\pi\nu)_{9}$ | 0.90 | $(\pi\nu)_{8}(\pi\nu)_{9}$ | 0.67 |
| 4 | $(\pi\nu)_{3}(\pi\nu)_{3}$ | 0.91 | $(\pi\nu)_{7}(\pi\nu)_{8}$ | 0.82 | $(\pi\nu)_{5}(\pi\nu)_{9}$ | 0.90 | $(\pi\nu)_{5}(\pi\nu)_{9}$ | 0.63 |
| 5 | $(\pi\nu)_{4}(\pi\nu)_{4}$ | 0.80 | $(\pi\nu)_{5}(\pi\nu)_{7}$ | 0.64 | $(\pi\nu)_{6}(\pi\nu)_{9}$ | 0.92 | $(\pi\nu)_{8}(\pi\nu)_{9}$ | 0.67 |

Table 5.2: Configurations with the largest probabilities for the two lowest states $^{94}\text{Ag}(0^+_1)$ and $^{94}\text{Ag}(7^+_1)$ corresponding to both $(\pi\nu) \otimes (\pi\pi\nu\nu)$ (left) and the tonsorial products of three pairs (right).

| State | n | Configuration | $|x|$ | Configuration | $|x|$ |
|-------|---|---------------|-----|---------------|-----|
| $^{94}\text{Ag}(0^+_1)$ | 1 | $(\pi\nu)_{9}(\pi\pi\nu\nu)_{9}$ | 0.971 | $(\pi\nu)_{9}(\pi\pi\nu\nu)_{9}$ | 0.981 |
|       | 2 | $(\pi\nu)_{0}(\pi\pi\nu\nu)_{0}$ | 0.971 | $(\pi\nu)_{0}(\pi\pi\nu\nu)_{0}$ | 0.778 |
|       | 3 | $(\pi\nu)_{8}(\pi\pi\nu\nu)_{8}$ | 0.917 | $(\pi\nu)_{8}(\pi\pi\nu\nu)_{8}$ | 0.739 |
| $^{94}\text{Ag}(7^+_1)$ | 1 | $(\pi\nu)_{5}(\pi\pi\nu\nu)_{16}$ | 0.970 | $(\pi\nu)_{5}(\pi\pi\nu\nu)_{16}$ | 0.815 |
|       | 2 | $(\pi\nu)_{5}(\pi\pi\nu\nu)_{4}$ | 0.835 | $(\pi\nu)_{1}(\pi\pi\nu\nu)_{2}$ | 0.475 |
|       | 3 | $(\pi\nu)_{1}(\pi\pi\nu\nu)_{1}$ | 0.747 | $(\pi\nu)_{2}(\pi\pi\nu\nu)_{8}$ | 0.435 |
This we will present later in Fig. 5.13. The reason is probably that the isoscalar $(\pi\nu)_{9}$ pair excitations play an important role in the low-lying yrast states of all these nuclei [42,44]. And while the isoscalar interaction $V_{9}$ vanishes, the dominant component switch to the normal pairing term.

The $T = 0$ states in $^{94}$Ag are especially interesting because they are the only states which can be coupled from three isoscalar $(\pi\nu)_{9}$ pairs. Indeed we found that most of the $T = 0$ yrast levels in Fig. 5.2, except the states $16^{+}_{1}$ and $18^{+}_{1}$, are dominated by the vector consisting of three spin-aligned $(\pi\nu)_{9}$ states.

The ground state of $^{94}$Ag is suggested to be $I^{\pi} = 4^{+}$ and $T = 1$ [46]. It may seems that in odd-odd system the isovector pairing mode retakes its predominance. We found that this is not the case by analyzing the wave function in terms of the tensor product of three pairs. The largest components of the ground state in terms of both $(\pi\nu) \otimes (\pi\nu) \otimes (\pi\nu)$ and the tonsorial products of three pairs are listed in Table 5.2. The most important configuration consists of two spin-aligned $(\pi\nu)_{9}$ pairs coupled to $|(\pi\nu)_{9}(\pi\nu)_{9}; 0\rangle$ (which was dominant in $^{96}$Cd) and an isovector state $(\pi\nu)_{0}$. An illustration of the construction with such configurations is given in Fig. 5.3.

![Figure 5.3: Structure of the main component in the ground state of $^{94}$Ag.](image)

Another interesting case is the first excited state $7^{+}$, which is also the lowest state in isospin $T = 0$ channel. The largest configurations are also given in Table 5.2. Clearly it is dominated by the three spin-aligned $(\pi\nu)_{9}$ pairs. More specifically, two spin-aligned $(\pi\nu)_{9}$ pairs which coupled to $|(\pi\nu)_{9}(\pi\nu)_{9}; 16\rangle$, with another $(\pi\nu)_{9}$ coupled to a total $7^{+}$ state. An illustration of such construction is in Fig. 5.4.

![Figure 5.4: Structure of the main component in $^{94}$Ag($7^{+}$).](image)

The probabilities $x^{2}$ corresponding to the spin-aligned proton-neutron pairing and normal pairing configuration as a function of $\delta$ for the ground state and $7^{+}$ state of $^{94}$Ag are shown in Fig. 5.5. One can see that the normal pairing configuration
CHAPTER 5. MULTISTEP SHELL MODEL DESCRIPTION OF SPIN-ALIGNED PROTON-NEUTRON PAIR COUPLING

Figure 5.5: Coefficients $x^2$ corresponding to the wave function of the ground state $0^+$ and the first excited state $7^+$ of $^{94}$Ag as a function of the controlling parameter $\delta$. Left frame: The red line indicates $|((\pi\nu)_0((\pi\nu)_0^2;0)$, and the blue line indicates $|((\pi\nu)_0(\pi\pi)_0(\nu\nu)_0;0)$. Right frame: The red line indicates $|((\pi\nu)_7(\pi\pi)_0(\nu\nu)_0;7)$, and the blue line indicates $|((\pi\nu)_7(\pi\pi)_0(\nu\nu)_0;7)$.

played a much less important role than the spin-aligned proton-neutron pairing one in both cases. The normal pairing becomes more important in $^{94}$Ag($^7_1^+$) only when the isoscalar interaction $V_9$ is very weak.

It has also been expected that a spin-trap isomer $21^+$ state exists at an excitation energy around 6.67 MeV [46]. Our calculation with the single $0g_9/2$ shell assigns a correct excitation energy. However, according to Fig. 5.2 the state $21^+$ is above the state $19^+$, which means the isomerism of the $21^+$ state is not reproduced. This pattern remains even if the shells $p_{3/2}$, $p_{1/2}$ and $f_{5/2}$ are also included, therefore the reason of this inversion is not clear. In Ref. [47] it is suggested that it may be related to core excitations across the $N = Z = 50$ shell gap.

Eight-particle system $^{92}$Pd

The calculation of the eight-particle system $^{92}$Pd was done within the MSM basis $\{|\alpha_4\beta_4;\alpha_0\}$. In this case the MSM basis is highly overcomplete and the calculation is extremely difficult. For instance there are only 36 shell model $0^+$ states in $^{92}$Pd while the corresponding MSM dimension is 915. Therefore only the ground state of $^{92}$Pd are evaluated for the coefficients $x$ corresponding to both $(\pi\pi\nu\nu) \otimes (\pi\pi\nu\nu)$ and the tensorial products of four pairs, in Table 5.3. Since many basis vectors are similar to each other in such overcomplete basis set, there is not a value of $x$ which is significantly larger than others. But still one can find that the most important configuration is the one corresponding to the four aligned $(\pi\nu)_0$ pairs. The second largest component is the combination of two aligned $(\pi\nu)_0$ pairs and two normal pairing states, which is not surprising since in the ground state of four particle system the second largest component is the normal pairing term. The configuration constructed with four normal pairing states $(\pi\pi)_0(\nu\nu)_0(\pi\pi)_0(\nu\nu)_0$
5.2. ISOSPIN SYMMETRY

Table 5.3: Configurations with the largest probabilities for the state $^{92}\text{Pd}(0^+_1)$ corresponding to the tensorial products of two $(\pi\pi\nu\nu)$ (left) and the tensorial products of four pairs (right).

| n | Configuration | $|x|$ | Configuration | $|x|$ |
|---|---|---|---|---|
| 1 | $(\pi\pi\nu\nu)_0(\pi\pi\nu\nu)_0$ | 0.975 | $(\pi\nu)_0(\pi\nu)_0(\pi\nu)_0(\pi\nu)_0$ | 0.921 |
| 2 | $(\pi\pi\nu\nu)_8(\pi\pi\nu\nu)_8$ | 0.937 | $(\pi\nu)_0(\pi\nu)_0(\pi\pi)_0(\nu\nu)_0$ | 0.870 |
| 3 | $(\pi\pi\nu\nu)_8(\pi\pi\nu\nu)_8$ | 0.915 | $(\pi\nu)_0(\pi\nu)_1(\pi\pi)_0(\nu\nu)_0$ | 0.746 |
| 4 | $(\pi\pi\nu\nu)_10(\pi\pi\nu\nu)_10$ | 0.813 | $(\pi\nu)_0(\pi\nu)_1(\pi\pi)_0(\nu\nu)_8$ | 0.746 |
| 5 | $(\pi\pi\nu\nu)_0(\pi\pi\nu\nu)_0$ | 0.776 | $(\pi\nu)_1(\pi\nu)_1(\pi\pi)_0(\nu\nu)_0$ | 0.723 |

has $x = 0.679$. It is a relatively small number and only occupies the 10th place in order of importance, which also reflects the dominance of the aligned configuration in this nuclear region.

5.2 Isospin symmetry

We performed a number of systematic calculations on four-particle, six-particle and eight-particle systems within this $0g_{9/2}$ region using the MSM basis which was constructed fulfilling the isospin symmetry. The calculations were done with the same single $0g_{9/2}$ hole shell and interaction matrix elements as before. The initial motivation was to inspect the results again under the isospin symmetry which was not spontaneously included during the former calculations. Besides, by introducing the isospin symmetry, the dimension of the corresponding MSM basis was to some extent reduced, which made the calculation less time consuming.

