Kinetic energy operator approach to the quantum three-body problem with Coulomb interactions

Xuguang Chi\textsuperscript{1}, Wuyi Hsiang\textsuperscript{2} and Ping Sheng\textsuperscript{1}\textsuperscript{†}

\textsuperscript{1}Department of Physics and the Institute of Nano Science and Technology, 
Hong Kong University of Science and Technology, 
Clear Water Bay, Kowloon, Hong Kong, China 
\textsuperscript{2}Department of Mathematics, Hong Kong University of Science and Technology, 
Clear Water Bay, Kowloon, Hong Kong, China

Abstract. We present a review of the quantum three-body problem, with emphasis on the different methodologies, different three-body atomic systems and their historical interest. With the review as the background, a more recently proposed non-variational, kinetic energy operator approach to the solution of quantum three-body problem is presented, based on the utilization of symmetries intrinsic to the kinetic energy operator, i.e., the three-body Laplacian operator with the respective masses. Through a four-step reduction process, the nine dimensional problem is reduced to a one dimensional coupled system of ordinary differential equations, amenable to accurate numerical solution as an infinite-dimensional algebraic eigenvalue problem. A key observation in this reduction process is that in the functional subspace of the kinetic energy operator where all the rotational degrees of freedom have been projected out, there is an intrinsic symmetry which can be made explicit through the introduction of Jacobi-spherical coordinates. A numerical scheme is presented whereby the Coulomb matrix elements are calculated to a high degree of accuracy with minimal effort, and the truncation of the linear equations is carried out through a systematic procedure. The resulting matrix equations are solved through an iteration process. Numerical results are presented for (1) the negative hydrogen ion H\textsuperscript{−}, (2) the helium and helium-like ions (Z = 3 \sim 6), (3) the hydrogen molecular ion H\textsubscript{2}\textsuperscript{+}, and (4) the positronium negative ion Ps\textsuperscript{−}. Up to thirteen-significant-figure accuracy is achieved for the ground state eigenvalues when double precision programming is used. Comparison with the variational and other approaches shows our ground state eigenvalues to be comparable, generally with less decimal digits than the variational results, but can yield highly accurate wavefunctions as by-products. Results on low-lying excited states and their wavefunctions are obtained simultaneously with the ground state properties, some at accuracies not achieved by other methods. In particular, for the doubly excited state \textsuperscript{3}P\textsuperscript{e} of H\textsuperscript{−} and the \textsuperscript{1,3}P\textsuperscript{e} states of helium, some results are obtained for the first time. Also, we have calculated fourteen H\textsubscript{2}\textsuperscript{+} excited states, up to its dissociation level. Analysis of the wavefunction characteristics, especially in relation to the electron-electron correlation effects, are presented. A significant advantage of the kinetic energy operator approach is its general applicability to different three-body systems, with only the charges, masses, and the symmetry of the desired state as the required inputs. Potential applications of the present approach to scattering and other problems are noted.

\textsuperscript{†} Corresponding author email: sheng@ust.hk
# CONTENTS

## Contents

1. **Introduction**  

2. **Review of the various approaches**  
   2.1 Variational method  
   2.2 Hyperspherical coordinates method  
   2.3 Perturbation, Hartree-Fock, and the finite element methods  

3. **Formulation**  
   3.1 Overview of the approach  
   3.2 Jacobi vectors and coordinate transformations  
   3.2.1 Rotationally invariant variables  
   3.2.2 Jacobi spherical coordinates  
   3.2.3 Interparticle distance $r_{ij}$ expressed in Jacobi spherical coordinates  
   3.3 Symmetries and angular momentum eigenfunctions  
   3.3.1 Wave function expansion  
   3.3.2 Reduced Schrödinger equation  
   3.4 Expansion of reduced Schrödinger equation in Jacobi-spherical coordinates  
   3.4.1 Reduced Schrödinger equations in terms of $(\rho, \xi, \beta)$  
   3.4.2 Eigenfunctions of the operator $A^{(l)}$  
   3.4.3 Matrices $B_1$ and $B_2$  
   3.4.4 Coulomb potential expressed in Jacobi-spherical coordinates $(\rho, \xi, \beta)$  
   3.4.5 Matrix elements of $U(\xi, \beta)$  
   3.5 Further reduction to a system of 1D ODEs  
   3.6 Conversion to a linear algebraic eigenvalue problem  
   3.6.1 Expansion of the ODE system in terms of the Laguerre polynomials  
   3.6.2 Infinite linear equations for the coefficients  

4. **Numerical scheme**  
   4.1 Solution of the linear eigenvalue problem  
   4.1.1 Matrix-vector product ($M_{Rv}$) evaluation  
   4.1.2 Calculation of $M_{r^{-1}v}$  
   4.2 Truncation and extrapolation procedures  
   4.2.1 Truncation path  
   4.2.2 Extrapolation procedure  

5. **Results on three-body systems**  
   5.1 Euler angles and wave functions  
   5.1.1 Euler angles and the distribution function  
   5.2 Negative hydrogen ion  
   5.2.1 The ground state  
   5.2.2 The $^3P^e$ state
1. Introduction

The dynamics of three interacting bodies constitutes one of the oldest challenges in physics. Studies in this field can be traced back to the work of Euler in the 18th century. In the beginning of the 20th century, the failure of the Bohr-Sommerfeld quantization to correctly describe the ground state of helium has stimulated the development of the “new” quantum theory, formulated by Schrödinger and Heisenberg. Almost 100 years after the founding of modern quantum mechanics, there is still a continuing effort to improve the solution methods or to invent new approaches for the seemingly simple three-body Coulomb system.

In the early calculations of the two-electron systems, the focus was usually on the bound-state spectra, with the helium and helium-like ions as the proving ground. The spectra could be calculated efficiently with the help of the Hartree-Fock self-consistent-field method based on the variational principle. Very high accuracy can be achieved for eigenvalues such that they may be compared with high precision measurements. Bether and Salpeter [1] have summarized the early works in this area. The more recent calculations of the bound states have extended such routines with new numerical schemes and judicious choices of basis functions.

In a seminal experiment by Madden and Codding [2], the discovery of strong electron-electron correlation effects in doubly excited resonance states of helium has triggered the development of group-theoretical and adiabatic quantum approximations to understand these effects. The two-electron dynamics were again at the forefront of a revival. As doubly excited resonant states could not be tracked by an effective single-particle method, over the past four decades the effort to understand doubly excited resonances has stimulated much of the theoretical research on two-electron atoms. The
role of electron correlation has become more important with increasing order of double excitations, and the correlated three-body Coulomb dynamics have been found to cause an extremely rich and complicated resonance spectrum. Hence two-electron atoms have come to represent a prototype of the few-body systems strongly affected by electronic correlation.

