THE ROLE OF THREE-BODY FORCES IN FEW-BODY SYSTEMS

by

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Contents

Declaration

I declare that **The role of three-body forces in few-body systems** is my work, and all the references quoted are legally accepted.

D.F. Masita, November 2006

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Bophelo ke lefeela la mafeela, empa bo eba le moelelo o motle ha motho ana le tjhebelopele, maikarabelo, le maikemisetso a ho etsa ntho tse molemo. Motho ya jwalo Modimo o emelana le yena nthong tsohle, mme ha Modimo a le hlakoreng la hae ke mang ya tla mo tswa?

Summary

Bound state systems consisting of three nonrelativistic particles are numerically studied. Calculations are performed employing two-body and three-body forces as input in the Hamiltonian in order to study the role or contribution of three-body forces to the binding in these systems. The resulting differential Faddeev equations are solved as three-dimensional equations in the two Jacobi coordinates and the angle between them, as opposed to the usual partial wave expansion approach. By expanding the wave function as a sum of the products of spline functions in each of the three coordinates, and using the orthogonal collocation procedure, the equations are transformed into an eigenvalue problem.

The matrices in the aforementioned eigenvalue equations are generally of large order. In order to solve these matrix equations with modest and optimal computer memory and storage, we employ the iterative Restarted Arnoldi Algorithm in conjunction with the so-called tensor trick method. Furthermore, we incorporate a polynomial accelerator in the algorithm to obtain rapid convergence. We applied the method to obtain the binding energies of Triton, Carbon-12, and Ozone molecule.

KEY WORDS : Three-body forces, differential Faddeev equations, eigenvalue equations, Restarted Arnoldi algorithm, orthogonal collocation procedure.

Chapter 1

Introduction

Calculations of the binding energies for few particle systems such as ^{3}H, ^{3}He, and ^{4}He, using as input two-body forces only show an underbinding relative to their corresponding experimental values. For example, the calculated binding energy of ^{3}H with various two-body potentials is found to be about 1.0 - 1.5 MeV less than the experimental value of -8.482 MeV [1, 2, 3, 4, 5, 6]. Similarly, the binding for ^{4}He is about 2.0 - 4.0 MeV less compared to the experimental value of -28.30 MeV [7]. This discrepancy between theory and experiment may be due to several sources, the main ones being the *neglect* of the

- off-energy shell effects in the two-body forces [8, 9],

- relativistic effects [10, 11], and

- three-body forces [12, 13].

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Investigations on the role of relativistic effects, for example, show that their inclusion in calculations increases the triton binding energy by about 0.25 MeV [14]. The role played by the neglect of the other sources have been previously investigated [8, 9, 10, 11]. In this work our concern is to investigate the role played by three-body forces, i.e. the contribution of a three-body force to the binding energy of a three-body system.

Within the nonrelativistic framework a three-body force is expected to have an appreciable contribution relative to the other two sources mentioned, especially for systems with cluster structures. To this end the inclusion of these forces in the Hamiltonian could address the discrepancies in binding energy between experimental data and predictions based on two-body forces only. For completeness we mention the following: The inclusion of three-body forces in four-body calculations warrant that they be considered as the basic point from which the necessary insight into more complex many-body interactions can be achieved [7]. In this way a full description of the properties of few-particle systems can be accomplished.

Next we address the question of solving the Schrödinger equation for three particles. It is well known that the Lippmann-Schwinger equations for three particles do not lead to a unique solution. This problem can be addressed by using the Faddeev formalism, in which the wave function is decomposed into a sum of the components describing the two-body subsystems. The resulting Faddeev equations are the most fundamental formulation of the nonrelativistic quantum three-body problem. Originally they were formulated in momentum space. The configuration space equations

were derived later by Fiedeldey and Noyes in [15], and further formulated to completion by Merkuriev [16]. Therefore the Faddeev equations may be used in three different forms, namely

- as the integral equations in momentum space [17, 18, 19, 20, 21, 22],

- as differential equations in configuration space [1, 23, 24], or

- as the combination of both configuration and momentum spaces [25].

In this work we use the differential Faddeev equations in configuration space, within the framework of total-angular-momentum formalism[26]. Our preference for working in configuration space is based on the following reasons:

- the system's wave function can be directly obtained.

- our intuition is stronger in configuration space than in momentum space;

It is worth mentioning, however, that over the past many years the integral Faddeev equations had had a comparatively wider use. Furthermore, the problem of the correct inclusion of the asymptotics does not exist in momentum space, albeit at the expense of having to deal with singularities. Nowadays though, for three-body bound systems these singularities can be easily handled.

In their original form Faddeev equations contain operators in six-dimension, and thus numerically impossible to solve. For a numerical solution to be realized these

equations are reduced to a more tractable form. In the total angular momentum representation considered here, the Faddeev equations are reduced to a set of coupled equations in three dimension. For three identical particles the coupled equations further reduce to a single three-dimensional equation defined on an infinite interval. For numerical implementation, the equations are reduced to finite equations by using, for example,

- a transformation procedure, where the infinite interval is mapped into a finite interval [27] without any approximation, or

- the cutoff method.

In our work we employ the latter method.

In order to reduce the dimension of the three-dimensional Faddeev equations to a manageable size, the tensor trick technique [26] is used. In this procedure the Faddeev eigenvalue equations are transformed into an "inverted" eigenvalue matrix equations which can be stored as tensor-products of simpler matrices, i.e. matrices with smaller dimensions or diagonal matrices. In this way the convergence rate of the iterative techniques are improved. For a further improvement on convergence rate the regularization polynomial accelerator techniques are usually incorporated in calculations.

For a description of the problem one must define the kinematics. Various coordinate systems such as the Cartesian or Polar coordinates are usually employed. The

choice of a particular coordinate system depend on, amongst other reasons, the type of a problem one is investigating. Cartesian coordinates are, for example, suitable in describing systems with nonlocal potentials. That is the Faddeev equations can be reduced into a homogeneous representation where all the potential terms may be moved to the left hand side of the equation. The polar coordinates, on the other hand, had the advantage that they reduce the matrix structure associated with the eigenvalue problem to matrices with band structure, which is easier and faster to solve.

Next we address the question of actually solving the set of Faddeev equations for three bound particles. Because of the huge matrices involved the equations cannot be solved directly. Therefore iterative methods are necessary. The most commonly used algorithms are the Lanczos-type methods, e.g. the Arnoldi method which is employed in this work. In the Arnoldi method the Faddeev equations are reduced to matrix equations of an upper Hessenberg form which is much more tractable to solve than full matrix equations. As mentioned elsewhere in this dissertation, the matrix equations involved are of large order, resulting in a huge numerical problem requiring huge spaces. To address this problem the restarting mechanism is incorporated in the Arnoldi method leading to what is known as the Restarted Arnoldi method. To improve convergence of the eigensolution we incorporate the Chebychev polynomial accelerator in the Arnoldi algorithm.

In our calculations for the binding energies of the systems considered we adopted the following two-step approach. First, we calculate the system's energy using only

two-body forces as input in the Hamiltonian. In the second step, the procedure is repeated with three-body forces included in addition to the two-body forces. The aim for these investigations is thus: to find how good enough a Hamiltonian with three-body forces included describes the problem, i.e. the role of three-body force. First we tested our numerical methods by calculating the binding energies for Triton and Carbon-12, the latter as a cluster of three alpha particles. Second, we calculated the ground and first excited states for the Ozone molecule.

This dissertation is organized as follows: In Chapter 2, we briefly describe the formalism of the three-dimensional configuration Faddeev equations for three particles, within the framework of the total angular momentum representation, i.e. without resort to partial wave decomposition. Chapter 3 outlines the numerical procedures used in solving the differential Faddeev equation. The type of splines used in this work as well as their use together with collocation procedure are discussed. In Chapter 4 we present the results. Finally, conclusions and discussions are presented in Chapter 5. In Appendix A, a further discussion on the necessary boundary conditions for three-body bound systems is discussed. In Appendix B we discuss the practical implementations of the algorithm. In Appendix C we give the explicit expressions of the interactions used in this work.