The quantities $x^2$ which indicate the importance of the corresponding MSM configuration in a physical state were calculated for different systems. The probabilities $x^2$ corresponding to the spin-aligned pairing and normal pairing configurations as a function of $\delta$ for different yrast states of $^{96}\text{Cd}$, $^{94}\text{Ag}$ and $^{92}\text{Pd}$ are plotted in Fig. 5.6, Fig. 5.7 and Fig. 5.8 respectively. The configurations are denoted in the form of $|(j^2)_J T_T \cdots : JT\rangle$, where we use $j$ to indicate the single hole shell $0g_{9/2}$, $J_j$ and $T_j$ are the angular momentum and isospin for two particles, and $J$ and $T$ are the total angular momentum and isospin. We found that the same features discussed before remains when introducing the isospin symmetry. When $\delta = 0$, which corresponds for the standard interaction, all these yrast states are dominated by the isoscalar spin-aligned pair $(j^2)_{90}$. The normal pairing configuration is important only when $V_5$ is very weak. And as $V_5$ becomes more and more attractive, the importance of the normal pairing configuration drops dramatically.

The MSM bases in the proton-neutron representation and the isospin symmetry representation are actually constructed differently. For instance, in the MSM basis of the four-particle system $^{96}\text{Cd}$, there are two vectors $|[(\pi\pi)_0(\nu\nu)_0]:0\rangle$
CHAPTER 5. MULTISTEP SHELL MODEL DESCRIPTION OF
SPIN-ALIGNED PROTON-NEUTRON PAIR COUPLING

Figure 5.6: Same as Fig. 5.1 but for the calculations with isospin symmetry. Upper left frame: The red line indicates \( |(j^2)_{00}; 00\rangle\), and the blue line indicates \( |(j^2)_{01}; 00\rangle\). Upper right frame: The red line indicates \( |(j^2)_{00}; 20\rangle\), and the blue line indicates \( |(j^2)_{01}(j^2)_{21}; 20\rangle\). Lower left frame: The red line indicates \( |(j^2)_{00}; 40\rangle\), and the blue line indicates \( |(j^2)_{01}(j^2)_{41}; 40\rangle\). Lower right frame: The red line indicates \( |(j^2)_{00}; 60\rangle\), and the blue line indicates \( |(j^2)_{01}(j^2)_{61}; 60\rangle\).

Figure 5.7: Same as Fig. 5.5 but for the calculations with isospin symmetry. Left frame: The red line indicates \( |(j^2)_{01}(j^2)_{00}; 01\rangle\), and the blue line indicates \( |(j^2)_{01}^3; 01\rangle\). Right frame: The red line indicates \( |(j^2)_{00}; 70\rangle\), and the blue line indicates \( |(j^2)_{01}(j^2)_{70}; 70\rangle\).
5.2. ISOSPIN SYMMETRY

Figure 5.8: Coefficients $x^2$ corresponding to the wave function of the ground state of $^{92}$Pd as a function of the controlling parameter $\delta$ with considering of the isospin symmetry. The red line indicates $|(j^2)^{90};00\rangle$, while the blue line indicates $|(j^2)^{01};00\rangle$.

Figure 5.9: Comparison of calculated and experimental energy levels in $^{96}$Ag and $^{96}$Pd. The negative parity experimental levels are outside our shell model space.
Figure 5.10: Same as Fig. 5.9 but for levels in $^{94}\text{Ag}$, $^{94}\text{Pd}$, $^{94}\text{Rh}$ and $^{94}\text{Ru}$. The negative parity experimental levels are outside our shell model space.
5.2. ISOSPIN SYMMETRY

Figure 5.11: Same as Fig. 5.9 but for levels in $^{92}$Rh, $^{92}$Ru, $^{92}$Tc and $^{92}$Mo. The negative parity experimental levels are outside our shell model space.
and \( |(\pi\nu)_{0}(\pi\nu)_{0}; 0\rangle \) in the proton-neutron representation, and two other vectors \( |((j^2)_{01})^2; 00\rangle \) and \( |((j^2)_{01})^2; 02\rangle \) in the isospin symmetry representation. Both sets of two vectors under their own representation are actually describing the same subspace: two \( J = 0 \) two-particle states coupled to a \( J = 0 \) four-particle state, while these four vectors are quite different from each other. Therefore it is not difficult to understand that the cosines of the angles between the physical vector and the basis vectors under different representations can be different.

5.3 Spectra

The calculated spectra of four-particle, six-particle and eight-particle systems are compared with the experimental energy levels in different nuclei within this \( 0g_{9/2} \) region. Most of the experimental data are obtained from NNDC [46], except for \( ^{92}\text{Pd} \) which is reported in Ref. [41]. The results are plotted in Fig. 5.9 - 5.12. From these figures we can see that our calculations with the only single \( 0g_{9/2} \) hole shell fit very well most of the experimental data of these nuclei. This can be an evidence that the single \( 0g_{9/2} \) shell is qualified enough to describe the property of the low-lying states in this region.

In Fig. 5.13 we plotted the evolution of the spectra in \( ^{96}\text{Cd} \) and \( ^{92}\text{Pd} \) as a function of the \( V_9 \) interaction changes. As the interaction is becomes more and more
attractive, the spectra appear approximately equidistant and reach vibrational-like structure. This can be understood as the dominant component in the spectra changed from the normal pairing term to the isoscalar aligned pairs. In the normal pairing mode, one has to break a pair in order to excite the nucleus from the ground state. Instead, no pair was broken in the aligned isoscalar mode, and the excitation of the nucleus is due to a reorientation of the isoscalar pairs. This could be the cause of the similar exciting energies [42].

Figure 5.13: Calculated spectra of $^{96}$Cd and $^{92}$Pd for different controlling parameter $\delta$. 
Chapter 6

Monte Carlo representation in the complex energy plane

The Berggren representation is a complete single particle basis in the complex energy plane [22]. It has been a successful representation for describing many-body states in the continuum. However, since the Berggren basis contains a large number of scattering states on the contour, the dimension of the many-body matrix usually gets too big for realizable calculations. In Chapter 4 we have reduced the matrix dimension by introducing the MSM method and selecting only the relevant states in the middle steps. But one has to be very careful on selecting the intermediate states, because it may brake the symmetry of the $T$ matrix and lead to unreliable results.

In this chapter we attempt to use the Monte Carlo method to evaluate the integral in the complete Berggren representation. In this case, only very few scattering states will be needed in the single particle basis for each run. The price of this is to repeat the calculation thousands of times. In Section 6.1 we will first give a brief introduction to the Monte Carlo method. Then we will perform a standard calculation of Ref. [22] (Section 6.2) and try to achieve the same accuracy by using the Monte Carlo method in the complex energy plane (Section 6.3). We will also apply this Monte Carlo method in the two-particle system $^{26}$O (Section 6.4).

6.1 Monte Carlo method

Monte Carlo method is a numerical algorithm which use random samplings and probability statistics to perform mathematical calculations. It is most suited to the calculation that infeasible to compute an exact result with a deterministic algorithm, and can be especially useful for complex systems with many coupled degrees of freedom [48].

A rather simple example of the Monte Carlo method is to obtain an estimate of the number $\pi$ by using a stochastic process. Consider a unit circle inscribed
CHAPTER 6. MONTE CARLO REPRESENTATION IN THE COMPLEX ENERGY PLANE

Figure 6.1: Approximation of the value $\pi$ by counting the number of points that landed inside the unit circle. After placing 10,000 random points, the estimate value is $\pi \approx 3.1376$.

in a square. The ratio of the area of the unit circle to the square is simply $\pi/4$. Therefore the value of $\pi$ can be approximated by the following steps:

- Generate $N$ pairs of random numbers $(x, y)$ in the interval $[-1, 1]$. Each pair indicates one random point in the square.
- Count the number of points $N_C$ that fall inside the unit circle, by checking if $x^2 + y^2 \leq 1$.
- Calculate the estimate value through $\pi \approx 4N_C/N$.

A typical run with 10,000 points is shown in Fig. 6.1. The estimate value of this run is $\pi \approx 3.1376$, which is within 0.13% the actual value. The estimates may vary for different runs, especially when only a few points are generated. But in general, as the number of points increases, the accuracy of the result becomes better.

6.2 Discretized Berggren representation

The Berggren representation is a proper complete basis in the complex energy plane. As already seen in Section 2.2, the complete Berggren representation is derived from the Dirac $\delta$ function, and has the form

$$\delta(r - r') = \sum_n w_n(r)w_n(r') + \int_{L^+} dE u(r, E)u(r', E)$$

(6.1)
where the summation runs over all the bound states plus the resonances inside the contour, and the integral includes all the scattering states on the contour $L^+$. In order to make the representation usable for shell model calculations, one approach is to discretize the integral into a summation over a limited number of selected scattering states on the contour. In Ref. [22], it has been shown that around 50 scattering states are needed to reproduce the exact results within the order of a few keV.

Our first attempt is to reproduce the results of Ref. [22] with three different contours, and find out an appropriate cutoff energy for the following calculations. We will use a realistic Hamiltonian $H_0$ to generate different orthonormal bases, corresponding to different truncations and different number of scattering states. Within each basis, we can diagonalize a certain target Hamiltonian $H$ and calculate the eigenvalues and eigenvectors. We can also evaluate exactly the eigenvalues and eigenvectors of $H$ by just solving the corresponding Schrödinger equation. We will do this by using the computer code GAMOW [49]. By comparing the calculated eigenvalues with the exact values, we will assess the completeness of each basis, and determine whether the approximation is good enough.