A more difficult problem is the three-body scattering, such as hydrogen-electron scattering. This problem has attracted much attention recently. By using the finite element method, Levin and Shertzer \[3\] analyzed the S-wave phase shifts for low-energy positron-hydrogen scattering. Botero and Shertzer \[4\] directly solved the Schrödinger equation for electron-hydrogen scattering, and Rescigno et al \[5\] and Baertschy et al \[6\] used supercomputers to obtain a complete numerical solution of the hydrogen atom ionization through electron collision.

Three-body systems, especially the two-electron systems, remain an active field of research today. This persistent interest can be traced to the fact that the three-body problem is just complex enough for rather sophisticated theoretical concepts, yet simple enough to provide accurate numerical and experimental tests.

More recently, Hsiang and Hsiang \[7, 8, 9, 10\] have outlined a new approach to the quantum three-body problem which was based on the systematic exploitation of all the intrinsic dynamic symmetries of the three-body kinetic energy operator (the three-body Laplacian with the respective masses), some of which not fully recognized previously. The purposes of this work are to implement this new mathematical formulation and to compare the present approach with the conventional variational approach in terms of numerical results for both eigenvalues and eigenfunctions of a number of quantum three-body systems.

The main conclusions of this work are that the present approach offers not only systematic computability, requiring minimal ad hoc inputs in the computational process, but also achieves numerical accuracy for both the eigenvalues and eigenfunctions. The latter advantage is particularly significant for excited states. In particular, the wave function characteristics of excited states with strong electron-electron correlation can be accurately delineated.

In what follows, we first review the various approaches to the quantum three-body problem in section 2, followed by a detailed presentation of the kinetic energy operator approach in section 3. The formulation essentially consists of a four-step reduction process, in which the dynamic symmetries intrinsic to the kinetic energy operator are fully utilized. The end result of the reduction is a one-dimensional coupled system of ordinary differential equations, solvable as an infinite-dimensional algebraic eigenvalue problem. In section 4 a scheme is presented for the numerical implementation of our approach. Due to the high precision required for the Coulomb matrix elements, a special integration technique is used to evaluate both the matrix elements as well as the product of the potential energy matrix with a vector. A sparse matrix solver is then applied to solve the linear equations iteratively. Truncation of the infinite linear system is carried out by following a rule implied by the asymptotic behavior of the eigenvalues, leading
to sequences of numerical data from which one can apply a systematic extrapolation procedure. The results for some typical Coulomb systems are presented in section 5 with comparisons to those obtained via other approaches. We also explore the properties of three-body wave functions, and discuss some of their physical significances. It should be noted that all the results were obtained by using the same program. Inputs are the symmetry of the state (i.e., $S$, $P$, $D$, or $F$), the mass ratios, and the sign of the charges. The article concludes by noting some potential applications of the present approach.

2. Review of the various approaches

2.1. Variational method

Quantum variational method is most suitable for obtaining accurate results for the ground state or low-lying states, and in this regard it is superior to the perturbation methods. The basic idea of the variational method, sometime also denoted as the Ritz variational method, named after the pioneer of the approach, is to write the trial wave function $\Psi_{tr}$ in some arbitrarily chosen mathematical form with variational parameters,

$$\Psi_{tr} = \Psi_{tr}(\alpha, \beta, \gamma, \cdots)$$ \hspace{1cm} (1)

and then adjust the parameters to obtain the minimum energy

$$E_{tr}(\alpha, \beta, \gamma, \cdots) = \frac{\int \Psi_{tr}^* H \Psi_{tr} d\tau}{\int |\Psi_{tr}|^2 d\tau}$$ \hspace{1cm} (2)

through the solution of a system of coupled equations:

$$\frac{\partial E_{tr}(\alpha, \beta, \gamma, \cdots)}{\partial \alpha} = 0$$

$$\frac{\partial E_{tr}(\alpha, \beta, \gamma, \cdots)}{\partial \beta} = 0$$

$$\frac{\partial E_{tr}(\alpha, \beta, \gamma, \cdots)}{\partial \gamma} = 0$$

$$\vdots$$ \hspace{1cm} (3)

It should be noted that the trial wave function(s) must satisfy the symmetry condition imposed by the Fermi-Dirac statistics. The solution to (3) yields minima of energy in the multidimensional parameter space. The lowest energy minimum is treated as the approximate ground state eigenvalue. As an example, a simple trial wave function for the ground state of helium-like atoms is $\psi(r_1, r_2, r_{12}) = \exp(-(Z - \sigma)(r_1 + r_2))$, where $\sigma$ represents the screening effect in an approximate way. Minimizing the energy functional gives $E = -(Z - 5/16)^2$, i.e., $E=-2.85$ a.u. for the helium ground state [11]. However, for $H^-$ this trial wave function is noted to fail in obtaining a bounded ground state. For the excited states, the Hylleraas-Undheim theorem states that the remaining energy minima of $\lambda_2$, $\lambda_3$, $\cdots$, are also upper bounds to the exact eigenvalues $E_2$, $E_3$, $\cdots$, provided that the spectrum is bounded from below. However, the calculation of precise excited state energies is more difficult compared to that of the ground state, due to
the appearance of the subsidiary condition that the eigenfunction of every excited state must be orthogonal to the eigenfunctions of all the lower-order states. This condition reduces considerably the number of available trial functions which may be chosen to approximate the eigenfunction (to be inserted in the variation integral) of the particular excited state. As a result, convergence is not nearly as good.

Historically, Kellner [11] was the first to use the variational principle to obtain a rather precise ground state energy, $E=-2.895$ a.u.. His results were improved upon by the variational calculations of Hylleraas [12, 13], who obtained $E=-2.9037$ a.u. using a trial wave function with 38 variational parameters. This method was later used by Kinoshita [14] in large-scale variational calculations. In a bold move, Frankowski and Pekeris [15] used more than 200 parameters in trial functions to obtain the energies of helium-like systems that were not surpassed for almost two decades. With the appearance of powerful modern computers, however, people can now include more than one thousand parameters in trial wave functions in order to obtain high accuracy results for the ground state of helium, hydrogen-like ions and some muonic molecular ions [16, 17, 18, 19, 20, 21].

As a modified version of the variational method, the complex rotation method, based on the dilatation analytic continuation [22, 23, 24], was extensively used to calculate the doubly excited states of the two-electron systems [25, 26, 27, 28, 29]. The basic idea is that after a complex rotation, $r \rightarrow re^{i\theta}$, is applied to the radial coordinate, the resulting Hamiltonian becomes complex, i.e., $H(\theta) = e^{-2i\theta}T + e^{-i\theta}V$, where $T$ is the kinetic energy operator and $V$ the Coulomb potential. The complex Hamiltonian will yield complex eigenenergies as a result of applying the Ritz variation, in which the real part would correspond to the position of the doubly excited state, and the imaginary part its life-time.