Chapter 2

Faddeev Equations for three bound particles

2.1 Kinematics

We consider a system of three particles in the center of mass, defined by a set of standard Jacobi coordinates $\{\mathbf{x}_\alpha, \mathbf{y}_\alpha\}$ represented in Figure 2.1, expressed in terms of the particles position vectors $\mathbf{r}_\alpha \in \mathbb{R}^3$, and their masses m_α (α = 1,2,3) [26] as follows:

$$\mathbf{x}_\alpha = \left[\frac{2m_\beta m_\gamma}{m_\beta + m_\gamma} \right]^{1/2} (\mathbf{r}_\beta - \mathbf{r}_\gamma) \tag{2.1}$$

$$\mathbf{y}_\alpha = \left[\frac{2m_\alpha(m_\beta + m_\gamma)}{m_\alpha + m_\beta + m_\gamma} \right]^{1/2} \left(\mathbf{r}_\alpha - \frac{m_\beta \mathbf{r}_\beta + m_\gamma \mathbf{r}_\gamma}{m_\beta + m_\gamma} \right) \tag{2.2}$$
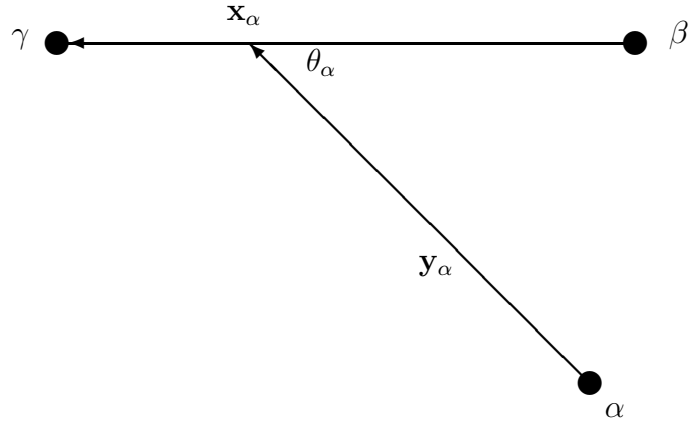
Figure 2.1: Jacobi coordinates in configuration space

The other pairs of independent variables for two particle subsystems γ and α are obtained from Eqs. (2.1) and (2.2) by cyclic permutation of the subscripts $\{\alpha, \beta, \gamma\}$. They are related to $\{x_\alpha, y_\alpha\}$ via an orthogonal transformation in $\mathbb{R}^6$ as follows

$$
\begin{pmatrix} \mathbf{x}_\beta \\ \mathbf{y}_\beta \end{pmatrix} = \begin{pmatrix} S_{\beta\alpha}^{11} & S_{\beta\alpha}^{12} \\ S_{\beta\alpha}^{21} & S_{\beta\alpha}^{22} \end{pmatrix} \begin{pmatrix} \mathbf{x}_\alpha \\ \mathbf{y}_\alpha \end{pmatrix} \tag{2.3}
$$

where the coefficients $S_{\beta\alpha}^{ij}$ are given by

$$
S_{\beta\alpha}^{11} = \left(\frac{m_\beta m_\alpha}{(m_\alpha + m_\gamma)(m_\beta + m_\gamma)} \right)^{1/2}, \tag{2.4}
$$

$$
S_{\beta\alpha}^{12} = (-1)^{\alpha-\beta}\text{sign}(\alpha - \beta) \left[\frac{m_\gamma(m_\alpha + m_\beta + m_\gamma)}{(m_\alpha + m_\gamma)(m_\beta + m_\gamma)} \right]^{1/2}, \tag{2.5}
$$

with $S_{\beta\alpha}^{22} = S_{\beta\alpha}^{11}$ and $S_{\beta\alpha}^{21} = \text{-}S_{\beta\alpha}^{12}$. For identical particles these coefficients are

$$
S_{\beta\alpha}^{11} = S_{\beta\alpha}^{22} = \frac{1}{2}, \quad \text{and} \quad S_{\beta\alpha}^{12} = -S_{\beta\alpha}^{21} = \frac{\sqrt{3}}{2}. \tag{2.6}
$$

2.2   Faddeev Equations

The Hamiltonian for three particles interacting via two-body forces is defined as

$$H = -H_0 + \sum_{\alpha=1}^{3} V_\alpha^{(2N)}(\mathbf{x}_\alpha), \tag{2.7}$$

where $\mathbf{x}_\alpha$ is the Jacobi coordinate for the two-particle subsystem α, $V_\alpha^{(2N)}(\mathbf{x}_\alpha)$ is the central potential, and H_0 is the free three particle Hamiltonian given as follows

$$H_0 \equiv -\nabla_\mathbf{X} = -\nabla_{\mathbf{x}_\alpha}^2 - \nabla_{\mathbf{y}_\alpha}^2, \tag{2.8}$$

Thus the Schrödinger equation for three-body system reads

$$\left[-\nabla_{\mathbf{x}_\alpha}^2 - \nabla_{\mathbf{y}_\alpha}^2 + \sum_{\alpha=1}^{3} V_\alpha^{(2N)}(\mathbf{x}_\alpha) \right] \Psi_{3N}(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = E_{3N} \Psi_{3N}(\mathbf{x}_\alpha, \mathbf{y}_\alpha), \tag{2.9}$$

where E_{3N} is the energy and $\Psi_{3N}(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ is the total wave function of the system. A direct numerical solution of Eq. (2.9) is cumbersome and difficult. In order to address this difficulty Faddeev proposed the idea that the total wave function of the system be decomposed into three components as follows [28] :

$$\Psi_{3N}(\mathbf{x}, \mathbf{y}) = \sum_{\alpha=1}^{3} \phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha), \tag{2.10}$$

where $\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ describes the two particle subsystem (β, γ) in which particle α is a spectator. Substitution of Eq. (2.10) into Eq. (2.9) leads to a set of six-dimensional three coupled differential equations for the components $\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$, namely

$$\left[H_0 + V_\alpha^{(2N)}(\mathbf{x}_\alpha) - E_{3N}\right]\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = -V_\alpha^{(2N)}(\mathbf{x}_\alpha)\left[\phi_\beta(\mathbf{x}_\beta, \mathbf{y}_\beta) + \phi_\gamma(\mathbf{x}_\gamma, \mathbf{y}_\gamma)\right]. \quad (2.11)$$

These equations are the `configuration space Faddeev equations` when only two-body forces are present. In the presence of three-body forces (i.e. in addition to the two-body forces) they read

$$\left[H_0 + V_\alpha^{(2N)}(\mathbf{x}_\alpha) + V_\alpha^{(3N)} - E_{3N}\right]\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha, \mathbf{z}_\alpha)$$
$$= -V_\alpha^{(2N)}(\mathbf{x}_\alpha)\left[\phi_\beta(\mathbf{x}_\beta, \mathbf{y}_\beta, \mathbf{z}_\beta) + \phi_\gamma(\mathbf{x}_\gamma, \mathbf{y}_\gamma, \mathbf{z}_\gamma)\right], \quad (2.12)$$

and are usually referred to as the `modified Faddeev equations` or Faddeev-Merkuriev equations [16].

For a system of three identical particles the Faddeev components have the same functional form. In this case the relationship between the components is

$$\phi_\beta(\mathbf{x}_\beta, \mathbf{y}_\beta) = P^+\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha), \quad (2.13)$$

$$\phi_\gamma(\mathbf{x}_\gamma, \mathbf{y}_\gamma) = P^-\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha). \quad (2.14)$$

where $P^\pm$ stands for cyclic and anti-cyclic permutation operators acting on the coordinates. Substituting Eqs. (2.13) and (2.14) into Eq. (2.11), and rearranging

terms leads to the equation

$$[H_0 + (I + P^+ + P^-)V_\alpha^{(2N)}(\mathbf{x}_\alpha) - E_{3N}]\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = 0. \tag{2.15}$$

where I is the identity operator. Similarly, when three-body forces are present, Eq (2.15) is modified to read

$$[H_0 + (I + P^+ + P^-)V_\alpha^{(2N)}(\mathbf{x}_\alpha) + V^{(3N)} - E_{3N}]\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = 0. \tag{2.16}$$

2.3 Faddeev Equations in fixed angular momentum representation

For fixed angular momentum L the wave function $\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha)$ can be expanded as

$$\phi_\alpha(\mathbf{x}_\alpha, \mathbf{y}_\alpha) = \sum_{L,m,n} \frac{\Phi^{Lmn}(x_\alpha, y_\alpha, z_\alpha)}{x_\alpha y_\alpha} D_{mn}^L(g). \tag{2.17}$$

where $\Phi^{Lmn}(x_\alpha, y_\alpha, z_\alpha)$ are the eigenfunctions of the total angular momentum L, $D_{mn}^L(g)$ is the Wigner function, and g refers to the coordinates describing collective angular motion of the system. The intrinsic coordinates x_α and y_α are given by

$$x_\alpha = |\mathbf{x}_\alpha|, \tag{2.18}$$

$$y_\alpha = |\mathbf{y}_\alpha|, \tag{2.19}$$

with z_α, the angle between $\mathbf{x}_\alpha, \mathbf{y}_\alpha$, given as

$$z_\alpha \quad = \quad \frac{(\mathbf{x}_\alpha, \mathbf{y}_\alpha)}{x_\alpha y_\alpha} = \cos(\mathbf{x}_\alpha, \mathbf{y}_\alpha) \tag{2.20}$$

Clearly $x_\alpha, y_\alpha \in [0, \infty), \quad z_\alpha \in (-1, 1)$. For fixed total angular momentum L, the projections of the Faddeev component correspond to the free Hamiltonian (H_0^L) as follows

$$H_0^L = D^L(g^{-1}) xy H_0 \frac{1}{xy} D^L(g) \tag{2.21}$$

where $D^L(g)$ correspond to the matrix constructed from the Wigner function. In this work we consider $L = 0$, and thus H_0^L reads

$$H_0^0 = -\frac{\partial^2}{\partial x_\alpha^2} - \frac{\partial^2}{\partial y_\alpha^2} - \left(\frac{1}{x_\alpha^2} + \frac{1}{y_\alpha^2} \right) \frac{\partial}{\partial z_\alpha} (1 - z_\alpha) \frac{\partial}{\partial z_\alpha}, \tag{2.22}$$