As in Ref. [22], we use a realistic potential corresponding to the states $h_{11/2}$ in $^{208}$Pb for generating the basis. The parameters of the Woods-Saxon potential are $V_0 = 44.4$, $r = 1.27$, $a = 0.7$ and $V_{sc} = 16.5$. It provides a bound state at $-14.960$ MeV and a resonance at $(2.251, -i0.026)$ MeV. The target Hamiltonian $H$ has the same Woods-Saxon parameters except that $V_0 = 40.4$ and $a = 0.6$. By solving the Schrödinger equation directly we found that it has one bound state at $-12.526$ MeV and one resonance at $(4.322 - i0.321)$ MeV.

We have chosen three contours with different cutoff energies in the complex energy plane. The nodes of each contour are listed as follows,

**Contour 1:** $(0, 0) \rightarrow (0, -5) \rightarrow (20, 0) \rightarrow (30, 0),$

**Contour 2:** $(0, 0) \rightarrow (0, -5) \rightarrow (20, 0) \rightarrow (30, 0) \rightarrow (100, 0),$

**Contour 3:** $(0, 0) \rightarrow (0, -5) \rightarrow (20, 0) \rightarrow (30, 0) \rightarrow (100, 0) \rightarrow (320, 0).$

For each contour, same number $n$ of discretized scattering states $u(r, E_p)$ are selected on the straight line of every segment, and their corresponding weight $h_p$ are calculated according to the Gaussian quadrature method. These weighted scattering states, together with the bound state and the resonance, form an orthonormal basis.

We diagonalized the target Hamiltonian $H$ within different bases, and the results thus obtained are shown in Table 6.1. One sees that as $n$ becomes larger and the cutoff energy goes higher, the results converge to the exact values. In Contour 1, the eigenvalues converge to the exact values within 2 keV. This implies that the scattering states with energies larger than 30 MeV have some importance. In Contour 2, the results agree with the exact ones within 1 keV. Which means the scattering states higher than 100 MeV do not affect appreciably the results, and 100 MeV is an appropriate cutoff.
CHAPTER 6. MONTE CARLO REPRESENTATION IN THE COMPLEX ENERGY PLANE

Table 6.1: The calculated one-particle eigenvalues under various bases with different contours and different number of scattering states. The energies are in units of MeV. Contour 1 has a cutoff at 30 MeV, contour 2 has a cutoff at 100 MeV, and contour 3 at 320 MeV.

| n   | Bound State | Resonance     |
|-----|-------------|---------------|
|     | Basis       | (2.251, -0.026) |
| 0   | -14.960     | (4.405, -0.133) |
| 2   | -12.519     | (4.442, -0.209) |
| 4   | -12.525     | (4.314, -0.372) |
| 8   | -12.525     | (4.343, -0.340) |
| Contour 1 16 | -12.524     | (4.329, -0.321) |
| 32  | -12.524     | (4.324, -0.322) |
| 64  | -12.524     | (4.324, -0.322) |
| 128 | -12.524     | (4.324, -0.322) |
|     | 2           | (4.429, -0.209) |
| 4   | -12.527     | (4.312, -0.372) |
| 8   | -12.526     | (4.341, -0.339) |
| Contour 2 16 | -12.526     | (4.327, -0.321) |
| 32  | -12.526     | (4.322, -0.321) |
| 64  | -12.526     | (4.322, -0.321) |
| 128 | -12.526     | (4.322, -0.321) |
|     | 2           | (4.438, -0.209) |
| 4   | -12.527     | (4.312, -0.371) |
| 8   | -12.527     | (4.341, -0.339) |
| Contour 3 16 | -12.526     | (4.327, -0.321) |
| 32  | -12.526     | (4.322, -0.321) |
| 64  | -12.526     | (4.322, -0.321) |
| 128 | -12.526     | (4.322, -0.321) |
| Exact| -12.526     | (4.322, -0.321) |

When \( n \) is small, we see that the result corresponding to the resonance has a larger deviation from the exact value than the one corresponding to the bound state. This is because the scattering states affect more to the resonance than to the ground state, as expected. Their wave functions are more alike, and the overlap between them are relatively larger. For instance when \( n = 0 \), which means the basis we diagonalized the target Hamiltonian within contains no continuum, the bound state we obtained has an error of 10 keV while the resonance has an error about 100 keV. This particular example shows that the continuum in the basis gives a non-negligible correction to the calculation, especially for the calculations of the resonances.
6.3 MC method for one-particle system

Instead of using the summation of discretized scattering states over the contour, we use the Monte Carlo method to evaluate the integral. We took the same Hamiltonian $H_0$ and $H$ in the previous section as example. We chose three segments for the contour: $(0,0) \rightarrow (0,-5) \rightarrow (20,0) \rightarrow (100,0)$, and randomly picked up one point on each segment for each run. Now the basis consists of only one bound state, one resonance and three random scattering states from different segments on the contour. Within this basis, we did the same diagonalization of the target Hamiltonian $H$ as in the previous section. For each run we picked a different basis and obtained different eigenvalues. After repeating this procedure many times (e.g. 50,000 runs), we took the average of all the corresponding eigenvalues from every individual run.

The results from the Monte Carlo method thus obtained are the bound state at $-12.526$ MeV and the resonance at $(4.324 - i0.328)$ MeV after 50,000 individual runs. The convergency of these results are shown in Fig. 6.2 and 6.3. We found that the actual error of the bound state energy we got is less than 1 keV, and the error of the resonance energy is about 3 keV. The error of this calculation is slightly bigger than the former calculation, but considering that we are taking only three scattering states on the contour in total, this small systematic error is acceptable.

![Figure 6.2: Convergency of the one-particle Monte Carlo calculation for the bound state in 10,000 runs. The black solid line denotes the average value given by Monte Carlo calculation, and the red dots indicate the estimated error bar of the result. The black dashed line gives the exact solution of target Hamiltonian.](image-url)
CHAPTER 6. MONTE CARLO REPRESENTATION IN THE COMPLEX ENERGY PLANE

6.4 MC method for two-particle system

In this section we will apply our Monte Carlo method on the two-particle system $^{26}\text{O}$, which has two neutrons outside the closed shell $^{24}\text{O}$. The single particle energy of the two neutrons are produced by a Woods-Saxon potential which is fitted to the experimental single particle levels in Ref. [50]. The parameters are $V_0 = 40.5$, $r_0 = 1.29$, $a = 0.57$ and $V_{sa} = 22$. In $^{26}\text{O}$ the lowest valence shells are $d_{3/2}$, $f_{7/2}$ and $p_{3/2}$. Therefore the basis will need to contain the resonances $d_{3/2}$ at $(1.30 - i 0.12)$ MeV, $f_{7/2}$ at $(2.66 - i 0.11)$ MeV, and the scattering states corresponding to the shells $d_{3/2}$, $f_{7/2}$ and $p_{3/2}$.

We first used the Complex Shell Model Method (CXSM) to calculate the $0^+$ states of $^{26}\text{O}$ as exact results. From the binding energy, we know that the ground state of $^{26}\text{O}$ is an unbound $0^+$ state which has an energy at $0.193$ MeV. By fitting the ground state energy to the experimental value, the separable interaction strength $G$ can be obtained, and so the excited $0^+$ states. We chose contour $(0,0) \rightarrow (0,-5) \rightarrow (20,0) \rightarrow (100,0)$ MeV for $d_{3/2}$ and $f_{7/2}$, and $(0,0) \rightarrow (20,0) \rightarrow (40,0) \rightarrow (100,0)$ MeV for $p_{3/2}$. We took 15 scattering states on each segment, which means 135 scattering states plus 2 resonances in the basis. The results of the calculation are shown in Table 6.2.

For comparison, we also calculated the same but without including the continuum states. In this case the basis we used only contains the resonances $d_{3/2}$ and $f_{7/2}$. The results are also shown in Table 6.2. We can see that the ground state we obtained has a positive imaginary part of the energy, which is not physical. The first excited $0^+$ state has an error which is more than 100 keV in comparison to
6.4. MC METHOD FOR TWO-PARTICLE SYSTEM

Table 6.2: The calculated $0^+$ states of two-particle system $^{26}\text{O}$ by different methods. The energies are in units of MeV.

|                | $^{26}\text{O}(0^+_1)$ | $^{26}\text{O}(0^+_2)$ |
|----------------|-------------------------|-------------------------|
| Exact          | $0.193 - i 0.000$       | $3.726 - i 0.337$       |
| Without Continuum | $0.193 + i 0.878$     | $3.621 - i 0.182$       |
| Monte Carlo Method | $0.193 - i 0.000$      | $3.726 - i 0.332$       |

the exact value. Such inaccuracy is due to the non-completeness of the basis. This again tells us the importance of the continuum spectrum in the Berggren basis in the calculations of resonances.

For the Monte Carlo calculation, we used the same contour as in the CXSM calculation, except that we randomly picked up one point on each segment for each run. That is, we included only 2 resonances and 9 random scattering states in each run. The dimension of the basis is only 11. This is a huge improvement comparing to the dimension in the CXSM calculation which is 137. We repeated the procedure 10,000 times and the results (in Table 6.2) are the average of all individual runs. One can see that the accuracy of our Monte Carlo calculation is very good. The real energy of the resonance has an error of only 0.2 keV. The imaginary energy has an error about 5 keV, which is acceptable. The convergency of the results is shown in Fig. 6.4.

Figure 6.4: Convergency of the two-particle Monte Carlo calculation for the first excited $0^+$ resonance in 10,000 runs. In left panel it shows the real part of the energy, while in right panel it is the imaginary part.
Chapter 7

Summary

The multistep shell model method (MSM) in the complex energy plane (CXMSM) was introduced to study nuclear excitations in the continuum. The MSM solves the shell model equations in terms of correlated basis. The elements of this basis consist of states in nuclei with less particles. For instance, a nucleus with \( s = m + n \) particles is described in terms of the tensorial product of states in the \( m \)-particle nuclei times states in the \( n \)-particle nuclei. The advantage of the MSM is that it provides a deep insight into the structure of nuclei. Besides, it might allow to drastically reduced the dimensions of the shell model basis.

