R-Matrix and Dynamical Theory of Three-Body Resonances

Amy Jane Bartlett MPhys

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Department of Physics
Faculty of Engineering and Physical Sciences
University of Surrey
Guildford
Surrey
GU2 7XH
United Kingdom.

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Abstract

R-matrix theory is applied to three-body resonances by treating the decay as two sequential two-body decays. This allows the decay to proceed through up to three different decay routes, each with an associated width. From the literature it is unclear whether these widths should be combined incoherently or coherently, especially in the case of two-neutron emission.

In this work three-body R-matrix theory is applied to the 1.8 MeV $2^+$ resonance in $^6$He, as the interactions of the two-body subsystems are well known. This resonance can decay via two possible routes, each going through an intermediate state:

(i) $^6$He($2^+$) $\rightarrow$ $^5$He($3/2^-$ g.s.) + $n$ $\rightarrow$ $\alpha + n + n$
(ii) $^6$He($2^+$) $\rightarrow$ $^2n(0^+)$ + $\alpha$ $\rightarrow$ $\alpha + n + n$

Limiting cases of the theory are explored, in particular the sensitivity to the shape of the probability density function (PDF) which describes the shape of the intermediate state. A new formula is developed for the PDF which allows for the choice of optimised boundary conditions. This is particularly important where the intermediate state is a virtual state.

In order to determine whether the widths from the R-matrix decay routes interfere coherently or incoherently, fully dynamical three-body hyperspherical harmonic (HH) calculations are also performed. The HH calculations produce a single value for the total width of the three-body decay. It was found that the coherent and HH widths are in agreement, but both fall short of the experimentally measured value. This is consistent with the calculations for two-proton decay found in the literature.
It seems to me that you need one of two things to successfully complete a PhD, (i) excellent supervision or (ii) the support of family and friends. I have been very fortunate and received both. Consequently there are a lot of people that I need to thank.

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Chapter 1

Introduction

\(^6\)He is considered to be a halo nuclide due to its large interaction radius in collisions with a target nucleus. In [1], Tanihata et al. extracted an interaction radius of 2.18 ± 0.02 fm from the total interaction cross-section. This was much larger than expected, 35% larger than the \(^4\)He interaction radius and 4% larger than that of the \(^6\)Li isobar. The \(^6\)He matter radius is larger than the charge radius, indicating the large radius is due to a ‘neutron skin’ or neutron halo. The halo nature of \(^6\)He has meant that it has been extensively modelled as three bodies; an α-particle core and two valence neutrons. Figure (1.1) illustrates \(^6\)He modelled as these three bodies. \(^6\)He is also called a Borromean nucleus because no two of its constituent bodies form bound states, i.e. \(^5\)He and the ‘di-neutron’. However, \(^6\)He is bound and relatively long-lived as a result of the (weak interaction) β-decay path. It has a half-life of 0.807 seconds. By comparison, the half-life of the particle unbound \(^5\)He, based on its resonance width, is just 7.6 × 10\(^{-22}\) seconds\(^2\). This means that \(^6\)He could be important astrophysically, as will now be explained.

Element production, such as in Big Bang nucleosynthesis and the astrophysical r-process (rapid-neutron-capture process), is impeded by the lack of bound nuclei with

Figure 1.1: \(^6\)He modelled as three-bodies; an α-particle core and two valence neutrons, together with its ground to first excited state and two-neutron separation energies.
mass numbers of 5 and 8. These “mass gaps” can be overcome by the three-particle fusion processes of 3α’s and 2α + n. However, these reactions are relatively slow and so r-process simulations require unphysically high entropy conditions to reproduce observed heavy element abundances. Two-neutron capture reactions on $^4$He and $^6$He could enhance the flow towards heavy nuclei[3, 4].

Görres et al. first estimated the $^4$He($2n,\gamma)^6$He reaction rate[4]. Subsequently, Terasawa et al. found the reaction rate was insufficient to provide a substantial flow towards heavier nuclei[5]. Later, Bartlett et al. re-estimated the reaction rate, taking into account an approximate treatment of a ‘di-neutron’ capture component[6]. This rate was 2-3 orders of magnitude larger than the Görres rate. However, in r-process simulations of the neutrino-heated material above a nascent proto-neutron star, this increase did not significantly affect final element abundances. It was found that $^6$He rapidly photodisintegrated in this high temperature and high entropy environment. Nevertheless, in other possible r-process environments, such as neutron star mergers and prompt supernova shocks, where the entropy and temperature are lower, the $^4$He($2n,\gamma)^6$He reaction may still play an important role.

In the Bartlett work, the resonant component of the reaction rate was calculated by treating the three-body reaction as two sequential two-body reactions, which could proceed by either

\[
\begin{align*}
^4\text{He} + n & \rightarrow ^5\text{He} \\
^5\text{He} + n & \rightarrow ^6\text{He}^* \\
^6\text{He}^* & \rightarrow ^6\text{He} + \gamma,
\end{align*}
\]

or

\[
\begin{align*}
n + n & \rightarrow ^2\text{n} \\
^4\text{He} + ^2\text{n} & \rightarrow ^6\text{He}^* \\
^6\text{He}^* & \rightarrow ^6\text{He} + \gamma.
\end{align*}
\]

Both reactions pass through the well known $2^+$ resonance in $^6$He. In the second case a localised di-neutron, $^2\text{n}$, is assumed to be formed and then captured on to the $^4$He. The “di-neutron” was approximated as a resonant state occurring at zero energy. One of the questions addressed by this work is how realistic is this treatment of the two-neutron system?

In the same way that the $^6$He $2^+$ state could decay by two-neutron emission, proton rich nuclei can decay by the emission of 2 protons; so called two-proton radioactivity. In 1960 Goldansky first predicted the existence of nuclei which naturally decay by the emission of one or two protons[7]. It was not until 1982 that the first experimental evidence of proton decay was found[8]. Then, in 2002, the first two-proton radioactivity
was observed in \(^{45}\text{Fe}\)^{[9, 10]. Since then, several proton rich nuclei have been shown to decay in this way, including \(^{94}\text{Ag}\) which has both one- and two-proton decay open to it\(^{[11]}\). If both protons are emitted simultaneously this is considered to be “true” two-proton radioactivity. The experimental signature of this for spherical nuclei is predicted to be that both protons will have almost the same energy\(^{[7, 12, 13]}\).

A theory that has been applied extensively to two-body reactions is R-matrix theory. One of the approximations built into traditional R-matrix theory is that three-body reactions do not occur. However, Lane and Thomas\(^{[14]}\) suggest that three-body reactions can be considered within the R-matrix framework if treated as two sequential two-body reactions. Barker has further developed the three-body R-matrix formalism\(^{[15]}\) and applied it to various nuclei\(^{[15, 16, 17]}\), including two-proton radioactive ones. These nuclei are modelled as a core with two valence protons. Since these reactions are treated as two sequential (two-body) decays, a valence proton or the core may be emitted first. This is called sequential and simultaneous emission of the two protons, respectively. Both the sequential and simultaneous decays have an associated decay lifetime and width. These must then be combined to get the total decay width. It is in general unclear if the two widths combine coherently or incoherently\(^{[18]}\).

Barker has found that in general the maximally coherent width is less than or equal to the experimental width in the case of di-proton decay\(^{[18]}\). This is better agreement than that obtained from the incoherent width. In the one di-neutron case looked at by Barker of \(^{5}\text{H}\), it is found that the coherent width is too large and the incoherent width agrees better with the experimental value\(^{[18]}\). Barker also investigates resonances in \(^{6}\text{Be}\) and \(^{7}\text{B}\), which can be modelled as \(\alpha + \alpha + n\) and \(\alpha + \alpha + p\) respectively. In this case it was found that for most of these resonances the coherent width gave a value closer to the experimental width\(^{[18]}\). Barker concludes that agreement with experimental values is possible using R-matrix theory if coherence is assumed. However this then reduces the predictive power of R-matrix theory unless one of the decay routes is dominant\(^{[18]}\).

The \(^{5}\text{H}\) result is at odds with Barker’s findings for the other resonances. Therefore in this work the theory will be applied to the better understood \(2^+\) resonance in \(^{6}\text{He}\), and compared with the results from fully dynamical three-body calculations in an attempt to ascertain how quantitative the R-matrix theory is, and how the R-matrix widths should be combined to get the total width.

The width of the 1.8 MeV \(^{6}\text{He}\) \(2^+\) state was measured in 1965 by Ajzenberg-Selove et al. to be \(\Gamma = 113 \pm 20\) keV\(^{[19]}\). Although the \(2^+\) state has been observed many times since then, there does not seem to be any other published values for the width of this state. Although Aumann et al. found that the width they observe is “consistent with the known width of the state”\(^{[20]}\). Various theoretical methods have been employed to calculate the width of this three-body resonance. In \([21]\), Csótó finds a width of \(\Gamma = 60\) keV using the complex scaling method. This width is only \(\approx 50\%\) of the experimental width. In \([22]\), Tanaka et al. calculate a width of \(\Gamma = 70\) keV using the analytical-continuation-in-the-coupling-constant method. This is 40\% less than the experimental width. In \([23]\), an algebraic model is used to determine the width by Vasilievsky et al. of the \(2^+\) state. They calculate a value of \(\Gamma = 168\) keV, which is \(\approx 50\%\) too large. In \([23]\) it is suggested that the differences in the results from the different models could be caused by different
descriptions of the system and different assumed neutron-neutron interactions.

In this work the method that will be directly compared with the R-matrix method is the Hyperspherical Harmonic (HH) Method. Previous calculations of the $^6\text{He} \, 2^+$ width have been made using this method. In [24], Danilin et al. calculate a width of $\Gamma = 40$ keV, which is 65\% less than the experimentally measured width. Later, in [25], Ershov et al. use the HH method to find a width of $\sim 60$ keV. In this work it will be possible to ensure that the same interactions are used in both the R-matrix and HH calculations, enabling a fair comparison to be made. The HH method is a fully dynamical three-body calculation. Therefore there are none of the coherent / incoherent concerns that are associated with the R-matrix theory. The main aim of this work is to compare HH calculations of the width of the $2^+$ state in $^6\text{He}$ with R-matrix calculations, in order to help clarify whether the R-matrix widths should be combined coherently or incoherently to get the total width of the state.

Chapter Two of this thesis presents some basic scattering theory and establishes an appropriate $\alpha + n$ interaction. Chapter Three investigates how to correctly treat the $n+n$ ("di-neutron") system and establishes an $n+n$ interaction. Chapter Four introduces traditional two-body R-matrix theory and applies it to the $\alpha + n$ system. In particular to the $p_{3/2}$ and $p_{1/2}$ resonances in $^5\text{He}$. R-matrix theory is used to obtain resonance energies and widths for these states and compared with other published values. This chapter also establishes R-matrix boundary conditions for the $p_{3/2}$ state. Chapter Five establishes interactions and boundary conditions for the $^5\text{He}+n$ and $\alpha + ^3\text{n}$ systems. Boundary conditions for the $n+n$ system are also discussed. Chapter Six introduces the three-body R-matrix theory and applies it to the decay of the $^6\text{He} \, 2^+$ state. Limiting cases of the theory are also presented. Chapter Seven summarises the pertinent points of the HH Method and applies this method to the $^6\text{He} \, 2^+$ state. The results of which are then compared with the results from the R-matrix calculations of the preceding chapter. Chapter Eight concludes this work and makes suggestions for further study.
Chapter 2

Resonances in the $\alpha+n$ system

The decay of the $2^+$ state in $^6$He is a three-body decay in which $^6$He decays into an $\alpha$-particle and two neutrons. If this three-body decay is modelled as two sequential two-body decays, a neutron can initially be lost to form the $p_{3/2}$ (ground state) resonance in $^6$He. Therefore, in this chapter, the $\alpha$-neutron interaction is studied and different ways of extracting the resonance energy and width of a state are investigated.

1 The S-Matrix

Due to the Heisenberg uncertainty principle,

$$\Delta E\Delta t \geq \frac{\hbar}{2},$$

(2.1)

a resonant state with a lifetime $\tau$ has an associated energy width, $\Gamma$, given by the relation

$$\Gamma = \frac{\hbar}{\tau},$$

(2.2)

Figure 2.1: The scattering of a valence particle of mass $m_v$ and charge $Z_v$ from a core of mass $m_c$ and charge $Z_c$. 

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Figure 2.2: Illustration of the angle defined as the phase shift, $\delta_E$, in the presence of an S-Matrix pole in the positive real and negative imaginary quadrant of the complex energy plane at $E_R - i\Gamma/2$.

$\Gamma$ can often be determined experimentally by measuring the full-width-half-maximum (FWHM) of an isolated resonant cross-section peak. A resonant state can also be described, theoretically as a pole in the S-matrix. The partial wave S-matrix, $S_\ell(E)$, can be written as \cite{26},

$$S_\ell(E) = e^{2i\delta_\ell(E)}, \quad (2.3)$$

where $\delta_\ell(E)$ is the phase shift\footnote{For further explanation of the phase shift please see Section 2 of this Chapter.}. The value of $|S_\ell(E)|^2$ gives the probability of transmission of the scattered wave. In the case of real potentials, as used in this work, and for real positive $E$, $|S_\ell(E)|^2 = 1$. The S-matrix in the region of an isolated resonance in partial wave $l$ can also be expressed as

$$S_\ell(E) = \frac{E - E_R - i\Gamma/2}{E - E_R + i\Gamma/2}, \quad (2.4)$$

In this form it can be seen that there will be a pole in the S-matrix at an energy $E = E_R - i\Gamma/2$ of the complex energy plane. Figure (2.2) shows a pole in the complex energy plane and the angle that is defined by the phase shift. Using this Figure it is possible to prove the equivalency of Equations (2.4) and (2.3).

Poles in the energy plane have corresponding poles in the complex $k$-plane, where $k$ is the wave number. The non-relativistic relationship between energy and wave number is described by

$$E = \frac{\hbar^2 k^2}{2\mu}, \quad (2.5)$$

where $\mu$ is the reduced mass,

$$\mu = \frac{m_cm_v}{m_c + m_v}. \quad (2.6)$$
Figure 2.3: The top diagram shows the complex $k$-plane or momentum plane, containing several S-matrix poles. The bottom diagram shows the complex energy plane and the corresponding location of the S-matrix poles. The pole labelled 1 is a bound state, pole 3 is a virtual state, poles 4 and 5 are resonances and pole 2 is a pole conjugate to the resonant state of pole 4.
Poles at different locations in the \( k \)-plane have different physical meanings, as shown in Figure (2.3). Poles, such as those labelled 4 and 5, located in the lower right quadrant (positive real \( k \) and negative imaginary \( k \)) are resonances. However, pole number 1 on the positive imaginary \( k \)-axis is a bound state. Whereas pole number 3 on the negative imaginary \( k \)-axis is a virtual state. Pole number 2 is a pole 'conjugate to the resonant state'\(^{[27]}\) of pole 4.

If pole number 1 is an \( s \)-wave bound state, and the potential binding that state is weakened, then the pole would move down the imaginary \( k \)-axis\(^{[26]}\). If the potential continues to weaken, the pole will pass through the origin onto the negative imaginary \( k \)-axis, becoming a virtual state, like pole 3. A virtual state close to the origin causes a large cross-section at low energy. A bound state pole with angular momentum \( l > 0 \) would also move down the imaginary \( k \)-axis should its binding potential weaken. However at the origin the pole would split into two poles, both continuing to move downwards but in opposite directions away from the imaginary axis. One pole forms a resonant state, like pole 4, the other is a pole conjugate to the resonant state, like pole 2.

Combining Equations (2.3) and (2.4), and rearranging to get an expression for the phase shift, gives

\[
\tan \delta_{l}(E) = \frac{\Gamma}{2(E - E_{R})}. \tag{2.7}
\]

This formula can be fitted to experimental phase shift data for real energies with \( \Gamma \) and \( E_{R} \) as parameters. However the discontinuity in the arctan function makes this numerically impractical. By looking at Figure (2.2) it can be seen that

\[
\sin^{2}(\delta_{l}(E)) = \frac{\Gamma^{2}}{4(E - E_{R})^{2} + \Gamma^{2}}. \tag{2.8}
\]

We will see that \( \sin^{2}(\delta_{l}(E)) \) is related to \( \sigma_{l}(E) \) and the famous Breit-Wigner expression for a resonant cross-section peak\(^{[26]}\).

## 2 Nuclear Phase Shift

In the absence of a potential a particle has a radial wave function like that shown in the top graph of Figure (2.4). The distance between the nodes of the wave function is constant. If a particle is influenced by a potential then outside the range of that potential the nodes of the wave function will be shifted with respect to those of the free particle. The wave function has the same form as the free particle but it has experienced a phase shift\(^{[28]}\). In the case of an attractive potential, the wave function is drawn into the potential and the wave function experiences a positive phase shift, as illustrated in the middle graph of Figure (2.4). A wave function in the region of a repulsive potential will be excluded from the region of the potential and experience a negative phase shift, like the wave function in the bottom graph of Figure (2.4).
Figure 2.4: Diagrammatic representation of the effect of a short range potential (indicated by the grey shaded area) on a scattering s-wave radial wave function. The top graph shows a scattering wave function in the absence of a potential. The middle graph shows a scattering wave function under the influence of an attractive square well potential near the origin. The bottom graph shows a scattering wave function under the influence of a repulsive square well potential near the origin.
2.1 The Potential Model

Using standard separation of variables methods\(^\text{[29]}\), the full scattering wave function, \(\Psi_{jm}(r)\), can be separated into radial and angular components as

\[
\Psi_{jm}(r) = r^{-1}\psi_{j\ell}(r)Y_{\ell m}(\theta, \phi), \tag{2.9}
\]

where \(Y_{\ell m}(\theta, \phi)\) is a spherical harmonic. The radial wave function \(\psi_{j\ell}(r)\), for a particle moving in a potential \(V_{j\ell}(r)\) with orbital angular momentum \(j\) and orbital angular momentum \(\ell\), is found by solving the radial Schrödinger Equation,

\[
\hat{H}\psi_{j\ell}(r) = E\psi_{j\ell}(r), \tag{2.10}
\]

where \(E\) is the centre of mass energy and \(\hat{H}\) is the radial Hamiltonian given by

\[
\hat{H} = -\frac{\hbar^2}{2\mu} \left[ \frac{d^2}{dr^2} - \frac{\ell(\ell + 1)}{r^2} \right] + V_{j\ell}(r), \tag{2.11}
\]

in one dimension. The potential \(V(r)\), is a sum of three other components,

\[
V_{j\ell}(r) = V_{ws}(r) + V_{so}(r)(\ell, s) + V_{coul}(r). \tag{2.12}
\]

The subscripts \(ws\), \(so\) and \(coul\) indicate Woods-Saxon, spin-orbit and coulomb potentials respectively.

Woods-Saxon Potential

The Woods-Saxon Potential\(^\text{[30]}\) is given by

\[
V_{ws}(r) = \frac{-V_{ws}^0}{1 + e^{(r-r_{ws})/\alpha_{ws}}}, \tag{2.13}
\]

where \(V_{ws}^0\) is the potential strength in MeV, \(r_{ws}\) is the radius of the potential in fm and \(\alpha_{ws}\) is the diffuseness and also in fm.

Spin-Orbit Potential

The spin-orbit potential is given by\(^2\)

\(^2\)This is not the standard parameterisation for the spin-orbit potential, often a factor of 4 is included. Therefore in this work the spin-orbit strength is a factor of 4 larger than the values often quoted in the literature.
\[ V_{so}(r) = -\frac{V_{so}^0}{\alpha_{so}^r} \left( \frac{e^{(r-r_{so})/\alpha_{so}}}{(1 + e^{(r-r_{so})/\alpha_{so}})^2} \right) \] (2.14)

so \( V_{so}(r) \propto \frac{1}{r} \frac{dV_{so}}{dr} \) and is therefore primarily a surface term. Here \( V_{so}^0 \) is the potential strength, \( r_{so} \) is the spin-orbit potential radius and \( \alpha_{so} \) is the diffuseness. For a particle with total angular momentum \( \ell \), the \( \langle \ell, s \rangle \) term is given by

\[ \langle \ell, s \rangle = \frac{1}{2} \left[ \ell(\ell + 1) - s(s + 1) - \ell(\ell + 1) \right], \] (2.15)

where \( s \) is the spin of the valence particle, \( \ell \) is the core-valence relative angular momentum and \( \ell = \ell \pm s, \ell \geq 0 \).

Coulomb Potential

The Coulomb potential involves the charge of both the valence, \( Z_v \), and the core, \( Z_c \). Therefore, where one or both of the particles are neutrons, the Coulomb potential is absent. The Coulomb potential is given by

\[ V_{coul}(r) = \begin{cases} \frac{Z_c Z_v e^2}{r}, & r > r_{coul}, \\ \frac{Z_c Z_v e^2}{r_{coul}} \left[ 3 - \frac{1}{2} \left( \frac{r}{r_{coul}} \right)^2 \right], & r \leq r_{coul}. \end{cases} \] (2.16, 2.17)

where \( r_{coul} \) is the radius of the core modelled as a uniformly charged sphere. This work involves only neutrons and their interactions with Helium nuclei, therefore \( V_{coul}(r) \) is only mentioned here for completeness.

2.2 Calculating the Phase Shift

A radial wave function outside a distance, \( R \), beyond which the interaction potential is negligible, has the form\(^{29}\)

\[ \psi_{\ell}(r) = A(F_\ell(\eta, \rho) \cos \delta_\ell + G_\ell(\eta, \rho) \sin \delta_\ell). \] (2.18)

Here \( A \) is a constant, \( \rho = kr \) and \( \eta \) is the Sommerfeld parameter,

\[ \eta = a c Z_c Z_v \sqrt{\frac{\mu}{2E}}, \] (2.19)
where $\alpha$ is the fine structure constant and $c$ is the speed of light (in a vacuum). The functions $F_\ell(\eta, \rho)$ and $G_\ell(\eta, \rho)$ are the Coulomb functions\(^3\). In this work $\eta = 0$ and $F_\ell(\rho) \equiv F_\ell(\eta = 0, \rho)$ and $G_\ell(\rho) \equiv G_\ell(\eta = 0, \rho)$ and are the regular and irregular solutions to the field free equation

$$\left[ \frac{d^2}{dr^2} + k^2 - \ell(\ell + 1) \right] u_\ell(kr) = 0. \quad (2.20)$$

Inside $R$, the Schrödinger Equation can be solved numerically. The Runge Kutta method and the Numerov algorithm are two such methods which solve ordinary differential equations. The wave function is calculated iteratively in step sizes of $\hbar$, using the knowledge that the regular solution has the boundary condition $u_\ell(r = 0) = 0$ and behaves as $u_\ell(r) \propto r^{\ell+1}$ near the origin.

The calculated wave function should match on to the asymptotic form given in Equation (2.18). The wave function is evaluated at 2 distances beyond $R$, $r_1$ and $r_2$. (Correspondingly $\rho_1 = kr_1$ and $\rho_2 = kr_2$.) This produces 2 simultaneous equations,

$$\begin{align*}
\psi_\ell(r_1) &= A [F_\ell(\rho_1) \cos \delta_\ell + G_\ell(\rho_1) \sin \delta_\ell], \\
\psi_\ell(r_2) &= A [F_\ell(\rho_2) \cos \delta_\ell + G_\ell(\rho_2) \sin \delta_\ell],
\end{align*} \quad (2.21)$$

where $A \cos \delta_\ell$ and $A \sin \delta_\ell$ are the unknowns. This can be expressed in matrix form,

$$\begin{pmatrix} \psi_\ell(r_1) \\ \psi_\ell(r_2) \end{pmatrix} = \begin{pmatrix} F_\ell(\rho_1) & G_\ell(\rho_1) \\ F_\ell(\rho_2) & G_\ell(\rho_2) \end{pmatrix} \begin{pmatrix} A \cos \delta_\ell \\ A \sin \delta_\ell \end{pmatrix}, \quad (2.23)$$

which can be solved for $A \cos \delta_\ell$ and $A \sin \delta_\ell$ and rearranged to give

$$\tan \delta_\ell = \frac{F_\ell(\rho_1) \psi_\ell(r_2) - F_\ell(\rho_2) \psi_\ell(r_1)}{G_\ell(\rho_2) \psi_\ell(r_1) - G_\ell(\rho_1) \psi_\ell(r_2)}. \quad (2.24)$$

### 3 $\alpha+n$ resonances

In [31] $\alpha$-phase shift data for the $s_{1/2}$, $p_{1/2}$ and $p_{3/2}$ states in $^5$He are fitted using the same Woods-Saxon and spin-orbit potential for all 3 states. The fit obtained was “quite satisfactory”\(^3\) up to $\approx 40$ MeV. It was found that a depth of $V_{ws}^0 = 43.0$ MeV, a diffuseness of $\alpha_{ws} = 0.70$ fm and a radius of $r_{ws} = 2.00$ fm was required for the Woods-Saxon and $V_{so}^0 = 40.0$ MeV, $\alpha_{so} = 0.35$ fm and $r_{so} = 1.50$ for the spin-orbit. For reference purposes this potential is called the Bang potential.