Substituting Eqs. (2.17) and (2.22) into Eq. (2.15) and using the orthogonality properties of the Wigner function we obtain three-dimensional equations

$$\left[H_0^0 + V^{2N}(x)(1 + P^+ + P^-) - E_{3N} \right] \Phi^0(x, y, z) = 0, \tag{2.23}$$

where

$$P^+ \Phi^0(x, y, z) \equiv xy \left(\frac{\Phi^0(x^+, y^+, z^+)}{x^+ y^+} \right) \tag{2.24}$$

$$P^-\Phi^0(x,y,z) \equiv xy\left(\frac{\Phi^0(x^-,y^-,z^-)}{x^-y^-}\right), \tag{2.25}$$

and $x^\pm(x,y,z)$, $y^\pm(x,y,z)$, and $z^\pm(x,y,z)$ are the permuted Jacobi coordinates, with the now superfluous subscript α dropped. Explicit expressions for these coordinates are

$$x^\pm(x,y,z) = \left(\frac{1}{4}x^2 + \frac{3}{4}y^2 \mp \frac{\sqrt{3}}{2}xyz\right)^{1/2}, \tag{2.26}$$

$$y^\pm(x,y,z) = \left(\frac{3}{4}x^2 + \frac{1}{4}y^2 \mp \frac{\sqrt{3}}{2}xyz\right)^{1/2}, \tag{2.27}$$

$$z^\pm(x,y,z) = \frac{\pm\frac{\sqrt{3}}{4}x^2 \mp \frac{\sqrt{3}}{4}y^2 - \frac{1}{2}xyz}{x^\pm(x,y,z)y^\pm(x,y,z)}.$$

Assuming that there is only one bound state in each two-body subsystem, the Faddeev components Φ^0 has the following boundary conditions (which are further discussed in a little more detail in Appendix A):

$$\Phi^0(x,y,z) \sim \varphi_2(x)e^{-k_y y} + A(x,y,z)\frac{e^{-k_3(x^2+y^2)^{1/2}}}{(x^2+y^2)^{1/4}}, \tag{2.28}$$

where $\varphi_2(x)$ represents the two-particle bound state wave function, while k_y and k_3 are the energy dependent wave numbers, and $A(x,y,z)$ is the scattering amplitude. The first term in Eq. (2.28) corresponds to the virtual decay of the system into a particle and a two-particle bound state while the second term corresponds to the virtual decay into three single particles. The latter term decreases much faster

than the first one. For this reason, and in the context of the present work, we only consider the first term. Thus at sufficiently large distances R_x and R_y the asymptotic boundary conditions for the Faddeev component reduce to

$$\frac{\partial}{\partial x} \ln \Phi^0(x, y, z)\bigg|_{x=R_x} = -k_x \equiv i\sqrt{E}_{2N}, \tag{2.29}$$

$$\frac{\partial}{\partial y} \ln \Phi^0(x, y, z)\bigg|_{y=R_y} = -k_y. \tag{2.30}$$

Chapter 3

Numerical Method

3.1 Eigenvalue equation

In order to obtain a numerical solution to Eq. (2.23), the equation is first transformed into an eigenvalue equation. To this end we discretize the domain in each of the three coordinates, and expand the Faddeev component in terms of a set of basis functions B_i in each direction as follows

$$\Phi^0(x, y, z) = \sum_{\ell=1}^{L} \sum_{m=1}^{M} \sum_{n=1}^{N} C_{\ell m n} B_\ell(x) B_m(y) B_n(z) \,, \tag{3.1}$$

where the subscripts L, M, and N stand for the number of basis functions in the three variables (x, y, z), respectively, whilst $\mathrm{C}_{\ell m n}$ are the expansion coefficients. Substituting Eq. (3.1) into Eq. (2.23), followed by orthogonal collocation method [29],

reduces the Faddeev equations (in the presence of two-body forces only) to a system of linear algebraic equations for the coefficients $C_{\ell mn}$, namely

$$\left[\hat{H}_0^0 + \hat{V}^{(2N)}(\hat{I} + P^+ + P^-) - E_{3N}\hat{I}\right]\mathbf{C} = 0, \tag{3.2}$$

where $\hat{I}$ stands for the unit matrix, and $\mathbf{C}$ is a vector of the expansion coefficients $C_{\ell mn}$. To obtain the eigensolution (iteratively), we treat E_{3N} as a parameter, E_0 say, and rewrite Eq. (3.2) as an eigenvalue equation

$$-(\hat{H}_1 - E_0\hat{I})^{-1}\hat{H}_2\mathbf{C} = \lambda(E_0)\mathbf{C}, \tag{3.3}$$

where

$$\hat{H}_1 = \hat{H}_0^0 + \hat{V}^{(2N)}, \tag{3.4}$$

$$\hat{H}_2 = \hat{V}^{(2N)}\left(P^+ + P^-\right). \tag{3.5}$$

λ is an eigenvalue corresponding to the energy E_0. Clearly, $\lambda(E_0)$ equals 1 corresponds to a physical solution of Eq (3.3).

3.2 Handling convergence of solutions

Three-body bound state calculations are highly demanding in terms of computer memory and numerical stability, and hence convergence toward the correct solution

is in general a huge challenge. Thus in order to make numerics tractable, innovative techniques or approaches are necessary. In this work, we are interested in making our numerical methods capable of handling calculations, in which the underlying two-body potentials have strong repulsive core. Strong repulsion lead to a plethora of negative eigenvalues being generated which lie close to unity. This accumulation of eigenvalue around unity retard the convergence rate toward a physical solution of the iterative algorithm. In order to address this problem a modifying potential $\hat{V}_m$ is introduced so that the Hamiltonian reads [26]

$$\hat{H}_{negative} = \hat{H}_0 + 2\hat{V}_m + \hat{V}^{(2N)}[1 - (P^+ + P^-)], \tag{3.6}$$

compared to the Hamiltonian in Eq. (3.2). Similar to the discussion leading to Eqs. (3.4) and (3.5), $\hat{H}_{negative}$ is decomposed into $\hat{H}_1$ and $\hat{H}_2$ as follows

$$\hat{H}_1 = \hat{H}_0 + \hat{V}^{(2N)} + \hat{V}_m, \tag{3.7}$$

$$\hat{H}_2 = -\hat{V}^{(2N)}(P^+ + P^-) + \hat{V}_m. \tag{3.8}$$

In other words the problem of calculating the eigensolutions to Eq. (2.23) now reduces to that of finding the discrete spectrum of the operator $\hat{\chi}$

$$\hat{\chi}(\epsilon) = -(\hat{H}_0 + \hat{V}^{(2N)} + \hat{V}_m - \epsilon)^{-1}(\hat{V}_m - \hat{V^{2N}}\hat{P}). \tag{3.9}$$

where ϵ is an eigenvalue. In the presence of three-body forces the equivalent expression reads

$$\hat{\chi}(\epsilon) = -(\hat{H}_0 + \hat{V}^{(2N)} + \hat{V}^{3N} + \hat{V}_m - \epsilon)^{-1}(\hat{V}_m - \hat{V}^{(2N)}\hat{P}). \tag{3.10}$$

3.3 Basis functions

In this work we employed, as basis functions, the piecewise quintic Hermite splines $B_i \equiv \phi_{im}$ $(m = 0, 1, 2)$. These splines are nonzero only on two adjoining subintervals, e.g. $[x_{i-1}, x_i] \cup [x_i, x_{i+1}]$ in the x-grid and $[y_{i-1}, y_i] \cup [y_i, y_{i+1}]$ in the y-grid, which means they have good convergence rate properties. Another advantage for using the Hermite splines is that their analytical expressions are known, and hence their first and second derivatives can be obtained *a priori* analytically, which helps the numerics tremendously. The explicit expressions of these splines are

$$\phi_{im}(x) = (1 - \delta)^3(x - x_i)^m \cdot \begin{cases} 6\delta^2 + 3\delta + 1, & \text{for} \quad m = 0, \\ 3\delta + 1, & \text{for} \quad m = 1, \\ \frac{1}{2}, & \text{for} \quad m = 2, \end{cases} \tag{3.11}$$

where $x \in [x_{i-1}, x_{i+1}]$, and δ is defined by

$$
\delta =
\begin{cases}
\dfrac{x - x_i}{x_{i-1} - x_i}, & x_{i-1} \leq x \leq x_i \\[4mm]
\dfrac{x - x_i}{x_{i+1} - x_i}, & x_i \leq x \leq x_{i+1}.
\end{cases}
\tag{3.12}
$$

Thus, for $m = 0, 1,$ and 2 we have, respectively

$$
\phi_{i0}(x) =
\begin{cases}
6\left(\dfrac{x - x_i}{x_{i-1} - x_i}\right)^2 + 3\left(\dfrac{x - x_i}{x_{i-1} - x_i}\right) + 1, & x_{i-1} \leq x \leq x_i \\[4mm]
6\left(\dfrac{x - x_i}{x_{i+1} - x_i}\right)^2 + 3\left(\dfrac{x - x_i}{x_{i+1} - x_i}\right) + 1, & x_i \leq x \leq x_{i+1},
\end{cases}
\tag{3.13}
$$

$$
\phi_{i1}(x) =
\begin{cases}
3\left(\dfrac{x - x_i}{x_{i-1} - x_i}\right) + 1, & x_{i-1} \leq x \leq x_i \\[4mm]
3\left(\dfrac{x - x_i}{x_{i+1} - x_i}\right) + 1, & x_i \leq x \leq x_{i+1},
\end{cases}
\tag{3.14}
$$

$$
\phi_{i2}(x) = \frac{1}{2}.
\tag{3.15}
$$

Chapter 4

Numerical Results

4.1   Procedure

Our procedure for calculating binding energies, as mentioned in the Introduction, is a two step process in the following sense: First we obtain the spectrum of the operator defined by Eq. (3.9) (i.e. using as input only two-body forces, and the Restarted Arnoldi algorithm [30] with its necessary changes as discussed in Chapter 3). In the second step we repeat the procedure but with the three-body potentials included; in other words we now obtain eigensolutions corresponding to the operator defined by Eq. (3.10).