2.2. Hyperspherical coordinates method

Hyperspherical coordinates were first introduced into atomic physics by Gronwall [30] to study the analytic structure of the Schrödinger equation for the ground state of helium atom. The basic idea of the hyperspherical approach to the three-body systems is to express the two relative (to center of mass) coordinates as a single six-dimensional vector, and the nonrelativistic Schrödinger equation in the six-dimensional space is to be solved without reference to the “wave functions” associated with individual particles. The condition of particle exchange symmetry then becomes a boundary condition on the three-body wave function on the hypersurface.

The hyperspherical approach has been applied to solve bound states and scattering problems in many different fields of physics and chemistry. Many of the earlier works dealt with the basic structure of the mathematical functions encountered in hyperspherical coordinates. Here we introduce the hyperspherical coordinates for two-electron atomic systems such as helium and hydrogen negative ions where the mass of the nucleus is treated as infinite. The hyperspherical coordinates are then obtained by
defining
\[ \rho = \sqrt{r_1^2 + r_2^2}, \quad \alpha = \arctan(r_2/r_1), \] (4)
where \( \rho \) is the hyperradius which measures the size of the system, and \( \alpha \) is the hyperangle. Thus the two vectors \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) are replaced by six coordinates \((\rho, \Omega)\), where \( \Omega = (\alpha, \theta_1, \phi_1, \theta_2, \phi_2) \) denotes collectively the five angles, with \((\theta_i, \psi_i)\) being the spherical angles of electron \( i \). In hyperspherical coordinates the two-electron equation is given by
\[ \left( -\frac{1}{2} \Delta_1 - \frac{1}{2} \Delta_2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} - E \right) \Psi(\mathbf{r}_1, \mathbf{r}_2) = 0. \] (5)
After eliminating the first-order derivatives in the differential operators by expressing
\[ \Psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\rho, \Omega)/(\rho^{5/2} \sin \alpha \cos \alpha), \] (6)
an equation in terms of \( \psi(\rho, \Omega) \) is obtained:
\[ \left( -\frac{\partial^2}{\partial \rho^2} + \frac{\Lambda^2}{\rho^2} + \frac{2C}{\rho} + 2E \right) \psi(\rho, \Omega) = 0, \] (7)
where
\[ \Lambda^2 = \left( -\frac{\partial^2}{\partial \alpha^2} + \frac{l_i^2}{\cos^2 \alpha} + \frac{l_i^2}{\sin^2 \alpha} \right) - \frac{1}{4} \] (8)
is the grand angular momentum operator, \( l_i \) being the angular momentum operator for electron \( i \) and \( C/\rho \) is the total Coulomb interaction potential among the three charged particles, with \( C \) given by
\[ C(\alpha, \theta) = -\frac{Z}{\cos \alpha} - \frac{Z}{\sin \alpha} + \frac{1}{\sqrt{1 - \sin 2\alpha \cos \theta_{12}}}. \] (9)
Here \( \theta_{12} \) is the angle between the two electrons with respect to the nucleus (as the origin).

The straightforward solution approach is to expand \( \psi(\rho, \Omega) \) by the eigenfunctions of \( \Lambda^2 \), called hyperspherical harmonics. This method has been applied by a number of authors to \( \text{H}^- \) and \( \text{He} \) systems \cite{31, 32, 33, 34}, but the rate of convergence is rather slow. To improve the rate of convergence, Haftel and Mandelzweig \cite{35, 36, 37, 38, 39} introduced an exponential factor in the expansion, \( \psi = \chi \Phi \), where \( \chi \) is chosen to be of the form \( \chi = \exp\{-a(r_1 + r_2) + br_{12}\} \), with \( a \) and \( b \) to be obtained variationally or by some ansatz. If \( a \) and \( b \) are appropriately chosen, the singularity in the Coulomb potential can be removed, and it is then possible to expand \( \Phi \) in terms of hyperspherical harmonics with rapid convergence. Another common approach, the adiabatic expansion, was introduced by Fano and first applied by Macek \cite{41}. Details of this method can be found in the review article by Fano \cite{43} and a relevant book \cite{44}. 


2.3. Perturbation, Hartree-Fock, and the finite element methods

In the perturbation method, the Hamiltonian is split into two parts, \( H = H_0 + \lambda H_1 \), where the perturbation term \( \lambda H_1 \) is small in a relative sense. For the Hamiltonian equation

\[
(H_0 + \lambda H_1 - E) \Psi = 0, \tag{10}
\]

the eigenfunction \( \Psi \) and eigenvalue \( E \) are expanded in powers of the small parameter \( \lambda \), namely

\[
E = \sum_{n=0}^{\infty} \lambda^n E_n, \quad \Psi = \sum_{n=0}^{\infty} \lambda^n \Psi_n. \tag{11}
\]

Substitution of these expansions into the Schrödinger equation and equating the coefficients for each power of \( \lambda \) to zero lead to an infinite set of coupled linear equations:

\[
H_0 \Psi_0 - E_0 \Psi_0 = 0 \tag{12}
\]

\[
H_0 \Psi_1 + H_1 \Psi_0 - E_0 \Psi_1 - E_1 \Psi_0 = 0 \tag{13}
\]

\[
.................................
\]

\[
H_0 \Psi_n + H_1 \Psi_{n-1} - \sum_{m=0}^{n} E_m \Psi_{n-m} = 0. \tag{14}
\]

If we consider \( \Psi_0 \) and \( E_0 \) as known, we can obtain the first order perturbation energy

\[
E_1 = \int \Psi_0^* H_1 \Psi_0 d\tau. \tag{15}
\]

For the calculation of \( E_2, E_3, \cdots \), more efforts are needed. There is no theorem to clearly tell one how to choose the perturbation \( \lambda H_1 \), and there can be different choices for the same problem. For large \( Z \) in helium-like ions, the interaction \( 1/r_{12} \) between the electrons can be treated as the perturbation; for the excited state, there is the unsymmetrical choice \[ \Pi \], \( H_0 = T + V_1 + V_2 \) and \( \lambda H_1 = W \), where

\[
V_1(r_1) = -\frac{Z}{r_1}, \quad V_2(r_2) = -\frac{Z - 1}{r_2}, \quad W = \frac{1}{r_{12}} - \frac{1}{r_2}. \tag{16}
\]