---

\(3\)In this work, the functions $F_\ell(\eta, \rho)$ and $G_\ell(\eta, \rho)$, will still be referred to as Coulomb functions, even in the absence of a Coulomb potential, $\eta = 0$. 

12
The Bang potential was used in the program POLER\(^{32}\) which calculates a scattering wave-function, \(\psi_\ell\), and matches it onto the asymptotic forms

\[
\psi_\ell(r) = \frac{i}{2} (H_\ell^- - S_\ell H_\ell^+),
\]

\[
\frac{d\psi_\ell}{dr} = \frac{ik}{2} (H_\ell'^- - S_\ell H_\ell'^+),
\]

at some matching radius, \(a\). The functions \(H_\ell^-\) and \(H_\ell^+\) are linear combinations of Coulomb functions

\[
H_\ell^+ = G_\ell(\eta, \rho) + iF_\ell(\eta, \rho),
\]

\[
H_\ell^- = G_\ell(\eta, \rho) - iF_\ell(\eta, \rho).
\]

The functions \(H_\ell'^+\) and \(H_\ell'^-\) are the derivatives of \(H_\ell^+\) and \(H_\ell^-\) with respect to \(\rho\). In the case of \(\eta = 0\), the functions \(H_\ell^-\) and \(H_\ell^+\) are called Hankel functions.

From Equations (2.25) and (2.26), the logarithmic derivative of \(\psi_\ell(r)\) is given by

\[
\frac{d\psi_\ell}{dr} \psi_\ell(r) = \frac{k(H_\ell'^- - S_\ell H_\ell'^+)}{H_\ell^- - S_\ell H_\ell^+}.
\]

As an S-matrix pole is approached, \(S_\ell\) becomes very large, and so the \(H_\ell^-\) and \(H_\ell'^-\) terms in the above are small in comparison and can be neglected. In which case Equation (2.29) simplifies to

\[
\frac{d\psi_\ell}{dr} \psi_\ell(r) = \frac{kH_\ell'^+}{H_\ell^+}.
\]

Therefore at an S-matrix pole

\[
\frac{d\psi_\ell}{dr} \psi_\ell(r) - \frac{kH_\ell'^+}{H_\ell^+} = 0.
\]

POLER\(^{32}\) produces contour data of

\[
\log_{10} \left| \frac{d\psi_\ell}{dr} \psi_\ell(r) - k\frac{H_\ell'^+}{H_\ell^+} \right|,
\]

for either the complex energy-plane or \(k\)-plane, where the \(\log_{10}\) is included for clarity of graphing.
Figure 2.5: Contour plot of Equation (2.32) showing the S-matrix pole corresponding to the $p_{3/2}^5\text{He}$ state in the complex energy plane.

Figure 2.6: Contour plot of Equation (2.32) showing the S-matrix pole corresponding to the $p_{1/2}^5\text{He}$ state in the complex energy plane.
Figure 2.7: Contour plot of Equation (2.32) showing the S-matrix pole corresponding to the $^5$He $s_{1/2}$ Pauli forbidden bound state in the complex $k$-plane.

Figure (2.5) is a contour plot of the complex energy-plane showing a pole in the S-matrix corresponding to the $p_{3/2}$ ground state resonance in $^5$He. A matching radius of 7 fm was used. From the pole's position in the energy plane the resonance was found to be at $E_R=0.90$ MeV above threshold with a width of $\Gamma=0.87$ MeV. The resonance energy agrees within 11% of the published value, $E_R=0.80$ MeV, from the [33] evaluation. The width is 25% larger than the published value of $\Gamma=0.648$ MeV.

Figure (2.6) shows a similar contour plot for the $p_{1/2}$ state. The S-matrix pole for this state was found to occur at $E_R=1.72$ MeV with $\Gamma=5.70$ MeV. The width agrees well (within 3%) of the published value of $\Gamma=5.57$ MeV[33]. The resonance energy agrees within 17% of the published value of $E_R=2.068$ MeV[33].

Unlike Figures (2.5) and (2.6), Figure (2.7) is a contour plot of Equation (2.32) in the complex $k$-plane rather than the energy-plane. This is because it is only possible to tell the difference between a virtual state and a bound state in the $k$-plane. Figure (2.7) shows an S-matrix pole at $E_R=-9.76$ MeV, $\Gamma = 0.0$ MeV. The location of this pole in the $k$-plane indicates a bound state. However this $s_{1/2}$ state is Pauli forbidden, if this were not so, this state would be the ground state of $^5$He.

4 The Derivative Method

The full expression for the energy dependent cross-section for a pure Breit-Wigner resonance[34] is
\[ \sigma_s(E) = \frac{4\pi}{k^2} (2l+1) \sin^2(\delta(E)) = \frac{4\pi(2l+1)}{k^2} \frac{\Gamma^2}{4(E-E_R)^2+\Gamma^2}. \] (2.33)

A Breit-Wigner resonance is a narrow isolated resonance[35]. A narrow resonance is one in which \( \Gamma \ll E_R \). An isolated resonance is one in which the energy separation to any other resonances is large in comparison with the width of the resonance. The factor peaks when \( \delta = \pi/2 \). Correspondingly, the right-hand-side of Equation (2.8) is at a maximum when the denominator is smallest, this occurs at \( E = E_R \). The energy at which \( \delta = \pi/2 \) is approximately equal to the energy at which the cross-section peaks, but not exactly due to the \( 1/k^2 \) dependence. Therefore for a pure Breit-Wigner resonance the point at which the phase shift passes through \( \pi/2 \) gives the resonance energy. Also for \( E > E_R \) the phase shift should go asymptotically to a maximum value of \( \pi \) for a pure Breit-Wigner resonance.

For a pure Breit-Wigner resonance the point at which the phase shift passes through \( \pi/2 \) is also the point at which the derivative, \( d\delta_s/dE \), is at a maximum. From Equation (2.7), the derivative of the phase shift with respect to energy is

\[ \frac{d\delta_s(E)}{dE} = \frac{2\Gamma}{4(E-E_R)^2+\Gamma^2}. \] (2.34)

Evaluating this at \( E = E_R \) gives

\[ \left. \frac{d\delta_s(E)}{dE} \right|_{E=E_R} = \frac{2}{\Gamma}, \] (2.35)

which means that both the width and the resonance energy can be determined from studying the phase shift.

However not all resonant states are pure Breit-Wigner resonances, in that their phase shift may not increase all the way to \( \pi \). In fact the phase shift need not necessarily increase to a value greater than \( \pi/2 \), let alone pass through it. Equation (2.34) also shows that the derivative of the phase shift is at its maximum value at \( E = E_R \). Therefore in cases where the phase shift does not meet the criteria for a Breit-Wigner resonance the point at which the derivative of the phase shift is a maximum and the value of the derivative could be used to estimate the resonance energy and width.

Figure (2.8) shows the phase shift and the derivative of the phase shift for the \( p_{3/2} \), \( p_{1/2} \) and \( s_{1/2} \) states in \(^5\)He calculated from the Bang potential. The top left graph of Figure (2.8) shows the \( p_{3/2} \) phase shift which is the only phase shift to pass through the \( \delta = 90^\circ (\pi/2) \) point. This gives a resonance energy \( E_R = 1.27 \) MeV and width \( \Gamma = 1.657 \) MeV. This does not compare well with the published values of \( E_R = 0.80 \) MeV and \( \Gamma = 0.65 \) MeV[33] or the S-matrix pole values of \( E_R = 0.90 \) MeV and \( \Gamma = 0.87 \) MeV.

The top right graph of Figure (2.8) shows the derivative of the phase shift with respect to energy for the \( p_{3/2} \) state. The point at which the derivative is a maximum
Figure 2.8: Phase shifts calculated from the Bang potential for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^5$He. Also shown are the derivatives of these phases with respect to energy.


<table>
<thead>
<tr>
<th>Method</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Published[33]</td>
<td>0.80</td>
<td>0.65</td>
<td>2.07</td>
<td>5.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S-matrix Pole</td>
<td>0.90</td>
<td>0.87</td>
<td>1.72</td>
<td>5.50</td>
<td>-9.76</td>
<td>0.00</td>
</tr>
<tr>
<td>$\delta_e = 90^\circ$</td>
<td>1.27</td>
<td>1.66</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d\delta_e/dE$</td>
<td>0.91</td>
<td>0.94</td>
<td>1.95</td>
<td>8.42</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.1: Summary of energies and widths obtained for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^5$He from different methods.

gives $E_R = 0.91$ MeV and $\Gamma = 0.94$ MeV which compares well with published values and also the S-Matrix pole values.

The middle left graph of Figure (2.8) shows that the $p_{1/2}$ phase shift does not pass through $\delta_e=90^\circ$ therefore only the point at which the derivative is at a maximum can be used to determine the resonance energy and width. The derivative for the $p_{1/2}$ state is shown in the middle right graph of Figure (2.8). This gives $E_R = 1.95$ MeV and $\Gamma = 8.42$ MeV. The resonance energy compares well with published energy $E_R = 2.07$ MeV (within 6%), but not so well with the S-Matrix pole energy $E_R = 1.72$ MeV (within 17%).

The bottom graphs of Figure (2.8) show the phase shift and its derivative for the $s_{1/2}$ state. The location of the $s_{1/2}$ S-matrix pole showed that this state is not a resonance. The phase shift also does not resemble a resonant phase shift. Therefore a resonance energy and width could not be determined for this state.

Table (2.1) summarises the energies and widths found for the different states in $^5$He using different methods. It shows that generally the S-Matrix pole values agree well with the published values, on average they agree to within 14%. The $\delta_e = 90^\circ$ values on average only agree to within 49% of the published values and to within 38% of the S-matrix pole values. The values from the maximum of $d\delta_e/dE$ compare much better. On average they agree to within 21% of the published values and 14% of the S-matrix pole values. This suggests that using the maximum derivative of the phase shift to obtain resonance energies and widths is a better method than simply using the $\delta_e = 90^\circ$ point.

5 Neutron-α Potential

The Bang potential[31] has been shown (see Sections (3) and (4)) to reproduce the published energies and widths of the $p_{3/2}$ and $p_{1/2}$ states states in $^5$He quite well. The Bang potential was fitted to experimental phase shift data measured in the 1950's[36, 37, 38]. More accurate phase shift data is now available; Bond and Pirk[39] measured the phase shift for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states up to a neutron lab energy of 20 MeV in 1977,
Figure 2.9: Graph showing the experimental phase shift data for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^3$He from [39]. Also shown is the SFRESCO fits to the phase shift.

with error bars typically less than 0.5%. The program SFRESCO\(^4\) can find a potential that best fits experimental phase shift data. The geometry from the $Bang$ potential (the diffuseness and radii for the Woods-Saxon and spin-orbit potentials) was kept constant but the strengths of the Woods-Saxon and spin-orbit potentials were varied to better fit the more recent experimental phase shift data. A better fit could probably be obtained by fitting each state individually, however a simple n-$\alpha$ interaction is required for use in future three-body calculations of $^6$He.

SFRESCO makes use of a function minimisation routine called minuit\(^{42, 43}\). To fit the experimental phase shift data the $\chi^2$ function is minimised. For $N$ data points this is given by

$$
\chi^2 = \sum_{i=1}^{N} \left( \frac{\delta_i^{\exp}(E_i) - \delta_i(E_i)}{\Delta \delta_i(E_i)} \right)^2,
$$

where $\delta_i(E_i)$ is the experimental value and $\Delta \delta_i(E_i)$ is the error in $\delta_i(E_i)$. Including the experimental errors serves to weight the fit towards the data points with the smallest error bars.

The experimental data\(^{39}\) is read into SFRESCO as a function of lab neutron energy. However the lab energies are easily converted to centre-of-mass energies by the relation

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\(^{4}\)The program SFRESCO is the search version of FRESCO, which was developed by Ian Thompson and uses a coupled channels model for nuclear reactions. Full documentation including the user’s manual for FRESCO can be found at [40]. A full description of the FRESCO formalism is outlined in [41].
Table 2.2: The $\chi^2/N$ values for the phase shift for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^6$He. The phase shift was calculated using the Bang and the fitted Bang potential and the percentage difference between the two values is given in the final column.

<table>
<thead>
<tr>
<th>State</th>
<th>$\chi^2/N$ Bang</th>
<th>$\chi^2/N$ Fitted Bang</th>
<th>Percentage decrease</th>
</tr>
</thead>
<tbody>
<tr>
<td>$p_{3/2}$</td>
<td>5381</td>
<td>106</td>
<td>98%</td>
</tr>
<tr>
<td>$p_{1/2}$</td>
<td>1987</td>
<td>1417</td>
<td>28%</td>
</tr>
<tr>
<td>$s_{1/2}$</td>
<td>1022</td>
<td>465</td>
<td>55%</td>
</tr>
</tbody>
</table>

and the results presented here are in the centre-of-mass frame for ease of comparison with previous phase shift plots.

If the fit agrees exactly with the experimental data then $\chi^2 = 0$. However the experimental data contains errors, the $\Delta\delta_t(E_i)$'s, which means that usually the best that can obtained is when $\delta_t^B(E_i) - \delta_t(E_i) \approx \Delta\delta_t(E_i)$ and the fraction $|\delta_t^B(E_i) - \delta_t(E_i)|/\Delta\delta_t(E_i)^2 \approx 1$. Therefore the best achievable value is $\chi^2 \approx N$. The phase shift for each state has 26 experimental measurements, therefore $N = 26$. However for ease of comparison between data sets with different numbers of data points it is usual for $\chi^2/N$ to be given, which for a good fit $\approx 1$.

Figure (2.9) shows the experimental data from [39] and the fitted phases. SFRESCO found a Woods-Saxon depth of $V_{ws} = 44.21$ MeV, and spin-orbit depth of $V_{so} = 38.91$ MeV produced the best fit. This is only a small change from the Bang potential depths of $V_{ws} = 43.0$ MeV and $V_{so} = 40.0$ MeV used in [31]. Table (2.2) shows the $\chi^2/N$ values for the phase shift calculated from the original Bang potential and the new fitted potential. Averaging over all three states there was a 76% reduction in $\chi^2/N$ for the fitted Bang potential in comparison with the unmodified Bang potential. The fit is particularly good for the $p_{3/2}$ state which fits the experimental data to within 2%. Table (2.2) shows that the fitted Bang potential does reproduce the experimental phase shift better than the original Bang potential, although the $\chi^2/N \gg 1$, which would usually indicate a bad fit to the data. The large $\chi^2/N$ is due to the very small errors in the experimental data (less than 0.5%), however Figure (2.9) shows that it is a good fit to the experimental data.

Table (6.6) shows the widths and energies obtained for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^6$He from different methods using the fitted Bang potential. For the $p_{3/2}$ state, the S-matrix pole values agree extremely well with published values. The energy agrees to within 3.8% and the width agrees to within 1.5%. This is an improvement on the Bang potential as this only agreed to within 11.1% and 25.3% respectively. For the $p_{1/2}$ state, the fitted Bang potential does slightly worse than the Bang potential. The S-matrix pole energy is 19.9% smaller than the published value and the width is 5.6% smaller. In general the fitted Bang potential gives S-matrix poles closer to the published energies and
Table 2.3: Summary of energies and widths obtained for the $p_{3/2}$, $p_{1/2}$ and $s_{1/2}$ states in $^5$He from different methods using the fitted Bang potential.

<table>
<thead>
<tr>
<th>Method</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
<th>$E_R$ (MeV)</th>
<th>$\Gamma$ (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Published[^33]</td>
<td>0.80</td>
<td>0.65</td>
<td>2.07</td>
<td>5.57</td>
<td></td>
<td></td>
</tr>
<tr>
<td>S-matrix Pole</td>
<td>0.77</td>
<td>0.66</td>
<td>1.72</td>
<td>5.26</td>
<td>-10.30</td>
<td>0.00</td>
</tr>
<tr>
<td>$\delta_\ell = 90^\circ$</td>
<td>1.01</td>
<td>1.11</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$d\delta_\ell/dE$ Maximum</td>
<td>0.75</td>
<td>0.71</td>
<td>1.90</td>
<td>7.54</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 2.4: Average percentage differences between energy and width values obtained from different methods using the Fitted Bang and Bang potential.

<table>
<thead>
<tr>
<th>Methods</th>
<th>Fitted Bang</th>
<th>Bang</th>
</tr>
</thead>
<tbody>
<tr>
<td>Published - S-matrix Pole</td>
<td>7.7%</td>
<td>13.7%</td>
</tr>
<tr>
<td>Published - $\delta_\ell = 90^\circ$</td>
<td>31.1%</td>
<td>48.9%</td>
</tr>
<tr>
<td>Published - $d\delta_\ell/dE$ Maximum</td>
<td>12.3%</td>
<td>20.7%</td>
</tr>
<tr>
<td>S-matrix Pole - $\delta_\ell = 90^\circ$</td>
<td>32.2%</td>
<td>38.4%</td>
</tr>
<tr>
<td>S-matrix Pole - $d\delta_\ell/dE$ Maximum</td>
<td>12.3%</td>
<td>13.8%</td>
</tr>
</tbody>
</table>

widths, indicating that the fitted Bang potential better represents the n-$\alpha$ interaction.

As with the Bang potential, the $\delta_\ell = 90^\circ$ values do not compare very well with either the published values or the S-matrix pole values. There is $\approx 20\%$ difference in the energy and $\approx 40\%$ difference in the width. The $d\delta_\ell/dE$ maximum values do considerably better than the $\delta_\ell = 90^\circ$ values. In the $p_{3/2}$ state the energy and width agree with the published values to within 6.2% and 8.5% respectively. There is also good correspondence in the $p_{1/2}$ resonance energy, that agrees with the published energy to within 8.2%, but is in fact slightly worse than the Bang potential which agreed within 5.8%. However there is a difference of 26.1% between the $p_{1/2}$ width and the published one. The $d\delta_\ell/dE$ maximum values also agree well with the S-matrix pole values. The $p_{1/2}$ energy and width agrees to within 2.6% and 7.0% respectively. However for the $p_{3/2}$ energy this is slightly worse than the Bang potential which agreed with the S-matrix pole to within 1.1%. The $p_{1/2}$ energy also compares well with the S-matrix pole, to within 9.5%, but the width only agrees to within 30.2%. This is further evidence of what was observed for the unmodified Bang potential in that the $d\delta_\ell/dE$ method gives values that are in better agreement with S-matrix pole energies and published values than the $\delta_\ell = 90^\circ$ method.

Table (2.4) contains the average percentage differences between resonance energies and widths obtained from different methods and using the two different potentials. It shows that on average the fitted Bang potential does better at giving the published resonance energies and widths. In particular the S-matrix pole values and $d\delta_\ell/dE$ maximum values agree well. The $\delta_\ell = 90^\circ$ has better agreement from the fitted Bang potential than from the Bang potential, but this method still does not agree well with experiment. Therefore using the $d\delta_\ell/dE$ maximum method to obtain resonance energies and widths from the
phase shift is better than the $\delta_t = 90^\circ$ method. The $d\delta_t/dE$ maximum method also has the benefit of being able to be applied to more states since it does not require the phase shift to rise through $90^\circ$. The $d\delta_t/dE$ maximum method also agrees better with the S-matrix pole values than the $\delta_t = 90^\circ$ method.

In general all the methods agree better for the $p_{3/2}$ state than the $p_{1/2}$ state. This is because the $p_{3/2}$ resonance is a narrower resonance and fits the criteria for a Breit-Wigner resonance better than the $p_{1/2}$ resonance. Since the sequential decay of the $2^+$ resonance in $^6$He goes through the $p_{3/2}$ ground state resonance in $^5$He, it is particularly important that the potential agrees well for the $p_{3/2}$ state. Since the fitted Bang potential agrees better with experimental data on the phase shift, and the resonance energies and widths than the Bang potential, the fitted Bang potential is the most suitable to be used in future three-body calculations of $^6$He.
Chapter 3

The ‘Di-Neutron’

When modelling the decay of the $2^+$ state in $^6$He as two ordered two-body decays, the first decay could be the emission of the $\alpha$-particle. This leaves a two-neutron system or ‘di-neutron’. The di-neutron is unbound and the correct treatment of the two-neutron system is looked at in this chapter.

1 Effective Range Expansion

The effective range expansion was first developed for the scattering of protons from neutrons\cite{44, 45}. In general the scattering of a particle from a potential can be described completely by the phase shift. In the case of low energy s-wave scattering, the phase shift can be parameterised by two other quantities; the ‘effective range’, $r_0$, and the ‘scattering length’, $a_s$\cite{46}. These quantities characterise the potential for low energy scattering. The effective range expansion is given by e.g. Wu\cite{46}, and in the thesis of Stott\cite{27}, as the low energy expansion of $k \cot (\delta_g)$ about $k \approx 0$,

$$k \cot \delta_{g=0}(k) = -\frac{1}{a_s} + \frac{1}{2} r_0 k^2 + \cdots \quad (3.1)$$

The scattering length, $a_s$, is thus defined by the limit

$$-\frac{1}{a_s} = \lim_{k \to 0} [k \cot \delta_{g=0}(k)], \quad (3.2)$$

and is negative for unbound states near threshold. It can be shown using l'Hôpital's Rule that $a_s$ is also

$$a_s = -\frac{d\delta_{g=0}(k)}{dk} \bigg|_{k=0}. \quad (3.3)$$

The scattering length and the effective range have units of length.
One-Term Effective Range Expansion

Using just the first term in the expansion of Equation (3.1) and rearranging for \( \delta_\ell \) gives

\[
\delta_{\ell=0}(k) = -\tan^{-1}(a_s k). 
\]  
(3.4)

A derivation for this Equation can be found in Bethe[44].

Two-Term Effective Range Expansion

Taking the first 2 terms of Equation (3.1) the phase shift is given by

\[
\delta_{\ell=0}(k) = \tan^{-1}\left(\frac{-2a_s k}{2 - \tau_0 a_s k^2}\right). 
\]  
(3.5)

The S-Matrix as a Function of \( k \)

In the same way that in Equation (2.4) the S-Matrix is described in terms of a pole in the complex energy plane, it can also be described in terms of its corresponding pole in the complex \( k \)-plane,

\[
S_\ell(k) = \frac{k - k_R + ik_I}{k - k_R - ik_I}, 
\]  
(3.6)

where \( k_I \) and \( k_R \) are the imaginary and real parts of the pole location in the complex \( k \)-plane. The above can be rearranged to give

\[
\delta_\ell(k) = -\tan^{-1}\left(\frac{k - k_R}{k_I}\right), 
\]  
(3.7)

which is analogous to Equation (2.7) since both expressions depend only on the location of the S-matrix pole in the complex energy- or momentum-plane. In the case of a virtual state, it is required that \( k_R = 0 \) and \( k_I = 1/\alpha_s \), where \( \alpha_s \) is the scattering length. Substituting this into the above Equation gives

\[
\delta_{\ell=0}(k) = -\tan^{-1}(a_s k). 
\]  
(3.8)

This equation is in agreement with Equation (3.4), the one term effective range expansion.
In [47] a simple Gaussian potential of the form

\[ V_{nn}(r) = -V_{nn}^0 \exp \left[ -\left( \frac{r}{r_{nn}} \right)^2 \right], \quad (3.9) \]

with a range of \( r_{nn} = 1.8 \text{ fm} \) and a depth of \( V_{nn}^0 = 31.0 \text{ MeV} \) is chosen to "reproduce the low energy scattering data" for two neutrons in a relative s-wave state; namely the neutron-neutron scattering length and the effective range. This simple gaussian is an approximation to the n+n interaction, but low energy (\( \leq 10 \text{ MeV} \)) scattering properties are insensitive to the shape of the potential\(^{[48]}\). In [49], the 1998 review of effective range parameters, the values of \( a_s = -18.5 \pm 0.3 \text{ fm} \) and \( r_0 = 2.75 \pm 0.11 \text{ fm} \) are recommended. In a 2006 experiment, Gonzalez et al. measured \( a_s = -18.7 \pm 0.7 \text{ fm} \)\(^{[50]}\). This value is in excellent agreement with [49], thus showing that the values given in [49] are still adequate today.

This nn-potential was used in the NNSCATTER program\(^1\) and the phase shifts were calculated. Figure (3.1) shows the derivative of the phase shift with respect to \( k \). From Equation (3.3) the value of \( d\delta_l/dk \) as \( k \to 0 \) determines the scattering length. The inset in Figure (3.1) shows \( d\delta_l/dk \) as \( k \) approaches zero, giving a value of \( a_s = -18.6 \text{ fm} \), in

\(^1\)The NNSCATTER program is a modified version of the program SCAT developed by Jeff Tostevin\(^{[51]}\).
Figure 3.2: The nnscatter phase shift and phase shifts calculated from the two-term effective range expansion (Equation (3.5)) for different effective ranges, \( r_0 \). A value of \( a_s = -18.6 \) fm was used.

agreement with both [49] and [50].