Several parameters must be adjusted to achieve optimality when implementing the procedure. We mention the main ones only. The first is the length parameter

(hereunder denoted a_0) that defines the distance from the origin to the first nonzero value of the x-grid. This parameter must be properly chosen so that:

- the correct boundary conditions are satisfied, otherwise one gets pathologies, associated with incorrect truncating of the space.

- the effects of repulsive core of the potential are counteracted (together with the background potential V_m, of course) and thus makes the numerics stable.

Other parameters of importance are the number of the collocation points associated with the $x-$, $y-$, and $z-$grid, as well as the size of the Krylov subspace and the cutoff lengths (x_{max}, y_{max}) which determine the range of the potential. These must be chosen to obtain a balance between accuracy of the results and computational cost. We now consider specific systems.

4.2   Triton

The simplest three-body bound nuclear system is triton. This system is to nuclear physics, what hydrogen atom is to atomic physics. It can therefore be used as a testing ground for numerical techniques in few-body calculations. For this reason several studies on this system are aplenty. In addition the input models, both two- and three-body potentials, are well known. The study of triton also provides more information on the nucleon-nucleon interaction.

4.2.1 Interactions

For the two-body input, we employed two s-projected Malfliet-Tjon type potentials[31, 32], with parameters given in Table C.1. These potentials had been widely used by other researchers, and thus offer us a platform for testing the reliability, stability and applicability of our numerical methods unambiguously. The Malfliet-Tjon (MT) potential is a superposition of a repulsive and attractive Yukawa interactions. It is a realistic interaction. With respect to three-body forces we employ the Urbana type potential given by Eqs. (C.2) and (C.4).

4.2.2 Results

The first step, in accordance with the procedure pointed above, is to determine the a_0 using the two-body forces only. It is worth mentioning that this a_0 is the first estimate. The optimal value is obtained in conjunction with other parameters, such as the number of basis functions in the different Jacobi coordinates. Fig. 4.1 show the triton binding energy as a function of the a_0 using the so-called MT-V potential with parameters taken from [33]. In Fig. 4.2 we show the results, obtained by using same two-body force with three-body force added. With two-body forces included, $a_0 = 0.038$ fm, whereas when the three-body force (Urbana) is included, $a_0 = 0.045$ fm, as can be seen from Fig. 4.2. Similar results were obtained with the MT potential of Ref. [34]. In Fig. 4.3 we show the results with two-body forces only whereas in Fig. 4.4 the results are with the three-body force added. With only two-body force of Ref. [34] included $a_0 = 0.05$ fm, and when the three-body force is included, the a_0 is shifted to the left and is found to be $a_0 = 0.047$ fm, as can be
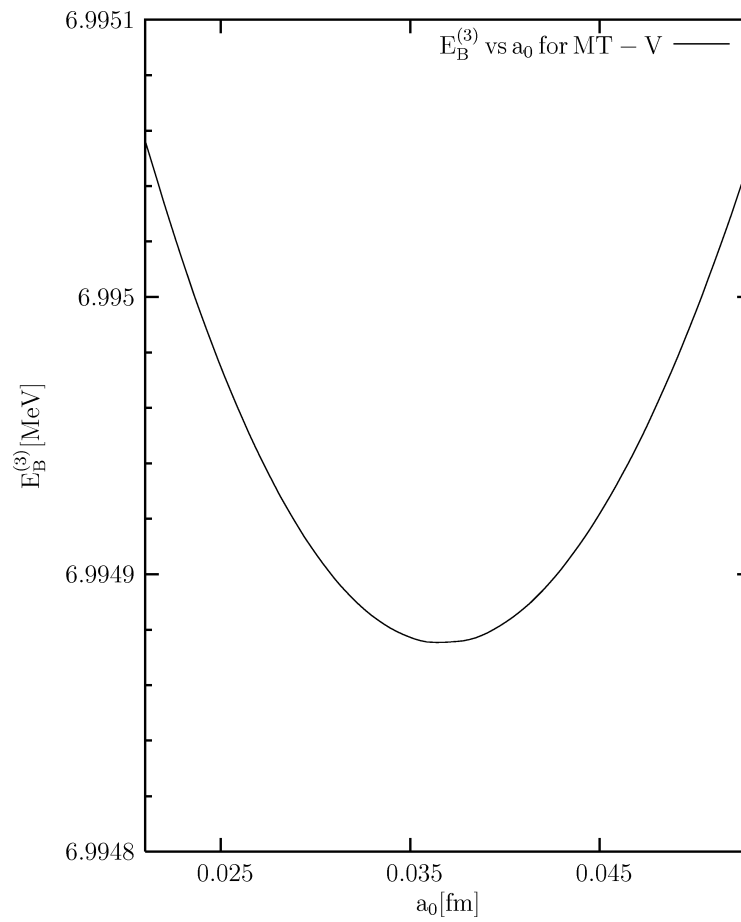
seen from Figure 4.4.

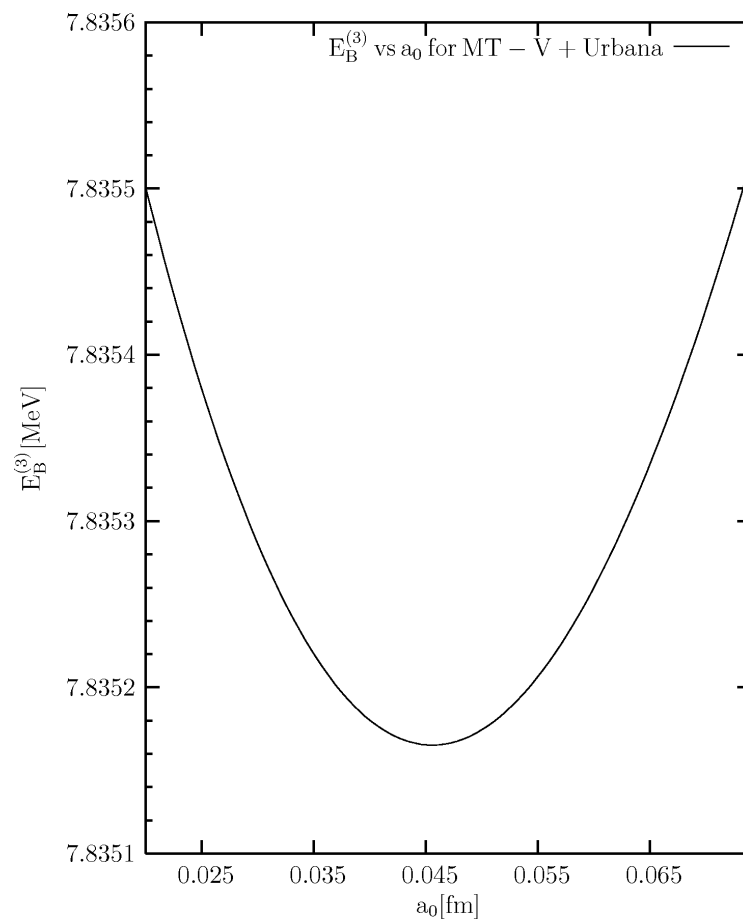Figure 4.1: Triton binding energy, $E_B^{(3)}$, as a function of a_0, for MT potential of Ref. [33]