In the Hartree-Fock method, the wave functions for the two-electron atom must obey overall antisymmetry. That means

\[
\Psi = \frac{1}{\sqrt{2}} [\psi_1(r_1)\psi_2(r_2) \pm \psi_1(r_2)\psi_2(r_1)], \tag{17}
\]

where the + sign in the above equation is used when the spin state has antisymmetry. The form of the trial wave functions \( \psi_1(r) \) or \( \psi_2(r) \) is unknown, but the aim is to find the most accurate form possible for the two functions \( \psi_1(r) \) or \( \psi_2(r) \) that would minimize the expectation value of the Hamiltonian, which is regarded as a functional of the two trial wave functions. The application of the general variational principle leads to two coupled differential-integral equations (the Euler-Lagrange equations). In essence, the Hartree-Fock method is a mean-field theory. It differs from the Ritz variational approach in that the variation in the Ritz method is carried out by using parameters, whereas in the Hartree-Fock method the variation is carried out by solving coupled integral-differential equations.
Recently, the finite element method (FEM) \[45\] has been used to directly solve the Schrödinger equation, especially for the $S$ state of some systems. The domain of the wave function is segmented into tetrahedrons, each serving as the domain of a local polynomial basis set. The approximation of the wave function as a linear combination of these local polynomials is called a finite-element description. FEM treatment for the helium atom in the infinite nuclear mass approximation \[46, 47, 48, 49, 50\], and the hydrogen molecular ion $H_2^+$ in the Born-Oppenheimer approximation, have been presented by several authors \[51, 52, 53, 54, 55, 56\]. An adaptable FEM approach was used by Ackermann \[57\] and co-workers to obtain the energy values to a precision of $10^{-11}$ with moderate computational effort. The advantage of FEM lies in its flexibility because of the local basis, but the drawback is that one often has to face huge sparse matrices.

3. Formulation

In a three-body Coulomb system, the position vectors and the masses of the three particles are denoted by $r_j$ and $M_j$, $j = 1, 2, 3$. The relative masses are defined as $m_j = M_j/M$, where $M$ is the total mass, $M = \sum M_j$, and $\sum m_j = 1$. Schrödinger equation is given by

$$-\frac{1}{2M}\Delta \Psi + V \Psi = E \Psi,$$

$$\Delta = \sum_{j=1}^{3} \frac{\Delta_j}{m_j}, \quad (18)$$

where $\Delta_j$ is the Laplacian operator with respect to the $j$-th particle, $\Delta$ is defined as the kinetic energy operator, and $V$ is the Coulomb potential of the three interacting particles:

$$V = \frac{Z_2Z_3}{|r_2 - r_3|} + \frac{Z_3Z_1}{|r_3 - r_1|} + \frac{Z_1Z_2}{|r_1 - r_2|}. \quad (19)$$

Here $Z_j$ is the electric charge of the $j$-th particle. In the above and in what follows, the length unit is the Bohr radius, $\hbar^2/m_e c^2$, $m_e$ is the electron mass, also the mass unit, and $m_e c^2/\hbar^2$ is the energy unit. The above system is uniquely determined by the six parameters, \{${m_j, Z_j, j = 1, 2, 3}$\}. The Coulomb potential depends only on the distance between each pair of particles, and the system is invariant under spatial translation, rotation, and inversion. Furthermore, if the system consists of identical particles, invariance with respect to the permutation of identical particles must be imposed.

3.1. Overview of the approach

As implied by the name, the focus of the present approach is on the kinetic energy operator $\Delta$. Before delving into the details, it would be helpful to give an overview of the formulation, which in essence consists of four reduction steps. In the first
step (section 3.2), we reduce the nine dimensional problem to a six dimensional problem by simply using coordinates relative to the center of mass. Jacobi vectors will be introduced at this stage to facilitate later developments. In the second step (section 3.3), angular momentum eigenfunctions will be presented which are in the null space of the kinetic energy operator. That is, when the angular momentum eigenfunctions are operated on by the kinetic energy operator, the result is zero. Thus when the total wave function is expanded in terms of the angular momentum eigenfunctions, the coefficients of the expansion, which are rotationally invariant, satisfy a reduced Schrödinger equation which is three-dimensional. The set of functions that satisfy this reduced Schrödinger equation constitutes a subspace in which all the rotational degrees of freedom have been projected out. In the third step of the reduction (section 3.4), this 3D reduced Schrödinger equation is expressed in terms of the Jacobi-spherical coordinates, leading to a form with an angular operator whose eigenfunctions are the Jacobi polynomials (hence the denotation of Jacobi-spherical coordinate). It should be emphasized that the Jacobi-spherical symmetry is particular only to the kinetic energy operator and not to the Coulomb potential, in contrast to the rotational symmetry. Hence the total Hamiltonian does not have this symmetry. However, the Coulomb potential becomes separable in the Jacobi-spherical coordinates. That is, the Coulomb potential can be expressed as a product of two terms, one of which depends only on the radial coordinate of the Jacobi-spherical coordinates. The wave functions of this reduced Schrödinger equation can therefore be expanded in terms of the Jacobi polynomials with coefficients depending only on the radial coordinate of the Jacobi-spherical coordinates. In the fourth and last reduction step (section 3.5), the substitution of the this expansion into the reduced Schrödinger equation leads to a set of coupled ordinary differential equations (ODEs) which is now only one dimensional, i.e., the solution depends only on the radial coordinate. The solution to the set of ODEs can be expanded in terms of the Laguerre polynomials, and the coefficients of this expansion satisfy an infinite linear system which is amenable to numerical solution (section 3.6).

3.2. Jacobi vectors and coordinate transformations

The configuration space of a given three-body system is a nine-dimensional space consisting of a triplet of position vectors,

\[ \mathcal{R}^9 = \{ \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 \}, \]

where \( \mathbf{r}_j \) is the position vector of \( j \)-th particle. Without the loss of generality, one can assume that the center of gravity is fixed at the origin, thus reducing the configuration space to the following six-dimensional reduced configuration space:

\[ \mathcal{R}^6 = \{ (\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3); \sum m_j \mathbf{r}_j = 0 \}. \]
Following Jacobi, we introduce the kinematic metric on the reduced configuration space by defining the inner product as

\[ \langle \{a_j\}, \{b_j\} \rangle := \sum_{j=1}^{3} m_j a_j \cdot b_j. \]  

(22)

This definition is related to the Lagrange’s least-action principle, which was reformulated by Jacobi, leading to the geometric explanation of mechanics. The metric \( ds^2 \) is defined in terms of the kinetic energy \( T \) by setting

\[ ds^2 = \frac{2T}{M} dt^2. \]  

(23)

For example, in the case of an n-body system

\[ ds^2 = \sum_{i=1}^{n} m_i \left( dx_i^2 + dy_i^2 + dz_i^2 \right), \]  

(24)

where \( M \) is the total mass, and \( m_i \) is the percentage of mass for the \( i \)-th particle. Lagrange’s least-action principle of classical mechanics has a simple geometric explanation: trajectories of a given mechanical system are exactly those geodesic curves in the metric space of \( ds^2 \), defined in the configuration space.

To each given m-triangle, i.e., triplet \( \{r_j\} \) with \( \sum m_j r_j = 0 \), we define a pair of Jacobi vectors \( x = (x_1, x_2, x_3) \) and \( y = (y_1, y_2, y_3) \) in the reduced space \( \mathbb{R}^6 \), given by

\[ x = \sqrt{\frac{m_1}{1 - m_1}} \left( m_2 (r_1 - r_2) + m_3 (r_1 - r_3) \right), \quad y = \sqrt{\frac{m_2 m_3}{1 - m_1}} (r_2 - r_3). \]  

(25)

It should be noted here that in this work, indices 2, 3 are used to label identical particles in our three-body system (e.g., the two electrons in the two-electron systems). Hence the exchange antisymmetry of the Fermi-Dirac statistics is manifest in letting \( y \to -y \).