Figure (3.2) shows the phase shift calculated by the nnscatter program and some phase shifts calculated from Equation (3.5) using different values for the effective range, \( r_0 \), and \( a_s = -18.6 \) fm. Figure (3.2) shows that a value of \( r_0 = 2.8 \) fm gives the best fit to the nnscatter phase shift. This value is in agreement with the recommended value in [49].

This shows that this simple Gaussian potential does indeed reproduce low energy neutron-neutron s-wave scattering data as stated by [47]. Therefore this potential is suitable for use in future three-body calculations of \(^{6}\text{He}\).

2 Previous Treatment of The Two-Neutron System

Figure (3.3) shows an S-matrix scan of the complex \( k \)-plane using the program POLER\(^{32}\) and the Gaussian n-n-potential. The S-matrix pole on the negative real \( k \)-axis shows the n+n virtual state. The pole occurs at \( E_R = -0.12 \) MeV and \( \Gamma = 0.00 \) MeV. In [6] and [52], Bartlett et al. do not treat the n+n virtual state explicitly, instead the n+n system is treated as a Breit-Wigner resonance occurring at zero energy, \( E_R = 0.0 \) MeV. The width of this "resonance", \( \Gamma = 0.10 \) MeV, was given by the FWHM of the neutron-neutron scattering cross-section peak. This section looks at the adequacy of this approximation.

A Breit-Wigner resonance at 0.0 MeV would be characterised as having \( \delta_t(E = 0.0) = 90 \) degrees and \( d\delta_t/dE|_{E=0.0} \) at a maximum. Figure (3.1) shows the derivative of the phase
shift, \( d\delta_k/dk \), against \( k \). Since \( d\delta_k/dk \propto E_k^{1/2}d\sigma_k/dE \), and \( E_k^{1/2} \) is a smooth slowly varying function, then \( d\delta_k/dk \) peaks at approximately the same energy as \( d\sigma_k/dE \). Figure (3.1) shows that \( d\delta_k/dk \) peaks at \( k = 0 \) which corresponds to \( E = 0.0 \) MeV, which is consistent with a Breit-Wigner resonance at zero energy.

The assumed values for the resonance energy, \( E_R = 0.0 \) MeV, and width, \( \Gamma = 0.10 \) MeV, can be used to calculate the phase shift using Equation (2.7). Figure (3.4) shows a comparison between this phase shift and the NNSCATTER phase shift. The NNSCATTER phase shift reproduces the low energy nn-scattering data very well, thus a comparison with this gives an indication of how well the phase shift calculated from the [52] values reproduces the experimental data. Figure (3.4) shows that the phase shift from [52] does not reproduce the experimental data and is a bad fit to the NNSCATTER phase shift. Since Equation (2.7) was derived for a Breit-Wigner Resonance and it does so badly at reproducing the experimental data, it shows that treating the n+n state as a resonance is an inadequate approximation.
Figure 3.4: The nn-scattering phase shift produced using the Gaussian potential in the NNSCATTER program and that produced using $E_R = 0$ and $\Gamma = 0.10$ MeV from [6] (labelled Bartlett et al.) in Equation (2.7).
Chapter 4

The R-Matrix

In this Chapter traditional two-body R-matrix theory is applied to the $p_{3/2}$ and $p_{1/2}$ states in $^5$He. R-matrix theory is used to estimate the widths of these states and a comparison is made with the previous estimates obtained in Chapter 2 and the published values. Appropriate boundary conditions are also discussed with a view to the later three-body R-matrix calculations.

1 R-matrix Theory: An Introduction

R-matrix theory is highly flexible and can be adapted to study any type of nuclear reaction\cite{14}. The theory is unconcerned with the detailed physical mechanisms of a reaction inside the nucleus\cite{26}, only surface properties such as the logarithmic derivative of the wave function at the surface are used. No assumptions about the wave function inside the nucleus are made. The theory is especially suitable for studying compound nuclear reactions\cite{14}, and has been applied extensively to such reactions, in particular to resonance ones\cite{26}, such as those looked at in this work.

There are four assumptions at the basis of traditional R-matrix theory\cite{14}:

(1) "Applicability of nonrelativistic quantum mechanics"
This assumption is justified for low energy reactions as the nucleon kinetic energies inside the nucleus are only a few percent of the rest mass energy.

(2) "Absence or unimportance of all process in which more than two product nuclei are formed"
This means the theory cannot be used immediately for three body decays.

(3) "Absence or unimportance of all processes of creation or destruction"
This assumption basically excludes reactions involving photons, therefore processes such as particle production and annihilation are not included.
The existence, for any pair of nuclei $c$, of some finite radial distance of separation $a_c$, beyond which neither nucleus experiences any polarizing potential field from the other.

Here $a_c$ is the matching radius, which in this work is simply $a$. This assumes that beyond $a$ the potential describing the interaction between two nuclei can be written as a function of radial distance only. The matching radius is discussed further in Section 2.

In R-matrix theory the matching radius, $a$, marks the boundary between the “internal” and the “external” regions. The internal region is that for which $r < a$ and the external region is that for which $r > a$. The scattering wave function, $\psi(r)$, here written as $\psi(r)$, can be expanded in terms of a complete set of orthonormal eigen functions in the internal region,

$$\psi(r) = \sum_p C_p \tilde{\psi}_p(r), \quad r \leq a. \tag{4.1}$$

The wave functions, $\tilde{\psi}_p(r)$, are R-matrix eigenfunctions, and are calculated from the Schrödinger Equation for a given two-body potential,

$$\hat{H} \tilde{\psi}_p(r) = \epsilon_p \tilde{\psi}_p(r). \tag{4.2}$$

Figure (4.1) is a diagram showing a central potential and the $\tilde{\psi}_p(r)$ and $\psi(r)$ calculated from it. Figure (4.1) illustrates that the index, $p$, relates to the number of radial nodes, $n$, in the internal wave function, $p = n + 1$. The $\tilde{\psi}_p(r)$ are calculated using the boundary conditions

$$\tilde{\psi}_p(r = 0) = 0 \quad \text{and} \quad \beta = \left( \frac{1}{\psi_p(r)} \frac{d\tilde{\psi}_p}{dr} \right)_{r = a}, \tag{4.3}$$

where $\beta$ is a constant. The fixed value of $\beta$ ensures the $\tilde{\psi}_p$ are orthonormal by rendering the kinetic energy Hermitian over the finite region $0 \leq r \leq a$. $\beta$ has units of inverse length and therefore use of a dimensionless constant of

$$b = a \beta \tag{4.4}$$

is convenient. The $\tilde{\psi}_p$ are normalised over the internal region,

$$\int_0^a |\tilde{\psi}_p(r)|^2 dr = 1. \tag{4.5}$$

The R-matrix, $R \equiv R_d(E)$, is defined in terms of $\psi(r)$ and $\beta$ as follows,
Figure 4.1: A central potential, $V(r)$, and the corresponding R-matrix eigenstate energies, $\varepsilon_p$, and wave functions, $\psi_p(r)$. 

- $\varepsilon_1$, $\varepsilon_2$, $\varepsilon_3$, $\varepsilon_4$ 
- $V(r)$ 
- $\psi_p(r)$
\[
R = \frac{1}{a} \left( \frac{\psi'(r)}{d\psi/dr - \beta \psi(r)} \right)_{r=a},
\]

where the \(1/a\) factor is included so that \(R\) is dimensionless. The coefficients, \(C_p\), of Equation (4.1) can be calculated from the relation,

\[
C_p = \int_0^a \psi \bar{\psi}_p^* \, dr.
\]

Using Equations (2.10) and (4.2), the above integral can be rearranged to give

\[
C_p(E) = \int_0^a \frac{(\bar{H} \bar{\psi}_p^*) \psi - \bar{\psi}_p(\bar{H}\psi)}{\epsilon_p - E} \, dr.
\]

It follows that

\[
C_p = -\frac{\hbar^2}{2\mu} \frac{1}{\epsilon_p - E} \int_0^a \left( \frac{d^2 \bar{\psi}_p^*}{dr^2} \psi - \bar{\psi}_p^* \frac{d^2 \psi}{dr^2} \right) \, dr,
\]

and using the product rule this can be rearranged,

\[
C_p = -\frac{\hbar^2}{2\mu} \frac{1}{\epsilon_p - E} \int_0^a \frac{d}{dr} \left( \frac{d\bar{\psi}_p^*}{dr} \psi - \bar{\psi}_p^* \frac{d\psi}{dr} \right) \, dr.
\]

Evaluating this integral, then

\[
C_p = -\frac{\hbar^2}{2\mu} \frac{1}{\epsilon_p - E} \left( \frac{d\bar{\psi}_p^*}{dr} \psi(a) - \bar{\psi}_p^* \frac{d\psi(a)}{dr} \right),
\]

and upon applying the boundary conditions given in Equation (4.3),

\[
C_p = -\frac{\hbar^2}{2\mu} \frac{\bar{\psi}_p^*(a)}{\epsilon_p - E} \left( \beta \psi(a) - \frac{d\psi(a)}{dr} \right).
\]

Substituting this back into Equation (4.1), evaluating at \(r = a\),

\[
\psi(a) = \sum_p \frac{-\hbar^2 |\bar{\psi}_p(a)|^2}{2\mu} \left( \beta \psi(a) - \frac{d\psi(a)}{dr} \right),
\]

and rearranging, gives
Substituting in from the Equation (4.6) definition of the R-matrix,

\[
\frac{\psi(a)}{\beta \psi(a) - d\psi(a)/dr} = \sum_p \frac{-\hbar^2 |\tilde{\psi}_p(a)|^2}{2\mu \epsilon_p - E}.
\]  

(4.14)

Therefore there are poles in the R-matrix for \( E = \epsilon_p \). This means that the \( \epsilon_p \) are not only the R-matrix eigenstate energies, they are also R-matrix pole energies. The reduced width, \( \gamma^2_p \), has units of energy and \( \gamma_p \) is known as the reduced width amplitude. The pole energy and reduced width are analogous to, but not equal to, the \( E_R \) and \( \Gamma \) of the S-matrix. In this work the exact scattering wave function will be approximated by the lowest energy R-matrix eigenfunction, \( p = 1 \), together with an appropriate value of \( b \). In this case the approximation to the R-matrix is

\[
R = \sum_p \frac{\gamma^2_p}{\epsilon_p - E}.
\]  

(4.17)

2 Hard-Sphere Phase Shift and Matching Radius

In order to apply the R-matrix to the \( \alpha + n \) system it is necessary to choose an appropriate R-matrix radius. The R-matrix radius marks the boundary between the “internal” and “external” regions\(^{[14]}\). A commonly used value is the sum of the radii of the colliding nuclei, \( \tau_0(A^{1/3}_c + A^{1/3}_v) \), where \( \tau_0 \) has a value in the range 1.4 \( \to \) 1.5 fm\(^{[14]}\). In the case of \(^5\)He this gives values in the range \( a = 3.62 \to 3.88 \) fm. Lane and Thomas\(^{[14]}\) define the matching radius as “The minimum radial distance beyond which neither nucleus experiences any polarising force from the other”. In other words the matching radius “marks the edge of a potential field which is smooth and refractive in character”, like
Figure 4.2: The total phase shift, $\delta_l(E)$, for the $p_{3/2}$ resonance in $^5\text{He}$, calculated using the fitted Bang potential. Also shown is the hard-sphere phase shift, $\phi_l$, calculated using a matching radius of $a = 7.0$ fm, and the R-matrix phase shift, $\varphi_l = \delta_l - \phi_l$.

the fitted Bang potential used in this work. Therefore, for all choices of matching radius greater than $a$, the deduced position of the S-matrix pole in the complex energy plane should have a converged value. In this section the effect of the matching radius on the resonance energy and width is investigated.

This section also introduces the hard-sphere and R-matrix phase shifts. In [54], Descouvemont suggests that it is the energy at which the R-Matrix phase shift rises through $\pi/2$ that should be used to determine the resonance energy and width of a state, rather than the point at which total phase shift is equal to $\pi/2$. This method of extracting the resonance energy and width information from the phase shift is compared with the methods previously considered in Chapter 2.

By definition, the matching radius, $a$, is outside the range of the potential. A radial wave function outside the range of the interaction potential has the form given in Equation (2.18), therefore at $r = a$,

$$\psi_l(a) = A[F_l(\rho) \cos \delta_l + G_l(\rho) \sin \delta_l], \quad (4.19)$$

where $\rho = ka$. If waves were incident on an impermeable sphere of radius, $a$, then the wave function, $\psi_l$, must satisfy $\psi_l(a) = 0$. The resulting phase shift is called the hard-sphere phase shift, $\phi_l$. Applying this boundary condition to the general form above gives
\[
\begin{align*}
\phi_0 &= -\rho \\
\phi_1 &= \tan^{-1} \left( \frac{\rho - \rho}{3} \right) \\
\phi_2 &= \tan^{-1} \left( \frac{3\rho - \rho^3}{3} \right) - \rho
\end{align*}
\]

Aside 4.1: Analytical expressions of the hard-sphere phase shift for different values of \( \ell \) for \( \eta = 0 \).

\[
\tan \phi_\ell = \frac{F_\ell(\rho)}{G_\ell(\rho)}. \tag{4.20}
\]

The phase shift, \( \delta_\ell \), can always be expressed as a sum of two terms,

\[
\delta_\ell = \phi_\ell + \varphi_\ell, \tag{4.21}
\]

where \( \varphi_\ell \) is called the R-matrix phase shift. Figure (4.2) shows the total phase shift calculated for the \( p_{3/2} \) resonance in \( ^{3}\mathrm{He} \) calculated using the fitted \( \text{Bang} \) potential. Also shown in Figure (4.2) is the hard-sphere phase shift calculated using a radius of \( a = 7.0 \) fm and the R-matrix phase shift. Analytical expressions for the hard-sphere phase shift when \( \eta = 0 \) can be found in Aside 4.1 for \( \ell = 0 \rightarrow 2 \).

The S-matrix can therefore be expressed as

\[
S_\ell = e^{2i\phi_\ell} e^{2i\varphi_\ell}. \tag{4.22}
\]

The S-matrix can also be expressed in terms of the tangent of the phase shift,

\[
S_\ell(k) = \frac{1 + i \tan \delta_\ell}{1 - i \tan \delta_\ell}, \tag{4.23}
\]

which is equivalent to the definition of the S-matrix given in Equation (2.3). It can be shown from Equations (2.18) and (4.6), that the R-matrix is related to the phase shift by

\[
\tan \delta_\ell = \frac{\rho F_\ell'(\rho) - F_\ell(\rho)(1 + Rb)}{G_\ell(\rho)(1 + Rb) - \rho RG_\ell'(\rho)}, \tag{4.24}
\]

where \( \rho = ka \) and the \( ' \) indicates derivatives with respect to \( \rho \). Substituting this into Equation (4.23) and using the definition of the Hankel functions given in Equation (2.28), then

\[
S_\ell(k) = \frac{(1 + Rb) - \rho RH_\ell''(\rho)/H_\ell(\rho)}{(1 + Rb) - \rho RH_\ell''(\rho)/H_\ell(\rho)} \times \frac{H_\ell'(\rho)}{H_\ell'(\rho)}. \tag{4.25}
\]
Comparing this with Equation (4.22) gives

\[ e^{2i\phi_\ell} = \frac{H_\ell^-(\rho)}{H_\ell^+(\rho)} \quad \text{and} \quad e^{2i\varphi_\ell} = \frac{(1 + R\ell) - \rho RH_\ell^-'(\rho)/H_\ell^+(\rho)}{(1 + R\ell) - \rho RH_\ell^-'(\rho)/H_\ell^+(\rho)}. \] (4.26)

An alternative derivation for the \( e^{2i\phi_\ell} \) part of Equation (4.26) can be found in Appendix A.

The nuclear phase shift from the program POLER\textsuperscript{32} was used to obtain resonance energies and widths for different matching radii. The resonance energy is obtained from the energy at which the derivative of the phase shift is a maximum and the width can be obtained from Equation (2.35). Also investigated is whether there is a difference between the values calculated from the total phase shift, \( \delta_\ell \), and those calculated from just the R-matrix phase shift, \( \varphi_\ell \). These values are then compared with the published values and S-matrix pole energies. Therefore resonance energies and widths could be found from the potential using 4 different methods:

1. **The S-matrix Pole**
   The resonance energy and width calculated from the S-matrix pole will be referred to as the S-energy and S-width.

2. **The Total Phase Shift**
   The resonance energy and width calculated from the derivative of the total phase shift will be referred to as the \( \delta \)-energy and \( \delta \)-width.

3. **The R-matrix Phase Shift**
   The resonance energy and width calculated from the R-matrix phase shift will be referred to as the \( \varphi \)-energy and \( \varphi \)-width.

4. **The Derivative of the R-matrix Phase Shift**
   The resonance energy and width calculated from the derivative of the R-matrix phase shift will be referred to as the \( d\varphi \)-energy and \( d\varphi \)-width.

Figure (4.3) shows the different resonance energies for a range of matching radii, \( 3 \leq a \leq 10 \) fm, for the \( p_{3/2} \) state in \(^{5}\text{He}\). Three of the methods agree with each other to within a few keV; these are the S-energy, the \( \delta \)-energy and the \( d\varphi \)-energy. However the choice of matching radius has a profound effect on \( E_R \). The derived \( E_R \) for \( a = 3 \) fm is \( \approx 2.5 \) times larger than the asymptotic values found for larger \( a \). All three methods give a converged result of \( E_R = 0.76 \) MeV for \( a \geq 6 \) fm, which is consistent within 5% of the published result\textsuperscript{33} of \( E_R = 0.80 \) MeV. The \( \varphi \)-energy does not converge with others until \( a \geq 9 \) fm.

Figure (4.4) shows the width calculated from the 4 different methods in the same range of matching radii. The widths follow the same trend as the resonance energies in Figure (4.3) with much larger values found for small values of \( a \). The S-width and
Figure 4.3: Resonance energies, $E_R$, calculated for the $p_{3/2}$ state in $^5\text{He}$ from different matching radii, $a$. For reference the horizontal line indicates the value published in the [33] evaluation.

Figure 4.4: Widths, $\Gamma$, calculated for the $p_{3/2}$ state in $^5\text{He}$ from different matching radii, $a$. For reference the horizontal line indicates the value published in the [33] evaluation.
Figure 4.5: Resonance energies, $E_R$, calculated for the $p_{1/2}$ state in $^5$He from different matching radii, $a$. For reference the horizontal line indicates the value published in the [33] evaluation.

$\delta$-width converge at $\Gamma=0.66$ MeV and $\Gamma=0.70$ MeV respectively. These values agree with the published width\cite{33} of $\Gamma=0.65$ MeV within 2% and 6% respectively.

It is interesting to note that in the region $a \leq 5$ fm the $d\varphi$-width agrees much better with the S-width than the $\delta$-width. Then in the region $a \geq 7$ fm the $\delta$-width agrees much better with the S-width than the $\varphi$-width.

Figures (4.5) and (4.6) for the $p_{1/2}$ state show the same trend as shown in Figure (4.4) for the $p_{3/2}$ width. The resonance energy and width for the S-method and $\delta$-method reach converged values but those for the $\varphi$-method and $d\varphi$-method continue to decrease. From Figure (4.5); the converged $\delta$-energy, $E_R = 1.88$ MeV, is closest to the published resonance energy, $E_R = 2.07$ MeV. The converged S-energy of $E_R = 1.70$ MeV also agrees quite well with the published value. In this converged region the $\delta$-energy is consistently $\approx 0.2$ MeV higher in energy than the S-energy.

Figure (4.6) shows that the converged S-width, $\Gamma = 5.26$ MeV, agrees within 6% of the published value $\Gamma = 5.57$ MeV. The $\delta$-width reaches a converged value of $\Gamma = 7.54$ MeV. Again the $\varphi$- and $d\varphi$-widths do not converge.

The S-method and $\delta$-method values for $E_R$ and $\Gamma$ converge beyond 6 fm for both the $p_{3/2}$ and $p_{1/2}$ states. This is due to the shape of the nuclear part of the potential used. Figure (4.7) shows the fitted Bang on-potential. For $a \geq 6$ fm the potential is small and slowly varying, causing the results to converge. The minimum value of $a$ that gives a suitably converged result is 7 fm. This is consistent with the definition of matching radius given by Lane and Thomas\cite{14} and quoted at the beginning of this section. Therefore a
matching radius of $a = 7$ fm is suitable for use in future three-body R-matrix calculations.

In general all the methods for obtaining the resonance energy and width agreed better for the $p_{3/2}$ state than the $p_{1/2}$ state. The $p_{3/2}$ is a narrower, lower energy resonance and as such is much closer to being described as a Breit-Wigner resonance than the $p_{1/2}$ state.

The $\varphi$- and $d\varphi$-values did not converge. Figure (4.8) shows that the hard-sphere phase shift, $\varphi$, does not converge with increasing values of $a$. This means that the R-matrix phase shift, $\delta_R$, also does not converge. Whereas the total phase shift, $\delta_T$ does converge. Due to the lack of convergence of the $\varphi$- and $d\varphi$-values, and their poor agreement with published values, the R-matrix phase shift is not suitable for the determination of resonance parameters, contrary to the discussion of [54].

3 Penetrability and Shift Function

In this section the relationships between the resonance energy and R-matrix pole energy and the resonance width and R-matrix reduced width are derived. This requires two functions to be introduced and defined; the penetrability, $P(E)$, and shift function, $S(E)$).

Looking at the $\rho H_T^{-1}(\rho)/H_T^{-1}(\rho)$ term of Equation (4.25)

\footnote{In [14], the penetrability and shift functions are referred to as the penetration and shift factors.}
Figure 4.7: The fitted Bloch Woods-Saxon potential used for the $p_{3/2}$ and $p_{1/2}$ states in $^5$He.

Figure 4.8: Hard-sphere phase shifts, $\phi_\ell$, for $\ell = 1$ (p-wave) for matching radii in the range $a = 3.0 \rightarrow 10.0$ fm.
\[
\frac{\rho H_{\ell}^{\ell'}(\rho)}{H_{\ell}^{\ell'}(\rho)} = \frac{G_{\ell}^*(\rho) - iF_{\ell}^*(\rho)}{G_{\ell}(\rho) - iF_{\ell}(\rho)},
\]
\[
= \frac{G_{\ell}^*(\rho)G_{\ell}(\rho) + F_{\ell}^*(\rho)F_{\ell}(\rho)}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2} - \frac{i\rho}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2} \left[ F_{\ell}(\rho)G_{\ell}(\rho) - F_{\ell}(\rho)G_{\ell'}(\rho) \right].
\]

(4.27)

(4.28)

(4.29)

Using the Wronskian relation \( F_{\ell}(\rho)G_{\ell}(\rho) - F_{\ell}(\rho)G_{\ell'}(\rho) = 1 \) this simplifies to

\[
\frac{\rho H_{\ell}^{\ell'}(\rho)}{H_{\ell}^{\ell'}(\rho)} = \frac{G_{\ell}^*(\rho)G_{\ell}(\rho) + F_{\ell}^*(\rho)F_{\ell}(\rho)}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2} - \frac{i\rho}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2},
\]

(4.30)

where this last equation defines the shift function, \( S(E) \), and the penetrability, \( P(E) \), as

\[
S(E) = \frac{\rho G_{\ell}(\rho)G_{\ell}(\rho) + F_{\ell}(\rho)F_{\ell}(\rho)}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2} \quad \text{and} \quad P(E) = \frac{\rho}{G_{\ell}(\rho)^2 + F_{\ell}(\rho)^2}.
\]

(4.32)

Similarly

\[
\frac{H_{\ell}^{\ell'}(\rho)}{H_{\ell}^{\ell'}(\rho)} = S(E) + iP(E),
\]

(4.33)

therefore Equation (4.25) becomes

\[
S_{\ell} = e^{2i\phi} \frac{(1 + Rb) - R[S(E) - iP(E)]}{(1 + Rb) - R[S(E) + iP(E)]}.
\]

(4.34)

Upon substituting for \( R \), the one term approximation from Equation (4.18), and rearranging, gives

\[
S_{\ell} = e^{2i\phi} \frac{E - (\epsilon - \gamma^2(S(E) - b)) - i\gamma^2 P(E)}{E - (\epsilon - \gamma^2(S(E) - b)) + i\gamma^2 P(E)}.
\]

(4.35)

There are no poles in the hard-sphere phase shift factor, therefore a comparison between the above equation and Equation (2.4) gives

\[
E_R = \epsilon - \gamma^2(S(E) - b) \quad \text{and} \quad \Gamma = 2\gamma^2 P(E).
\]

(4.36)

The shift function, \( S(E) \), is so called because it shifts the R-matrix pole, \( \epsilon \), to the resonance energy, \( E_R \). The width, \( \Gamma \), is known as the formal width, as it is not the FWHM of the resonant cross-section peak. From Chapter 2 Equation (2.8),
Figure 4.9: Penetrability functions for $\ell = 0, 1, 2$. Curves for the $\alpha+n$ system are solid and for the $n+n$ system are dashed.

\[
\sigma_\ell(E) \propto \frac{\Gamma^2}{4(E - E_R)^2 + \Gamma^2},
\]

making the substitution $E_R = \epsilon_p - \gamma^2(S(E) - b)$,

\[
\sigma_\ell(E) \propto \frac{\Gamma^2}{4(E - \epsilon - \gamma^2(S(E) - b))^2 + \Gamma^2}.
\]

As the shift and penetrability functions are functions of energy, their inclusion in $\sigma_\ell(E)$ means that it no longer has a Lorentzian form and $\Gamma$ is not the FWHM of the peak. This is explained in more detail in Chapter 6. A value closer to the FWHM is actually given by a quantity called the “observed width” which is derived in the next section.