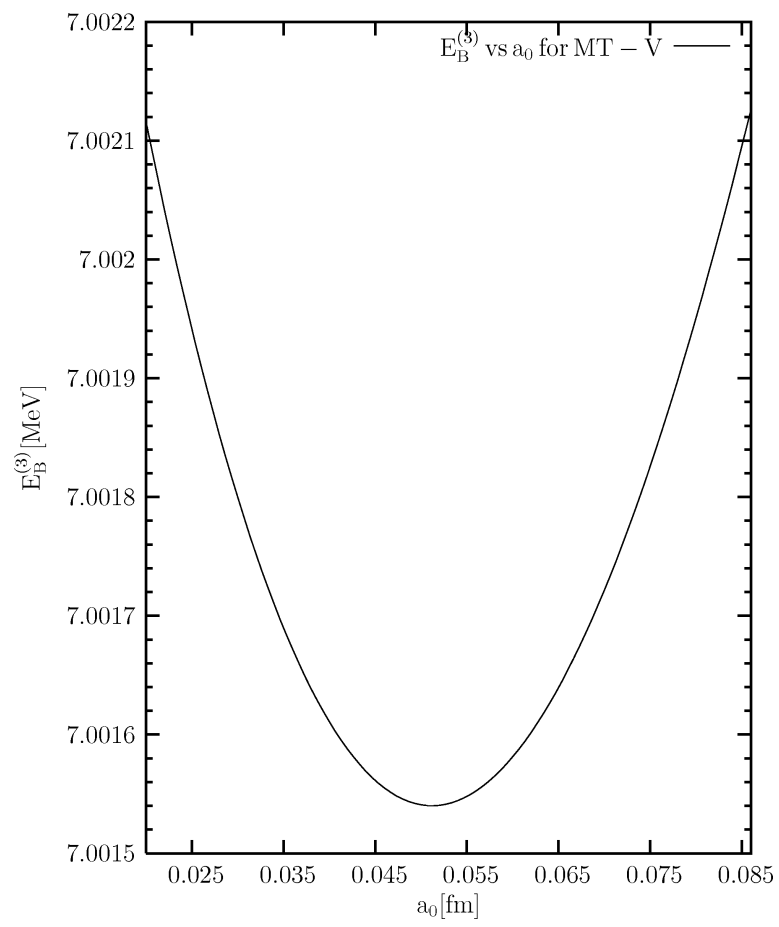Figure 4.2: Same as in Figure 4.1, but with three-body forces included

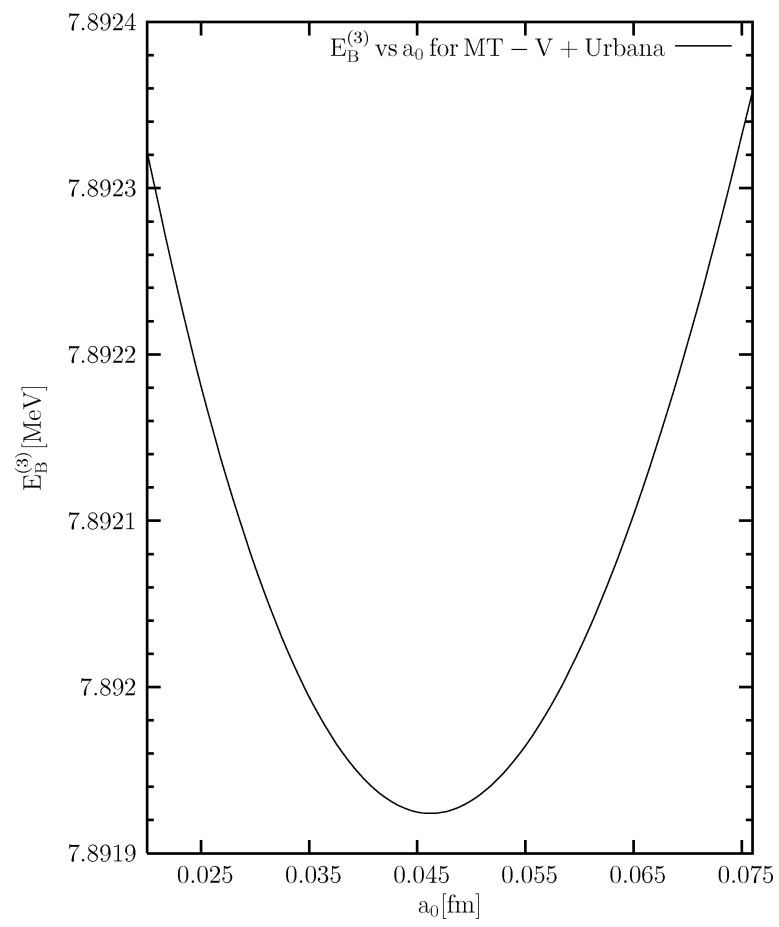Figure 4.3: Triton binding energy $E_B^{(3)}$ as a function of a_0 for the MT potential of Ref. [34]

Figure 4.4: .Same as in Figure 4.3, but with three-body forces included

Once the a_0's are determined and optimized, calculations for binding energy are performed. Our results, together with the literature results, are given in Tables 4.1 and 4.2. In our calculations we used $\frac{\hbar^2}{M} = 41.47$ MeV·fm^2.

Model	Ref. [90]	Ref. [40]	This work
Two-body force only	-7.736	-7.73661	-7.728
Two- + three-body force	–	–	-8.555

Table 4.1: Binding energy, in MeV, results for triton using the MT potential with parameters taken from Ref. [33]. The experimental value is -8.482 MeV [36]

Model	Ref. [34]	This work
Two-body force only	-8.26	-8.255
Two- + three-body force	-9.05	-8.782

Table 4.2: Same as in Table 4.1 but for the potential with parameters from Ref. [34]. The results of [34] are obtained with Green Function Monte Carlo approach.

4.3 Carbon-12

The triple-α reaction is suggested as one of the mechanisms for helium burning during the primordial nucleosynthesis epoch. The helium burning, in turn describes the observed abundance of the elements in the universe. When the alpha particles are close to one another, which is possible at temperatures that were existent during the primordial nucleosynthesis period, a bound state of three alpha particles, i.e. ^{12}C, may be formed. From this point of view, the ^{12}C nucleus, modeled as a bound state of three alpha particles, plays a very important role in the understanding of the primordial nucleosynthesis. Indeed the 3α model has been used before by many researchers to describe the resonance states in triple-α reactions. Thus one can use the 3α bound state model to study the spectrum of ^{12}C. Several low-lying states for this system are known to exist, but in this work we consider only the 0_1^+ ground state. The reason for this limited investigation is that our objective is to test the numerics in situations when the three-body forces are present, which is usually used in the calculations for ^{12}C.

4.3.1 Interactions

We employ the phenomenological s-wave Ali-Bodmer $\alpha - \alpha$ potential given by Eq. C.5, with parameters in Table C.2. We use $\frac{\hbar^2}{m_\alpha} = 10.4465$ MeV·fm^2 in our calculations. It is well known that the $\alpha\alpha$ potential does not adequately describe the cluster structure of Carbon-12 as 3α system, especially the ground state. This deficiency is usually addressed by introducing, in addition to $\alpha\alpha$, an attractive three-

alpha potential $V_{3\alpha}$. In this work we use the $V_{3\alpha}$ potential, given by Eq. C.6.

4.3.2 Results

Using the s-wave potential for the 3α system given in the Appendix C, we obtain the results in Table 4.3. In a similar manner as for the case of triton, we first calculated the binding with two-body forces only, and repeat the same with three-body included. It is to be noted that the repulsion among the alpha particles is taken care of by the inclusion of the Coulomb, as given by Eq. C.7.

Model	Ref. [37] ($\ell \leq 4$)	Ref. [38] (HHE)	This work
ABd0	-5.126	-5.12209	-5.123
ABd0 + $V_{3\alpha}$	-7.283	–	-7.301

Table 4.3: Binding energy, in MeV, for the ground state (0_1^+) of ^{12}C modelled as a 3α system, obtained with two-, three-body models. Note that the Coulomb contribution is included in the calculations in the second row. HHE means Hyperspherical harmonics expansion method. Values are relative to the 3α threshold. The experimental value is -7.27 MeV [39].

4.4   Ozone

The Ozone molecule, being a bound state of three atoms with spin zero, can be treated as a bosonic system. In [40] its low-lying states were determined. In this work we repeat the calculations, but for the ground and the first excited states only. This is done in order to check and test the new changes implemented in the numerics used in the aforementioned work.

4.4.1   Results

We employ the interactions given in [40, 41], which are reproduced in the Appendix C for completeness, and obtain the results in Table 4.4.

State	Two-body force only	Two- plus three-body forces
0	-10.049	-13.422
1	-9.921	-12.009

Table 4.4: Binding energies (in eV) for the ground and first excited states for Ozone molecule. We used $\frac{\hbar^2}{m} = 2.614 \times 10^{-4} \mathring{A}^{-2}$

Chapter 5

Concluding Remarks

We now pass some remarks in respect of the work of this dissertation.

- **On Formalism and Method**

  We presented a formalism for the configuration space Faddeev equations within the framework of the so-called total-angular-momentum representation. In this formalism no explicit partial wave decomposition is performed. For this reason this formalism is useful in calculations where a plethora of partial waves would be necessary in order to achieve convergence.

  The formalism in a straight-forward way, permits the incorporation of three-body potentials in the Hamiltonian, leading to the so-called modified Faddeev equations, which retains the important characteristics associated with the original Faddeev equations for short-range interactions. This is very important for

few-body systems with cluster structures where the role of three-body forces to the binding (or other properties) might be significant.