The reduced configuration space can be represented by \( \mathbb{R}^3 \oplus \mathbb{R}^3 = \{(x, y); x, y \in \mathbb{R}^3\} \), and the metric \( ds^2 \), becomes

\[ ds^2 = dx \cdot dx + dy \cdot dy, \]  

(26)

with the kinetic energy operator given by

\[ \Delta = \Delta_x + \Delta_y. \]  

(27)

Also, the total angular momentum operator is given by

\[ L = L_x + L_y = -i (x \times \nabla_x + y \times \nabla_y). \]  

(28)

By using the Jacobi vectors \( x \) and \( y \), the motion of the center-of-mass is removed from (18), leading to a six-dimensional equation:

\[ -\frac{1}{2M} (\Delta_x + \Delta_y) \Psi + V \Psi = E \Psi. \]  

(29)
3.2.1. **Rotationally invariant variables**  For given two vectors \( \mathbf{x} \) and \( \mathbf{y} \), we can construct three rotationally invariant polynomials,

\[
f_1 = \mathbf{x} \cdot \mathbf{x}, \quad f_2 = \mathbf{y} \cdot \mathbf{y}, \quad f_3 = \mathbf{x} \cdot \mathbf{y}.
\]

Any rotationally invariant quantity with respect to \( \mathbf{x} \) and \( \mathbf{y} \) should be a function of \( (f_1, f_2, f_3) \). Since the metric \( ds^2 \) is rotationally invariant, thus it can be expressed as

\[
ds^2 = \sum_{i,j} g_{ij} \, df_i \, df_j,
\]

where \( (g_{ij}) \) is the inverse matrix of the following \( (g^{ij}) \):

\[
(g^{ij}) = (\nabla f_i \cdot \nabla f_j).
\]

The three variables \( (f_1, f_2, f_3) \) will be used to express the reduced Schrödinger equation below.

3.2.2. **Jacobi spherical coordinates**  The Hamiltonian of the three-body problem (Laplacian plus Coulomb potential) has space-rotation symmetry, but the symmetry of the kinetic energy operator is higher than that of the potential energy (Coulomb interaction). Moreover, there is a direct relation between the kinetic energy operator and the kinetic metric \( ds^2 \). It is obvious that \( (f_1, f_2, f_3) \) is not orthogonal; hence terms \( \{g_{ij} \, df_i \, df_j, i \neq j\} \) do not vanish in \( ds^2 \). By making use of the following coordinate transformation \[9, 10\], namely

\[
\rho = \sqrt{f_1 + f_2}, \quad \cos \theta = 2(f_1 f_2 - f_3^2)^{1/2}(f_1 + f_2)^{-1},
\]

\[
tan \beta = 2f_3(f_2 - f_1)^{-1}, \quad \sin \beta = 2f_3 \left[ (f_2 - f_1)^2 + 4f_3^2 \right]^{-1/2},
\]

\[(0 \leq \rho < \infty, \quad 0 \leq \theta \leq \pi/2, \quad -\pi \leq \beta \leq \pi),\]

the metric \( ds^2 \) becomes

\[
ds^2 = d\rho^2 + \frac{1}{4} \rho^2 (d\theta^2 + \sin^2 \theta d\beta^2).
\]

It is thus obvious that there is a semi-spherical structure in \( ds^2 \), which implies some form of symmetry of the kinetic energy operator, beyond those associated with rotational symmetries. We will soon learn the importance of this symmetry. Moreover, it is easy to get the inversion of the transform, namely

\[
f_1 = \frac{\rho^2}{2} (1 - \xi \cos \beta), \quad f_2 = \frac{\rho^2}{2} (1 + \xi \cos \beta), \quad f_3 = \frac{\rho^2}{2} \xi \sin \beta,
\]

where \( \xi = \sin \theta \). For convenience, we shall use \( (\rho, \xi, \beta) \) instead of \( (\rho, \theta, \beta) \) throughout this work, and call them the Jacobi spherical coordinates for reason that will become obvious later (see \[78\] and \[79\]).
3.2.3. Interparticle distance $r_{ij}$ expressed in Jacobi spherical coordinates. From the cyclic permutations of three sets of Jacobi coordinate vectors, i.e.,

$$x^{(1)} = \sqrt{\frac{m_1}{1 - m_1}}(m_2(r_1 - r_2) + m_3(r_1 - r_3)), \quad y^{(1)} = \sqrt{\frac{m_2m_3}{1 - m_1}}(r_2 - r_3),$$

$$x^{(2)} = \sqrt{\frac{m_2}{1 - m_2}}(m_3(r_2 - r_3) + m_1(r_2 - r_1)), \quad y^{(2)} = \sqrt{\frac{m_3m_1}{1 - m_2}}(r_3 - r_1),$$

$$x^{(3)} = \sqrt{\frac{m_3}{1 - m_3}}(m_1(r_3 - r_1) + m_2(r_3 - r_2)), \quad y^{(3)} = \sqrt{\frac{m_1m_2}{1 - m_3}}(r_1 - r_2).$$

(36)

and two simple relations

$$\begin{pmatrix} x^{(2)} \\ y^{(2)} \end{pmatrix} = \begin{pmatrix} \cos \beta_2 & \sin \beta_2 \\ -\sin \beta_2 & \cos \beta_2 \end{pmatrix} \begin{pmatrix} x^{(1)} \\ y^{(1)} \end{pmatrix},$$

$$\begin{pmatrix} x^{(3)} \\ y^{(3)} \end{pmatrix} = \begin{pmatrix} \cos \beta_3 & \sin \beta_3 \\ -\sin \beta_3 & \cos \beta_3 \end{pmatrix} \begin{pmatrix} x^{(1)} \\ y^{(1)} \end{pmatrix},$$

(37)

where

$$\cos \beta_2 = \sqrt{\frac{m_1m_2}{m_3 + m_1m_2}}, \quad \sin \beta_2 = -\sqrt{\frac{m_3}{m_3 + m_1m_2}},$$

$$\cos \beta_3 = \sqrt{\frac{m_1m_3}{m_2 + m_1m_3}}, \quad \sin \beta_3 = \sqrt{\frac{m_2}{m_2 + m_1m_3}},$$

(38)

we can write $|r_{ij}|^2$ in the Jacobi-spherical coordinates $(\rho, \xi, \beta)$:

$$|r_{23}|^2 = k_1 \rho^2(1 + \xi \cos \beta),$$

$$|r_{31}|^2 = k_2 \rho^2(1 + \xi \cos(\beta + 2\beta_2)), $$

$$|r_{12}|^2 = k_3 \rho^2(1 + \xi \cos(\beta + 2\beta_3)),$$

(39)

with

$$k_1 = \frac{1 - m_1}{2m_2m_3}, \quad k_2 = \frac{1 - m_2}{2m_3m_1}, \quad k_3 = \frac{1 - m_3}{2m_1m_2}.$$ 