Figure (4.9) shows the penetrability, as a function of centre-of-mass energy, calculated for $\ell = 0, 1, 2$ in the $\alpha+n$ and $n+n$ systems. Matching radii of 7.0 fm and 5.02 fm were used, respectively. The penetrability is zero for negative energies for all values of $\ell$. Figure (4.10) shows the shift functions calculated for the $\alpha+n$ and $n+n$ systems using the same matching radii and over the same range of $\ell$. For positive energies the shift function is always zero for $\ell = 0$. For negative energies the shift function is calculated in terms of
Figure 4.10: Shift functions for $\ell = 0, 1, 2$. Curves for the $\alpha+n$ system are solid and for the $n+n$ system are dashed.

the Whittaker function$^2$, $W$,$^{14, 55}$, as

$$S(E) = \rho \frac{W'}{W}. \quad (4.39)$$

Here $W'$ is the derivative of $W$ with respect to $\rho$. Equation (4.39) is the appropriate expression for negative energies since the only solution of the field free equation (Equation (2.20))$^3$ with physical significance is the Whittaker function$^{14}$.

4 The Observed Width

This section introduces the observed width and its relation to the formal width (discussed in the previous section). The observed width is more suitable for comparison with experimental values than the formal width, as it is the observed width that gives the FWHM of a cross-section peak. (This will be shown later in Chapter 6 Section 1.)

$^2$For $\eta = 0$, which is the case in this work, the Whittaker function reduces down to a modified Bessel function of the second kind$^{14}$. However, the $\eta = 0$ solution will be referred to as a Whittaker function in this work.

$^3$The Coulomb functions $F_{\ell}$ and $G_{\ell}$ are also solutions of the field free equation.
Equation (4.35) gives an expression for the R-matrix phase shift, \( \varphi \),

\[
\tan \varphi = \frac{\gamma^2 P}{(\epsilon - \gamma^2(S(E) - b)) - E} \quad (4.40)
\]

Differentiating \( \varphi \) with respect to energy gives

\[
\frac{d\varphi}{dE} = \frac{\gamma^2 P (1 + \gamma^2 \frac{dS}{dE})}{(\epsilon - \gamma^2[S(E) - b] - E)^2 + (\gamma^2 P)^2} \quad (4.41)
\]

where the penetrability, \( P \), has been approximated to be independent of energy over the width of the resonance. Evaluating at \( E = E_R = \epsilon - \gamma^2(S(E_R) - b) \) gives

\[
\frac{d\varphi}{dE} \bigg|_{E=E_R} = \frac{1 + \gamma^2 \frac{dS}{dE} \bigg|_{E=E_R}}{\gamma^2 P} \quad (4.42)
\]

From Equations (2.35) and (4.21) the derivative of the phase shift with respect to energy at the resonance energy is given by,

\[
\frac{d\delta}{dE} \bigg|_{E=E_R} = \frac{d\varphi}{dE} \bigg|_{E=E_R} + \frac{d\phi}{dE} \bigg|_{E=E_R} = \frac{2}{\Gamma^0} \quad (4.43)
\]

Here \( \Gamma^0 \) is the observed width. If the hard-sphere phase shift is approximated to be constant over the width of the resonance then

\[
\frac{d\phi}{dE} \bigg|_{E=E_R} \approx 0, \quad (4.44)
\]

and Equation (4.43) becomes

\[
\frac{d\delta}{dE} \bigg|_{E=E_R} = \frac{d\varphi}{dE} \bigg|_{E=E_R} \quad (4.45)
\]

\[
\frac{d\phi}{dE} \bigg|_{E=E_R} = \frac{2}{\Gamma^0} \quad (4.46)
\]

Substituting the above into Equation (4.42), and rearranging defines \( \Gamma^0 \) as

\[
\Gamma^0 = \frac{2\gamma^2 P}{1 + \gamma^2 \frac{dS}{dE} \big|_{E=E_R}},
\]

\[
= \frac{1}{\Gamma} \frac{1 + \gamma^2 \frac{dS}{dE} \bigg|_{E=E_R}}{1 + \gamma^2 \frac{dS}{dE} \bigg|_{E=E_R}} \quad (4.47)
\]
where $\Gamma^0$ is the observed width and its relation to the formal width, $\Gamma$, has been derived. (See Equation (4.36) for the definition of the formal width.) An alternative derivation of the observed width can be found in Appendix B of this thesis and in [53].

5 Boundary Conditions

In order to use R-matrix theory to estimate the width for the $p_{3/2}$ and $p_{1/2}$ states in $^5$He a suitable choice of the boundary condition $b$ must also be made.

In one pole approximated R-matrix theory the scattering wave function is approximated by just the lowest energy R-matrix eigenstate wave function. Therefore a suitable choice of $b$ is the value that produces an R-matrix eigenstate wave function that best approximates the full scattering wave function calculated at the S-matrix pole energy. In the case of the $^5$He $p_{3/2}$ resonance the S-matrix pole energy is $E_R = 0.77$ MeV, and the scattering wave function at this energy has a logarithmic derivative of $\beta = -0.029$ fm$^{-1}$ at $a = 7.0$ fm. This gives a value of $b = a\beta = -0.2$. Figure (4.11) shows the lowest R-matrix eigenstate wave functions calculated for different values of $b$ and the scattering wave function for the $p_{3/2}$ state calculated at the S-matrix pole energy. The wave functions have all been normalised to the same peak height so that the shape of the curves can be compared. Figure (4.11) shows that indeed $b = -0.2$ best fits the scattering wave function...
Figure 4.12: Lowest R-matrix eigenstate state wave functions calculated for different boundary conditions, $b$, for the $p_{1/2}$ state. The scattering wave function calculated at the $p_{1/2}$ S-matrix pole energy of $E_R = 1.72$ MeV is also shown. All the wave functions have been normalised to 1 as in Equation (4.5).

$$\begin{array}{cccccc}
\hline
b & \epsilon (\text{MeV}) & \gamma^2 (\text{MeV}) & \Gamma (\text{MeV}) & \Gamma_0 (\text{MeV}) \\
\hline
p_{3/2} & -0.2 & 0.76 & 0.52 & 0.72 & 0.62 \\
p_{1/2} & 0.6 & 1.66 & 1.33 & 3.56 & 3.10 \\
\hline
\end{array}$$

Table 4.1: R-matrix pole parameters, boundary conditions and formal and observed widths for the $p_{3/2}$ and $p_{1/2}$ states in $^5\text{He}$ derived from the fitted Bang potential.

function. The fitted Bang potential was used in these calculations.

Similarly, Figure (4.12) shows the scattering wave function for the $p_{1/2}$ state calculated at the S-matrix pole energy, $E_R = 1.72$ MeV. The lowest R-matrix eigenstate wave functions calculated for different values of $b$ are also shown. The curves have been normalised using Equation (4.5). Figure (4.12) shows that $b = 0.6$ produces the R-matrix wave function that best fits the exact scattering wave function.

Table (4.1) contains the values of $b$ found for each state and the resulting R-matrix pole parameters found, as well as the formal and observed widths for each state. In each case the observed width is smaller than the formal width. This is because the shift functions always have a positive gradient, as shown in Figure (4.10). Table (4.2) shows the formal and observed widths as well as some of the other widths calculated in Chapter 2 for both the $p_{3/2}$ and $p_{1/2}$ states. Table (4.2) shows that the observed width for the $p_{3/2}$ state does indeed agree better with the published value than the formal width. The
Table 4.2: Summary of resonance widths calculated from different methods.

<table>
<thead>
<tr>
<th></th>
<th>( \Gamma_{\text{pub}} ) (MeV)</th>
<th>( \Gamma_{S} ) (MeV)</th>
<th>( \Gamma_{\delta} ) (MeV)</th>
<th>( \Gamma ) (MeV)</th>
<th>( \Gamma^{0} ) (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( p_{3/2} )</td>
<td>0.65</td>
<td>0.66</td>
<td>0.71</td>
<td>0.72</td>
<td>0.62</td>
</tr>
<tr>
<td>( p_{1/2} )</td>
<td>5.57</td>
<td>5.26</td>
<td>7.54</td>
<td>3.56</td>
<td>3.10</td>
</tr>
</tbody>
</table>

\( \Gamma_{\text{pub}} \) indicates the published widths from [33]. \( \Gamma_{S} \) indicates the width from the S-matrix pole. \( \Gamma_{\delta} \) is the width from the maximum derivative of the phase shift. \( \Gamma \) and \( \Gamma^{0} \) are the formal and observed widths. These widths were all calculated using the fitted \( V_{t} \) potential.

The observed width agrees within 6% of the published and S-matrix pole values. In the case of the \( p_{1/2} \) state, the observed width has worse agreement with the published value than the formal width. The observed width only agrees within 45% of the published and S-matrix pole values. However, since the sequential decay of \( {}^{6}\text{He} \) goes through the \( p_{3/2} \) state, this is the primary concern and a good estimate for the width of this state can be obtained using R-matrix theory.

Chapter 2 established a suitable potential to describe the \( \alpha + n \) interaction. This Chapter has shown that a good estimate for the width of the \( p_{3/2} \) state in \( {}^{6}\text{He} \) can be obtained using this potential and an appropriate boundary condition of \( b = -0.2 \). In the next Chapter potentials and R-matrix boundary conditions are discussed for the remaining two-body sub-systems of \( {}^{6}\text{He} \). This will enable three-body R-matrix calculations of \( {}^{6}\text{He} \) to be performed.
Chapter 5

The $^2n+\alpha$ and $^5$He+$n$ Interactions

In the next chapter a three-body, successive decay formulation of R-matrix theory is applied to the $2^+$ resonance in $^6$He. The decay is treated as two ordered two-body decays that can proceed via two different routes,

I: $^5$He($2^+$) $\to$ $^5$He($3/2^-$) + $n$ $\to$ ($\alpha$ + $n$) + $n$,
II: $^6$He($2^+$) $\to$ $\alpha$ + $^2n$($0^+$) $\to$ $^4$He + ($n$ + $n$).

This means that four sets of interaction potentials and R-matrix boundary conditions need to be established. The four potentials are:

(1) $^5$He+$n$ (I)
(2) $\alpha$+$n$ (I)
(3) $^2n$+$\alpha$ (II)
(4) $n$+$n$ (II)

The $\alpha$+$n$ potential has already been discussed in Chapter 2 and boundary conditions were established in Chapter 4. The $n$+$n$ potential was also discussed in Chapter 3. This chapter will establish the R-matrix boundary conditions for this interaction, and the $^5$He+$n$ and the $^2n$+$\alpha$ potentials are considered for the first time, and the boundary conditions established.

1 $^5$He+$n$ Potential

The $^6$He+$n$ potential was based on the $\alpha$+$n$ potential. Therefore the Woods-Saxon geometry and spin-orbit potential of the $Bang$ potential were used. The S-matrix pole of the $^5$He $p_{3/2}$ state is at 0.765 MeV above the $\alpha$+$n$ threshold. The $2^+$ state in $^6$He is experimentally placed 0.824 MeV above the $\alpha$+$n$+$n$ threshold[33]. Therefore the Woods-Saxon potential depth was tuned to place the S-matrix pole, for the $^5$He+$n$ $p_{1/2}$ state, at $E_R = 0.824 - 0.765 = 0.059$ MeV. This yielded a depth of $V_{ws}^0 = 46.601$ MeV.
The exact scattering wave function at the S-matrix pole energy has a logarithmic
derivative of $\beta = -0.13$ fm$^{-1}$ at 7.0 fm. From Equation (4.4), this gives a boundary
condition $b = -0.13 \times 7.0 = -0.9$. Therefore this potential and these boundary conditions
can be used in future three-body R-matrix calculations.

2 $^2\text{n+}\alpha$ Potential

Since the $s = 0$ n+n system has a near-threshold virtual state but no bound states there
are no $^3\text{n+}\alpha$ scattering data. In the absence of scattering data three different $^2\text{n+}\alpha$
potential models were considered:

(1) The Point Di-neutron (or "2($\alpha+n$)"") Potential

This potential is just twice the $\alpha+n$ fitted Bang potential discussed in Chapter 2,
with $V_{\alpha n} = 0$, as the n+n system has $s = 0$.

(2) The "$\alpha+d$" Potential

This potential is based on the $\alpha$-deuteron interaction used in the $^6\text{Li}$ two-body
calculations performed in [56] and [57].

(3) The Bin Potential

This is a folded potential based on a description of the n+n system using a continuum bin. It thus uses inputs from both the $\alpha+n$ and n+n interactions.

The S-matrix pole for the nn-virtual state occurs at $E_R = -0.12$ MeV below threshold. This places the $2^+$ resonance in $^6\text{He}$ at 0.944 MeV above this state. Therefore all three
of the $^2\text{n+}\alpha$ potential models had their depths tuned to place the $^2\text{n+}\alpha$ S-Matrix pole at
this energy.

The Point Di-neutron Potential

This potential is approximately twice the fitted Bang potential. It has the same radius
and diffuseness of 2.00 fm and 0.70 fm respectively. Initially double the depth, $V_{\alpha n}^0 = \frac{2 \times 44.21}{2} = 88.42$ MeV was used. However this potential was then too deep
and the S-matrix pole in the $^2\alpha$ relative d-waves, corresponding to the $^6\text{He}$ $2^+$ state, was bound.
The depth of the potential was then tuned to place the $2^+$ state at 0.944 MeV above
threshold. It was found that a depth of $V_{\alpha n}^0 = 71.26$ MeV was required to do this.

The exact scattering wave function calculated at the S-matrix pole energy has a logarithmic
derivative of $\beta = -0.14$ fm$^{-1}$ at the matching radius of $a = 7.0$ fm. This
gives a boundary condition of $b = a\beta = 7.0 \times -0.14 = -1.0$. The potential parameters
are summarised in Table (5.1).
Table 5.1: Summary of the potential parameters and boundary conditions deduced for use in both steps of the two decay routes. The $\alpha+n$ and $^5$He+n potential included the spin-orbit potential from the fitted Bang potential, discussed in Chapter 2.

Note the nn-potential is a Gaussian and not a Woods-Saxon potential.

The $^{\alpha+d}$ Potential

$^6$Li has often been modelled as two-bodies; an $\alpha$-particle core with a valence deuteron. In [56] and [57], a Woods-Saxon binding potential, in relative s-waves, with $a_{ws}=0.65$ fm, $r_{ws}=1.90$ fm and $V_{ws}^0=78.50$ MeV was used as this potential was found to reproduce scattering data. This potential was found to be slightly too shallow for the present application as the $^6$He($2^+$) state S-matrix pole was too high in energy. A depth of $V_{ws}^0=80.25$ MeV was required to place the S-Matrix pole at the correct energy.

The scattering wave function at the S-matrix pole energy was calculated using this potential. This wave function had a logarithmic derivative of $\beta=-0.16$ fm$^{-1}$ at 7.0 fm. This gives an R-matrix boundary condition of $b=a\beta=-1.1$. Table (5.1) summarises the potential parameters and boundary conditions found.
Figure 5.2: The folded Bin potential proposed for the $^2\text{n} + \alpha$ interaction potential. The Graph also shows a Woods-Saxon fit to the Bin potential.

The Bin Potential

The Bin potential is calculated using a program called BIN\textsuperscript{[58]}. This program uses both the nn-interaction and the no-interaction to calculate an $\alpha + ^2\text{n}$ interaction. Initially, the Gaussian potential used to describe the n+n relative s-wave state is used to calculate a linear superposition of nn-scattering states over an energy (relative wave number) range. This range of $k$ is divided into $n$ quadrature intervals. In this case an energy range of 0 → 2 MeV and 200 integration points are used. So, the wave number, $k$, is integrated over a bin of width $\Delta k$. The n+n s-wave bin wave function, $\phi_{nn}(r)$, is given by

$$
\phi_{nn}(r) = \frac{U_{\Delta k}(r)}{r} Y_0(\theta),
$$

with the radial part, $U(r)$\textsuperscript{[59]},

$$
U_{\Delta k}(r) = \sqrt{\frac{2}{\pi N}} \int_{\Delta k} w(k) f(k, r) dk.
$$

Here $w(k)$ is a weight function, chosen to be

$$
w(k) = \sin \delta(k),
$$

for reasons given in [60, 61]. The $N$ is a normalisation constant given by

51
The \( f(k, r) \) are the real \( nn \)-scattering states, and are defined such that as \( r \to \infty \)

\[
f(k, r) \rightarrow \cos \delta_t(k) F_t(k, r) + \sin \delta_t(k) G_t(k, r).
\] (5.5)

The bin wave function is also normalised,

\[
\langle \phi_{nn} | \phi_{nn} \rangle = 1.
\] (5.6)

To calculate the bin potential, \( V_{\text{bin}}(\mathbf{R}) \), the bin wave functions are folded with the np-potential,

\[
V_{\text{bin}}(\mathbf{R}) = \langle \phi_{nn} | V_{\text{np}}(\mathbf{r}_1) + V_{\text{np}}(\mathbf{r}_2) | \phi_{nn} \rangle,
\] (5.7)

where the vectors, \( \mathbf{r}_1, \mathbf{r}_2, \mathbf{R} \) and \( \mathbf{r} \) are shown in Figure (5.1). The vector \( \mathbf{R} \) joins the \( \alpha \)-particle to the centre of mass of the \( n+n \) system.

For convenience the Bin potential was fitted with a Woods-Saxon. Figure (5.2) shows both the Bin potential and its fit. This potential is more shallow, extended and diffuse and was fitted by a potential with \( a_{\text{ws}} = 1.14 \text{ fm}, r_{\text{ws}} = 2.38 \text{ fm} \) and \( V_{\text{ws}}^0 = 30.61 \text{ MeV} \). However this potential was too shallow to place the \( {}^6\text{He} \) \( 2^+ \) state at the correct energy. A depth of \( V_{\text{ws}}^0 = 39.75 \text{ MeV} \) was required to lower the \( 2^+ \) state to the correct energy.

The \( \alpha + {}^2\text{n} \) scattering wave function, calculated at the S-matrix pole energy, has a logarithmic derivative of \( \beta = -0.13 \text{ fm}^{-1} \) at 7.0 fm. This gives an R-matrix boundary condition of \( b = -0.9 \).

Table (5.1) shows the potential parameters for this potential and the other two candidates for the \( {}^2\text{n}+\alpha \) potential, as well as the appropriate R-matrix boundary conditions.

**\( {}^2\text{n}+\alpha \) Potential Comparison**

Figure (5.3) shows all three candidates discussed here for the \( \alpha + {}^2\text{n} \) potential. All three of these potentials have been tuned to place the \( {}^6\text{He} \) \( 2^+ \) resonance at the same energy, 0.944 MeV.

Figure (5.3) shows that the bin potential is very different from the point di-neutron and "\( \alpha+d \)" potentials. This is due to how correlated the two neutrons are assumed to be within the models. Figure (5.4) shows the radial part of the deuteron wave function, \( |U_d(r)|^2 \) (like that found in [62]), and the \( n+n \) bin wave function, \( |U_{\Delta k}(r)|^2 \). The \( n+n \) wave function is more spatially extended than that of the deuteron, thus showing that the 2 neutrons in the bin potential are less spatially correlated than a deuteron. In the
Figure 5.3: The three proposed $^2n+\alpha$ potentials.

Figure 5.4: The n+n bin wave function, $|U_{\Delta\epsilon}(r)|^2$, and for comparison a deuteron wave function, $|U_d(r)|^2$, is also shown. The deuteron wave function was calculated using the analytic form found in [62].
limit that the 2 neutrons form a point-like di-neutron then the nn bin wave functions\(^3\) \(|\phi_{\text{nn}}(r)|^2 \to \delta(r)\). Upon substituting this into Equation (5.7) then

\[
V_{\text{bin}}(R) \to \int [V_{\text{na}}(|R + r/2|) + V_{\text{na}}(|R - r/2|)]\delta(r)dr \quad (5.8)
\]

\[
= 2V_{\text{na}}(R). \quad (5.9)
\]

So, in the limit that the 2 neutrons form a point-like di-neutron, the potential between the \(\alpha\)-particle and the di-neutron is double the neutron-\(\alpha\) potential; this is the \(2(\alpha + n)\) potential discussed here. Therefore the bin and point di-neutron potentials are at two physical extremes. The "\(\alpha+d\)" potential is an intermediate situation. However this phenomenological potential is quite similar to the \(2(\alpha + n)\) potential, since the deuteron is bound and the neutron and proton are strongly correlated. That the bin potential is so much shallower and wider than the \(2(\alpha + n)\) potential reveals that the two neutrons are less localised in the bin wave function. This is intuitively what one might expect for \(^6\text{He}\) with its Borromean halo nature.

All three of these potentials can be used in the three-body R-matrix calculations. All three potentials are used and their results compared with experimental data on the width of the \(2^+\) state. In this way we assess the sensitivity of the calculations to the choice of the assumed \(\alpha + 2n\) potential.

### 3 The \(n+n\)-Potential

The \(n+n\)-potential does not exhibit a resonant state, it has a virtual state at \(E_R = -0.121\) MeV, therefore a different method of establishing \(b\) is employed. The \(\alpha+n\) fitted Bang potential produces an R-matrix pole at \(\epsilon_p = 0.76\) MeV, which is close to the S-matrix pole energy, \(E_R = 0.77\) MeV, for the \(^3\text{He} p_{3/2}\). Therefore a value of \(b=0.27\) was chosen for the \(n+n\)-potential as this placed the R-matrix pole at \(\epsilon_p = E_R = -0.121\) MeV.

Now that the potentials and boundary conditions have been established for all the required two-body channels and decay steps in the three-body decay of \(^6\text{He}\), three-body R-matrix theory can now be applied to the \(2^+\) resonance in \(^6\text{He}\). This is the subject of the next chapter.

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\(^3\)See Equation (5.2).
Chapter 6

Three-Body R-Matrix Theory Applied to $^6\text{He}$

The 1.797 MeV $2^+$ first excited state in $^6\text{He}$ decays to $\alpha+n+n$, this is a three-body decay. Traditional R-matrix theory only includes two-body decays\cite{14}, but Lane and Thomas suggested that the theory could be extended to three-body decays by treating them as two ordered two-body decays. Lane and Thomas presented some initial formalism which has been developed further by Barker\cite{15}. In the case of $^6\text{He}$, the ordered two-body decay of the 1.797 MeV $2^+$ state can proceed in two ways:

I: $^6\text{He} \rightarrow ^5\text{He} + n \rightarrow ^4\text{He} + n + n$, 
II: $^6\text{He} \rightarrow ^4\text{He} + ^2n \rightarrow ^4\text{He} + n + n$. \hspace{1cm} (6.1)

Here $^2n$ indicates the un-bound, spin singlet, 2-neutron system or 'di-neutron'. Decay route I will be known as the sequential decay route since the neutrons are emitted sequentially. This is shown in Figure (6.1). Decay route II will be known as the simultaneous decay route as both neutrons are emitted simultaneously. This decay is shown in Figure (6.2).

In this Chapter the Barker formalism is presented and then derived in order to investigate its validity when applied to the decay of the $2^+$ state in $^6\text{He}$. Estimates of the width of this state are obtained. These will be compared with fully dynamical three-body calculations in the following Chapter.

1 Barker's formalism

In this section Barker's R-matrix formalism for the treatment of a three-body decay as two ordered two-body decays is presented.