Working in configuration space has some advantages. For example, as mentioned elsewhere in the dissertation, our intuition is more stronger in this space than in momentum space. More importantly, in configuration space the Coulomb potential is easily incorporated in a straightforward way. Thus in respect to the calculations on ^{12}C, it was possible notwithstanding the numerical instabilities, to incorporate the attractive Coulomb potential in the numerics.

- ## On Numerics

In implementing the algorithm described in this dissertation, a fair amount of time is spend in trying to obtain an optimal value for the a_0 parameter (i.e. the first nonzero value of the $x-$grid from the origin). This step is time consuming since, although guided by some physical intuition, is in the main a trial and error step. For this reason, towards the end of this research, we started to correct this deficiency by allowing the optimal search to be done numerically and iteratively (see Future Work below).

- ## On Results

The role of three-body forces in the few-particle systems investigated here was done systematically as explained in the text. With respect to the determination of a_0, it appears that the presence of three-body forces shifted the value to the right. This feature may be the result of the repulsiveness nature of the

underlying forces. However, caution must be exercised in the use of this value in the following sense: The use of the underlying mesh with an a_0 is obtained when three-body forces are employed must ensure that the two-body binding is reproduced, otherwise the a_0 from step one of the algorithm must be used, at the expense of a slow convergence.

Our results, first with respect to model Triton calculations, are highly comparable with other results from the literature. Thus we can conclude in the positive concerning the stability of our numerics, at least for the systems considered in this work. The results of the ^{12}C are the next relatively more stringent test for our methods in term of complexity, because of the cluster nature of the system. The binding energy of the ground states obtained is in agreement with others in the literature. When three-body forces are included we obtain the results that are close but slightly different to, for example, those found in [37]. This discrepancy need further calculations to pinpoint, but we are obliged to conclude that the difference might lie in the fact that in our method all partial waves are implicitly included since no partial wave decomposition is performed in contrast to other works cited. The expansion of our method is underway to permit the investigation of other low-lying excited resonant states of ^{12}C, such as 0_2^+, [40].

For Ozone molecular system we encountered problems with the convergence rate and instability of the Arnoldi method, due to the presence of various excited states in this system. In order to address these problems we incorporated the Arnoldi method with the so called `minimization` method, to reduce the number of excited states to a reasonable range for calculations. The latter

procedure proved to be effective in addressing the mentioned problems, and we finally obtained results which are well comparable to those found in [40] for the ground and first excited states respectively.

- ## On Future Work

The objective of repeating the work of [40] with respect to the Ozone system, was to test the stability of the numerics, with regard to some changes made to the codes, employed for systems that are weakly bounded. Further work is needed in this direction in future, specifically on the van der Waals clusters.

The procedure to obtain optimal parameters, in particular a_0 will be automated in order to remove the tedious work of 'trial-and-error' as applied in the present work. The scheme envisaged works by adapting the mesh such that the two-body binding, that is fixed *a priori* set is reproduced exactly. This aspect is still ongoing, and at a trial stage.

Appendix A

Further discussion on boundary conditions

The boundary conditions, Eqs. (2.28) and (2.30) mentioned in Chapter 2 of this work, are energy dependent. Here, we show how such boundary conditions were derived. If we assume that in each of the two-body subsystem, only one bound state exist, then the asymptotic behavior of the Faddeev component can be written as a sum of two terms, namely, the $(2 + 1)$- and the $(1 + 1 + 1)$- configurations [42], as follows

$$\Phi^0(x, y, z) \sim \varphi_2(x) \exp(-k_y y) + A(x, y, z) \frac{\exp\left\{-k_3(x^2 + y^2)^{1/2}\right\}}{(x^2 + y^2)^{1/4}}, \tag{A.1}$$

where $\varphi_2(x)$ is the two-body bound state in the two-body subsystem, corresponding to the two-body bound state energy E_2, and A is the scattering amplitude. With

the wave numbers k_y and k_3 being related to both three-body, E_3, and two-body binding energies by $(E_2 - E_3)^{1/2}$, and $(-E_3)^{1/2}$.

For sufficiently, large large distances we neglect the term corresponding to the $(1 + 1 + 1)$- configuration, since it decreases much faster than the $(2 + 1)$- configuration term. Thus the asymptotic boundary conditions for ϕ read

$$\Phi(x, y, z) \sim \varphi_2(x) \exp\left\{-(E_2 - E_3)^{1/2}\right\}. \tag{A.2}$$

Furthermore, the ϕ_2 behaves asymptotically as

$$\phi_2 \sim \exp\left\{-(E_2)^{1/2}\right\}. \tag{A.3}$$

Hence, for sufficiently large distances x_{max} and y_{max}, the asymptotic boundary conditions for the Faddeev ϕ are simplified to

$$\frac{\partial \phi}{\partial x} \ln \Phi(x, y, z)|_{x=x_{max}} = -(E_2)^{1/2}, \tag{A.4}$$

$$\frac{\partial \phi}{\partial x} \ln \Phi(x, y, z)|_{y=y_{max}} = -(E_2 - E_3)^{1/2}, \tag{A.5}$$

In addition Φ must satisfy the regularity conditions

$$\Phi(x, y, z)|_{x=0,\infty} = 0, \tag{A.6}$$

$$\Phi(x, y, z)|_{y=0,\infty} = 0. \tag{A.7}$$

Appendix B

Practical Implementation of the Algorithm

The configuration Faddeev equations, i.e., Eqs. (3.3) in matrix form are defined on an infinite interval. Hence, for their numerical solution with an iterative algorithm (which is the Arnoldi method for this work) such equations should first be expressed on a finite interval. There are several ways, that can be used for this task. One way is a direct transformation of the infinite interval onto a finite interval [27]. Another approach, employed in this work is the radius cutoff method.

In using the radius cutoff approach, first we assume that the wave function approaches zero at some finite cutoff radius R which is roughly of the order of the size of the bound system. This radius may also be slightly larger than the range of the potential. In this way the potential is expected to be zero for large distances

close to R, otherwise the system will under bind. It is therefore, also necessary to approximate the wave function to its asymptotic form for distances larger than R.

In other to avoid the error in the wave function and under binding. First we define the infinite domain of the system for both $x-$ and $y-$ coordinates respectively as Ω_x and Ω_y. These domains are then subdivided into regions of interactions, namely, the inner and outer domains which are defined as follows

$$\Omega_x = \Omega_{x,I} + \Omega_{x,J}, \qquad \text{for} \quad 0 \le R$$

$$\Omega_y = \Omega_{y,I} + \Omega_{y,J}, \qquad \text{for} \quad 0 \le R$$

where the inner domains, $\Omega_{x,I}$ and $\Omega_{y,I}$ are defined for $[0, R)$, while the outer domains (asymptotic region), $\Omega_{x,J}$ and $\Omega_{y,J}$ associated with large R outside the range of potential are defined for $[R, \infty)$.

Of the aforementioned domains, Ω_x is of the most important one, since the x- grids associated with it must be optimized, to reproduce the two-body binding as well. For this purpose we define the x- grids on the interval $[a_0, x_{max}]$ for $\Omega_{x,I}$, i.e., we generate a partition:

$$a_0 = x_0 < x_1 < \ldots < x_B \ldots < x_{N_x} = x_{\max},$$

where a_0 is a measure of the distance from $x = 0$ carefully chosen to eliminate numerical noise associated with the $x \to 0$ behavior, and x_B is the break-point separating the interior and exterior domains. The large part of our numerical solution for the Faddeev equations is mainly based in the interior domain, $\Omega_{x,I}$. This is where more of the wave functions structure is covered, due to the following reasons: First, $\Omega_{x,I}$ is relatively dense compared to $\Omega_{x,J}$. Second, the small grid points in this domain have small separations.

Moreover, as the last reason, $\Omega_{x,I}$ must contain a sufficient number of points to describe well the most important ranges affecting the binding energy and wave function. Most of the important feature of the wave function, is covered in grids between a_0 and point x_B in $\Omega_{x,I}$. This means that x_B, as required should be chosen in such a way that roughly more of the x-grid points are in $\Omega_{x,I}$. Otherwise, the important structure of the wave function may be lost.

The asymptotic part of the wave function, i.e., where the interaction between particles is no longer active is then covered from point x_B up to points in $\Omega_{x,J}$. The interactions in the interior domain, $\Omega_{x,I}$, may clearly be observed, and explained through the following simple analytical transformation

$$x_{i+1} = a_0 + i\Delta x_i^{(I)}, \qquad i = 1, 2, \ldots, N_{x,I} - 1, \tag{B.1}$$

$$x_i = x_{i-1} + \Delta x_i^{(J)}, \qquad i = N_{x,I}, \ldots, N_x, \tag{B.2}$$

where the $\Delta x_i's$ are the scaling functions, and $N_{x,I}$ is the number of the interior points in the $\Omega_{x,I}$.