(40)

For the special case of helium-like ions with infinite nuclear mass, we take

$$x = \frac{r_1 + r_2}{\sqrt{2}}, \quad y = \frac{r_2 - r_1}{\sqrt{2}},$$

(41)

as the Jacobi coordinate vectors, where $r_1$ and $r_2$ are the position vectors of two electrons, and the distances become

$$|r_1|^2 = \frac{1}{2} \rho^2(1 - \xi \sin \beta),$$

$$|r_2|^2 = \frac{1}{2} \rho^2(1 + \xi \sin \beta),$$

$$|r_{12}|^2 = \rho^2(1 + \xi \cos \beta).$$

(42)

From (39) and (40), it is straightforward to express the Coulomb potential in terms of $(\rho, \xi, \beta)$. It will be seen that the Coulomb potential becomes separable in the Jacobi-spherical coordinates.
3.3. Symmetries and angular momentum eigenfunctions

Schrödinger equation is invariant under the spatial rotation and coordinate inversion. That means both the total angular momentum operator \( L^2 (= L_1^2 + L_2^2 + L_3^2) \), its \( z \)-direction component \( L_3 \), and the parity operator commute with the Hamiltonian, therefore one has the angular momentum quantum numbers \((l, m)\), where \( m \) characterizes the azimuthal component of the angular momentum, plus the parity quantum number \( \lambda = 0, 1 \) for even and odd parities, respectively. In addition, the wavefunctions must also satisfy the Fermi-Dirac statistics, manifest as antisymmetry under the exchange of two electrons. It should be noted that since the antisymmetry applies to the product of spin state with the wavefunction, hence the wavefunction can be either symmetric (for antisymmetric spin state) or antisymmetric (for symmetric spin state).

In this section, we use a set of bi-harmonic functions as the eigenfunctions of \( L^2 \) and \( L_3 \), and expand the wave functions in these basis functions so as to separate out the rotational degrees of freedom from the Schrödinger equation.

The system is independent of the choice of \( z \)-direction, hence it is enough to consider the special case, \( m = l \). As is well known, \( Y^l_m(r) = r^l Y^l_m(\theta, \phi) \), where the set \((r, \theta, \phi)\) denotes the spherical coordinates of a vector, is a homogeneous polynomial of degree \( l \) with respect to the components of \( r \), and satisfies the Laplace equation. It is the eigenfunction for the angular momentum operator. The polynomials \( Y^l_m(x)Y^{l-q}_m(y) \) can be combined to form the eigenfunctions of the total angular momentum \( L^2 (L = L_x + L_y) \) by the Clebsch-Gordan coefficients [58]. For the special case, \( m = l \), one has two types of bi-homogeneous functions [8, 9] with respect to \( x \) and \( y \):

\[
\begin{align*}
 h^{(0)}_{a,b}(x, y) &= \frac{1}{a!b!} u^a v^b, \quad a, b \geq 0, \\
 h^{(1)}_{a,b}(x, y) &= \frac{1}{(a-1)!(b-1)!} u^{a-1} v^{b-1} w, \quad a, b \geq 1,
\end{align*}
\]

(43)

where

\[
\begin{align*}
 u &= x_1 + i x_2, \quad v = y_1 + i y_2, \\
 w &= (x_2 y_3 - x_3 y_2) + i(x_3 y_1 - x_1 y_3).
\end{align*}
\]

(44)

This specific family of basis functions, \( h^{(\lambda)}_{a,b}(x, y) \) (\( \lambda = 0 \) or 1), has the following properties.

(i) They are in the null space of the kinetic energy operator. In particular, they have zero eigenvalues for the operators \( \Delta_x, \Delta_y \) and \( \Delta_{xy} \), i.e., they exhibit bi-harmonicity:

\[
\Delta_x h^{(\lambda)}_{a,b}(x, y) = \Delta_y h^{(\lambda)}_{a,b}(x, y) = \Delta_{xy} h^{(\lambda)}_{a,b}(x, y) = 0,
\]

(45)

where

\[
\Delta_{xy} = \sum_{j=1}^{3} \frac{\partial^2}{\partial x_j \partial y_j}.
\]

(ii) They are bi-homogeneity in \( x_j \) and \( y_j \).
(iii) They are the common eigenfunctions of $L^2$ and $L_3$, i.e.,

$$L^2 h_{a, b}^{(\lambda)} = (a + b - \lambda)(a + b - \lambda + 1)h_{a, b}^{(\lambda)},$$

$$L_3 h_{a, b}^{(\lambda)} = (a + b - \lambda)h_{a, b}^{(\lambda)}.$$ (46)

(iv) They exhibit spatial inversion symmetry under $(x, y) \rightarrow (-x, -y)$:

$$h_{a, b}^{(\lambda)}(-x, -y) = (-1)^{a+b}h_{a, b}^{(\lambda)}(x, y).$$ (47)

(v) They exhibit symmetry under the permutation of particle 2 and particle 3, $y \rightarrow -y$:

$$h_{a, b}^{(\lambda)}(x, -y) = (-1)^b h_{a, b}^{(\lambda)}(x, y).$$ (48)

By using the ladder operator $L_\pm = L_1 - i L_2$, it is easy to construct the common eigenfunctions of $L^2$, $L_3$, and the parity operator from $h_{a, b}^{(\lambda)}$:

$$h_{a, b, k}^{(\lambda)} = L_k h_{a, b}^{(\lambda)}.$$ (49)

It is simple to verify that the set of functions

$$\{ h_{l-q+\lambda, q; l-m}^{(\lambda)}, \lambda \leq q \leq l \}$$

are the common eigenfunctions for $L^2$, $L_3$, and the parity operator with the eigenvalues $l(l+1)$, $m$, and $(-1)^{l+\lambda}$, respectively.

3.3.1. Wave function expansion For the special case of $m = l$, one can expand the wave function with parity $(-1)^{l+\lambda}$ in the following form:

$$\Psi^{(\lambda)} = \sum_{q=\lambda}^{l} \psi_q^{(\lambda)} h_{l-q+\lambda, q}^{(\lambda)}(x, y),$$ (51)

where $\lambda = 0$ or $1$, and $\{ \psi_q^{(\lambda)}, \lambda \leq q \leq l \}$ are $(l+1-\lambda)$-tuples of functions of the rotationally invariant variables $(f_1, f_2, f_3)$. They are the coefficients of the vector space $\{ h_{l-q+\lambda, q}^{(\lambda)}(x, y), \lambda \leq q \leq l \}$. This expansion is unique because of the orthogonality of $\{ h_{l-q+\lambda, q}^{(\lambda)}(x, y), \lambda \leq q \leq l \}$.