The Complex Shell Model (CXSM) is an extension of the shell model to the complex energy plane. The CXSM provides all bound energies plus complex energies which may have physical meaning if the imaginary parts of those energies are negative and small in absolute value. Calling the complex energy \( \tilde{E} = E - i\Gamma/2 \), then the mean life of the resonant state is \( T = h/\Gamma \). For this interpretation to be valid \( \Gamma \) has to be small, since otherwise the state is not a “resonance” but rather a part of the continuum background. Yet, the question remains of how small the imaginary part of the energy should be in order to call the corresponding state a “resonance”. Besides, there are scattering states which are very close to the real energy axis but have no physical meaning. We found that a better way of probing the validity of a complex state as physically meaningful, is to notice that the resonance is a manifestation of the trapping of the system within the nuclear volume. Therefore the corresponding wave function has to be localized and practically real inside the nucleus. We used this as criterion to decide whether a state was physically meaningful.

In this thesis the MSM was combined with the CXSM in order to be able to evaluate unstable nuclei. Within this framework the nuclei \(^{12}\text{Li}\) and \(^{13}\text{Li}\) will be analyzed, choosing \(^{9}\text{Li}\) as the core. The reason why this isotope, with three protons and six neutrons, can be considered a core is that the three protons lie deep in the interior of the nucleus and can be considered to be frozen in the range of energies to be studied. The six neutrons fill the shells \(0s_{1/2} \) and \(0p_{3/2} \), which can also be
considered frozen in these light nuclei.

The unusual feature in this nuclear region is that $^{10}\text{Li}$ is unbound but $^{11}\text{Li}$ is bound. It means that the single-particle states in this case, which are the levels in $^{10}\text{Li}$, are resonances.

The two-particle states will be determined by using a separable force. The corresponding potential strength $G$ will be obtained by fitting the experimental energy of $^{11}\text{Li}(gs)$ as a two-particle state.

The next step in the CXSM is the calculation of the three-particle states, which will be described in terms of a one-times two-nucleon basis. Besides $^{11}\text{Li}(gs)$, I found two physically meaningful two-particle states. They are the resonances $^{11}\text{Li}(1^-)$ and $^{11}\text{Li}(2^+)$, which have not been experimentally observed yet. With these two-particle states and the single-particle states, the CXSM was applied to calculate the three-particle states in $^{12}\text{Li}$.

Three physically meaningful states were thus found in $^{12}\text{Li}$. Of these the ground state $1/2^+$ is predicted to be an antibound state. The other three-particle states are a resonance $1/2^-$ lying at about 0.176 MeV and another resonance $5/2^+$ lying at about 2.380 MeV with a width of 760 keV. The antibound ground state was confirmed by several experiments [2, 4] and the resonance $5/2^+$ has probably been observed in Ref. [3].

The four-particle states in $^{13}\text{Li}$ were calculated in terms of the two-particle states themselves. No bound or antibound state was found physically meaningful in $^{13}\text{Li}$. Experimentally it is only known that this nucleus is unbound.

The MSM method was extended to the proton-neutron case of non-identical particles. But I also extended the formalism including isospin, such that the particles become again identical. This formalism was then used to study the recently proposed spin-aligned proton-neutron pair coupling scheme.

The great advantage of the MSM in these studies is that it allows us to identify simultaneously the roles played by different excitation modes. Of particular interest is to understand the interplay between the normal pairing mode and the aligned proton-neutron isoscalar mode.

The method has been applied to analyze four-particle, six-particle and eight-particle states in the $N = Z$ region below the core $^{100}\text{Sn}$. The calculation has been restricted to a basis provided by the single $0g_{9/2}$ hole shell only. The corresponding interaction matrix elements were taken from Refs. [42, 44].

It was found that the low-lying yrast states in the nuclei $^{96}\text{Cd}$, $^{94}\text{Ag}$ and $^{92}\text{Pd}$ are dominated by the isoscalar aligned mode instead of the normal pairing configuration. The most important configurations in these states are mainly constructed by the coupling of spin-aligned $(\pi\nu)_{9}$ pairs. The calculated spectra are in all cases in excellent agreement with the corresponding experimental data when available. This shows that the space spanned by only the single $0g_{9/2}$ hole shell is qualified enough to describe the low-lying states in this region.

To overcome the dimension problem in the CXSM, I also developed a novel
Monte Carlo representation in the complex energy plane. The Monte Carlo method was introduced to approach the integral in the complete Berggren representation, so that only few scattering states are needed in the single-particle basis for each run.

The MC method was applied to evaluate the eigenstates of a Woods-Saxon potential in terms of a representation provided by the exact diagonalization of another Woods-Saxon potential. This was already done in Ref. [22], but I considered it in order to probe the reliability of the MC method. The method was applied to a realistic potential corresponding to the $h_{11/2}$ states in the nucleus $^{208}$Pb. By using only 3 random scattering states in the contour with a cutoff energy of 100 MeV, the $h_{11/2}$ eigenvalues were obtained after 50,000 individual runs. The errors were less than 3 keV and the convergency was very stable. The Monte Carlo calculation was also extended to the two-particle system $^{26}$O with three valence shells. In this case the basis contains the resonances $d_{3/2}$ and $f_{7/2}$. To this I added 9 random scattering waves corresponding to the states $d_{3/2}, f_{7/2}$ and also $p_{3/2}$. After 10,000 runs, the energy of the first excited $0^+$ state was obtained within an error of less than 5 keV in comparison with the exact value. I also considered the effect induced by the proper continuum by including only the resonances in the basis. It was found that the bound state is rather well described within this basis, but the resonances are very poorly described without the scattering (continuum) waves.
Appendix A

A.1 Coupling of angular momenta

An useful relation between $6j$-symbol and $3j$-symbols [51]

\[
\sum_{M_3} \left( \begin{array}{ccc} J_1 & J_2 & J_3 \\ M_1 & M_2 & M_3 \end{array} \right) \left( \begin{array}{ccc} J_4 & J_5 & J_6 \\ M_4 & M_5 & -M_3 \end{array} \right) = \sum_{J_6 M_6} (-1)^{J_3+J_6+M_3+M_6(2J_6+1)} \left( \begin{array}{ccc} J_1 & J_2 & J_3 \\ J_4 & J_5 & J_6 \end{array} \right) \times \left( \begin{array}{ccc} J_6 \\ M_6 \end{array} \right) \left( \begin{array}{ccc} J_1 & J_5 & J_6 \\ M_1 & M_5 & -M_6 \end{array} \right) \right), \quad (A.1)
\]

Expansion of $9j$-symbol in $6j$-symbols

\[
\left\{ \begin{array}{ccc} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{array} \right\} = \sum_{j} (-1)^{2j}(2j + 1) \left\{ \begin{array}{ccc} J_{11} & J_{21} & J_{31} \\ J_{12} & J_{22} & J_{32} \\ J_{13} & J_{23} & J_{33} \end{array} \right\} \times \left\{ \begin{array}{ccc} J_{12} & J_{22} & J_{32} \\ J_{13} & J_{23} & J_{33} \end{array} \right\} \times \left\{ \begin{array}{ccc} J_{13} & J_{23} & J_{33} \\ J_{11} & J_{21} & J_{31} \end{array} \right\} \right), \quad (A.2)
\]

Expansion of $9j$-symbol in $3j$-symbols

\[
\left\{ \begin{array}{ccc} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{array} \right\} = \sum_{\text{all } m} \left( \begin{array}{ccc} J_{11} & J_{12} & J_{13} \\ M_{11} & M_{12} & M_{13} \end{array} \right) \left( \begin{array}{ccc} J_{11} & J_{21} & J_{31} \\ M_{11} & M_{21} & M_{31} \end{array} \right) \times \left( \begin{array}{ccc} J_{21} & J_{22} & J_{23} \\ M_{21} & M_{22} & M_{23} \end{array} \right) \left( \begin{array}{ccc} J_{12} & J_{22} & J_{32} \\ M_{12} & M_{22} & M_{32} \end{array} \right) \times \left( \begin{array}{ccc} J_{31} & J_{32} & J_{33} \\ M_{31} & M_{32} & M_{33} \end{array} \right) \left( \begin{array}{ccc} J_{13} & J_{23} & J_{33} \\ M_{13} & M_{23} & M_{33} \end{array} \right) \right), \quad (A.3)
\]
A.2 The MSM equations

Three-particle system

The MSM basis of three-particle system is
\[
\left\{ \left( c_p^\dagger P_\alpha^\dagger \right)_{\alpha_3} |0\right\}.
\]

The dynamical equation is given as
\[
(W(\alpha_3) - \epsilon_p - W(\alpha_2)) \langle \alpha_3 | (c_p^\dagger P_\alpha^\dagger(\alpha_2))_{\alpha_3} |0\rangle
= \sum_{q\beta_2} \left( \sum_r (W(\beta_2) - \epsilon_p - \epsilon_r) A(pq, q\beta_2; \alpha_3) \right) \langle \alpha_3 | (c_p^\dagger P_\beta^\dagger(\beta_2))_{\alpha_3} |0\rangle,
\]
where
\[
A(pq, q\beta_2; \alpha_3) = \hat{\alpha}_2 \hat{\beta}_2 \left\{ \begin{array}{ccc}
p & q & \beta_2 \\
\alpha_2 & \alpha_2 & \alpha_2
\end{array} \right\} Y(ij; \alpha_2) Y(k\ell; \beta_2),
\]
with \( \hat{\alpha}_2 = \sqrt{2J_{\alpha_2} + 1} \). The corresponding overlap matrix is
\[
\langle 0 | (c_p^\dagger P_\beta^\dagger(\beta_2))_{\alpha_3}^\dagger (c_p^\dagger P_\alpha^\dagger(\alpha_2))_{\alpha_3} |0\rangle = \delta_{pq} \delta_{\alpha_2,\beta_2} + \sum_r A(pq, q\beta_2; \alpha_3).
\]