If the three-body decay of the $2^+$ resonance in $^6\text{He}$ is treated as two ordered two-
Figure 6.1: The sequential decay of the $^6\text{He}$ 1.797 MeV $2^+$ resonance through the unbound ground state resonance in $^5\text{He}$ to the ground state in $^4\text{He}$. The energies of the intermediate state and final state are relative to the $^6\text{He}$ ground state, in MeV. $Q_{2n}$ and $Q_{1n}$ are the energies of the $^6\text{He}$ ($2^+$) and $^5\text{He}$ ($3/2^-$) states relative to the $^4\text{He}+n+n$ threshold. The energies, $E$ and $U$, are arbitrary energies measured from threshold in $^6\text{He}$ and $^5\text{He}$ respectively.

body decays, the decay must proceed through an intermediate state. In the case of the sequential neutron decay route, this intermediate state is the $p_{3/2}$ resonance in $^5\text{He}$, the unbound $^5\text{He}$ ($3/2^-$) ground state. In the case of the simultaneous decay route, the intermediate state is the di-neutron (the $^1S_0$ n-n) virtual state. The Probability Density Function (PDF), $\rho(U)$, describes the shape of this intermediate state and is given by

$$\rho(U) = c \frac{\Gamma_2(U)}{[U - Q_{1n} - \Delta_2(U)]^2 + (1/4)\Gamma_2(U)^2}.$$  (6.2)

This allows the first step of the decay to proceed not just at the resonance energy but through the tail of the resonance as well, which is important for broad states. The probability density function\(^1\) gives the probability that the second step of the decay will occur at an energy, $U$. The energy, $Q_{1n}$, is the energy above threshold of the intermediate state, as shown in Figures (6.1) and (6.2). The width, $\Gamma_2(U)$, is the formal width of the second decay step.

$$\Gamma_2(U) = 2\gamma_2^2 P_2(U).$$  (6.3)

This is the same expression for the formal width as derived in Chapter 4 and given in Equation (4.36). The second step of the decay is from the intermediate to final state, which in the case of the sequential decay is $^5\text{He} \rightarrow ^4\text{He}+n$ and in the case of the simulta-

\(^1\)The origin and properties of the probability density function is discussed further in Section 2.
neous decay is $^2n \rightarrow n+n$. The subscript 2 indicates quantities associated with the second step of the decay.

The factor, $c$, in Equation (6.2) is a normalisation constant such that,

$$ \int_0^\infty \rho(U)dU = 1. \quad (6.4) $$

The integrand $\rho(U)$ gives the probability that the second step of the decay will occur. Normalising this integral to 1 means that this second step definitely occurs once the first step has occurred. Due to computational limitations $\rho(U)$ cannot be normalised over the range $0 \rightarrow \infty$ MeV, therefore $\rho(U)$ is normalised over the range $0 \rightarrow U_{\text{max}}$ MeV. Section 4 investigates an appropriate value of $U_{\text{max}}$ for both the sequential and simultaneous decay routes.

The quantity $\Delta_2(U)$ is a linear combination of shift functions $^{[14, 15]}$,

$$ \Delta_2(U) = -\gamma_2^2[S_2(U) - S_2(Q_{1n})]. \quad (6.5) $$

This is the familiar $-\gamma_2^2[S(E) - b]$ shift term, where the boundary condition, $b$, has been set equal to $S_2(Q_{1n})$. This choice means that from the expression $E_R = \epsilon - \gamma_2^2[S(E) - b]$, $E_R \approx \epsilon \approx Q_{1n}$. A boundary condition of $b = S_2(Q_{1n})$ gives a value of $b = -0.4$ for the $^5\text{He} \rightarrow \alpha + n$ step. It was shown in Chapter 4 that the optimal choice of $b$ for the $p_{3/2}$ state in $^5\text{He}$ is $b = -0.2$. Requiring $b = S_2(Q_{1n})$, is clearly in disagreement with the optimum choice of $b$. By comparing Equations (2.4) and (4.35), it can be seen that the approximation $b = S_2(Q_{1n})$ is only valid if the width of the intermediate state is narrow and the hard-sphere phase shift can be approximated to be non-changing across the width of the resonance. As shown in Figure (4.2) this is not the case for the $^5\text{He} p_{3/2}$ state. Therefore this form of $\rho(U)$, as presented by Barker in $^{[15]}$ is not expected to be appropriate for use in this case.

It is important to note that the inclusion of the energy dependent shift term in Equation (6.2) means that $\rho(U)$ does not have the form of a Lorentzian. This in turn means that the width, $\Gamma_2$, is not the width of $\rho(U)$, as has been previously stated in Chapter 4 Section 3.

The total formal width from each of the decay routes in Equation (6.1) is given by $^{[15]}$,

$$ \Gamma_{\text{tot}}(E) = \int_0^E \Gamma_1(E, U)\rho(U)dU, \quad (6.6) $$

where the energy, $E$, is an arbitrary energy in $^6\text{He}$ measured from threshold, as shown in Figures (6.1) and (6.2). The formal width of the first step, $\Gamma_1(E, U)$, of the decay is given by

$$ \Gamma_1(E, U) = 2\gamma_1^2 P_1(E - U). \quad (6.7) $$
Figure 6.2: Simultaneous decay of the $^6$He 1.797 MeV $2^+$ resonance through the di-neutron virtual state. Energies of the intermediate and final states are given relative to the $^6$He ground state, in MeV. $Q_{2n}$ and $Q_{1n}$ are the energies of the $^6$He ($2^+$) and $^2n$ ($0^+$) states relative to the $^4$He+$n+n$ threshold. The energies, $E$ and $U_1$, are arbitrary energies measured from threshold in $^6$He and $^3n$ respectively.

In the sequential route this is the $^6$He $\rightarrow$ $^5$He+$n$ step and in the case of the simultaneous route this is the $^6$He $\rightarrow$ $^4$He+$^2n$ step. Quantities with a subscript 1 refer to the first step of the decay.

2 The Probability Density Function

As discussed in the previous section, the form of the probability density function, $\rho(U)$, as presented in [15] may not be appropriate for the ordered decay of the $2^+$ state of $^6$He. This Section will therefore investigate the origin of this equation. Lane and Thomas provide a derivation of Equation (6.2) in [14]. A single channel version of this earlier multi-channel formulation is presented in this Section.

Lane and Thomas define the probability density function as the interior norm of the exact two-body scattering wave function at energy $U$, $\psi(r, U)$,

$$\rho(U) = \int_{r=0}^{a} |\psi(r, U)|^2 dr.$$  \hspace{1cm} (6.8)

This integral is a measure of the probability that the two nuclei will penetrate within the radius $a$. Here the scattering wave function is defined to have a different asymptotic (normalisation) form from that previously used and given in Equations (2.25) and (2.26). Lane and Thomas define the asymptotic form as

\[\text{...} \]
\[ \psi(r, U) = \frac{i}{\sqrt{v/2}}(H_e^r - S_{e}H_e^r) \quad \text{and} \quad \frac{d\psi(r, U)}{dr} = \frac{ik}{\sqrt{v/2}}(H_{e'}^r - S_{e}H_{e'}^r), \quad (6.9) \]

where the \( \ell \) indicates the derivative with respect to \( \rho \), where \( \rho = kr \). This definition differs from Equations (2.25) and (2.26) by a factor of \( 2/\nu^{-1/2} \), where \( \nu \) is the velocity. Using the relation \( \nu = \hbar k/\mu \), the above can be rewritten as

\[ \psi(r, U) = i\sqrt{\frac{\mu}{\hbar k}}(H_e^r - S_{e}H_e^r) \quad \text{and} \quad \frac{d\psi(r, U)}{dr} = \frac{ik}{\sqrt{\hbar k}}(H_{e'}^r - S_{e}H_{e'}^r). \quad (6.10) \]

The scattering wave function in the internal region can be expressed as the sum over a complete set of R-matrix eigenstate wave functions,

\[ \psi(r, U) = \sum_p C_p(U)\tilde{\psi}_p(r), \quad r \leq a, \quad (6.11) \]

as is also stated in Equation (4.1). Substituting this into Equation (6.8),

\[ \int_0^a |\psi(r, U)|^2 dr = \int_0^a \left| \sum_p C_p(U)\tilde{\psi}_p(r) \right|^2 dr, \quad (6.12) \]

\[ = \sum_p |C_p(U)|^2 \int_0^a |\tilde{\psi}_p(r)|^2 dr, \quad (6.13) \]

\[ = \sum_p |C_p(U)|^2. \quad (6.14) \]

Applying the one pole approximation to the above gives

\[ \int_0^a |\psi(r, U)|^2 dr = |C_1(U)|^2. \quad (6.15) \]

Therefore the interior norm of the scattering wave function can be calculated from the R-matrix coefficient, \( C_1 \equiv C_{p-1} \), which is given in (4.12) as

\[ C_1(U) = \frac{-\hbar^2}{2\mu} \frac{\psi_p(a)}{e - U} \left( \psi(a, U) - \frac{d\psi(a, U)}{dr} \right), \quad (6.16) \]

where \( e \equiv \epsilon_{p-1} \). The asymptotic form of the scattering wave function is defined in terms of the S-matrix, \( S \), using the definition of the formal width and defining
\[
\Delta_2(U) = \gamma_2^2 (S_2(U) - b),
\]

Equation (4.35) can be rearranged to give

\[
S = \frac{H^-_\ell}{H^+_\ell} \left( 1 - \frac{i\Gamma_2(U)}{U - (\epsilon + \Delta_2(U) - i\Gamma_2(U)/2)} \right).
\]

This definition can also be found in \cite{53}. Substituting this into the expression for \(d\psi/dr\) given in Equation (6.10) and using the definition of the Hankel functions given in Equation (2.28), the definitions of the penetrability and shift functions from Equation (4.32) and the Wronskian relation \(F'_\ell(\rho) G_\ell(\rho) - F_\ell(\rho) G'_\ell(\rho) = 1\), gives

\[
\frac{d\psi(a, U)}{dr} = -\frac{k}{\hbar} \sqrt{\frac{\mu}{\hbar \Delta_2(U)}} \left( \frac{-2(U - \epsilon) + 2\gamma^2 b}{U - (\epsilon + \Delta_2(U) - i\Gamma_2(U)/2)} \right).
\]

In the same way the \(\beta\psi(a, U)\) term in Equation (6.16) can be rewritten as

\[
\beta\psi(a, U) = -\beta \sqrt{\frac{\mu}{\hbar \Delta_2(U)}} \left( \frac{H^-_\ell(\rho) \Gamma_2(U)}{U - (\epsilon + \Delta_2(U) - i\Gamma_2(U)/2)} \right).
\]

Substituting the above and Equation (6.19) into Equation (6.16) and simplifying,

\[
C_1(U) = \frac{\hbar \beta^2}{\mu a} \sqrt{\frac{\mu}{\hbar \Delta_2(U)}} \left( \frac{U - \epsilon}{U - (\epsilon + \Delta_2(U) - i\Gamma_2(U)/2)} \right).
\]

Taking the square modulus of \(C_1\), and using the definition of the reduced width given in Equation (4.16), gives

\[
|C_1(U)|^2 = \frac{\hbar \Gamma_2(U)}{(U - \epsilon - \Delta_2(U))^2 + (\Gamma_2(U))^2/4}.
\]

Substituting into Equation (6.15),

\[
\int_0^a |\psi(\tau, U)|^2 d\tau = \frac{\hbar \Gamma_2(U)}{(U - \epsilon - \Delta_2(U))^2 + (\Gamma_2(U))^2/4},
\]

therefore by Equation (6.8),

\[
\rho(U) = \frac{\hbar \Gamma_2(U)}{(U - \epsilon - \Delta_2(U))^2 + (\Gamma_2(U))^2/4}.
\]

This agrees with the Barker Equation\cite{15} for \(\rho(U)\) given in Equation (6.2), where \(\epsilon = Q_{1n}\) and \(b = S(Q_{1n})\) and the \(\hbar\) is lost in the normalisation.

60
As mentioned in the previous section, the energy dependence of the penetrability and
the shift term, $\Delta_2(U)$, means that this expression for $\rho(U)$ is not a Lorentzian, so that
$\Gamma$ does not give the width of $\rho(U)$. However applying a linear approximation to the shift
function means that the observed width, $\Gamma^0$, gives a better measure of the width of $\rho(U)$.
This will be shown in the next Section.

3 Observed Widths

The Thomas Approximation or Linear Approximation (LA) is the approximation that
the shift function is locally linear. Assuming the shift function, $S_2(U)$, is a linear function
of energy, it can be expanded using just the first 2 terms of the Taylor Series,

$$S_2(U) = S_2(Q_{1n}) + \frac{dS_2(U)}{dU} \bigg|_{U=Q_{1n}} (U - Q_{1n}). \quad (6.25)$$

Substituting the above into Equation (6.17)

$$\Delta_2(U) = -\gamma_2^2 \left( S_2(Q_{1n}) + (U - Q_{1n}) \frac{dS_2}{dU} \bigg|_{U=Q_{1n}} - b \right). \quad (6.26)$$

and substituting this into Equation (6.24) and rearranging gives

$$\rho(U) = \frac{c \Gamma_2(U) \left( \frac{1}{1 + \gamma_2^2 \frac{dS_2}{dU} \bigg|_{U=Q_{1n}}} \right)^2}{\left[ (U - Q_{1n}) + \gamma_2^2 \frac{dS_2}{dU} \bigg|_{U=Q_{1n}} \right]^2 + \frac{1}{4} \left( \Gamma_2(U) \right)^2 \left( \frac{1}{1 + \gamma_2^2 \frac{dS_2}{dU} \bigg|_{U=Q_{1n}}} \right)^2}. \quad (6.27)$$

Using the definition of the observed width from Equation (4.47),

$$\Gamma_2^0(U) = \frac{\Gamma_2(U)}{1 + \gamma_2^2 \frac{dS_2}{dU} \bigg|_{U=Q_{1n}}}, \quad (6.28)$$

that was derived in Chapter 4, Section 4, and defining a new constant, $c'$, as

$$c' = \frac{c}{1 + \gamma_2^2 \frac{dS_2}{dU} \bigg|_{U=Q_{1n}}}, \quad (6.29)$$

Equation (6.27) becomes
\[ \rho(U) = \frac{c \Gamma_2^0(U)}{\left[U - Q_{1n} + \frac{\gamma_2^2(S_2(Q_{1n}) - b)}{1 + \gamma_2^2 \frac{d S_2}{d \gamma}} \bigg|_{U=Q_{1n}} \right]^2 + \left(\Gamma_2^0(U)\right)^2 / 4}. \]  

Then by defining a new (constant) shift term,

\[ \Delta_2^0 = \frac{-\gamma_2^2(S_2(Q_{1n}) - b)}{1 + \gamma_2^2 \frac{d S_2}{d \gamma}} \bigg|_{U=Q_{1n}}, \]  

Equation (6.30) can be further simplified to give

\[ \rho(U) = \frac{c \Gamma_2^0(U)}{\left[U - Q_{1n} - \Delta_2^0\right]^2 + \left(\Gamma_2^0(U)\right)^2 / 4}. \]  

Despite the observed width having some energy dependence through the penetrability, the above form of \( \rho(U) \) is closer to having the form of a Lorentzian. This means that the observed width is a better measure of the width of \( \rho(U) \). In the Barker limit that \( b = S_2(Q_{1n}) \), the \( \Delta_0 \) term vanishes and Equation (6.32) becomes,

\[ \rho(U) = \frac{c \Gamma_2^0(U)}{\left[U - Q_{1n}\right]^2 + \left(\Gamma_2^0(U)\right)^2 / 4}. \]  

The above formula gives the shape of the intermediate state and the observed width, \( \Gamma_2^0 \), gives the width of this state. However it is the width of the initial \( 2^+ \) state in \( \textsuperscript{6} \)He that is required. In [15], Barker gives an expression similar to Equation (6.2), that describes the shape of the initial state,

\[ N(E, U) \sim \frac{\Gamma_1(E, U)}{[E - Q_{2n} - \Delta_{\text{tot}}(E)]^2 + (1/4) \Gamma_{\text{tot}}^2}. \]  

Here \( \Delta_{\text{tot}}(E) \) is given by\[15\]

\[ \Delta_{\text{tot}}(E) = \int_{\infty}^{\infty} -\gamma_1^3 \left[S_1(E - U) - S_1(Q_{2n} - U)\right] \rho(U) dU. \]  

This is again the familiar shift term, \( S(E) - b \), where the boundary condition, \( b \), has been set equal to \( S_1(Q_{2n} - U) \). The shift function, \( S_1(E - U) \), can be Taylor expanded about \( S_1(Q_{2n} - U) \). If only the first two terms of the expansion are used and the following expression for the observed width,

\[ \Gamma_1^0(E, U) = \frac{\Gamma_1(E, U)}{1 + \gamma_1^2 \int_{\infty}^{\infty} [d S_1(E - U)/d E]_{E=Q_{2n}} \rho(U) dU}, \]  

\[ \text{62} \]
is used along with the expression for the observed total width, \( \Gamma^0_{\text{tot}}(E) \),

\[
\Gamma^0_{\text{tot}}(E) = \int_0^E \Gamma^0_1(E, U) \rho(U) dU, \tag{6.37}
\]

then \( N(E, U) \) can be re-written as

\[
N(E, U) \sim \frac{\Gamma^0_1(E, U)}{|E - Q_{2n}|^2 + (1/4)[\Gamma^0_{\text{tot}}]^2}.
\tag{6.38}
\]

This expression is consistent with the work by Kryger et al. \cite{63}. Equation (6.38) shows that it is the observed width, rather than the formal width, which gives the width of the function \( N(E, U) \) and therefore also the width of the initial state. Equation (6.37) should be evaluated at \( E = Q_{2n} \) to get the total observed width of the \(^6\text{He} \ 2^+\) state.

Several different Equations have been introduced for the calculation of the PDF, \( \rho(U) \). It is convenient at this point to introduce notation corresponding to these different methods:

- \( \rho_B \) Barker\ Equation (6.33)
- \( \rho_{\text{IN}} \) Interior Norm\ Equation (6.8)
- \( \rho_{\text{L&T}} \) Lane and Thomas\ Equation (6.24)
- \( \rho_{\text{LA}} \) Linear Approximation\ Equation (6.32)

Figure (6.3) shows the PDF for the sequential decay route calculated using the IN, L&T and LA methods. The PDF's were all normalised to 1 over the range \( U = 0 \rightarrow 10 \) MeV. Figure (6.3) shows that the LA and L&T curves agree well, indicating that the linear approximation of the shift function holds for the sequential PDF. The IN curve has a high energy tail that the L&T and LA curves do not have. This is investigated in Section 4. The lack of this tail means that the peak is enhanced for the LA and L&T curves, however in general they agree well with the IN calculation.

Figure (6.4) shows PDF's calculated for the simultaneous decay route. These PDF's were also normalised to 1 over the range \( U = 0 \rightarrow 10 \) MeV. The LA calculation does not agree well with the IN calculation in this case. The linear approximation holds well for the sequential PDF but Figure (6.4) shows this is not the case for the simultaneous PDF. This is because the neutron-neutron system has a negative value of \( Q_{1n} \) and is in an \( \ell = 0 \) state. In this case \( S(U) \) is zero for positive energies and negative and finite for negative energies, with a discontinuity in the gradient occurring at zero (see Figure (4.10)). As the energy, \( U \), is always positive then the two-term Taylor expansion given in Equation (6.25) of

\[
S(U) \approx S(Q_{1n}) + \left. \frac{dS(U)}{dU} \right|_{U=Q_{1n}} (U - Q_{1n}), \tag{6.39}
\]
is only true for positive values of $Q_{1n}$ but not for negative values. A better approximation in this case is that $S(U) = 0$. Applying this approximation to (6.24) gives

$$
\rho(U) = c \frac{\Gamma_2}{(U - Q_{1n} - \gamma_2 b)^2 + \Gamma_2/4}. \quad (6.40)
$$

Since the energy dependence of the shift term has been removed, then in this case it is the formal width that gives the width of $\rho(U)$ and therefore the intermediate state, and not the observed width.\(^2\)

This introduces a 5th method for the calculation of $\rho(U)$, this method will be referred to with the following notation;

$$
\rho_{S=0}(U) \quad \text{Zero Shift Approximation} \quad \text{Equation (6.40)}
$$

However, this method is only appropriate for the simultaneous decay route, it is not a good approximation for a general case.

\(^2\)Although if the shift function was Taylor expanded about a positive energy, then $dS/dE|_{\epsilon=Q_{1n}} = 0$ in this case, so the formal width and the observed width would give the same result, $\Gamma_2 = \Gamma_{2}^{p}$. 

---

Figure 6.3: The PDF calculated for the sequential decay route using the interior norm (IN), the Lane and Thomas form (L&T) and the linear approximation (LA).
Figure 6.4: The PDF calculated for the simultaneous decay route using three different methods, the interior norm (IN), the linear approximation (LA) and the zero-shift approximation \((S = 0)\), Equation (6.40).

### 4 Normalisation of the PDF

The probability density function (PDF), \(\rho(U)\), should be normalised to 1 over the range \(U = 0 \to \infty\), as is shown in Equation (6.4). However for reasons of practicality the integral needs to be truncated to a maximum value, \(U_{\text{max}}\). In [15], Barker normalises \(\rho(U)\) up to \(U_{\text{max}} = 20.0\) MeV as the “one-level (or one-pole) approximation is not expected to be valid above this energy” in the case of \(^{12}\)O. Table (6.1) contains the first 10 R-matrix pole energies calculated for the \(p_{3/2}\) resonance in \(^{5}\)He, and shows that the 2nd pole is quite low in energy and that therefore the one pole approximation may not be good for \(^{5}\)He up to the Barker value of \(U_{\text{max}} = 20.0\) MeV.

Figure (6.5) shows the PDF calculated from the interior norm (IN) of the scattering wave function, as given in Equation (6.8). Figure (6.5) also shows the PDF calculated from the first 2 R-matrix poles using the linear approximation (LA) given in Equation (6.32). This is not a full multi-pole calculation as no interference affects are taken into account between the two poles. The IN curve has been normalised to 1 in the range \(U = 0 \to 10.0\) MeV. The sum of the two LA curves has been normalised to 1 over the same range. The IN curve exhibits a high energy tail which means that a minimum of 2 R-matrix poles are required to account for this shape. The first R-matrix pole, \(\epsilon_1\), is the resonant pole, the other poles, \(\epsilon_{p>1}\), are considered to be background poles.

Figure (6.6) shows the sequential PDF normalised over \(U = 0 \to U_{\text{max}}\) for values of \(U_{\text{max}} = 2.5, 5.0, 10.0\) and \(20.0\) MeV calculated from both the IN and single-pole LA methods. The IN and LA methods agree best when \(U_{\text{max}}\) is small as the high energy tail
<table>
<thead>
<tr>
<th>Pole number</th>
<th>Energy (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\epsilon_1$</td>
<td>0.76</td>
</tr>
<tr>
<td>$\epsilon_2$</td>
<td>9.61</td>
</tr>
<tr>
<td>$\epsilon_3$</td>
<td>33.82</td>
</tr>
<tr>
<td>$\epsilon_4$</td>
<td>69.71</td>
</tr>
<tr>
<td>$\epsilon_5$</td>
<td>116.67</td>
</tr>
<tr>
<td>$\epsilon_6$</td>
<td>174.31</td>
</tr>
<tr>
<td>$\epsilon_7$</td>
<td>242.51</td>
</tr>
<tr>
<td>$\epsilon_8$</td>
<td>321.30</td>
</tr>
<tr>
<td>$\epsilon_9$</td>
<td>410.67</td>
</tr>
<tr>
<td>$\epsilon_{10}$</td>
<td>510.62</td>
</tr>
</tbody>
</table>

Table 6.1: R-matrix pole energies calculated for the $\alpha$-n system with $a = 7.0$ fm and $b = -0.2$.

Figure 6.5: The PDF calculated from the interior norm (IN) and the linear approximated (LA) contribution to the PDF from the first 2 R-matrix poles.
Figure 6.6: The sequential PDF normalised to different maximum energies, $U_{\text{max}}$, calculated using the interior norm (IN) method and linear approximation (LA).

of the IN curve is truncated.

Figure (6.7) shows the sequential width calculated from the different PDF’s shown in Figure (6.6). It shows that the high energy tail of the IN calculation makes it impossible for a converged result to be obtained. The width calculated from the LA PDF’s does converge, a value of $U_{\text{max}} = 10.0$ MeV is sufficient to obtain a converged result.

Figure (6.8) shows simultaneous PDF’s calculated from both the IN and LA methods and normalised over the range $U = 0 \rightarrow U_{\text{max}}$ for values of $U_{\text{max}} = 2.5, 5.0, 10.0, 20.0$ and 30.0 MeV. The IN curves exhibit a smaller high energy tail than in the sequential case. However this still has the effect that the $S = 0$ curve agrees best with the IN curve when $U_{\text{max}}$ is small and the high energy tail is truncated.

Figure (6.9) shows the widths obtained from the different PDF’s plotted in Figure (6.8). The high energy tail of the IN calculation means that it is difficult to obtain a converged result. The $S = 0$ width converges more easily and a value of $U_{\text{max}} = 20$ MeV is sufficient.

Due to the difficulty in normalising $\rho_{\text{IN}}(U)$, $\rho_{\text{LA}}(U)$ will be used to calculate the width from the sequential decay and $\rho_{S=0}(U)$ will be used to calculate the width from the simultaneous decay. The normalisation of $\rho(U)$ and having used the one pole R-matrix approximation means that the second step of the decay definitely occurs and it only occurs through the resonance, not through any background contribution.
Figure 6.7: The sequential width, $\Gamma^0_{00\infty}$, calculated from different PDF's normalised to different maximum energies, $U_{\text{max}}$. Results from both the interior norm (IN) calculation and the linear approximation (LA) are shown.