In the case of Ω_y, the value of a_0 is not important and is set equal to zero. In addition, the density of the points in $\Omega_{y,I}$ and $\Omega_{y,J}$ is not required to be as in the x-grid, meaning that convergence is not dependent on the y-grid. On the other hand the z-grid, $z_0 < z_1 < \ldots < z_{N_z}$, is obtained by the transformation

$$z_i = g(t_i), \qquad i = 0, \ldots\ldots, N_z, \tag{B.3}$$

where $t_i = -1 + i\Delta z$ and the function g is given by

$$g(t) = \frac{t + C_0 t^3}{1 + C_0}, \tag{B.4}$$

with $z_0 = -1$ and $z_{N_z} = 1$, and the control parameter is chosen within $-1 < C_0 \leq 0$. A typical of C_0 used in our calculations is -0.3333. The function $g(t)$ should be chosen carefully to satisfy the condition $g(0) = 0$ and $g(1) = 1$.

Appendix C

Interactions used in this work

C.1   Malfliet-Tjon potential

The Malfliet-Tjon potential is given by[31, 32]

$$V^{(2N)}(r) = V_R \frac{\exp(-\mu_R r)}{r} - V_A \frac{\exp(-\mu_A r)}{r} \ . \tag{C.1}$$

For the models used in this work, the parameters given in Table C.1.

Ref	V_A [MeV·fm]	μ_A [fm^{-1}]	V_R [MeV·fm]	μ_R [fm^{-1}]
[33]	570.316	1.550	1438.4812	3.110
[34]	578.09	1.550	1458.05	3.110

Table C.1: Parameters for the Malfliet-Tjon potential

C.2 Urbana potential

The Urbana IX potential[34] is given by the expression

$$
V^{(3N)}(r_{12}, r_{23}, r_{31}) = \sum_{cyc} \left[0.003 T_\pi^2(r_{12}) T_\pi^2(r_{23}) \right.
$$

$$
\left. + 4.5 T_\pi(r_{12}) T_\pi(r_{23}) \left\{ \frac{1}{2}(3c_2{}^2 - 1) \right\} \right], \tag{C.2}
$$

$$
\text{where} \quad T_\pi(r) = \frac{\exp(-0.7r)}{r} \left(1 + \frac{3}{0.7r} + \frac{3}{(0.7r)^2} \right) (1 - \exp(-2r^2))^2, \tag{C.3}
$$

$$
c_2 = \frac{(r_{12}^2 + r_{23}^2 - r_{31}^2)}{(2r_{12}r_{23})} = \cos(\theta_1). \tag{C.4}
$$

The summation runs over the three cyclic permutations of particles 1,2, and 3. The coordinate r_{ij} means the vector between particle i and j.

C.3 Ali-Bodmer s-wave $\alpha\alpha$ potential (ABd0)

The *s*-wave Ali-Bodmer $\alpha\alpha$ potential is given by

$$
V_{2\alpha}(r) = V_1 \exp\left(-\mu_1 r\right)^2 - V_2 \exp\left(-\mu_2 r\right)^2. \tag{C.5}
$$

Its parameters are given in Table C.2.

V_1 [MeV·fm]	μ_1 [fm^{-1}]	V_2 [MeV·fm]	μ_2 [fm^{-1}]
500	0.7	130	0.475

Table C.2: Parameters for the Ali-Bodmer $\alpha\alpha$ potential

C.4 Three-body potential for 3α system

The three-body potential for the 3α system used in this work is

$$V_{3\alpha}(x, y) = -V_1 \exp -(\rho/3.315)^2 \tag{C.6}$$

where ρ is the hyperadius $\rho = x^2/2 + 2/3y^2$ and $V_1 = 18.45$ MeV·fm.

C.5 Coulomb potential among 3 α particles

The Coulomb potential among the three α particles is given by

$$V^C = \frac{\eta}{x} + \frac{\eta}{x'} + \frac{\eta}{x''} \tag{C.7}$$

where $\eta = 4e^2/(\hbar^2/m_\alpha)$. x' and x'' are the permuted inter-particle coordinates.

C.6   Ozone Interactions

The interactions employed in the Ozone calculations are those cited in Ref.[40] (and references therein). Here we give, for completeness, the analytical expression for the long-range triple-dipole three-body interaction[43]

$$V^{(3N)}(r_\alpha, r_\beta, r_\gamma) = C\left[\frac{1 + 3\cos\theta_\alpha\cos\theta_\beta\cos\theta_\gamma}{(r_\alpha r_\beta r_\gamma)^3}\right], \tag{C.8}$$

where C is the constant characteristic of a system, and the coordinates r_i , θ_i, (i = α, β, γ) are, respectively, the internuclear distances, and internal angles of the triangle formed by the three atoms making up the system. In terms of the symmetry-adapted coordinates Q's, the three-body Ozone potential, in the ground state, may be expressed as [41]

$$V^{(3N)}(r_\alpha, r_\beta, r_\gamma) = [P(r_\alpha, r_\beta, r_\gamma) + G(r_\alpha, r_\beta, r_\gamma)][1 - \tanh\gamma_0 Q_1/2]; \tag{C.9}$$

where

$$
\begin{aligned}
P(r_\alpha, r_\beta, r_\gamma) &= a_1 + a_2 Q_1 + a_3 Q_1^3 + a_4(Q_2^2 + Q_3^2) + a_5 Q_1(Q_2^2 \\
&\quad + Q_3^2) + a_6(Q_3^3 - 3Q_2^2 Q_3) + a_7(Q_2^2 + Q_3^2)^2,
\end{aligned} \tag{C.10}
$$

$$G(r_\alpha, r_\beta, r_\gamma) = (b_1 + b_2)\left[b_3 + \sum_{i=\alpha,\beta,\gamma} \frac{r_i^2 - r_j^2 - r_k^2}{2r_j r_k}\right]^5 \mathrm{e}^{(-b_4(Q_2^2 + Q_3^2))}. \tag{C.11}$$

The parameters are given in TableC.3.

Parameter	Value
R_0	1.5698
γ_0	4.4
a_1	7.9920
a_2	6.1872
a_3	12.4339
a_4	-15.1314
a_5	-3.2418
a_6	2.6323
a_7	12.4195
b_1	3941.4453
b_2	3909.5196
b_3	1.2527
b_4	0.8

Table C.3: Parameters for the ozone potential

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Bibliography

[1] A. Laverne and C. Gignoux, Nucl. Phys. **A203**, 597 (1973) .

[2] A. Brandenburg, Y. E. Kim, and A. Tubis, Phys. Rev. **C 12** 1368 (1975) .

[3] N. D. Birrell and I. R. Afnan, Phys. Rev. **C 17**, 326 (1978) .

[4] R. A. Brandenburg, P. U. Sauer, and R. Machleidt, Z. Phys. **A280** 93 (1977) .

[5] J. L. Friar, B. F. Gibson, and G. L. Payne, Annu. Rev. Nucl. Part. Sci. **34**, 403 (1984) .

[6] S. Ishikawa, T. Sasakawa, T. Sawada, and T. Ueda, Phys. Rev. letters **53**, 20 (1984) .

[7] A. Nogga, H. Kamada, W. Glöckle; arXiv:nucl-th/0004023, **2**, (2000) .

[8] Muslim, Y. E. Kim and T. Ueda, Phys. Lett. **115 B** , 273 (1982) .

[9] M. Fabre de la Ripelle, C. R. Acad. Sci. **288B**, 325 (1979) .

[10] E. Hadjimichael, Nucl. Phys. **A294**, 513 (1978) .

[11] C. Hajduk, P. U. Sauer, H. Arenhóvel, D. Dreschel, M. M. Gianini, *ibid.* **A352**, 413 (1981).

[12] M. R. Robilotta, Few-Body Syst. Suppl. **2**, 35 (1987).

[13] S. A. Coon et al., Nucl. Phys. **A317**, 242 (1979).

[14] A. D. Jackson, and J. A. Tjon; Phys. Lett. **32 B**, 9.

[15] H. P. Noyes and H. Fiedeldey, in *Three-Particle Scattering in Quantum Mechanics. Proceedings of Texas A and M Conference*, Edited by J. Gillespie and J. Nutall (Benjanim, New York, 1968), pp. 195-294.

[16] S. P. Merkuriev, C. Gignoux, A. Laverne, Annals of physics **99**, 30-71 (1976), and references therein.

[17] A. Picklesimer, R. A. Rice, R. Brandenburg, Phys. Rev. **C 45**, 2045 (1992).

[18] A. Picklesimer, R. A. Rice, R. Brandenburg, Phys. Rev. **C 45**, 547 (1992).

[19] A. Picklesimer, R. A. Rice, R. Brandenburg, Phys. Rev. **C 44**, 1359 (1991).

[20] A. Stadler, W. Glöcle, P. U. Sauer, Phys. Rev. **C 44**, 2319 (1991).

[21] A. Stadler, P. U. Sauer, Phys. Rev. **C 46**, 64 (1992).

[22] A. Nogga, D. Hüber, H. Kamada, W. Glöckle, Phys. Lett. **B409**, 19 (1997).

[23] J. L. Friar, B. F. Gibson, and G. L. Payne, Z. Phys. **A301**, 309 (1981).

[24] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. **C 31**, 2266 (1985).