Four-particle system

The four-particle MSM basis is
\[
\left\{ \left( P_\alpha^\dagger(\alpha_2) P_\beta^\dagger(\beta_2) \right)_{\alpha_4} |0\right\},
\]
in which \( \alpha_2 \leq \beta_2 \). The dynamical matrix is
\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | (P_\alpha^\dagger(\alpha_2) P_\beta^\dagger(\beta_2))_{\alpha_4} |0\rangle
= \sum_{\gamma_2,\delta_2} \left( \sum_{ijkl} \frac{-1}{1 + \delta_{\gamma_2,\delta_2}} \sum \right) \left( W(\gamma_2) + W(\delta_2) - \epsilon_i - \epsilon_j - \epsilon_k - \epsilon_l \right)
\times A(ijkl, \alpha_2 \beta_2 \gamma_2 \delta_2; \alpha_4) \langle \alpha_4 | (P_\beta^\dagger(\gamma_2) P_\delta^\dagger(\delta_2))_{\alpha_4} |0\rangle,
\]
where
\[
A(ijkl, \alpha_2 \beta_2 \gamma_2 \delta_2; \alpha_4) = \hat{\alpha}_2 \hat{\beta}_2 \hat{\gamma}_2 \hat{\delta}_2
\times Y(ij; \alpha_2) Y(kl; \beta_2) Y(ik; \gamma_2) Y(jl; \delta_2) \left\{ \begin{array}{ccc}
i & j & \alpha_2 \\
k & l & \beta_2 \\
\gamma_2 & \delta_2 & \alpha_4
\end{array} \right\},
\]
and the overlap matrix is

\[
\langle 0 | (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4}^{\dagger} (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle = \delta_{\alpha_2 \gamma_2} \delta_{\beta_2 \delta_2} \\
+ (-1)^{\alpha_2 + \beta_2 - \alpha_4} \delta_{\alpha_2 \gamma_2} \delta_{\beta_2 \delta_2} - \sum_{ijkl} A(ijkl; \alpha_2 \beta_2 \gamma_2 \delta_2). \tag{A.7}
\]

### A.3 The MSM with proton-neutron pair

#### Two-proton two-neutron system

The MSM basis of two-proton two-neutron system is constructed as

\[
\left\{ \langle P^\dagger(\alpha_2)P^\dagger(\beta_2) \rangle_{\alpha_4} | 0 \rangle \right\} \oplus \left\{ \langle P^\dagger(\alpha_2)P^\dagger(\beta_2) \rangle_{\alpha_4} | 0 \rangle \right\},
\]

where \( \alpha_2 \leq \beta_2 \). The corresponding dynamical matrix is

\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle \\
= \sum_{\gamma_2 \leq \delta_2} \left\{ \sum_{p_1 p_2 n_1 n_2} (-1)^{\frac{(W(\gamma_2) + W(\delta_2) - \epsilon_{p_1} - \epsilon_{p_2} - \epsilon_{n_1} - \epsilon_{n_2})}{1 + \delta_{\gamma_2 \delta_2}}} \right. \\
\times \langle \mathcal{A}_1 + \mathcal{A}_2 \rangle \left\langle \alpha_4 | (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} | 0 \rangle \right\} \\
+ \sum_{\gamma_2 \leq \delta_2} \left\{ \sum_{p_1 p_2 n_1 n_2} (W(\gamma_2) + W(\delta_2) - \epsilon_{p_1} - \epsilon_{p_2} - \epsilon_{n_1} - \epsilon_{n_2}) \\
\times \mathcal{B}_1 \right\} \langle \alpha_4 | (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} | 0 \rangle;
\]

\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2)) \langle \alpha_4 | (P^\dagger(\alpha_2)P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle \\
= \sum_{\gamma_2 \leq \delta_2} \left\{ \sum_{p_1 p_2 n_1 n_2} \frac{(W(\gamma_2) + W(\delta_2) - \epsilon_{p_1} - \epsilon_{p_2} - \epsilon_{n_1} - \epsilon_{n_2})}{1 + \delta_{\gamma_2 \delta_2}} \right. \\
\times \mathcal{B}_2 \left\langle \alpha_4 | (P^\dagger(\gamma_2)P^\dagger(\delta_2))_{\alpha_4} | 0 \rangle \right\}.
\tag{A.8}
\]

where

\[
\mathcal{A}_1 = (-1)^{2p_1 + n_1 + n_2 + \beta_2 + \delta_2} \hat{\alpha}_2 \hat{\beta}_2 \hat{\gamma}_2 \hat{\delta}_2 \\
\times \left\{ \begin{array}{ccc}
\begin{array}{ccc}
p_1 & n_1 & \alpha_2 \\
n_2 & p_2 & \beta_2 \\
\gamma_2 & \delta_2 & \alpha_4
\end{array}
\end{array} \right\}
\times X(p_1 n_1; \alpha_2) X(p_2 n_2; \beta_2) X(p_1 n_2; \gamma_2) X(p_2 n_1; \delta_2),
\]
\[ A_2 = (-1)^{2p_1+n_1+n_2+\beta_2+\delta_2+\alpha_4} \alpha_2 \beta_2 \hat{\gamma}_2 \hat{\delta}_2 \begin{pmatrix} \frac{p_1 n_1}{n_2} & \frac{n_1}{p_2} & \frac{n_1}{\beta_2} & \frac{n_1}{\delta_2} & \frac{n_1}{\alpha_4} \\ \frac{p_2}{n_2} & \frac{n_2}{\beta_2} & \frac{n_2}{\delta_2} & \frac{n_2}{\alpha_4} \end{pmatrix} \times X(p_1 n_1; \alpha_2) X(p_2 n_2; \beta_2) X(p_2 n_1; \gamma_2) X(p_1 n_2; \delta_2), \]

\[ B_1 = \hat{\alpha}_2 \hat{\beta}_2 \hat{\gamma}_2 \hat{\delta}_2 \begin{pmatrix} \frac{p_1}{n_1} & \frac{n_1}{\beta_2} & \frac{n_1}{\alpha_2} & \frac{n_1}{\alpha_2} \\ \frac{p_2}{n_2} & \frac{n_2}{\beta_2} & \frac{n_2}{\alpha_2} \end{pmatrix} \times X(p_1 n_1; \alpha_2) X(p_2 n_2; \beta_2) Y(p_1 p_2; \gamma_2) Y(n_1 n_2; \delta_2), \]

\[ B_2 = \hat{\alpha}_2 \hat{\beta}_2 \hat{\gamma}_2 \hat{\delta}_2 \begin{pmatrix} \frac{p_1}{n_1} & \frac{n_1}{\beta_2} & \frac{n_1}{\alpha_2} & \frac{n_1}{\alpha_2} \\ \frac{p_2}{n_2} & \frac{n_2}{\beta_2} \end{pmatrix} \times Y(p_1 p_2; \alpha_2) Y(n_1 n_2; \beta_2) X(p_1 n_1; \gamma_2) X(p_2 n_2; \delta_2). \]

The overlap matrices are given as

\[
\langle 0 \mid \left( P^\dagger(\gamma_2) P^\dagger(\delta_2) \right)^\dagger \left( P^\dagger(\alpha_2) P^\dagger(\beta_2) \right) \alpha \mid 0 \rangle = \delta_{\alpha_2, \gamma_2} \delta_{\beta_2, \delta_2} + (-1)^{\alpha_2 + \beta_2 + \alpha_4} \delta_{\alpha_2, \gamma_2} \delta_{\beta_2, \delta_2} - \sum_{p_1 p_2 n_1 n_2} (A_1 + A_2) \]

\[
\langle 0 \mid \left( P^\dagger(\gamma_2) P^\dagger(\delta_2) \right)^\dagger \left( P^\dagger(\alpha_2) P^\dagger(\beta_2) \right) \alpha \mid 0 \rangle = \sum_{p_1 p_2 n_1 n_2} B_1 \]

\[
\langle 0 \mid \left( P^\dagger(\gamma_2) P^\dagger(\delta_2) \right)^\dagger \left( P^\dagger(\alpha_2) P^\dagger(\beta_2) \right) \alpha \mid 0 \rangle = \delta_{\alpha_2, \gamma_2} \delta_{\beta_2, \delta_2}. \]

(A.9)

**Three-proton three-neutron system**

The MSM basis of three-proton three-neutron system is

\[
\left\{ \left( P^\dagger(\alpha_2) P^\dagger(\alpha_4) \right) \alpha_6 \mid 0 \rangle \right\}.
\]
A.3. THE MSM WITH PROTON-NEUTRON PAIR

The full dynamical matrix is

\[
(W(\alpha_0) - W(\alpha_2) - W(\alpha_4)) \langle \alpha_0 | (P^\dagger(\alpha_2)P^\dagger(\alpha_4))_{\alpha_0} | 0 \rangle \\
= \sum_{\beta_2, \beta_4} \langle \alpha_0 | (P^\dagger(\beta_2)P^\dagger(\beta_4))_{\alpha_0} | 0 \rangle \left\{ \sum_{A_2} (W(\alpha_0) - W(\alpha_2) - W(A_2)) \times \hat{A} \\
+ \sum_{p_1 p_2 p_3 n_1 A_2 p_2 B_2 n_1} (W(\beta_2) + W(C_{2p}) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{p_3} - \varepsilon_{n_1}) \times \hat{B}_1 \\
+ \sum_{p_1 n_1 n_2 n_3 A_2 p_2 B_2 n_2 D_{2n}} (W(\beta_2) + W(D_{2n}) - \varepsilon_{p_1} - \varepsilon_{n_1} - \varepsilon_{n_2} - \varepsilon_{n_3}) \times \hat{B}_2 \right\},
\]