Figure 6.8: The simultaneous PDF normalised to different maximum energies, $U_{\text{max}}$, calculated using the interior norm (IN) method and zero-shift approximation ($S = 0$).
5 Spectroscopic Factors

So far in this work spectroscopic factors of unity have been assumed. Spectroscopic factors are a measure of the probability that the nucleus is in a particular spatial configuration.

The definition of the reduced width given in Equation (4.16) of

\[ \gamma^2 = \frac{\hbar^2}{2\mu a} |\tilde{\psi}(a)|^2, \]  

must then be modified to include the spectroscopic factor, \( S \), as \(^{15, 64}\):

\[ \gamma^2 = \frac{\hbar^2}{2\mu a} S|\tilde{\psi}(a)|^2. \]  

For every occurrence of the reduced width in this Chapter, this redefined reduced width, which includes the spectroscopic factor, is used in preference to the definition given in Equation (4.16).

If \(^6\text{He}\) is assumed to have a pure \((p_{3/2})^2\) configuration the spectroscopic factor for the \(^6\text{He} \rightarrow ^5\text{He}+\text{n}\) step would be 2. However, the \(^6\text{He}(2^+)\) resonance may be modelled as \(^5\text{He}\) and a neutron in different angular momentum states, coupling to form the \(2^+\) state. Three-body dynamical calculations of \(^6\text{He}\) were performed using the Hyperspherical


Table 6.2: The spectroscopic factors used for the different decay steps.

<table>
<thead>
<tr>
<th>Decay Step</th>
<th>Sequential</th>
<th>Simultaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^6\text{He} \rightarrow ^6\text{He} + n$</td>
<td>1.64</td>
<td></td>
</tr>
<tr>
<td>$^6\text{He} \rightarrow ^4\text{He} + ^2n$</td>
<td>0.39</td>
<td></td>
</tr>
<tr>
<td>$^5\text{He} \rightarrow ^4\text{He} + n$</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$^2n \rightarrow n + n$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 6.3: Sequential and simultaneous widths (in keV) for the decay of the $^6\text{He}$ $2^+$ resonance. These widths were calculated using $\rho_{LA}(U)$ for the sequential decay route and $\rho_{S=0}(U)$ for the simultaneous route.

<table>
<thead>
<tr>
<th>Width</th>
<th>Sequential</th>
<th>Simultaneous</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_{col}^{\text{seq}}$ (keV)</td>
<td>34.8</td>
<td>4.29</td>
</tr>
<tr>
<td>$\Gamma_{col}^{\text{sim}}$ (keV)</td>
<td>11.2</td>
<td>3.54</td>
</tr>
</tbody>
</table>

Harmonic (HH) method$^{65, 66}$, these calculations are fully present in Chapter 7. From these three-body calculations, it is deduced that there is an 84% probability that the $2^+$ state has the $[\alpha \otimes 3/2^+]_0 \otimes 3/2^+]_0$ structure. This spectroscopic factor must then be multiplied by the number of valence neutrons, which in this case is 2. Therefore this gives a final spectroscopic factor for the $^6\text{He} \rightarrow ^5\text{He} + n$ decay step of $2 \times 0.84 = 1.68$. Similarly for the $^6\text{He} \rightarrow ^4\text{He} + ^2n$ step, it is deduced from the dynamical three-body calculations, that there is an 39% probability the $2^+$ state has a $[n \otimes n]_0 \otimes \alpha]_2^+$ structure. This gives a spectroscopic factor of 0.39 for this step. The spectroscopic factors for the other two steps, $^5\text{He} \rightarrow ^4\text{He} + n$ and $^2n \rightarrow n + n$, are both 1.0. Table (6.2) summarises these values.

Table (6.3) shows the widths calculated for both the simultaneous and sequential decay routes. These widths were calculated using the fitted Bang $\alpha + n$ potential discussed in Chapter 2, the $n + n$ potential discussed in Chapter 3, the $^5\text{He} + n$ potential discussed in Chapter 5 and the three assumed $\alpha + ^2n$ potentials, also discussed in Chapter 5. All of the widths calculated are considerably smaller than the experimentally measured width of $113 \pm 20$ keV, indicating that a combination of these decay routes is needed to account for the full width of the state. This is discussed further in Section 8. The sequential width is more than 3 times larger than the largest estimate of the simultaneous width, indicating that sequential decay is the dominant decay method. The $2(\alpha + n)$ potential, which assumes a point like di-neutron, and the $\alpha + d$ potential, produces a much smaller width than the bin potential in which the neutrons are less spatially correlated, as was previously discussed in Chapter 5.

6 Dependence on $Q_{1n}$

It was shown in Chapter 3 that the $nn$-system forms a virtual state at $E_R = -0.121$ MeV. This gives a negative value of $Q_{1n}$, as shown in Figure (6.2). A negative value of $Q_{1n}$ is also consistent with a bound state, which the $nn$-system is not. In the intermediate $^2n + \alpha$ state there is some ambiguity as to how to define the most appropriate $Q_{1n}$. Therefore this section looks at the $Q_{1n}$ dependence of the simultaneous width.
Table 6.4: Values used/found in the fixed potential calculation in comparison with the values used/found in the fixed energy calculation for the sequential decay of $^6\text{He}$. The $\rho_{PLA}$ was used in these calculations.

<table>
<thead>
<tr>
<th></th>
<th>Fixed Potential</th>
<th>Fixed Energy</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$^6\text{He} \rightarrow ^5\text{He} + n$</td>
<td>$^6\text{He} \rightarrow ^4\text{He} + n$</td>
</tr>
<tr>
<td>$b$</td>
<td>-0.90</td>
<td>-0.20</td>
</tr>
<tr>
<td>$V_{\text{eff}}^0$ (MeV)</td>
<td>46.6</td>
<td>44.2</td>
</tr>
<tr>
<td>$E_R$ (MeV)</td>
<td>0.06</td>
<td>0.76</td>
</tr>
<tr>
<td>$\Gamma^0_{\text{tot}}$ (keV)</td>
<td>34.84</td>
<td></td>
</tr>
</tbody>
</table>

The previous calculations have all used fixed boundary conditions and fixed potentials and found the R-matrix eigenstate energies. An alternative way of performing the same calculation is to fix the boundary condition and the energy and then adjust the potential depth. Such a calculation is required in order to investigate the dependence of the width on $Q_{1n}$. In the previous calculations the boundary condition, $b$, was chosen in order to obtain a good fit to the scattering wave function calculated at the S-matrix pole energy. This procedure would be time-consuming to perform for a range of values of $Q_{1n}$. Therefore it is necessary and convenient to automate the choice of boundary condition, $b$, for each value of $Q_{1n}$. From Equation (4.36),

$$E_R = \varepsilon - \gamma^2 (S(E_R) - b),$$

therefore by fixing $b = S(Q_{1n})$, $E_R \approx \varepsilon$. Barker used this relation in his work, as is explained in Section 1 and used in Equation (6.33) for $\rho(U)$. Once the boundary condition has been fixed a Newton-Raphson iterative procedure can be used to find the correct potential depth.

Table (6.4) shows the values from the previous fixed potential calculations and the values from the fixed energy calculation for the sequential decay route. In general there is good agreement between the two sets of calculations. The only significant variation is in $b$ for the second step in the decay, $^5\text{He} \rightarrow ^4\text{He} + n$. This is caused by the hard-sphere phase shift being significant in the $^5\text{He} p_{3/2}$ resonance, as is shown in Figure (4.2). From Equation (4.35), it is possible to see that the relation given in Equation (6.43) will only hold if the hard sphere phase shift is not changing across the width of the resonance. Although using Equation (6.43) is not ideal for the $p_{3/2}^5\text{He}$ resonance, there is only a 13% difference in the width, $\Gamma^0_{\text{tot}}$.

Table (6.5) compares the values from the fixed potential calculation and the fixed energy calculation for the simultaneous decay route using the previously discussed "a+d" potential for the $^4\text{He} + ^2n$ potential. It was found that setting the boundary condition $b = S(Q_{1n})$ was not suitable for the $^3n \rightarrow n + n$ step in the decay. The program located potentials that bound the di-neutron since a negative value of $Q_{1n}$ could correspond to a bound state. It was found that setting $b = -S(Q_{1n})$ was a suitable boundary condition for the di-neutron virtual state.
Table 6.5: Values used/found in the fixed potential calculation in comparison with the values used/found in the fixed energy calculation for the simultaneous decay of $^6\text{He}$. The $\rho_{S=0}(U)$ was used to calculate these widths.

Table (6.5) shows that the two calculations agree extremely well for the sequential route, with only a 2% difference in the width, $\Gamma_{\text{tot}}^0$. Having established a method for automating the choice of suitable boundary conditions and potential depths, the fixed energy calculations can now be used to vary $Q_{1n}$ and investigate the dependence of the width on this quantity.

Figure (6.10) shows the simultaneous width obtained for different values of $Q_{1n}$. Widths were calculated using $\rho_{IN}(U)$ and $\rho_{S=0}(U)$ [Equations (6.8) and (6.40)]. It was not possible to calculate the width at $Q_{1n} \approx 0$ due to numerical instability where the program switches from calculating the shift function using Whittaker functions for negative energies and the Coulomb functions at positive energies. The curves are asymmetric about $Q_{1n}=0$ because the behaviour of the shift function changes at that energy for $\ell = 0$. The shift function is finite for negative values of $Q_{1n}$ and zero for positive values. Since the boundary condition, $b$, is dependent upon the shift function, the behaviour of the PDF is also affected. Figure (6.11) shows the PDF's used to calculate the widths for $Q_{1n} = -0.121$, 0.020 and 0.121 MeV. Both $\rho_{IN}(U)$ and $\rho_{S=0}(U)$ have a peaked shape for $Q_{1n} = -0.121$ MeV. Whereas the curves for $\rho_{IN}(U)$ and $\rho_{S=0}(U)$, for both $Q_{1n} = 0.020$ and 0.121 MeV, have a maximum value at $U = 0$. The total width for the decay route is clearly significantly affected by the shape of the PDF. In order to further understand these effects a systematic study of how the total width is affected by the shape of $\rho(U)$ would be helpful. This is looked at in the next section.

7 Width of $\rho(U)$

The previous section posed some interesting questions about how the shape of the probability density function (PDF), $\rho(U)$, of the intermediate state affects the total decay width, $\Gamma_{\text{tot}}^0$. Due to the uncertainty in how best to treat the $n$-virtual state, it is clearer to examine how the width of the $\rho(U)$ distribution affects the width of the sequential decay route.

An extreme would be that $\rho(U)$ has zero width and becomes a delta function,
Figure 6.10: Dependence of the total width on the value of $Q_{1n}$ for the simultaneous decay route.

Figure 6.11: Probability Density functions calculated assuming different values of $Q_{1n}$. 

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Figure 6.12: Width calculated in the limit that $p(U)$ is a delta function. Also shown for comparison is the width calculated from $p_B(U)$.

\[ \rho_\delta(U) = \delta(U - Q_{1n}), \quad (6.44) \]

where $Q_{1n}$ is the energy of the intermediate state above threshold. In this case the formalism presented in Section 1 simplifies extensively. The total width of the state depends only on the width of the first step in the sequential decay,

\[ \Gamma_0^{\text{tot}} = \Gamma_1^0(E, Q_{1n}). \quad (6.45) \]

The expression for $\Gamma_1^0$ given in Equation (6.36) also simplifies to become

\[ \Gamma_1^0(E, Q_{1n}) = \frac{\Gamma_1(E, Q_{1n})}{1 + \gamma_1^0 [dS(E - Q_{1n})/dE]_{E = Q_{2n}}}. \quad (6.46) \]

Substituting this into Equation (6.45) gives

\[ \Gamma_0^{\text{tot}} = \frac{\Gamma_1(E, Q_{1n})}{1 + \gamma_1^0 [dS(E - Q_{1n})/dE]_{E = Q_{2n}}}. \quad (6.47) \]

Figure 6.12 shows widths calculated in the limit that the probability density function is a delta function, $\rho_\delta(U)$. Also shown is the width calculated from $p_B(U)$. The widths are calculated for a range of energies, $E_1$, which is the energy of the $^8\text{He} \ 2^+$ resonance above the intermediate state, as shown in Figure (6.1). As the delta function has zero
width the decay is unable to proceed through the tail of the resonance. Figure (6.12) shows that this is particularly important as \( E \to 0 \). In the delta reduced formalism, \( \Gamma^0_{\text{tot}} \propto P(E_1) \) and the penetrability, \( P(E_1) \), is zero for \( E_1 \leq 0 \). This means that the decay cannot occur at all at \( E = 0 \) unless it can proceed through the tail of the resonance. Figure (6.12) shows that in all cases the width increases with increasing \( E_1 \).

At the physical value of \( E_1 = 0.026 \text{ MeV} \), \( \Gamma_\delta = 7.3 \text{ keV} \), in comparison with the full calculation which gives a value of \( \Gamma_B = 40.3 \text{ keV} \). This illustrates how important the width of \( \rho(U) \) is for small values of \( E_1 \), if the decay could not go through the tail of the intermediate state resonance in \(^5\text{He} \) the width would be less than half the value.

The functional form of the probability density function given in Equation (6.32) allows the width of \( \rho_{LA} \) to be controlled directly by fixing the reduced width, \( \gamma_2^2 \). Figure (6.13) shows different \( \rho_{LA} \)'s for increasing \( \gamma_2^2 \)'s and Figure (6.14) shows the total widths calculated using these different \( \rho_{LA} \)'s. This shows that as \( \rho(U) \) becomes wider, less like a delta function and more constant, the larger the width becomes. Interestingly, Figure (6.14) shows that the total width is converging \( \approx 40 \text{ keV} \). This shows that no matter how wide the intermediate state is the sequential width will never reach a value close to the experimental width of \( 113 \pm 20 \text{ keV}^\text{[19]} \).
Figure 6.14: Total sequential width against the assumed reduced width, $\gamma_2^2$. 

\[
\begin{array}{c}
\text{physical} \\
\end{array}
\]
8 Interference

By extending R-Matrix theory to include three-body decays, assumption (2), which states that three-body reactions are absent or unimportant\(^3\), has been relaxed. Including three-body decay in the theory means that assumption (4) which states that for a pair of nuclei there is a distance beyond which the potential becomes negligible, may no longer hold. This has the effect that the two decay routes discussed here for $^6$He, the sequential and simultaneous emission of the two neutrons, may not be independent of one another. If they were independent the widths from each decay route could simply be summed incoherently.

$$\Gamma_{inc} = \sum_c \Gamma_c^0$$

(6.48)

to obtain the total width of the $2^+$ resonance. If they are not independent then interference can occur between the 2 widths. Assuming interference, the maximum possible total width is given by the coherent sum,

$$\Gamma_{coh} = \left[ \sum_o (\Gamma_o^0)^{1/2} \right]^2$$

(6.49)

Figure (6.15) shows the $^6$He $2^+$ resonance widths calculated using the three different $^2n+\alpha$ potentials discussed in Chapter 5 and Table (6.6) contains the tabulated values for these widths. The observed sequential width, $\Gamma_{n+n}$, in Figure (6.15) is the same for all three $^2n+\alpha$ potentials since it does not require a $^2n+\alpha$ potential for its calculation.

It is the coherent and incoherent sums of the sequential and simultaneous observed widths that give the "total" width of the state and can therefore be compared with experimental measurements. The experimental value for the width is $113 \pm 20$ keV\(^{19}\). The solid horizontal line represents this experimental value and the dashed lines indicate the error bars. Figure (6.15) shows that none of the data points are in this experimental region. The closest is the coherent Bin width of 85.4 keV, but there is a 24\% difference between this and the experimental width. However, for all three proposed $^2n+\alpha$ potentials, the coherent width is closer to, but still less than the experimental value. This is consistent with Barker's findings for "di-proton" decay\(^{18}\).

Since R-matrix theory is unable to give a result closer to the experimental width, it would be useful to compare these results with others from more rigorous three-body calculations. Also, without being able to narrow the choice of $\alpha+^2n$ potential, a comparison with experimental results will not resolve whether the R-matrix widths should be summed coherently or incoherently. Therefore, in the next chapter, fully dynamical three-body calculations of $^6$He are undertaken, where ordered decay routes are not assumed and where interference will be taken into account intrinsically.

\(^3\)See Chapter 4
Potential | $\Gamma_{\text{inc}}$ (keV) | %age $\Gamma_{\text{exp}}$ | $\Gamma_{\text{coh}}$ (keV) | %age $\Gamma_{\text{exp}}$
---|---|---|---|---
2($\alpha+n$) | 39.1 | 35% | 63.5 | 56%
Bin | 46.0 | 41% | 85.4 | 76%
"$\alpha+d$" | 38.4 | 34% | 60.6 | 54%

Table 6.6: Tabulated values for the coherent and incoherent sums of the sequential and simultaneous decay widths for different $^2n+\alpha$ potentials.

Figure 6.15: Calculated decay widths for the $^6$He $2^+$ resonance when using different $^2n+\alpha$ potentials. The $\Gamma_{n+n}$ is the observed width calculated from the sequential decay route. The $\Gamma_{n+n}$ are the observed widths calculated from the simultaneous decay route. The $\Gamma_{\text{inc}}$ are the incoherent sums of the sequential and simultaneous widths and the $\Gamma_{\text{coh}}$ are the maximally coherent sums. The solid horizontal line indicates the experimentally measured width and the dotted lines indicate the error boundaries.
Chapter 7

Hyperspherical Harmonics

The hyperspherical harmonic method enables a fully three-body dynamical calculation of the states of $^6\text{He}$. Unlike in the previous discussion of R-Matrix theory, presented in Chapter 6, only one width is calculated which is the total width of the $2^+$ state. Therefore this width can be compared with that from R-matrix theory to determine the degree to which the two R-Matrix widths interfere with one another or can be summed incoherently. The Hyperspherical Harmonic calculations presented in this chapter were performed using the two programs EFADDY and STURMXX, as developed by Thompson et al.\cite{65, 66}.

1 Jacobi Coordinates

A two-body problem with a central potential can be simplified by separating the radial and angular dependent parts of the wave function\cite{67}, as

$$\Psi(r, \theta, \phi) = \psi(r)Y^m_\ell(\theta, \phi). \quad (7.1)$$

The Hyperspherical Harmonic (HH) method simplifies the wave function of a three-body problem in a similar way. The radial variable in this case is the hyper-radius, $p_r$, and there are five angular variables, collectively known as $\Omega_5$.

Figure (7.1) shows the coordinates in which the physical two-body interactions are defined, these are labelled $r_{ij}$. In order to simplify the kinetic energy operator of the three-body system, it is convenient to define a new coordinate system called Jacobi coordinates. Figure (7.1) shows one possible set of Jacobi coordinates, in which $r$ links two of the particles, $b$ and $c$, and $R$ joins the centre-of-mass of the two-body sub-system to the third particle, $a$. It is useful to scale the coordinates $r$ and $R$ to give

$$x_{bc} = \sqrt{\mu_{bc}} r_{bc} \quad \text{and} \quad y_{bc,a} = \sqrt{\mu_{bc,a}} R_{bc,a}, \quad (7.2)$$
Figure 7.1: A nucleus modelled as three distinct bodies, $a$, $b$ and $c$, where body $a$ is designated the core and $b$ and $c$ are valence particles. Two sets of coordinates are shown; (i) the physical valence-core coordinates in which the two-body interactions are defined, $r_{ab}$ and $r_{ac}$ and (ii) a set of Jacobi coordinates, $R$ and $r$.

Figure 7.2: The three possible sets of Jacobi coordinates for a nucleus modelled as three-bodies. The first Jacobi coordinate, $x_{ij}$ joins two arbitrary particles. The second coordinate, $y_{ij,k}$ joins the centre of mass of the first two particles $i$ and $j$ to the third particle, $k$. 
where the $\mu$'s are the reduced masses,

$$\mu_{bc} = \frac{A_b A_c}{A_b + A_c} \quad \text{and} \quad \mu_{bc,a} = \frac{(A_b + A_c)A_a}{A_b + A_b + A_c},$$

(7.3)

and the $A_i$ are massless ratios, $A_i = m_i/\mu$. Here $\mu$ is a unit mass, for example the atomic mass unit. Figure (7.2) shows that when modelling a nucleus as three distinct bodies, there are three possible sets of Jacobi coordinates. The first radial coordinate, $x_{ij}$, joins any arbitrary pair of particles, $ij$, in the three-body system. The second radial coordinate, $y_{ij,k}$, joins the centre of mass of the pair to the third particle, $k$. Each of the two radial coordinates have associated spherical polar angular coordinates; $\theta_x, \phi_x$ and $\theta_y, \phi_y$. These four angles are four of the $\Omega_5$ set of angles. The fifth angle, $\Theta_{ij}$, is called the hyperangle and is defined as

$$\tan \Theta_{ij} = \frac{x_{ij}}{y_{ij,k}},$$

(7.4)

and is therefore dependent upon which of the three Jacobi coordinate sets is chosen. Hence $\Omega_5$ is defined as the angle set

$$\Omega_5 \rightarrow \{\Theta_{ij}, \theta_x, \phi_x, \theta_y, \phi_y\}.$$ 

(7.5)

Unlike the hyperangle, the hyper-radius is the same for each coordinate set and can be defined as

$$\rho_r = \sqrt{x_{ij}^2 + y_{ij,k}^2}.$$ 

(7.6)

The hyper-radius can also be defined in terms of the distances, $r_i$, of the three particles from the overall centre of mass,

$$\rho_r^2 = \sum_{i=1}^{3} A_i r_i^2,$$

(7.7)

where $A_i$ is the massless ratio of each particle. The hyper-radius is thus invariant under translations and rotations. The hyper-radius gives an indication of the overall size of the nucleus. If the hyper-radius is large then at least one of the distances between two of the constituent particles is large. Similarly, a small hyperangle, $\Theta_{ij}$ corresponds to particle configurations in which the pair $ij$ are in close proximity. Following from Equation (7.7), the square of the hyper-radius would be proportional to the moment of inertia of the three-body system were it composed of point particles.

In the case of $^8$He the two valence particles are both neutrons. This reduces the number of Jacobi coordinate sets required from three to two. Looking at Figure (7.2), the two
right-hand coordinate sets become equivalent under exchange of the two neutrons, particles b and c. This coordinate set is called the ‘Y-type’. The left-hand set in Figure (7.2) is called a ‘T-type’ set. This is because when the valence particles are indistinguishable the centre of mass of the pair is equidistant from both particles.

2 Coupled Hypperradial Equations

The Schrödinger Equation, written in terms of hyperspherical coordinates, is[70]

$$\left[ -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{\rho^2} \frac{d}{d\rho} \left( \rho^2 \frac{d}{d\rho} \right) - \frac{\hat{K}^2(\Omega_5)}{\rho_5^2} \right\} + V(\rho, \Omega_5) - E \right] \Psi_{J\ell_M}(\rho, \Omega_5) = 0. \quad (7.8)$$

Here \( \hat{K}^2 \) is the hypermomentum operator[70],

$$\hat{K}^2(\Omega_5) = -\frac{d^2}{d\Omega_{ij}^2} - 4 \cot(2\Theta_{ij}) \frac{d}{d\Theta_{ij}} + \frac{1}{\sin^2 \Theta_{ij}} \hat{l}^2(\mathbf{x}) + \frac{1}{\cos^2 \Theta_{ij}} \hat{l}^2(\mathbf{y}), \quad (7.9)$$

where \( \hat{l}^2(\mathbf{x}) \) and \( \hat{l}^2(\mathbf{y}) \) are the squares of the orbital angular momenta associated with \( x_i \) and \( y_i \) motions. The hyperspherical harmonics, \( y_{KLM}^{l_xli_y}(\Omega_5) \), are eigenfunctions of \( \hat{L}^2 \) with \( \hat{L} = \hat{l}(\mathbf{x}) + \hat{l}(\mathbf{y}) \). The hyperspherical harmonics are also eigenfunctions of \( \hat{K}^2 \),

$$\hat{K}^2(\Omega_5) y_{KLM}^{l_xli_y}(\Omega_5) = K(K + 4) y_{KLM}^{l_xli_y}(\Omega_5), \quad (7.10)$$

where \( K(K + 4) \) is the eigenvalue and \( K \) is an integer called the hypermomentum. The hypermomentum is independent of the choice of coordinate system. The hypermomentum is a conserved quantity in the case of either non-interacting particles or interactions that are only \( \rho_\tau \) dependent. This is approximately true for nuclei, therefore \( K \) is considered to be a “good” quantum number[69]. The hyperspherical harmonics are calculated from coupling 2 ordinary spherical harmonics[71],

$$y_{KLM}^{l_xli_y}(\Omega_5) = \zeta_{KLM}^{l_xli_y}(\Theta_{ij}) \left[ Y_{l_x}(\hat{\mathbf{x}}) \otimes Y_{l_y}(\hat{\mathbf{y}}) \right]_{LM}. \quad (7.11)$$

The hyperangular dependent part, \( \zeta_{KLM}^{l_xli_y}(\Theta_{ij}) \), of the hyperspherical harmonic has the form

$$\zeta_{KLM}^{l_xli_y}(\Theta_{ij}) = N_{KLM}^{l_xli_y}(\sin \Theta_{ij})^l (\cos \Theta_{ij})^M P_{n}^{l_x+1/2,l_y+1/2}(\cos 2\Theta_{ij}), \quad (7.12)$$

where the \( P_{n}^{l_xl_y} \)'s are Jacobi polynomials and \( N_{KLM}^{l_xli_y} \) is a normalisation factor.