3.3.2. Reduced Schrödinger equation These operators of $\Delta_x$, $\Delta_y$, $\nabla_x$ and $\nabla_y$, on $\psi(f_1, f_2, f_3)$ may be expressed in terms of $f_i$ derivatives as

$$\Delta_x \psi = \left( 4 f_1^2 \frac{\partial^2}{\partial f_1^2} + 4 f_3 \frac{\partial^2}{\partial f_1 \partial f_3} + 6 \frac{\partial}{\partial f_1} \right) \psi,$$

$$\Delta_y \psi = \left( 4 f_2^2 \frac{\partial^2}{\partial f_2^2} + 4 f_3 \frac{\partial^2}{\partial f_2 \partial f_3} + 6 \frac{\partial}{\partial f_2} \right) \psi,$$

$$\Delta \psi = (\Delta_x + \Delta_y) \psi$$

$$= \left( 4 \left( f_1^2 \frac{\partial^2}{\partial f_1^2} + f_2^2 \frac{\partial^2}{\partial f_2^2} \right) + 4 f_3 \left( \frac{\partial^2}{\partial f_1 \partial f_3} + \frac{\partial^2}{\partial f_2 \partial f_3} \right) + (f_1 + f_2) \frac{\partial^2}{\partial f_3^2} + 6 \left( \frac{\partial}{\partial f_1} + \frac{\partial}{\partial f_2} \right) \right) \psi,$$

$$\nabla_x \psi = \left( 2x_1 \frac{\partial}{\partial f_1} + y_1 \frac{\partial}{\partial f_3}, 2x_2 \frac{\partial}{\partial f_1} + y_2 \frac{\partial}{\partial f_3}, 2x_3 \frac{\partial}{\partial f_1} + y_3 \frac{\partial}{\partial f_3} \right) \psi,$$

$$\nabla_y \psi = \left( 2y_1 \frac{\partial}{\partial f_2} + x_1 \frac{\partial}{\partial f_3}, 2y_2 \frac{\partial}{\partial f_2} + x_2 \frac{\partial}{\partial f_3}, 2y_3 \frac{\partial}{\partial f_2} + x_3 \frac{\partial}{\partial f_3} \right) \psi.$$ (52)
From (51) and (52), one has

\[
\Delta \Psi^{(\lambda)} = \sum_{q=\lambda}^{l} \left( \Delta \psi_{q}^{(\lambda)} h_{l-q+\lambda,q}^{(\lambda)} + 2 \nabla \psi_{q}^{(\lambda)} \cdot \nabla h_{l-q+\lambda,q}^{(\lambda)} \right)
\]

\[
= \sum_{q=\lambda}^{l} \left[ \left( \Delta + 4(l - q + \lambda) \frac{\partial}{\partial f_{1}} + 4q \frac{\partial}{\partial f_{2}} \right) \psi_{q}^{(\lambda)} + 2(q - \lambda) \frac{\partial \psi_{q-1}^{(\lambda)}}{\partial f_{3}} + 2(l - q) \frac{\partial \psi_{q+1}^{(\lambda)}}{\partial f_{3}} \right] h_{l-q+\lambda,q}^{(\lambda)},
\]

(53)

where \( \lambda = 0 \) or 1. Substituting (53) into the Schrödinger equation, one obtains a system of coupled partial differential equations (PDEs) for the \((-1)^{l+\lambda}\) parity states, in terms of the expansion coefficients:

\[
- \frac{1}{2M} \left\{ \Delta \psi_{q}^{(\lambda)} + 4(l - q + \lambda) \frac{\partial \psi_{q}^{(\lambda)}}{\partial f_{1}} + 4q \frac{\partial \psi_{q}^{(\lambda)}}{\partial f_{2}} \right\} + V \psi_{q}^{(\lambda)} = E \psi_{q}^{(\lambda)},
\]

(54)

where \( \lambda = 0 \) or 1, and \( \lambda \leq q \leq l \). For a given angular momentum \( l \), one has \( l + 1 \) coupled PDEs for the \((-1)^{l}\) parity state, and \( l \) coupled PDEs for the \((-1)^{l+1}\) parity state. In terms of atomic spectrum, these \((-1)^{l+1}\) parity states are called doubly excited states (DES), such as the spectra \( 2p^{2} 3P_{e} \) and \( 2p3d \ 1,3D^{o} \). Below we note three special cases of interest.

(i) The case of \( l = 0 \)

In this case, the wave function is a rotationally invariant function, and the Schrödinger equation becomes

\[
- \frac{1}{2M} \Delta \psi + V \psi = E \psi.
\]

(55)

(ii) The even parity case of \( l = 1 \)

In this case, the wave function

\[
\Psi = \psi h_{l,1}^{(1)},
\]

(56)

and the coupled PDEs reduce to one single PDE:

\[
- \frac{1}{2M} \left\{ \Delta \psi + 4 \frac{\partial \psi}{\partial f_{1}} + 4 \frac{\partial \psi}{\partial f_{2}} \right\} + V \psi = E \psi.
\]

(57)

(iii) The odd parity case of \( l = 1 \)

In this case, the wave function

\[
\Psi = \psi_{0} h_{l,0}^{(0)} + \psi_{1} h_{l,0}^{(0)},
\]

(58)

and the coupled PDEs become

\[
- \frac{1}{2M} \left\{ \Delta \psi_{0} + 4 \frac{\partial \psi_{0}}{\partial f_{1}} + 2 \frac{\partial \psi_{1}}{\partial f_{3}} \right\} + V \psi_{0} = E \psi_{0},
\]

\[
- \frac{1}{2M} \left\{ \Delta \psi_{1} + 4 \frac{\partial \psi_{1}}{\partial f_{2}} + 2 \frac{\partial \psi_{0}}{\partial f_{3}} \right\} + V \psi_{1} = E \psi_{1}.
\]

(59)
In the above form of (54), the rotational degrees of freedom have been completely projected out from the Schrödinger equation. This is achieved by expanding the wave function in the bi-harmonic basis,
\[ \{ h^{(\lambda)}_{l-q+\lambda,\lambda}(x,y), \lambda \leq q \leq l \}, \]
leading to a set of coupled PDEs for the expansion coefficients functions \( \{ \psi^{(\lambda)}_q, \lambda \leq q \leq l \} \), expressed with respect to the three rotationally invariant variables \( (f_1, f_2, f_3) \). The problem is hence three dimensional. The number of the coupled PDE system is noted to be finite, \( l + 1 \) or \( l \), and there are no singularities, which is noted to contrast with the case if the Euler angles were used.