(A.10)

with

\[
\hat{A} = \hat{a}_4 \hat{b}_4 \left\{ \frac{\alpha_2}{\beta_2} \frac{A_2}{\alpha_6} \frac{\alpha_4}{A_4} \right\} Y(\alpha_2; \beta_2; \alpha_4)F(A_2; \alpha_2; \beta_4),
\]

\[
\hat{B}_1 = \sum_{X_4} (-1)^{p_3 + n_1 + \alpha_2 + \beta_2 + A_{2p} + X_4} \hat{a}_4 \hat{b}_4 \hat{C}_2p \hat{d}_4 \hat{X}_4
\]

\[
\times \left\{ \frac{p_1}{\beta_2} \frac{n_1}{\alpha_4} \frac{\alpha_2}{A_2p} \frac{A_2}{C_{2p}} \frac{X_4}{X_4} \right\}
\times \left\{ \frac{\alpha_2}{\beta_2} \frac{A_2}{\alpha_6} \frac{X_4}{X_4} \right\}
\times \left\{ \frac{\beta_2}{\beta_2} \frac{C_{2p}}{\alpha_6} \frac{X_4}{X_4} \right\}
\times X(p_1 n_1; \alpha_2)X(p_3 n_1; \beta_2)Y(p_2 p_3; A_{2p})Y(p_1 p_2; C_{2p})
\times X(A_{2p}; B_{2n}; \alpha_4)F(C_{2p}; B_{2n}; \beta_4),
\]

\[
\hat{B}_2 = \sum_{X_4} (-1)^{n_2 + n_1 + \alpha_2 + \beta_2 + B_{2n} + \alpha_4 + \beta_4} \hat{a}_4 \hat{b}_4 \hat{B}_{2n} \hat{D}_{2n} \hat{\beta}_4 \hat{X}_4
\]

\[
\times \left\{ \frac{p_1}{\beta_2} \frac{n_1}{\alpha_4} \frac{\alpha_2}{B_{2n}} \frac{B_{2n}}{B_{2n}} \frac{X_4}{X_4} \right\}
\times \left\{ \frac{\alpha_2}{\beta_2} \frac{B_{2n}}{\alpha_6} \frac{X_4}{X_4} \right\}
\times \left\{ \frac{\beta_2}{\beta_2} \frac{D_{2n}}{\alpha_6} \frac{X_4}{X_4} \right\}
\times X(p_1 n_1; \alpha_2)X(p_1 n_3; \beta_2)Y(n_2 n_3; B_{2n})Y(n_1 n_2; D_{2n})
\times X(A_{2p}; B_{2n}; \alpha_4)F(A_{2p}; D_{2n}; \beta_4),
\]

where \(X_4\) is a integer runs through all the possible angular momentum in the 9\(j\) coefficients. The overlap matrix can be written as

\[
\langle 0 | (P^\dagger(\beta_2)P^\dagger(\beta_4)) \rangle_{\alpha_0} \langle (P^\dagger(\alpha_2)P^\dagger(\alpha_4)) \rangle_{\alpha_0} | 0 \rangle = \delta_{\alpha_2 \beta_2} \delta_{\alpha_4 \beta_4} + \sum_{A_2} \hat{A}'
\]

\[
+ \sum_{p_1 p_2 p_3 n_1 A_{2p} B_{2n} C_{2p}} \hat{B}_1 + \sum_{p_1 n_1 n_2 n_3 A_{2p} B_{2n} D_{2n}} \hat{B}_2 + \sum_{A_{2p} B_{2n} C_{2p}} \hat{C}, \quad (A.11)
\]
APPENDIX A. APPENDIX

with

\[ \hat{A}' = \hat{a}_4 \beta_4 \left\{ \begin{array}{ccc} a_2 & A_2 & \beta_4 \\ \beta_2 & \alpha_6 & \alpha_4 \end{array} \right\} F(A_2 \beta_2; \alpha_4) F(A_2 \beta_2; \beta_4), \]

\[ \mathbb{C} = \sum_{X_i} \hat{a}_4 \beta_4 X_i \left\{ \begin{array}{ccc} a_2 & A_2 & X_4 \\ \beta_2 & \alpha_6 & \alpha_4 \end{array} \right\} \left\{ \begin{array}{ccc} \beta_2 & C_2 & X_4 \\ \beta_4 & \alpha_6 & \beta_4 \end{array} \right\} \times Y(A_2 B_2; \alpha_4) F(C_2 B_2; \beta_4) \Omega(A_2 \alpha_2, C_2 \beta_2; X_4). \]

The projection of the MSM basis with three pairs of two-particle states has the form

\[ F(\alpha_2 \beta_2 \gamma_2; \alpha_6) = \sum_{\alpha_4} F(\alpha_2 \alpha_4; \alpha_6) F(\beta_2 \gamma_2; \alpha_4). \quad (A.12) \]

The cosine of the angle between a three pairs MSM basis and the physical state is

\[ x(\alpha_2 \beta_2 \gamma_2; \alpha_6) = F(\alpha_2 \beta_2 \gamma_2; \alpha_6)/N(\alpha_2 \beta_2 \gamma_2; \alpha_6), \quad (A.13) \]

where \( N(\alpha_2 \beta_2 \gamma_2; \alpha_6) \) is the norm of the basis vector and can be obtained from

\[ N^2(\alpha_2 \beta_2 \gamma_2; \alpha_6) = \sum_{\alpha_4} F(\beta_2 \gamma_2; \alpha_2) |\langle \alpha_2 \alpha_4; \alpha_6 | \alpha_2 \beta_4; \alpha_6 \rangle F(\beta_2 \gamma_2; \beta_4). \quad (A.14) \]

**Four-proton four-neutron system**

The MSM basis of four-proton four-neutron system is

\[ \left\{ |(P^1(\alpha_4)P^1(\beta_4))_\alpha \rangle |0 \rangle \right\}, \]

where \( \alpha_4 \leq \beta_4 \). The dynamical equation can be expressed as

\[ (W(\alpha s) - W(\alpha_4) - W(\beta_4))(\alpha_8 |(P^1(\alpha_4)P^1(\beta_4))_\alpha \rangle |0 \rangle) \]

\[ = \sum_{\gamma_4 \leq \delta_4} \frac{1}{1 + \delta_4} \langle \alpha_8 |(P^1(\gamma_4)P^1(\delta_4))_\alpha \rangle |0 \rangle \sum_{A_2 p, B_2 n, C_2 p, D_2 n} \times \left\{ (W(\gamma_2) + W(\delta_2) - W(A_2 p) - W(B_2 n) - W(C_2 p) - W(D_2 n))(A_1 + A_2) \right. \]

\[ + \sum_{E_2 p, G_2 p, P_1 p, P_3 P_4} (W(E_2 p) + W(G_2 p) - \varepsilon_{p_1} - \varepsilon_{p_2} - \varepsilon_{p_3} - \varepsilon_{p_4})(B_1 + B_2) \]

\[ + \sum_{F_2 n, H_2 n, n_1 n_2 n_3 n_4} (W(F_2 n) + W(H_2 n) - \varepsilon_{n_1} - \varepsilon_{n_2} - \varepsilon_{n_3} - \varepsilon_{n_4})(C_1 + C_2) \left. \right\}. \quad (A.15) \]
where

\[
\mathbb{A}_1 = (-1)^{B_{2n} + D_{2n} + \beta_i + \delta_i} \delta_4 \gamma_4 \delta_4 \left\{ \begin{array}{ccc} A_{2p} & B_{2n} & \alpha_4 \\ D_{2n} & C_{2p} & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{array} \right\} \\
\times X(A_{2p} B_{2n}; \alpha_4) X(C_{2p} D_{2n}; \beta_4) F(A_{2p} D_{2n}; \gamma_4) F(C_{2p} B_{2n}; \delta_4),
\]

\[
\mathbb{A}_2 = (-1)^{B_{2n} + D_{2n} + \beta_i + \delta_i} \delta_4 \gamma_4 \delta_4 \left\{ \begin{array}{ccc} A_{2p} & B_{2n} & \alpha_4 \\ D_{2n} & C_{2p} & \beta_4 \\ \delta_4 & \gamma_4 & \alpha_8 \end{array} \right\} \\
\times X(A_{2p} B_{2n}; \alpha_4) X(C_{2p} D_{2n}; \beta_4) F(C_{2p} B_{2n}; \gamma_4) F(A_{2p} D_{2n}; \delta_4),
\]

\[
\mathbb{B}_1 = \sum_{X_4 Y_4} (-1)^{A_{2p} \epsilon_2 p_2 C_2 p_2 \epsilon_4 \gamma_4 \delta_4 \hat{X}_4 \hat{Y}_4^2} \\
\times \left( \begin{array}{ccc} p_1 & p_2 & A_{2p} \\ p_3 & p_4 & C_{2p} \end{array} \right) \left( \begin{array}{ccc} A_{2p} & B_{2n} & \alpha_4 \\ D_{2n} & C_{2p} & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{array} \right) \\
\times X(A_{2p} B_{2n}; \alpha_4) X(C_{2p} D_{2n}; \beta_4) F(E_{2p} D_{2n}; \gamma_4) F(G_{2p} D_{2n}; \delta_4) \\
\times Y(p_1 p_2; A_{2p}) Y(p_3 p_4; C_{2p}) Y(p_1 p_3; E_{2p}) Y(p_2 p_4; G_{2p}),
\]