The hyperspherical harmonics can be used to construct a set of hyperspherical basis functions, \( \gamma_{J\ell_M}^{l_xli_y} \)[71], of a given total angular momentum \( J_M \), as
\[ \mathcal{T}_{J K L S M J}^{\ell \ell_y} (\Omega_5) = \left[ y_{K L M}^{\ell \ell_y} \otimes X_{S \sigma} \right]_{J M J}, \tag{7.13} \]

where in Equations (7.11) and (7.13) the \([\otimes]\) notation indicates vector coupling. These basis functions are also eigenfunctions of the operator \(\hat{K}^2\). The quantity \(X_{S \sigma}\) is the total spin of the system resulting from the coupling of the two neutron spinors, \(\chi_i\).

\[ X_{S \sigma} = [\chi_{1/2} \otimes \chi_{1/2}]_{S \sigma}. \tag{7.14} \]

The wavefunction \(\Psi_{J M J}(\rho, \Omega_5)\), for a given \(J^\pi\), can be expanded in terms of a complete set of the hyperspherical basis functions[70],

\[ \Psi_{J M J}(\rho, \Omega_5) = \sum_{K \gamma} \frac{\psi_{K \gamma}(\rho)}{\rho^{5/2}} \mathcal{T}_{K \gamma}(\Omega_5). \tag{7.15} \]

The quantum numbers \(l_x, l_y, L, S\) and \(\pi\) are included in the set \(\gamma \rightarrow \{l_x, l_y, L, S, \pi\}\). So as not to complicate the notation, the dependence of the \(\psi_{K \gamma}\) on \(J\), and \(\mathcal{T}_{K \gamma}\) on \(J\) and \(M_j\), is implicit. The wave function, \(\psi_{K \gamma}(\rho_r)\), has the asymptotic form given in Equation (2.21) of [69]. The above equation can be substituted into Equation (7.8) to give

\[ \sum_{K \gamma} \left[ \frac{-\hbar^2}{2\mu} \left( \frac{d^2}{d\rho_r^2} \right) - \frac{15}{4\rho_r^2} \frac{\hat{K}^2(\Omega_5)}{\rho_r^2} \right] + V(\rho, \Omega_5) - E \] \[ \psi_{K \gamma}(\rho) \mathcal{T}_{K \gamma}(\Omega_5) = 0, \tag{7.16} \]

where the \(\rho^{-5/2}\) term in Equation (7.15) has been included to remove the first derivative in Equation (7.8). Replacing \(\hat{K}^2\) by its eigenvalue (Equation (7.10)) and making the substitution \(K = L - 3/2\) gives

\[ \sum_{K \gamma} \left[ \frac{-\hbar^2}{2\mu} \left( \frac{d^2}{d\rho_r^2} - \frac{L(L + 1)}{\rho_r^2} \right) \right] + V(\rho, \Omega_5) - E \] \[ \psi_{K \gamma}(\rho) \mathcal{T}_{K \gamma}(\Omega_5) = 0. \tag{7.17} \]

The hyperspherical basis functions are orthonormal,

\[ \int \mathcal{T}_{K' \gamma'}^* \mathcal{T}_{K \gamma} d\Omega_5 = \delta_{KK'} \delta_{\gamma \gamma'}. \tag{7.18} \]

Multiplying Equation (7.17) by \(\mathcal{T}_{K' \gamma'}^*\) and integrating over \(d\Omega_5\) gives
\[ 0 = \left[ \frac{-\hbar^2}{2\mu} \left( \frac{d^2}{d\rho_r^2} - \frac{L(L + 1)}{\rho_r^2} \right) - E \right] \psi_{K\gamma}(\rho_r) + \sum_{K'\gamma'} \int \gamma_{K'\gamma'}(\Omega_6) V(\rho_r, \Omega_6) Y_{K\gamma}(\Omega_6) \psi_{K'\gamma'}(\rho_r) d\Omega_6, \tag{7.19} \]

\[ = \left[ \frac{-\hbar^2}{2\mu} \left( \frac{d^2}{d\rho_r^2} - \frac{L(L + 1)}{\rho_r^2} \right) - E \right] \psi_{K\gamma}(\rho_r) + \sum_{K'\gamma'} V_{K'\gamma',K\gamma} \psi_{K'\gamma'}(\rho_r). \tag{7.20} \]

where

\[ V_{K'\gamma',K\gamma}(\rho_r) = \langle \gamma_{K'\gamma'} | V(\rho_r, \Omega_6) | \gamma_{K\gamma} \rangle = \int \gamma_{K'\gamma'}(\Omega_6) V(\rho_r, \Omega_6) Y_{K\gamma}(\Omega_6) d\Omega_6. \tag{7.21} \]

By separating the diagonal and off diagonal elements of \( V_{K'\gamma',K\gamma} \) and rearranging, the following set of coupled hyper-radial equations is obtained\(^6\) for each \( J^n \),

\[ \left[ \frac{-\hbar^2}{2\mu} \left( \frac{d^2}{d\rho_r^2} - \frac{L(L + 1)}{\rho_r^2} \right) + V_{K\gamma,K\gamma} - E \right] \psi_{K\gamma}(\rho_r) = - \sum_{K'\gamma' \neq K\gamma} V_{K'\gamma',K\gamma} \psi_{K'\gamma'}(\rho_r). \tag{7.22} \]

For a reaction with a total of \( N = K\gamma \) reaction channels, there are \( N \) coupled hyper-radial equations.

The potential used to calculate \( V_{K'\gamma',K\gamma} \) is the sum of the two-body interactions of the constituent particles,

\[ V(\rho_r, \Omega_6) = V_{an_1}(r_{an_1}) + V_{an_2}(r_{an_2}) + V_{nn}(r_{n_1n_2}) + V_{3B}(\rho_r), \tag{7.23} \]

where \( V_{3B}(\rho_r) \) is a three-body potential of the form

\[ V_{3B}(\rho_r) = \frac{V_{3B}^0}{1 + (\rho_r/\rho_0)^3}. \tag{7.24} \]

Here \( \rho_0 \) is the radius of the potential. In [69] this was given the value of 5 fm, as the mean value of the hyper-radius corresponding to the r.m.s. radius of the lowest shell model configuration for \(^2\)He falls in the range \( \rho_r = 4.0 \to 5.0 \) fm. The depth, \( V_{3B}^0 \), is tuned to place the \(^2\)He \( 2^+ \) resonance at the experimental energy, 0.824 MeV above threshold\(^33\). This tuning is required for comparison with the three-body R-matrix calculations performed in the previous Chapter, for which the \( 2^+ \) resonance position was fixed. The three-body potential is discussed further in Section 6.
Figure 7.3: The total decay width of the $2^+$ state in $^6$He against the maximum hypermomentum used, $K_{\text{max}}$. The data points are annotated with the depth of the three-body potential (in MeV) required to place the $2^+$ state at 0.824 MeV above threshold.

The other potentials, $V_{an}$ and $V_{nn}$, are the fitted Bang and Gaussian potentials discussed in Chapters 2 and 3 respectively. The fitted Bang potential contains both central and spin-orbit terms.

The summation over $K$ given in Equation (7.15) is in principle infinite, however for practicality it is necessary to truncate it to a maximum value, $K_{\text{max}}$. Figure (7.3) shows the width\(^1\) of the $2^+$ state calculated for different values of $K_{\text{max}}$. The data points are annotated with the depth of the three-body potential, $V_{3BP}^0$, needed to place the $2^+$ resonance at the experimental energy. Figure (7.3) shows that a value of $K_{\text{max}} = 30$ is sufficient to obtain a converged result for the width.

3 Solving the Coupled Hyper-Radial Equations

In this section the formalism for solving the coupled hyper-radial equations given in Equation (7.22) is explained. In order to do this, multi-channel S- and R-matrices are introduced. As was the case in the two-body calculations performed in Chapter 4, the R-matrix has an associated matching radius, $\rho_{\text{max}}$, and this section investigates the value of $\rho_{\text{max}}$ necessary for a converged calculation. An appropriate value of $\rho_{\text{max}}$, as well as depending upon the potentials involved, also depends on the number of channel basis functions used, $Q$. Therefore convergence calculations are performed for increasing values of $\rho_{\text{max}}$.

\(^1\)How the width is extracted from the HH calculations is discussed later in Section 5.
of both $\rho_{\text{max}}$ and $Q$.

For an outgoing channel, $i$, labelled by the set of quantum numbers $i \rightarrow \{K, \gamma\}$, and an incoming channel, $j$, the coupled radial wave function, $\psi_{ij}(\rho_r)$, (Equation (7.22)) can be expanded in terms of a complete set of multi-channel $R$-matrix eigenstates, $\phi^q_r(\rho_r)$, as

$$\psi_{ij}(\rho_r) = \sum_p A^p_{ij} \phi^p_r(\rho_r). \quad (7.25)$$

As described in [66], the $\phi^q_r$'s can, in turn, be expressed as a sum over a complete set of channel basis functions, $f^q_i(\rho_r)$,

$$\phi^q_r(\rho_r) = \sum_{q=1}^Q C_{ij}^{pq} f^q_i(\rho_r), \quad (7.26)$$

where the $f^q_i(\rho_r)$'s can be chosen to be the solutions of the diagonal part of the Hamiltonian in Equation (7.22) in each channel $i$,

$$\left\{ -\frac{\hbar^2}{2\mu} \frac{d^2}{dp_r^2} - \frac{L_i(L_i + 1)}{p_r^2} \right\} + V_{ii}(\rho_r) - \xi_q \right\} f^q_i(\rho_r) = 0. \quad (7.27)$$

The sum over $q$ in Equation (7.26) is in principle infinite, however for reasons of practicality must be truncated to a maximum value, $Q$. A reasonable value of $Q$ depends on the matching radius, $\rho_{\text{max}}$, for the calculation of the $f^q_i(\rho_r)$'s. The $f^q_i$ basis functions are chosen to have a fixed logarithmic derivative, $\beta$, at $\rho_{\text{max}}$

$$\beta = \left. \frac{d \ln f^q_i(\rho_r)}{d \rho_r} \right|_{\rho_r = \rho_{\text{max}}}. \quad (7.28)$$

The choice of a constant value for $\beta$ produces an orthonormal set of $f^q_i(\rho_r)$'s in the range $\rho_r = 0 \rightarrow \rho_{\text{max}}$ for each channel $i$.

The coefficients, $A^p_{ij}$, in Equation (7.25) can be calculated from

$$A^p_{ij} = \frac{\hbar^2}{2\mu \epsilon_p - \mathcal{E}_L} \sum_i \phi^p_i \left[ \delta_{ij} \left( \hat{H}_L^{-}(k_i \rho_{\text{max}}) - \beta \hat{H}_L^{+}(k_i \rho_{\text{max}}) \right) - S_{ij} \left( \hat{H}_L^{+}(k_i \rho_{\text{max}}) - \beta \hat{H}_L^{-}(k_i \rho_{\text{max}}) \right) \right], \quad (7.29)$$

where, as before, the $\hat{H}_L$ are the Hankel functions, but the $\hat{H}_L$ are the derivatives of the Hankel functions with respect to $\rho_r$. This equation is the multi-channel analogue of Equation (4.12), where the asymptotic behaviour of the wave function from Equations (2.25) and (2.26) has been substituted in. By writing the Hankel functions as diagonal
matrices, $H^\pm$, the S-matrix, $S$, can be calculated from a relation similar to Equation (4.25),

$$S = \frac{H^- - \rho_{\text{max}} R (H^- - \beta H^-)}{H^+ - \rho_{\text{max}} R (H^+ - \beta H^+)}.$$  \hfill (7.30)

This is the same as Equation (4.25) except the relations $H'_c = \frac{1}{\hbar} H_L$ and $b = \rho_{\text{max}} \beta$ have been used. In this case the R-matrix, $R$, is given by

$$R_{ij}(E) = \frac{\hbar^2}{2\mu \rho_{\text{max}}} \sum_{p=1}^{P} \frac{\phi_p^p(\rho_{\text{max}})\phi_p^p(\rho_{\text{max}})}{e_p - E}.$$  \hfill (7.31)

With the calculation of the multi-channel S-matrix, the eigenphases can be calculated, and the width of the resonance obtained. The eigenphases are discussed further in Section 5.

Figure (7.4) shows the width of the $2^+$ state obtained for different numbers of basis functions, $Q$, (see Equation (7.26)) and for different maximum values of the hyper-radius, $\rho_{\text{max}}$. Figure (7.4) shows that to obtain a converged result for a particular $\rho_{\text{max}}$, the number of basis functions $Q \approx \rho_{\text{max}} - 5$. Figure (7.4) also shows that the converged width is also converging as $\rho_{\text{max}}$ is increased. The results from $\rho_{\text{max}} = 25$ fm and 30 fm lie on top of one another and indicate that $\rho_{\text{max}} = 30$ fm and $Q = 25$ will yield the converged result. These widths for different values of $Q$ and $\rho_{\text{max}}$ are tabulated in Table (7.1) and the converged calculation is highlighted in bold. Table (7.1) also contains the depth of the three-body potential, $V_{32}^0$, required to place the $2^+$ resonance at the experimental energy. The table shows that as $Q$ and $\rho_{\text{max}}$ increase, $V_{32}^0$ decreases. Therefore the minimum values of $Q$ and $\rho_{\text{max}}$ required in order to obtain a converged result are $Q = 25$ and $\rho_{\text{max}} = 30$ fm. These values will be used in the fully converged calculation to obtain an estimate of the width of the $2^+$ state in $^6\text{He}$ for comparison with the results from the three-body R-matrix calculations performed in Chapter 6.

### 4 Pauli Exclusion

The Pauli Exclusion Principle (PEP) states that no two identical fermions in a given system may occupy the same quantum state\textsuperscript{[72]}. This means that some nuclear configurations, such as the $s_{1/2}$ state in $^5\text{He}$, are Pauli forbidden. Failing to take into account the PEP would mean that it would be possible for one of the valence neutrons to scatter into already occupied core states. In the K-convergence calculations of Section 2, and the $\rho_{\text{max}}$ and $Q$-convergence calculations of Section 3, the PEP was taken in account by applying a simple repulsive potential, $V_{\text{rep}}$, to the n-$\alpha$ sub-system in s-wave states, of the form.
<table>
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<th>$\rho_{\text{max}}$ (fm)</th>
<th>$Q$</th>
<th>$V_{3B}^\text{0}$ (MeV)</th>
<th>$\Gamma$ (keV)</th>
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<td>-0.324</td>
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</tr>
</tbody>
</table>

Table 7.1: Widths of the 1.8 MeV ($2^+$) resonance in $^8\text{He}$ obtained for different matching radii, $\rho_{\text{max}}$, and different numbers of channel basis functions, $Q$. The depth of the three-body potential, $V_{3B}^\text{0}$, required to place the resonance at 0.824 MeV above the $\alpha + n + n$ threshold, is also shown.
Figure 7.4: Widths of the 1.8 MeV (2+) resonance in $^6$He obtained from the HH calculations for different matching radii, $p_{\text{max}}$, and number of channel basis functions, $Q$.

\[ V_{\text{res}} = 50 \exp \left[ - \left( \frac{r}{2.3} \right)^2 \right]. \]  

However, a more accurate method is to apply Pauli Projection Operators (PPO's). The PPO’s move the forbidden eigenstates to a large positive energy (eg: 1000 MeV) so they can not affect the states of interest\(^7\).

For a system with one or more occupied nucleon states, $|u_m\rangle$, of the core nucleus, flexible three-body functions can be constructed, $U_{mn}(x, y)$, defined by

\[ U_{mn}(x, y) = u_m(x) s_n(y), \]

Here the $m$ labels the (forbidden) occupied state and $n$ labels one of a complete set of fitting (spline) functions. The vectors $x$ and $y$ refer to the $y$-type set of Jacobi coordinates, for example the right hand coordinate set shown in Figure (7.2). For a state of spin-parity, $J^\pi$, the $U_{mn}$ can be expressed in terms of the hyperspherical basis functions, $f_i^q(\rho_r)$, of Equation (7.27), by

\[ U_{mn}(x, y) = \sum_{ij} u_{mn}^q f_i^q(\rho_r) Y_j(\Omega_s). \]

Following [66], to satisfy $\langle u_m(x)|\psi_{ij}\rangle = 0$, (i.e. that the $\psi_{ij}$ has no forbidden component

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Figure 7.5: The total decay width, $\Gamma_{\text{rsp}}$, of the $2^+$ state in $^6$He calculated using a repulsive s-wave potential against that calculated using Pauli projection operators, $\Gamma_{\text{ppo}}$, for different values of $K_{\text{max}}$. The dashed line is the $\Gamma_{\text{ppo}} = \Gamma_{\text{rsp}}$ line.

in each multichannel eigenstate $p$), requires the solution of the linear equations

$$\sum_{q_{\text{i}} \overline{m}} w^q_{mni} C^p_{q_{\text{i}}} = 0, \quad (7.35)$$

for the expansion coefficients $w^q_{mni}$ in terms of the $C^p_{q_{\text{i}}}$ of Equation (7.26).

Having thus determined the $U_{mn}$ for all forbidden states, $m$, and splines, $n$, these are used, as discussed in [66], to construct the projection operator of the occupied states. The three-body problem is then solved in the allowed subspace of states by introduction of the projection operator, the forbidden eigenstates being removed by attributing to them a large positive energy eigenvalue, commonly referred to as the Pauli Projection Operator (PPO) technique.

Figure (7.5) shows a comparison between the widths calculated using a repulsive s-wave potential, $\Gamma_{\text{rsp}}$, and those calculated using the PPO's, $\Gamma_{\text{ppo}}$, for different values of $K_{\text{max}}$. As indicated by the $\Gamma_{\text{ppo}} = \Gamma_{\text{rsp}}$ line in Figure (7.5), the two widths agree well, within 1% of each other. As was the case in the previous section, the depth of the three-body potential was tuned to place the $2^+$ resonance at the experimental energy. The PPO's required a slightly deeper potential, $\approx 0.016 \rightarrow 0.018$ MeV deeper, than the repulsive s-wave potential. The depths of the three-body potential required for the widths calculated using the repulsive s-wave potential are given in Figure (7.3).
Since $\Gamma_{gp}$ and $\Gamma_{pp}$ agree so well, either method can be used to take into account the PEP. However using the repulsive s-wave potential method requires less time for the program to run than using the PPO's. Therefore the repulsive s-wave potential method was used for the rest of the HH calculations performed in this work.

5. The Eigenphase Shift

This section introduces the eigenphase shift and establishes how the resonance width can be obtained using the multi-channel eigenphases in a similar way as the phase shift was used in the single channel, two-body calculations performed in Chapters 2 and 4.

5.1 Calculating the Eigenphases

Multi-channel resonances, such as those that arise as solutions of the three-body hyperspherical calculations, are normally too complicated to be described using Breit Wigner forms\cite{1973} in any single channel. Nevertheless eigenphase shifts can be used to characterise these resonances.

The unitary multi-channel S-matrix can be diagonalised,

$$\left(U^* S U\right)_{kk'} = e^{2i\delta_k} \delta_{kk'},$$

(7.36)

where $U$ is a unitary matrix and $\delta_k$ is the eigenphase in the $k$th channel\cite{1974}. The $e^{2i\delta_k}$ in the above Equation (7.36) are eigenvalues of unit norm, which therefore have corresponding eigenvectors. For a system with $n$ channels these are

$$e^k = \begin{pmatrix} e_1^k \\ \vdots \\ e_n^k \end{pmatrix}, \quad k = 1, \ldots, n,$$

(7.37)

which are orthogonal,

$$\sum_{i=1}^{n} e_i^k e_i^{k'} = \delta^{k'k},$$

(7.38)

and complete,

$$\sum_{k=1}^{n} e_i^k e_j^{*k} = \delta_{ij}.$$ 

(7.39)

Introducing the Hermitian matrices $E^k$, where $E^k$ is an $n \times n$ matrix with elements
\[ E_{k_l} = c_k c_{l}^{*} \]  

then from Equations (7.38) and (7.39) these matrices satisfy

\[ E^k E^{k'} = \delta^{kk'} E^{k'} \quad \text{and} \quad \sum_{k=1}^{n} E^k = I, \]  

where \( I \) is a unit matrix. Therefore, the S-matrix is given by

\[ S = \sum_{k=1}^{n} e^{2i\delta_k} E^k. \]  

In order to clarify this formalism, a two-channel example is elucidated in Appendix D. It is interesting to note that the unitarity of the S-matrix, \( S \), can be verified using the above Equation.

### 5.2 Eigenphases and Resonant Width

This section examines how the eigenphases can be used to obtain the width of a multi-channel resonant state. The total eigenphase shift for a state of given \( J^\pi \) in \( n \) channels, \( \Delta(E) \), is given by

\[ \Delta(E) = \sum_{k=1}^{n} \delta_k(E). \]  

On resonance only one of the eigenphases, as defined, passes through \( \pi/2 \) or \( N\pi + \pi/2 \) for some integer, \( N \). This particular eigenphase is called the resonant phase, \( \delta_r \). In \([75]\) it is shown that \( \Delta(E) \) has the same form of energy dependence as the phase shift in a single channel reaction, namely

\[ \Delta(E) = \Delta_0(E) + \delta_r(E), \]  

\[ = \Delta_0(E) + \tan^{-1} \left( \frac{\Gamma}{2(E_R - E)} \right) \]  

where \( \Delta_0(E) \) is the sum over all other (background) eigenphases,

\[ \Delta_0(E) = \sum_{k \neq r}^{n} \delta_k(E), \]  

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Figure 7.6: The total eigenphase shift, $\Delta(E)$, resonant eigenphase, $\delta_r$, and background eigenphases, $\Delta_0(E)$ against energy, are shown on the left, their derivatives (with respect to energy) are shown on the right. These eigenphases were calculated using $K_{\text{max}} = 30$, $\rho_{\text{max}} = 30$ fm and $Q = 25$. 
provided that $\Delta_0(E)$ is a slowly varying function of energy. This means that the resonance energy and width can be extracted from $\Delta(E)$ using Equation (2.35) in the same way as was used for the single channel phase shift, $\delta_i$. By taking the derivative of Equation (7.45)

$$\frac{d\Delta(E)}{dE} = \frac{d\Delta_0(E)}{dE} + \frac{2\Gamma}{4(E_R - E)^2 + \Gamma^2}$$

and under the assumption that $\Delta_0(E)$ is slowly varying, and evaluating at $E = E_R$

$$\left.\frac{d\Delta(E)}{dE}\right|_{E=E_R} = \frac{2}{\Gamma}.$$  

(7.48)

However, if $\Delta_0(E)$ is not a sufficiently slowly varying function of energy then

$$\frac{2}{\Gamma} = \left.\frac{d\Delta(E)}{dE}\right|_{E=E_R} - \left.\frac{d\Delta_0(E)}{dE}\right|_{E=E_R},$$  

(7.49)

which is the same as

$$\frac{2}{\Gamma} = \left.\frac{d\delta_r}{dE}\right|_{E=E_R}.$$  

(7.50)

Therefore either the total eigenphase or just the resonant phase can be used to determine the width depending on how $\Delta_0(E)$ varies with energy.

Figure (7.6) shows the total eigenphase shift, $\Delta(E)$, the resonant eigenphase, $\delta_r$, and background eigenphases, $\Delta_0(E)$ against energy. These phases were calculated using a repulsive s-wave potential to take into account Pauli exclusion, a maximum value of hypermomentum of $K_{max} = 30$, a matching radius of $\rho_{max} = 30$ fm and a maximum number of channel basis states of $Q = 25$. Figure (7.6) shows that the total eigenphase is indeed dominated by the resonant phase. The background eigenphases also vary only slightly over the width of the resonance. Thus indicating that the total eigenphase shift is adequate for establishing the width of a resonant state.

Figure (7.7) shows the converged widths, $\Gamma$, for different values of $\rho_{max}$ against the width calculated from just the resonant eigenphase, $\Gamma_r$. Figure (7.7) shows that as $\rho_{max}$ increases the agreement between $\Gamma$ and $\Gamma_r$ decreases, indicating that the background eigenphases become more significant. However, at worst, there is only a 7% difference.