[25] Y. Wu, S. Ishikawa, T. Sasakawa, Few-Body Systems **15**, 145 (1993).

[26] V. A. Roudnev, S. L. Yakovlev, and S. A. Sofianos, physics /0204025 v2 9 Apr 2002.

[27] N. W. Schellingerhout, L. P. Kok, and G. D. Bosveld, Phys. Rev. **A 40**, 5568 (1989).

[28] L. D. Faddeev, Sov. Phys. JETP **2**, 1014 (1961);
L. D. Faddeev, *Mathematical Aspects of the Three Body Problem in Quantum Scattering Theory* (Israel Program for Scientific Translation, Jerusalem , 1965).

[29] C. de Boor and B. Swartz, SIAM J. Numer. Anal. **10** , 582 (1973).

[30] Y. Saad, *Numerical methods for large eigenvalue problems*, Manchester University Press in Algorithms and architectures for Advanced Scientific Computing, NY (1992).

[31] R. A. Malfliet and J. A. Tjon, Nucl. Phys. **A127**, 161 (1969).

[32] R. A. Malfliet and J. A. Tjon, Ann. of Phys. **61**, 425 (1970).

[33] G. L. Payne, J. L. Friar, and B. F. Gibson, Phys. Rev. **C 26**, 4 (1982).

[34] J. G. Zabolitzky, K. E. Schmidt, and M. H. Kalos, Phys. Rev. **C 25**, 2, 1982.

[35] J. Carlson, V. R. Pandharipande, R.B. Wiringa, Nucl. Phys. **A401**, 59, (1983).

[36] H. T. Coelho, T. K. Das, M. R. Robilotta, Phys. Rev. **C 28**, 1812 (1983).

[37] I. Filikhin, V. M. Suslov, B. Vlahovic; J. Phys. G: Nucl. Part. **31** (2005) 1207-1224.

[38] E. M. Tursunov *et al*; Nucl. Phys. **A 723**, 365 (2003) .

[39] F. Ajzenberg-Selove, C. L. Busch; Nucl. Phys. **A 336**, 1 (1980).
F. Ajzenberg-Selove; Nucl. Phys. **A 490**, 1 (1988) .

[40] M. L. Lekala; PhD Thesis, University of South Africa, 2005 .

[41] A. J. C. Varandas, J. N. Murrell; Chem. Phys. Lett. **88**, 1 (1982) .

[42] A. A. Kvitsinsky, V. V. Kostrykin, S. P. Merkuriev, A. K. Motovilov, S. L. Yakovlev; Sov. J. Part. Nucl. **17**, 533 (1986) .

[43] B. M. Axilrod, E. J. Teller; J. Chem. Phys. **11**, 299 (1943), Y. Muto, Proc. Phys. Math. Soc. Japan **17**, 629 (1943) .

[44] E. Hadjimichael, A. D. Jackson, Nucl. Phys. **A180** ,217 (1972) .

[45] M. I. Haftel, Phys. Rev. **C 7**, 80 (1973) .

[46] P. U. Sauer and J. A. Tjon, Nucl. Phys. **A 216**, 541 (1973) .

[47] H. Fiedeldey; Phys. Letters **30B**, 603 (1961) .

[48] M. M. Hoenig, Phys. Rev. **C 3**, 1118 (1971) .

[49] Y. E. Kim, E. P. Harper, and Tubis; Phys. Rev. **C 6**, 1601 (1972) .

[50] M. Sato, Y. Akaishi, H. Tanaka; Suppl. Prog. Theor. Phys. **56**, 76 (1974) .

[51] M. Sato, and H. Tanaka, Prog. Theor. Phys. **51**, 1979L (1974) .

[52] Shin-Nam Yang, Phys. Rev. **C 10**, 2067 (1974) .

[53] L. M. Delves, Adv. Nucl. Phys. **5**, 1 (1972) .

[54] J. L. Ballot and M. Fabre de la Ripelle, Ann. Phys. (N.Y) **127**, 62 (1980).

[55] C.D. Lin and X. H. Liu, Phys. Rev. **A 37**, 2749 (1988).

[56] J. G. Zabolitzky and M. H. Kalos, Nucl. Phys. **A356**, 114, (1981).

[57] K. E. Schmidt, in *Models and Methods in Few-Body Physics, Proceedings, Lisboa, Portugal, 1986, Vol. 273 of Lecture Notes in Physics*, Edited by L. S. Ferreira, A. C. Fonseca, and L. Streit (Springer-Verlag, Berli, 1987), pp. 363-407.

[58] A. Kvitsynsky and C. Y. Hu, Few-Body Systems **12**, 7 (1992),
P. M. Prenter, *Splines and Variational Methods* (Wiley, New York, 1975).

[59] J. J. Benayoun, C. Gignoux, J. Chauvin, Phys. Rev. **C 23**, 1854 (1981).

[60] G. L. Payne, J. L. Friar, B. F. Gibson, Phys. Rev. **C 26**, 1385 (1982).

[61] G. L. Payne and L. Schlessinger, J. Comput. Phys. **13**, 266 (1973).

[62] P. Nunberg, D. Prosperi, and E. Pace, Nucl. Phys. **A285**, 58 (1977).

[63] J. Lomnitz-Adler and V. R. Pandhari-Pande, Nucl. Phys. **A342**, 404 (1980).

[64] V. V. Kostrykin, A. A. Kvitsinsky, and S. P. Merkuriev, Few-Body Systems **6**, 97 (1989).

[65] W. Glöckle and R. Offerman, Phys. Rev. **C 16** (1977) 2039.

[66] M. I. Haftel and W. M. Kloet, Phys. Rev. **C 15** (1977) 404.

[67] B. D. Day, Rev. Mod. Phys. **50** (1978) 495.

[68] B. D. Day, F. Coester and A. Goodman, Phys. Rev. **C 6** (1972) 1992.

[69] H. Kümmel, K. H. Lührmann and J. G. Zabolitzky, Phys. Reports **36C**, 674 (1978) 1.

[70] D. Hüber et al., Phys. Rev. **C 58**, 674 (1998).

[71] D. Hüber et al., LANL Report No. nucl-th/9910034. 68.

[72] J. L. Friar et al., Phys. Rev. **C 59**, 53 (1999).

[73] S. A. Coon et al., Phys. Rev. **C 48**, 2559 (1993).

[74] J. Fujita and H. Miyazawa, Prog. Theor. Phys. **17**, 360 (1957).

[75] S. A. Coon, M. D. Schadron, P. C. McNamee, B. R, Barrett, D. W. E. Blatt, and B. H. J. McKellar, Nucl. Phys. **A317**, 242 (1979).

[76] S. A. Coon, Few-Body Syst., Suppl. **1**, 41 (1984).

[77] S. A. Coon and J. L. Friar, Phys. Rev.**C 34**, 1060 (1060).

[78] S. A. Coon and M. T.Peña, Phys. Rev. **C 48**, 2559 (1993).

[79] S. A. Coon and W. Glöckle, Phys. Rev **C 23**, 1790 (1981).

[80] R. Schiavilla, V. R. Pandharipande, and R.B. Wiringa, Nucl. Phys. **A449**, 219, (1986).

[81] R. B. Wiringa, Phys. Rev. **C 43**, 1585 (1991).

[82] A. Kievsky, Phys. Rev. **C 60**, 034001 (1999).

[83] L. D. Knutson and A. Kievsky, Phys. Rev. **C 58**, 1 (1998).

[84] K. Sekiguchi, H. Sakai, and H. Witala, Phys. Rev. **C 65**, 034003 2002 .

[85] M. L. Lekala, S. A. Sofianos, V. Roudnev, and M. Braun, Few-Body Systems Suppl. **14**, 171-174 (2003) .

[86] O. Portilho and D. A. Agrello, Phys. Rev. **C 6**, 27 1983 .

[87] L. D. Faddeev, Tr. Mat. Inst. Akad. Nauk SSSR **69** (1969) .

[88] M. A. Hennell and L. M. Delves, Nucl. Phys. **A246**, 490 (1975) .

[89] J. Carbonell, C. Gignoux, and S. P. Merkriev, Few-Body Systems **15**, 15-23, (1993) .

[90] N. W. Schellingerhout, *Factorizability in the Numerical Few-Body Problem* (PhD Thesis, University of Gröningen, The Netherlands (1995)) .

[91] M. Born and R. Oppenheimer; Ann. Physik **84**, 457 (1927)

[92] Chi-Yu Hu, A. A. Kvitsinsky, and S. P. Merkuriev; Phys. Rev **A 45**, 5 (1992) .

[93] S. P. Merkuriev, S. L. Yakovlev, C. Gignoux; Nucl. Phys. **A431**, 125(1984) .

[94] J. L. Friar, B. F. Gibson, and G. L. Payne; Phys. Rev **C 24**, 5 (1981) .

[95] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson; Phys. Rev. C 31, 6 (1985) .

[96] C. R. Chen, G. L. Payne, J. L. Friar, and B. F. Gibson; Phys. Rev. **C 33**, 5 (1986) .

[97] M. L. Lekala; Private communication.