\[
\mathbb{B}_2 = \sum_{X_4 Y_4} (-1)^{1 + B_{2n} + D_{2n} + Y_4} \hat{A}_{2p} \epsilon_2 p_2 C_2 p_2 \epsilon_4 \gamma_4 \delta_4 \hat{X}_4 \hat{Y}_4^2 \\
\times \left( \begin{array}{ccc} p_1 & p_2 & A_{2p} \\ p_3 & p_4 & C_{2p} \end{array} \right) \left( \begin{array}{ccc} A_{2p} & B_{2n} & \alpha_4 \\ D_{2n} & C_{2p} & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{array} \right) \\
\times X(A_{2p} B_{2n}; \alpha_4) X(C_{2p} D_{2n}; \beta_4) F(E_{2p} D_{2n}; \gamma_4) F(G_{2p} B_{2n}; \delta_4) \\
\times Y(p_1 p_2; A_{2p}) Y(p_3 p_4; C_{2p}) Y(p_1 p_3; E_{2p}) Y(p_2 p_4; G_{2p}),
\]

\[
\mathbb{C}_1 = \sum_{X_4 Y_4} (-1)^{B_{2n} \epsilon_2 p_2 C_2 p_2 \epsilon_4 \gamma_4 \delta_4 \hat{X}_4 \hat{Y}_4^2} \\
\times \left( \begin{array}{ccc} n_1 & n_2 & B_{2n} \\ n_3 & n_4 & D_{2n} \end{array} \right) \left( \begin{array}{ccc} A_{2p} & B_{2n} & \alpha_4 \\ D_{2n} & C_{2p} & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{array} \right) \\
\times X(A_{2p} B_{2n}; \alpha_4) X(C_{2p} D_{2n}; \beta_4) F(A_{2p} F_{2n}; \gamma_4) F(C_{2p} H_{2n}; \delta_4) \\
\times Y(n_1 n_2; B_{2n}) Y(n_3 n_4; D_{2n}) Y(n_1 n_3; F_{2n}) Y(n_2 n_4; H_{2n}),
\]
The corresponding overlap matrix is

$$\mathbb{C}_2 = \sum_{X_4 Y_4} (-1)^{1+\alpha_{2p}+\alpha_{4}} X_{2n} \tilde{D}_{2n} \tilde{F}_{2n} \tilde{H}_{2n} \alpha_{4} \beta_{4} \gamma_{4} \delta_{4} \tilde{X}_{2} \tilde{Y}_{2}$$

$$\times \left\{ \begin{array}{ccc}
\alpha_{1} & \beta_{1} & \\
\gamma_{1} & \delta_{1} & \\
\alpha_{2} & \beta_{2} & \\
\gamma_{2} & \delta_{2}
\end{array} \right\} \left\{ \begin{array}{ccc}
\alpha_{3} & \beta_{3} & \\
\gamma_{3} & \delta_{3} & \\
\alpha_{4} & \beta_{4} & \\
\gamma_{4} & \delta_{4}
\end{array} \right\} \times X(A_{2p} B_{2n} C_{2p} D_{2n}) F(C_{2p} F_{2n} \gamma_{4}) F(A_{2p} H_{2n} \delta_{4})$$

$$\times Y(n_{1} n_{2}; B_{2n}) Y(n_{3} n_{4}; D_{2n}) Y(n_{1} n_{3}; F_{2n}) Y(n_{2} n_{4}; H_{2n}).$$

The corresponding overlap matrix is

$$\langle 0 \left| P^{\dagger} (\gamma_{4}) P^{\dagger} (\delta_{4}) \right| 0 \rangle_{\alpha_{8}} = \delta_{\alpha_{4} \gamma_{4}} \delta_{\beta_{4} \delta_{4}} (-1)^{\alpha_{4} + \beta_{4} + \alpha_{8} + \delta_{\alpha_{4} \delta_{4}} \gamma_{4}}$$

$$+ \sum_{A_{2p}, B_{2n}, C_{2p}, D_{2n}} \left\{ \begin{array}{ccc}
\alpha_{1} & \beta_{1} & \\
\gamma_{1} & \delta_{1} & \\
\alpha_{2} & \beta_{2} & \\
\gamma_{2} & \delta_{2}
\end{array} \right\} \left\{ \begin{array}{ccc}
\alpha_{3} & \beta_{3} & \\
\gamma_{3} & \delta_{3} & \\
\alpha_{4} & \beta_{4} & \\
\gamma_{4} & \delta_{4}
\end{array} \right\} \left\{ \begin{array}{c}
\alpha_{5} & \beta_{5} & \\
\gamma_{5} & \delta_{5}
\end{array} \right\} \left\{ \begin{array}{c}
\alpha_{6} & \beta_{6} & \\
\gamma_{6} & \delta_{6}
\end{array} \right\} + \sum_{E_{2p}, G_{2p}, p_{1}, p_{2}, p_{3}, p_{4}}$$

$$\times \sum_{F_{2n}, H_{2n}, n_{1}, n_{2}, n_{3}, n_{4}} \sum_{p_{1}, p_{2}, p_{3}, p_{4}} \sum_{n_{1}, n_{2}, n_{3}, n_{4}} \sum_{F_{2n}, H_{2n}, n_{1}, n_{2}, n_{3}, n_{4}} \sum_{E_{2p}, G_{2p}, p_{1}, p_{2}, p_{3}, p_{4}} \sum_{n_{1}, n_{2}, n_{3}, n_{4}} \sum_{F_{2n}, H_{2n}, n_{1}, n_{2}, n_{3}, n_{4}} \sum_{E_{2p}, G_{2p}, p_{1}, p_{2}, p_{3}, p_{4}} \sum_{n_{1}, n_{2}, n_{3}, n_{4}}$$

$$= \sum_{X_4 Y_4} \tilde{A}_{2p} \tilde{B}_{2n} \tilde{C}_{2p} \tilde{D}_{2n} \tilde{E}_{2p} \tilde{F}_{2n} \tilde{G}_{2p} \tilde{H}_{2n} \alpha_{4} \beta_{4} \gamma_{4} \delta_{4} \tilde{X}_{2} \tilde{Y}_{2}$$

$$\times \left\{ \begin{array}{ccc}
p_{1} & p_{2} & A_{2p} \\
p_{3} & p_{4} & C_{2p} \\
E_{2p} & G_{2p} & X_{4}
\end{array} \right\} \left\{ \begin{array}{ccc}
n_{1} & n_{2} & B_{2n} \\
n_{3} & n_{4} & D_{2n} \\
F_{2n} & H_{2n} & Y_{4}
\end{array} \right\} \left\{ \begin{array}{ccc}
A_{2p} & B_{2n} & \alpha_{4} \\
C_{2p} & D_{2n} & \beta_{4} \\
E_{2p} & F_{2n} & \alpha_{8} \\
G_{2p} & H_{2n} & \beta_{8} \\
X_{4} & Y_{4} & \gamma_{4} \\
\dot{\alpha}_{4} & \dot{\beta}_{4} & \gamma_{4} \\
\dot{\alpha}_{8} & \dot{\beta}_{8} & \gamma_{8}
\end{array} \right\} \times X(A_{2p} B_{2n} C_{2p} D_{2n}; \alpha_{4}) X(C_{2p} F_{2n}; \beta_{4}) F(E_{2p} F_{2n}; \gamma_{4}) F(G_{2p} H_{2n}; \delta_{4})$$

$$\times Y(p_{1} p_{2}; A_{2p}) Y(p_{3} p_{4}; C_{2p}) Y(p_{1} p_{3}; E_{2p}) Y(p_{2} p_{4}; G_{2p})$$

$$\times Y(n_{1} n_{2}; B_{2n}) Y(n_{3} n_{4}; D_{2n}) Y(n_{1} n_{3}; F_{2n}) Y(n_{2} n_{4}; H_{2n}).$$

The projection of the MSM basis with four pairs of two-particle states upon the physical state can be obtained by

$$F(\alpha_{2} \beta_{2} \gamma_{2} \delta_{2}; \alpha_{8}) = \sum_{\alpha_{4} \beta_{4}} F(\alpha_{4} \beta_{4}; \alpha_{8}) F(\alpha_{2} \beta_{2}; \alpha_{4}) F(\gamma_{2} \delta_{2}; \beta_{4}),$$

$$N^{2}(\alpha_{2} \beta_{2} \gamma_{2} \delta_{2}; \alpha_{8}) = \sum_{\alpha_{4} \beta_{4}} \sum_{\gamma_{4} \delta_{4}} F(\alpha_{2} \beta_{2}; \alpha_{4}) F(\gamma_{2} \delta_{2}; \beta_{4}) F(\gamma_{4} \delta_{4}; \alpha_{8})$$

$$\times F(\alpha_{2} \beta_{2}; \gamma_{4}) F(\gamma_{2} \delta_{2}; \beta_{4}),$$

and the cosine of the angle in between is given by

$$\cos(\alpha_{2} \beta_{2} \gamma_{2} \delta_{2}; \alpha_{8}) = F(\alpha_{2} \beta_{2} \gamma_{2} \delta_{2}; \alpha_{8}) / N(\alpha_{2} \beta_{2} \gamma_{2} \delta_{2}; \alpha_{8}).$$
A.4 The MSM with isospin symmetry