The total eigenphase, $\Delta(E)$, is also simpler to use than the resonant eigenphase, $\delta_r(E)$. This is because the program STURMXX does not write the eigenphase data for a channel, $k$, to one column. Figure (7.8) shows the eigenphase data from the first 8 columns of the data file. This means that the resonant eigenphase data must be pieced together after the program has finished. However the total eigen phase can be found by simply summing over all the columns of data.
Figure 7.7: Width of the $^6$He $2^+$ resonance calculated using only the resonant eigenphase, $\Gamma_r$, against the width calculated from the total eigenphase shift, $\Gamma$. The widths were calculated using different values of matching radius, $\rho_{\text{max}}$, with $Q > \rho_{\text{max}} - 5$ to obtain a converged result.

Figure 7.8: Eigenphases, $\delta_k(E)$, calculated by the program STURMXX. The eigenphase for a particular channel, $k$, is read out to a different column for different energies, $E$. The eigenphases from the first 8 data columns are shown here.
As it is easier to obtain the total eigenphase shift, and since there is little difference between the width obtained from the resonant eigenphase and that obtained from the total, it is the total eigenphase shift that is used to determine the width of the $2^+$ resonance in $^6$He. This width will then be compared with results from three-body R-matrix calculations.

## 6 Sequential Width

The R-matrix calculations performed in Chapter 6 treated the three-body decay of the $^6$He $2^+$ resonance as two ordered two-body decays. This meant there were two possible decay routes, either emitting the two neutrons sequentially or simultaneously. This section looks at using the HH method to obtain an estimate of the sequential width for comparison with the R-matrix calculations. To do this the n+n-potential strength is reduced so that the neutrons become less correlated within $^6$He, making it less likely that both neutrons will be emitted simultaneously. To compensate the three-body potential strength is increased to ensure that the $2^+$ is 0.824 MeV above threshold.

The full strength of the neutron-neutron interaction is $V_{nn}^0 = 31$ MeV. Figure (7.9) shows the width calculated for different percentage strengths of $V_{nn}^0$, ie: $V_{nn}$ is the percentage fraction of $V_{nn}^0$, where the three-body potential, $V_{3B}$, has a radius of $\rho_0 = 5.0$ fm. The Figure shows that as the strength $V_{nn}$ is decreased, the width initially decreases, but as $V_{nn}$ becomes repulsive the width increases. This is due to the radius of $V_{3B}$, Figure (7.10) shows $V_{3B}$ for $\rho_0 = 5.0$ fm and for $V_{nn} = V_{nn}^0$ and $V_{nn} = 0$. It shows that as $V_{nn}$ has
Figure 7.10: Three-body potentials, $V_{3B}$, for different radii $\rho_0 = 2.0$ fm and $5.0$ fm, required to place the $^6$He $2^+$ resonance $0.824$ MeV above threshold, both with and without neutron-neutron interaction.

decreased, the strength $V_{3B}^0$ has increased to keep the $2^+$ resonance at the correct energy, so that $V_{3B}$ exerts an influence over a large distance. This allows the two neutrons to interact despite the fact there is no neutron-neutron potential. In order to obtain an estimate of the sequential width it is necessary to reduce the range of the three-body potential so that the two valence neutrons cannot interact through the three-body potential. Therefore the same calculation was performed with a reduced three-body potential radius of $\rho_0 = 2.0$ fm and the results are also shown in Figure (7.9). Despite the three-body potential being significantly stronger in order to place the resonance at the correct energy, the width does not follow the trend observed in the $\rho_0 = 5.0$ fm results. Figure (7.10) shows the three-body potential used in the $\rho_0 = 2.0$ fm calculations for $V_{nn} = V_{2B}^0$ and $V_{nn} = 0$. The graph shows that these potentials are much less significant at larger radii than the $\rho_0 = 5.0$ fm, $V_{nn} = 0$ potential. Therefore the $\rho_0 = 2.0$ fm and $V_{nn} = 0$ calculation gives an estimate of the sequential width of $\Gamma = 46.5$ keV.

The dashed line in Figure (7.9) indicates the R-matrix sequential width from the previous Chapter. Figure (7.9) shows that the estimate of the sequential width calculated using the HH method is larger than the R-matrix width. There is a 25% difference between the HH value of $\Gamma = 46.5$ keV and the R-matrix value, $\Gamma_{1A} = 34.8$ keV. The removal of the neutron-neutron interaction in the HH calculation does not remove all correlation between the two neutrons because there is still the three-body potential acting between them. With this in mind, agreement of within 25% between the HH and R-matrix calculation of the sequential width is good.
Figure 7.11: Comparison between R-matrix and HH widths calculated for the $2^+$ resonance in $^6$He. $\Gamma_{n+n}$ is the sequential R-matrix decay width and $\Gamma_{2n}$ is the simultaneous R-matrix decay width. $\Gamma_{inc}$ and $\Gamma_{coh}$ are the incoherent and maximally coherent sums of the R-matrix sequential and simultaneous widths. These are shown for three different $\alpha+^3$n potentials. $\Gamma_{seq}$ is the estimate of the sequential width from the HH calculations and $\Gamma_{HH}$ is the full decay width of the state from the HH calculations.

7 Comparison with R-matrix Theory

Having established appropriate values for obtaining a converged result, the width of the $^6$He $2^+$ resonance can be calculated for comparison with the R-matrix results of the previous chapter. Therefore, using the repulsive s-wave potential to take into account the PEP, $K_{max} = 30$, $\rho_{max} = 30$ fm, $Q = 25$ and $\rho_0 = 2.0$ fm, a width of $\Gamma = 67.8$ keV was obtained. Figure (7.11) shows how this width agrees with the coherent and incoherent R-matrix widths obtained for the three different $\alpha+^3$n potentials. The HH width agrees within 6% of the coherent point-di-neutron width (labelled the 2(\alpha+n) potential). The HH width also agrees quite well with the coherent "\alpha+d" width, with an 11% difference. However the HH width does not agree well with the experimental width of $113 \pm 20$ keV. The HH width is 40% less than the experimental width.

The agreement between the HH calculation and the coherent width for the point-di-neutron potential indicates that interference does occur between the simultaneous and sequential widths in the R-matrix calculation. However the HH calculation, which is a full three-body dynamical calculation, does not agree well with the well established
experimental width for the state. The width that best agrees with the experimental width
is the $R$-matrix coherent width for the Bin potential, in which the two neutrons are much
less correlated than in the $2(\alpha+n)$ potential. One of the cases of “di-proton” decay
studied by Barker is the $^{12}$O ground state\cite{15, 16, 18, 76}. In this case the three-body $R$-
matrix theory and HH calculations\cite{77} also predict widths smaller than the experimentally
measured values\cite{63, 76, 78}. However, there has been some doubt expressed about these
experimental values\cite{15, 76}.

8 Comparison With Other Theoretical Results

The HH result from this work, $\Gamma = 67.8$ keV, compares quite well with the previous HH
result from Ershov et al. of $\Gamma \sim 60$ keV\cite{25}. Although it is significantly larger than the
earlier HH result from Danilin et al. of $\Gamma = 40$ keV\cite{24}. Other theoretical methods have
also been used to calculate the width of the $^6$He $(2^+)$ state. In [21], Csótó finds a width
of $\Gamma = 60$ keV using the complex scaling method, which also agrees well with the results
found in this work. Excellent agreement is found with the Tanaka et al. value of $\Gamma = 70$
keV\cite{22} using the analytical-continuation-in-the-coupling-constant method. The result of
$\Gamma = 168$ keV that Vasilevsky et al. calculate using an algebraic model\cite{23} is the only
result that significantly disagrees with the results from this work.

None of the theoretical results agree well with the experimental value. The average
theoretical value\footnote{This is an average of the theoretical results quoted here, the HH width from this work and the 3 coherent estimates from the three-body $R$-matrix theory, also from this work.} for the width is $\Gamma = 75$ keV. If the lowest and highest estimates for
the width are excluded, the average falls to $\Gamma = 67$ keV. There is a clear discrepancy
between what has been experimentally measured and what theory predicts. Since the
HH calculations performed here were fully converged, it is not obvious how a larger
estimate of the width could be obtained using this method.
Chapter 8

Conclusions

$^6$He is a Borromean halo nucleus and has often been modelled as three-bodies, an alpha-particle core and two valence neutrons. $^6$He exhibits a $2^+$ (three-body) resonance, 1.8 MeV above the ground state, with a measured width of $113 \pm 20$ keV$^{[13]}$. *Lane and Thomas*,$^{[14]}$ and later *Barker*,$^{[15]}$ have developed formalism for treating the decay of such a three-body system as two, ordered two-body decays. In this model the $2^+$ resonance in $^6$He could decay by one of two routes; (i) $^6$He $\to$ $^5$He + n $\to$ $^4$He + n + n, (ii) $^6$He $\to$ $^4$He + $^2$n $\to$ $^4$He + n + n. Decay route (i) is designated the sequential neutron decay route and goes through the $^5$He ground state ($^3p_{3/2}$) resonance as an intermediate state. Decay route (ii) is designated the simultaneous neutron decay route and goes through the "di-neutron" s-wave virtual state as an intermediate state. Each of the decay routes has an associated width which, in combination, determine the total width of the state. These decays, and their widths, may interfere with one another and it is therefore unclear whether they combine coherently or incoherently. In order to investigate this the Hyperspherical Harmonic (HH) expansion method is also applied to the $2^+$ resonance in $^6$He. The HH method enables a fully dynamical three-body calculation, in which any interference effects are automatically taken into account, directly producing a total width for the state.

In order to apply these models the two-body interactions of the two body sub-systems of $^6$He must be known. Both the R-matrix and HH methods require interactions for the $^4$He+n and n+n systems. In addition, the R-matrix model also requires interactions for the $^5$He+n and $^4$He+$^2$n systems.

The $^4$He+n potential used is based on a potential first used by *Bang et al.*$^{[31]}$. This central Woods-Saxon plus spin-orbit potential was fitted to $^4$He+n scattering phase shift data for the $^3p_{3/2}$, $^1p_{1/2}$ and $^1s_{1/2}$ states. The geometry of these potentials were taken and kept constant and the potential strengths varied to produce a fit to more recent phase shift data. On average, this "fitted Bang" potential was found to produce S-matrix poles that agree with accepted values for the resonance energy and width for all three states (within 8%).

For the s-wave n+n potential the simple Gaussian potential used in [47] was used. This potential produces a scattering length and effective range that agree with experimental values. The $^5$He+n potential was based on the $^4$He+n potential, the strength being tuned
to place the $^6\text{He} (2^+)$ resonance at the experimental energy. In [6], Bartlett et al. treat the “di-neutron” system as having a resonance at zero energy in order to obtain an estimate of the $^4\text{He}(2\pi,\gamma)^4\text{He}$ reaction rate. This work has shown this approximation is insufficient and does not adequately treat the $n+n$ virtual state at $E_R = -0.12$ MeV.

Since no scattering information exists for $^4\text{He}+^3\text{n}$, three different potentials are proposed; (i) a point di-neutron potential, this is approximately twice the $^4\text{He}+n$ potential, (ii) a phenomenological potential based on the $\alpha+d$ interaction, and (iii) a folded bin potential based on a description of the $n+n$ system using a continuum bin. All three $^4\text{He}+^3\text{n}$ potentials were tuned to place the $^6\text{He} (2^+)$ resonance at the correct energy. The point di-neutron potential and the folded bin potential are at two physical extremes, the two valence neutrons being highly spatially correlated in the point di-neutron potential but are less localised in the bin potential. The “$\alpha+d$” potential represents an intermediate case.

R-matrix theory approximates the exact scattering wave function using R-matrix eigenstate wave functions, which are normalised over the internal region, $r = 0 \to a$. In order to ensure that these form a complete orthonormal set, the eigenstate wave functions are chosen to have a fixed logarithmic derivative, $\beta$, at the matching radius, $a$. Therefore, appropriate values of $a$ and $\beta$ must be chosen for each potential. This work approximates the R-matrix by a single pole, therefore the lowest energy eigenstate wave function approximates the exact scattering solution in the internal region. So, a value of $\beta$ is chosen to best describe the scattering wave function. The radius, $a$, was chosen so that all the strength of the potential is within that radius. For all the potentials discussed here, excluding the $n+n$ potential, a value of $a = 7.0$ fm was found to be appropriate. In the case of the $n+n$ potential a value of $a = 5.0$ fm was used.

Different methods of extracting $\alpha+n$ resonant widths and energies from a potential for the $p_{3/2}$ and $p_{1/2}$ states were also examined. In [54] it is suggested that the point at which the R-matrix phase shift goes through 90° defines the resonance energy. The R-matrix phase shift is the scattering phase shift minus the hard-sphere phase shift. Values obtained from the R-matrix phase shift were compared with those obtained from finding the S-matrix pole and from using either the point at which the phase shift rises through 90° or the point at which the derivative of the phase-shfit is at a maximum. It was found that the S-matrix pole agreed most closely with the values published in the [33] evaluation. Values obtained from the maximum derivative of the phase shift gave values that agreed well with the S-matrix pole. This was especially the case for the $p_{3/2}$ state, as this is a narrower resonance and is therefore more Breit-Wigner-like in nature.

The three-body R-matrix theory has been applied to the $2^+$ state in $^6\text{He}$. In [15], Barker uses a probability density function (PDF) to describe the shape of the intermediate state. Barker’s prescription for the PDF fixes the R-matrix boundary condition, $\tilde{b} = a\beta$, to be equal to the shift function evaluated at the resonance energy, $\tilde{b} = S(E_R)$. In this work the PDF formalism was generalised to allow an optimum $b$ to be chosen to best match the exact scattering wave function. Also, this work showed that approximating the shift function to be linear with energy, is not adequate for the $n+n$ virtual state. A “zero-shift” prescription for the PDF was found to be more appropriate for this s-wave state. A sequential width of $\Gamma_{n+n} = 34.8$ keV was found. Using the three proposed
\( \alpha + 2n \) potentials, incoherent total widths were calculated (i) \( \Gamma_{2(\alpha+n)} = 39.1 \text{ keV} \), (ii) \( \Gamma_{2n} = 46.0 \text{ keV} \) and (ii) \( \Gamma_{\alpha+n} = 38.4 \text{ keV} \). As well as three maximally coherent widths for the state, (i) \( \Gamma_{2(\alpha+n)} = 63.5 \text{ keV} \), (ii) \( \Gamma_{2n} = 85.4 \text{ keV} \) and (ii) \( \Gamma_{\alpha+n} = 60.6 \text{ keV} \). The coherent width is closer to, but still less than, the experimental width for all three \( \alpha + 2n \) interactions. This is consistent with Barker's findings for two-proton decay\(^{[18]}\). In the one case of “di-neutron” decay studied by Barker\(^{[18]}\), that of \( ^5\text{H} \), it was found that the coherent width was too large and that the incoherent width gave better agreement with experiment. However, the interactions of the two-body sub-systems of \( ^6\text{He} \) are better understood.

The same \( n+n \) and \( \alpha + n \) interactions as used in the R-matrix calculations were then used in the HH calculations. Some parameters in the HH calculations are truncated to the minimum values required, in order to reduce run time, but consistent with obtaining a converged result. Therefore, a maximum hyper-radius of \( \rho_r = 30 \text{ fm} \), a maximum hypermomentum of \( K_{\text{max}} = 30 \), and \( Q = 25 \) R-matrix channel basis functions were used. The depth of a small three-body potential was tuned to place the \( ^6\text{He} \ (2^+) \) state at the correct energy. A 2\(^+ \) decay width of \( \Gamma_{\text{HH}} = 67.8 \text{ keV} \) was found which agrees well with the coherent results from the R-matrix calculations. However, this value is 40% smaller than the experimentally measured width of the state. The HH calculations were also used to obtain an estimate of the sequential width. This was achieved by reducing the strength of the \( n+n \) interaction, causing the two neutrons to be less correlated in the \( ^6\text{He} \) nucleus. An estimate of \( \Gamma_{n+n} = 46.5 \text{ keV} \) was obtained. This also agrees quite well with the R-matrix value of \( \Gamma_{n+n} = 34.8 \text{ keV} \) as the interaction between the two neutrons cannot be fully removed from the HH calculation (due to the three-body potential).

In summary, this work has shown that:

- In the case of resonances in \( ^5\text{He} \), the point at which the derivative of the phase shift reaches a maximum gives resonance energies and widths that best agree with the values from the location of the S-matrix pole in the complex plane. This is contrary to the recommendation in \([54]\), which states that the point at which the R-matrix phase shift rises through 90° should be used to determine the resonance energy and width.

- Approximating the \( n+n \) virtual state as a resonance at zero energy is inadequate. This approximation was used in \([6]\) and \([52]\) in order to estimate the \( ^4\text{He}(2n,\gamma)^6\text{He} \) reaction rate.

- Barker's R-matrix formalism can be generalised to allow for the choice of optimised boundary conditions. This generalisation is especially important for states where the hard-sphere phase shift changes across the width of the resonance.

- Coherence between the widths for the different ordered two-body decay routes for \( ^6\text{He} \) must be assumed in order to agree with fully dynamical three-body calculations of the state.

- Both the R-matrix and HH calculations of the width \( (\Gamma \approx 60 \rightarrow 70 \text{ keV}) \) of the \( ^6\text{He} \ (2^+) \) state do not fall within the error bars of the experimentally determined width \( (\Gamma = 113 \pm 20\text{keV}) \). Indicating further theoretical / experimental work is required.
In the future it would be interesting to apply the generalised three-body R-matrix formalism to other nuclei. It would be particularly interesting to apply it to some of the cases of two-proton decay already studied by Barker. This would enable limits to be established for when Barker's prescription is sufficient. In addition, it may also be possible to extend Barker's existing formalism to enable a cross-section to be calculated for the $^4\text{He}(2n,\gamma)^6\text{He}$ reaction, thus enabling a reaction rate to be calculated that could be compared with the previous estimate found in [6, 52].
Appendix A

Alternative Derivation of the Hard-Sphere Phase Shift

As given in Equation (2.25), the asymptotic behaviour of the scattering wavefunction can be expressed as a combination of Hankel functions,

$$
\psi_\ell(r) = \frac{i}{2} (H^-_\ell - S_\ell H^+_\ell).
$$

(A.1)

If this wave function were incident on an impermeable sphere of radius, $a$, the wave function must satisfy, $\psi_\ell(a) = 0$. The resulting phase shift is the hard-sphere phase shift, $\phi_\ell$, in this case the S-matrix is given by

$$
S_\ell = e^{2i\phi_\ell}.
$$

(A.2)

Using this definition of the S-matrix and the condition that $\psi_\ell(a) = 0$, Equation (A.1) can be rearranged to give

$$
e^{2i\phi_\ell} = \frac{H^-_\ell}{H^+_\ell},
$$

(A.3)

evaluated at $\rho = ka$. This is an alternative derivation for part of Equation (4.26).
Appendix B

Alternative Derivation of Observed Width

This appendix describes an alternative derivation for the relations

\[ E_R = \epsilon_p - \gamma^2 (S(E_R) - b) \quad \text{and} \quad \Gamma^0 = \frac{2\gamma^2 P(E_R)}{1 + \gamma^2 \frac{d\delta}{dE}} \bigg|_{E=E_R}, \]

from that which is presented in Chapter 4. There is a pole in the S-matrix when \( E = E_R - i\Gamma^0/2 \). Looking at the denominator of Equation (4.35) there is a pole in the S-matrix at \( E = \epsilon_p - \gamma^2 (S(E) - b) - i\gamma^2 P(E) \), therefore

\[ E_R - i\Gamma^0/2 = \epsilon_p - \gamma^2 (S(E_R - i\Gamma^0/2) - b) - i\gamma^2 P(E_R - i\Gamma^0/2). \]  

(B.2)

Using the first two terms of the Taylor expansion to expand the shift function and the penetrability,

\[ S(E_R - i\Gamma^0/2) = S(E_R) - i\Gamma^0/2 \frac{dS}{dE} \bigg|_{E=E_R} \]

(B.3)

and

\[ P(E_R - i\Gamma^0/2) = P(E_R) - i\Gamma^0/2 \frac{dP}{dE} \bigg|_{E=E_R}. \]

(B.4)

Substituting these into Equation (B.2) and rearranging,

\[ E_R - i\Gamma^0/2 = \epsilon_p - \gamma^2 (S(E_R) - b) - \gamma^2 \Gamma^0/2 \frac{dP}{dE} \bigg|_{E=E_R} - i \left( \gamma^2 P(E_R) - \gamma^2 \Gamma^0/2 \frac{dS}{dE} \bigg|_{E=E_R} \right). \]

(B.5)
Equating the real and imaginary parts,

\[ E_R = \epsilon_p - \gamma^2 (S(E_R) - b) - \gamma^2 \Gamma^0 / 2 \left. \frac{dP}{dE} \right|_{E=E_R}, \quad (B.6) \]

\[ \Gamma^0 / 2 = \gamma^2 P(E_R) - \gamma^2 \Gamma^0 / 2 \left. \frac{dS}{dE} \right|_{E=E_R}. \quad (B.7) \]

Solving Equation (B.7) for \( \Gamma^0 \),

\[ \Gamma^0 = \frac{2\gamma^2 P(E_R)}{1 + \gamma^2 \left. \frac{dS}{dE} \right|_{E=E_R}}. \quad (B.8) \]

Substituting Equation (B.8) into Equation (B.6),

\[ E_R = \epsilon_p - \gamma^2 (S(E_R) - b) - \gamma^2 \left. \frac{dS}{dE} \right|_{E=E_R} \left. \frac{dP}{dE} \right|_{E=E_R}. \quad (B.9) \]

The highest order term is usually ignored,

\[ E_R = \epsilon_p - \gamma^2 (S(E_R) - b). \quad (B.10) \]
Appendix C

Parameter Space Evaluation

In Barker's papers on the three-body R-matrix formalism no definition of the penetrability and shift functions are given. In order to check that the functions in this work have the same definitions as that used by Barker, some of the results from [15] were replicated. In particular the parameter space evaluation in Figure (1) of [15] for the sequential emission of 2 protons from $^{12}$O was studied.

Figure (C.1) shows both the original Barker figure from [15] (the upper graph) and parameter space evaluation performed here (the lower graph). Neither graph were calculated using a potential model, instead $Q_{1p}$, $Q_{2p}$, $\Gamma^0_2(Q_{1p})$ and $(\gamma_1)^2$ were given fixed values and $\Gamma^0_{tot}$ calculated from those. A value of $Q_{2p}=1.78$ MeV was used for all the calculations. In the lower graph of Figure (C.1) the different colours correspond to different values of $Q_{1p}$. On the upper graph of Figure (C.1) the values of $Q_{1p}$ are annotated on the curves. In both graphs the dotted lines correspond to $\Gamma^0_2(Q_{1p}) = 0.5$ MeV, the solid lines are $\Gamma^0_2(Q_{1p}) = 1.0$ MeV and the dashed are $\Gamma^0_2(Q_{1p}) = 1.5$ MeV. The lower graph has more curves plotted than the upper graph since $\Gamma^0_{tot}$ is plotted for every value of $Q_{1p}$ and $\Gamma^0_2(Q_{1p})$. Figure (C.1) shows that the parameter space evaluation performed in this work is in excellent agreement with Figure (1) of [15]. Therefore the penetrability and shift functions are being calculated in the same way.
Figure C.1: Top: Figure (1) from [15]. Bottom: Reproduction of Figure (1) from [15].
Appendix D

Two-channel example of Eigenphases

In Chapter 7 the eigenphases are used to deduce the width of the $^6\text{He} (2^+)$ three-body resonance. To clarify the use of the formalism presented in Section 5 of Chapter 7, a simple 2 channel example is worked through here. This is in the same style as [73]. In the 2 channel case $S$ is a $2 \times 2$ matrix with eigenvalues $e^{2\delta_1}$ and $e^{2\delta_2}$. If it is assumed that the eigenvectors corresponding to these eigenvalues are

$$e^1 = \begin{pmatrix} \frac{5}{13} \\ \frac{12}{13} \end{pmatrix} \quad \text{and} \quad e^2 = \begin{pmatrix} \frac{12}{13} \\ -\frac{5}{13} \end{pmatrix}, \quad (D.1)$$

then the $E^k$ matrices, from Equation (7.40), are

$$E^1 = \begin{pmatrix} 25 & 60 \\ 169 & 169 \end{pmatrix} \quad \text{and} \quad E^2 = \begin{pmatrix} 144 & -60 \\ 169 & 169 \end{pmatrix}. \quad (D.2)$$

Therefore, by Equation (7.42), the $S$-matrix is

$$S = \begin{pmatrix} 25 e^{2i\delta_1} + 144 e^{2i\delta_2} & 60 (e^{2i\delta_1} - e^{2i\delta_2}) \\ 60 (e^{2i\delta_1} - e^{2i\delta_2}) & 169 e^{2i\delta_1} + 25 e^{2i\delta_2} \end{pmatrix}. \quad (D.3)$$
Bibliography


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