We define special notations for 6j-symbols and 9j-symbols as

\[
\begin{bmatrix}
  c_1 & c_2 & \alpha_2 \\
  c_3 & c_4 & \beta_2 \\
  \gamma_2 & \delta_2 & \alpha_4
\end{bmatrix} = \hat{T}_{\alpha_2} \hat{T}_{\beta_2} \hat{T}_{\gamma_2} \hat{T}_{\delta_2}
\]

\[
\times \begin{bmatrix}
  J_{e_1} & J_{e_2} & J_{e_4} \\
  J_{e_3} & J_{e_4} & J_{e_6} \\
  J_{\gamma_2} & J_{\delta_2} & J_{\alpha_4}
\end{bmatrix}
\begin{bmatrix}
  T_{e_1} & T_{e_2} & T_{e_4} \\
  T_{e_3} & T_{e_4} & T_{e_6} \\
  T_{\gamma_2} & T_{\delta_2} & T_{\alpha_4}
\end{bmatrix}, \quad (A.20)
\]

\[
\begin{bmatrix}
  \alpha_2 & A_2 & \beta_4 \\
  \beta_2 & \alpha_6 & \beta_4 \\
  \gamma_2 & \delta_2 & \alpha_4
\end{bmatrix} = \hat{T}_{\alpha_4} \hat{T}_{\beta_4} \hat{T}_{\gamma_4} \hat{T}_{\delta_4}
\]

\[
\times \begin{bmatrix}
  J_{\alpha_2} & J_{A_2} & J_{\beta_4} \\
  J_{\beta_2} & J_{\alpha_6} & J_{\beta_4} \\
  J_{\gamma_2} & J_{\delta_2} & J_{\alpha_4}
\end{bmatrix}
\begin{bmatrix}
  T_{\alpha_2} & T_{A_2} & T_{\beta_4} \\
  T_{\beta_2} & T_{\alpha_6} & T_{\beta_4} \\
  T_{\gamma_2} & T_{\delta_2} & T_{\alpha_4}
\end{bmatrix}, \quad (A.21)
\]

**Four-particle system**

The dynamical matrix of four-particle system is

\[
(W(\alpha_4) - W(\alpha_2) - W(\beta_2))\langle \alpha_4 | (P^\dagger(\alpha_2)P^\dagger(\beta_2)) | \alpha_4 \rangle | 0 \rangle
= \sum_{\gamma_2 \leq \delta_2} \frac{-1}{1 + \delta_{\gamma_2 \delta_2}} \sum_{c_1, c_2, c_3, c_4} (W(\gamma_2) + W(\delta_2) - \varepsilon_{c_1} - \varepsilon_{c_2} - \varepsilon_{c_3} - \varepsilon_{c_4})
\times \mathbb{A} \times \langle \alpha_4 | (P^\dagger(\gamma_2)P^\dagger(\delta_2)) | \alpha_4 \rangle | 0 \rangle, \quad (A.22)
\]

with

\[
\mathbb{A} = Y(c_1 c_2; \alpha_2)Y(c_3 c_4; \beta_2)Y(c_1 c_3; \gamma_2)Y(c_2 c_4; \delta_2)
\begin{bmatrix}
  c_1 & c_2 & \alpha_2 \\
  c_3 & c_4 & \beta_2 \\
  \gamma_2 & \delta_2 & \alpha_4
\end{bmatrix}.
\]

And the overlap matrix is

\[
\langle 0 | (P^\dagger(\alpha_2)P^\dagger(\beta_2)) | \alpha_4 \rangle | 0 \rangle
= \delta_{\alpha_2 \gamma_2} \delta_{\beta_2 \delta_2} + (-1)^{J_{\alpha_2} + J_{\beta_2} + J_{\alpha_4} + T_{\alpha_2} + T_{\beta_2} + T_{\alpha_4}} \delta_{\alpha_2 \beta_2} \delta_{\beta_2 \gamma_2} - \sum_{c_1, c_2, c_3, c_4} \mathbb{A}. \quad (A.23)
\]

**Six-particle system**

The dynamical matrix of six-particle system is

\[
(W(\alpha_6) - W(\alpha_2) - W(\beta_4))\langle \alpha_6 | (P^\dagger(\alpha_2)P^\dagger(\beta_4)) | \alpha_6 \rangle | 0 \rangle
= \sum_{\beta_2 \beta_4} \sum_{A_2} (W(\beta_4) - W(\alpha_2) - W(A_2)) \mathbb{A} \times \langle \alpha_6 | (P^\dagger(\beta_4)P^\dagger(\beta_4)) | \alpha_6 \rangle | 0 \rangle, \quad (A.24)
\]
where
\[ \mathcal{A} = Y(A_2 \beta_2; \alpha_4) F(A_2 \alpha_2; \beta_4) \begin{bmatrix} \alpha_2 & A_2 & \beta_4 \\ \beta_2 & \alpha_6 & \alpha_4 \end{bmatrix}. \]

And the overlap matrix is
\[ \langle 0 | (P^\dagger(\beta_2) P^\dagger(\beta_4))_\alpha \langle P^\dagger(\alpha_2) P^\dagger(\alpha_4) \rangle_{\alpha_4} | 0 \rangle = \delta_{\alpha_2, \beta_2} \delta_{\alpha_4, \beta_4} + \sum_{A_2} \mathcal{A}' + \sum_{A_2 B_2 C_2} \mathbb{B}, \tag{A.25} \]

where
\[ \mathcal{A}' = F(A_2 \alpha_2; \alpha_4) F(A_2 \alpha_2; \beta_4) \begin{bmatrix} \alpha_2 & A_2 & \beta_4 \\ \beta_2 & \alpha_6 & \alpha_4 \end{bmatrix}. \]

\[ \mathbb{B} = \sum_{X_4} Y(A_2 B_2; \alpha_4) F(C_2 B_2; \beta_4) \Omega(A_2 \alpha_2, C_2 \beta_2; X_4) \times \begin{bmatrix} \alpha_2 & A_2 & X_4 \\ B_2 & \alpha_6 & \alpha_4 \end{bmatrix} \begin{bmatrix} \beta_2 & C_2 & X_4 \\ B_2 & \alpha_6 & \beta_4 \end{bmatrix}, \]

with
\[ \Omega(A_2 \alpha_2, C_2 \beta_2; X_4) = \langle 0 | (P^\dagger(A_2) P^\dagger(\alpha_2)) \langle X_4 | (P^\dagger(C_2) P^\dagger(\beta_2))_{\alpha_4} | 0 \rangle - \delta_{A_2 C_2} \delta_{\alpha_2, \beta_2} + (-1)^{J_{A_2} + J_{A_2} + J_{X_4} + T_{A_2} + T_{\alpha_2} + T_{\beta_2}} \delta_{A_2 \beta_2} \delta_{C_2 \alpha_2}. \]

**Eight-particle system**

The dynamical matrix of eight-particle system is
\[ (W(\alpha_8) - W(\alpha_4) - W(\beta_4)) \langle \alpha_8 | (P^\dagger(\alpha_4) P^\dagger(\beta_4)) \rangle_{\alpha_8} | 0 \rangle = \sum_{\gamma_4 \delta_4} \frac{1}{1 + \delta_{\gamma_4 \delta_4}} \left\{ \sum_{A_2 B_2 C_2 D_2} \left( W(\gamma_4) + W(\delta_4) - W(A_2) - W(B_2) - W(C_2) - W(D_2) \right) \times \mathcal{A}' \right\} \langle \alpha_8 | (P^\dagger(\gamma_4) P^\dagger(\delta_4)) \rangle_{\alpha_8} | 0 \rangle, \tag{A.26} \]

where
\[ \mathcal{A} = Y(A_2 B_2; \alpha_4) Y(C_2 D_2; \beta_4) F(A_2 C_2; \gamma_4) F(B_2 D_2; \delta_4) \begin{bmatrix} A_2 & B_2 & \alpha_4 \\ C_2 & D_2 & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{bmatrix}. \]

And the overlap matrix is
\[ \langle 0 | (P^\dagger(\alpha_4) P^\dagger(\beta_4)) \rangle_{\alpha_4} \langle (P^\dagger(\gamma_4) P^\dagger(\delta_4))_{\alpha_8} | 0 \rangle = \delta_{\alpha_4, \gamma_4} \delta_{\beta_4, \delta_4} + (-1)^{J_{\alpha_4} + J_{\beta_4} + J_{\alpha_8} + T_{\alpha_4} + T_{\beta_4} + T_{\alpha_8}} \delta_{\alpha_4, \delta_4} \delta_{\beta_4, \gamma_4} + \sum_{A_2 B_2 C_2 D_2} \mathcal{A}' + \sum_{A_2 B_2 C_2 E_2 F_2} \mathbb{B}_1 + \mathbb{B}_2, \tag{A.27} \]
A.4. THE MSM WITH ISOSPIN SYMMETRY

in which

\[ \mathcal{A}' = F(A_2 B_2; \alpha_4) F(C_2 D_2; \beta_4) F(A_2 C_2; \gamma_4) F(B_2 D_2; \delta_4) \begin{bmatrix} A_2 & B_2 & \alpha_4 \\ C_2 & D_2 & \beta_4 \\ \gamma_4 & \delta_4 & \alpha_8 \end{bmatrix}, \]

\[ \mathbb{B}_1 = \sum_{X_4 Y_4} \begin{bmatrix} A_2 & B_2 & \alpha_4 \\ C_2 & D_2 & \beta_4 \\ X_4 & Y_4 & \alpha_8 \end{bmatrix} \begin{bmatrix} E_2 & B_2 & \gamma_4 \\ F_2 & D_2 & \delta_4 \\ X_4 & Y_4 & \alpha_8 \end{bmatrix} \]

\[ \times Y(A_2 B_2; \alpha_4) Y(C_2 D_2; \beta_4) F(E_2 B_2; \gamma_4) F(F_2 D_2; \delta_4) \Omega(A_2 C_2; E_2 F_2; X_4), \]

\[ \mathbb{B}_2 = \sum_{X_4 Y_4} (-1)^J \gamma_4 + J_{\alpha_4 + J_{\alpha_4} + T_{\alpha_4} + T_{\alpha_4} + T_{\alpha_4}} \begin{bmatrix} A_2 & B_2 & \alpha_4 \\ C_2 & D_2 & \beta_4 \\ X_4 & Y_4 & \alpha_8 \end{bmatrix} \begin{bmatrix} E_2 & B_2 & \delta_4 \\ F_2 & D_2 & \gamma_4 \\ X_4 & Y_4 & \alpha_8 \end{bmatrix} \]

\[ \times Y(A_2 B_2; \alpha_4) Y(C_2 D_2; \beta_4) F(E_2 B_2; \gamma_4) F(F_2 D_2; \delta_4) \Omega(A_2 C_2; E_2 F_2; X_4). \]
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