3.4. Expansion of reduced Schrödinger equation in Jacobi-spherical coordinates

We introduce the Jacobi-spherical coordinates \((\rho, \xi, \beta)\) to rewrite the reduced Schrödinger equation. It will be seen that the present step naturally leads to the introduction of the Jacobi polynomials as the eigenfunctions of the angular differential operator, hence the denotation of Jacobi-spherical coordinates. It should be noted that the Jacobi-spherical coordinate has been used by Simonov [59] and Whitten [60], the latter used it to study the expression of pair potential. Mandelzweig and co-workers [61, 62, 63] have also used this coordinate system to calculate some properties of the Coulomb system. In the present case, the Jacobi-spherical coordinates are applied to the reduced Schrödinger equation for the three-body system. As such, it offers a natural coordinate system to delineate the intrinsic symmetry of the reduced three-body kinetic energy operator. We first note some physical interpretation and properties of this coordinate system.

(i) The variable \( \rho = \sqrt{I} \), where \( I = \sum_{j=1}^{3} m_j r_j^2 \) is the moment of inertia in the center-of-mass frame, thus \( \rho \) provides a natural measurement of the “size” of the system.

(ii) For the three sets of Jacobi coordinate vectors of (36), there are three simple relations among them:
\[
\begin{align*}
\rho^{(1)} &= \rho^{(2)} = \rho^{(3)} = \rho, \\
\xi^{(1)} &= \xi^{(2)} = \xi^{(3)} = \xi, \\
\beta^{(1)} &= \beta^{(2)} - 2\beta_2 = \beta^{(3)} - 2\beta_3 = \beta,
\end{align*}
\]
where \( \rho \) and \( \xi \) are unchanged, and \( \beta \) is shifted. This property has been used to express \( r_{ij} \).

(iii) For the permutation of particle 2 and particle 3, \( y \to -y, (\rho, \xi, \beta) \to (\rho, \xi, -\beta) \). This property will be useful for us to deal with the case in which there are identical particles in the system.

In terms of the coordinate system \((\rho, \xi, \beta)\), one has the following differential relations for the function \( \psi(f_1, f_2, f_3) \):
\[
\frac{\partial \psi}{\partial f_1} = \frac{1}{2\rho} \frac{\partial \psi}{\partial \rho} - \frac{1}{\rho^2} \left[ \xi \frac{\partial \psi}{\partial \xi} + \left( \cos \beta \frac{\partial \psi}{\partial \beta} - \frac{\sin \beta \partial \psi}{\xi} \right) \right],
\]
organized into the following two parts.

\[ \frac{\partial \psi}{\partial f_2} = \frac{1}{2\rho} \frac{\partial \psi}{\partial \rho} - \frac{1}{\rho^2} \left[ \xi \frac{\partial \psi}{\partial \xi} - \left( \cos \beta \frac{\partial \psi}{\partial \xi} - \sin \beta \frac{\partial \psi}{\partial \beta} \right) \right], \]

\[ \frac{\partial \psi}{\partial f_3} = \frac{2}{\rho^2} \left( \sin \beta \frac{\partial \psi}{\partial \xi} + \cos \beta \frac{\partial \psi}{\partial \beta} \right), \]

and

\[ \Delta \psi = \frac{\partial^2 \psi}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial \psi}{\partial \rho} + \frac{4}{\rho^2} A^{(0)} \psi, \]

where

\[ A^{(0)} \psi = (1 - \xi^2) \frac{\partial^2 \psi}{\partial \xi^2} + \frac{1}{\xi} \left( 1 - 3\xi^2 \frac{\partial \psi}{\partial \xi} + \frac{1}{\xi^2} \frac{\partial^2 \psi}{\partial \beta^2} \right). \]

3.4.1. Reduced Schrödinger equations in terms of \((\rho, \xi, \beta)\) In general, there are two quantum states of different parities for the special case of \(m = l\), whose wave functions are given by \(\Psi^{(\lambda)} = \sum_{q=0}^{l} \psi_q^{(\lambda)} h_{l-q+\lambda}^{(\lambda)}(x, y)\), where \(\lambda = 0\) or 1. Here \(\{\psi_q^{(\lambda)}, \lambda \leq q \leq l\}\) are \((l + 1 - \lambda)\)-tuples of rotationally invariant functions satisfying the systems of coupled PDEs. Substitution of the derivative relations, (61) and (62), into the reduced Schrödinger equation, the coupled PDEs of (54), leads to the following coupled PDEs in the Jacobi-spherical coordinates \((\rho, \xi, \beta)\):

\[
- \frac{1}{2M} \left\{ \frac{\partial^2 \psi_q^{(\lambda)}}{\partial \rho^2} + \frac{5 + 2l + 2\lambda \partial \psi_q^{(\lambda)}}{\rho \partial \rho} \right\} + \frac{4}{\rho^2} \left[ (1 - \xi^2) \frac{\partial^2 \psi_q^{(\lambda)}}{\partial \xi^2} + \frac{1}{\xi} \left( 1 - (l + \lambda + 3)\xi^2 \frac{\partial \psi_q^{(\lambda)}}{\partial \xi} \right) \right]
+ \frac{1}{\xi^2} \frac{\partial^2 \psi_q^{(\lambda)}}{\partial \beta^2} + (l - 2q + \lambda)B_1 \psi_q^{(\lambda)} + (q - \lambda)B_2 \psi_{q-1}^{(\lambda)} + (l - q)B_2 \psi_{q+1}^{(\lambda)} \right\} + V \psi_q^{(\lambda)} = E \psi_q^{(\lambda)}.
\]

\((\lambda = 0, 1; \lambda \leq q \leq l)\)

The above system of PDEs has remarkable simplicity and uniformly. Notice that the differential operators involving partial derivatives in \(\rho\) are the same for each component function \(\psi_q^{(\lambda)}\), i.e., \(\frac{\partial^2 \psi_q^{(\lambda)}}{\partial \rho^2} + \frac{5 + 2l + 2\lambda \partial \psi_q^{(\lambda)}}{\rho \partial \rho}\); while the partial derivatives in \(\xi\) and \(\beta\) can be organized into the following two parts.

(i) A uniform part for each component function \(\psi_q^{(\lambda)}\), denoted \(A^{(l+\lambda)}\), which comes from the angular part of the kinetic energy operator (see (63)):

\[ A^{(l+\lambda)} = (1 - \xi^2) \frac{\partial^2 \psi_q^{(\lambda)}}{\partial \xi^2} + \frac{1}{\xi} \left( 1 - (l + \lambda + 3)\xi^2 \frac{\partial \psi_q^{(\lambda)}}{\partial \xi} + \frac{1}{\xi^2} \frac{\partial^2 \psi_q^{(\lambda)}}{\partial \beta^2} \right). \]

(ii) A second part consisting of \((l - 2q + \lambda)B_1 \psi_q^{(\lambda)} + (q - \lambda)B_2 \psi_{q-1}^{(\lambda)} + (l - q)B_2 \psi_{q+1}^{(\lambda)}\),

where

\[ B_1 = \cos \beta \frac{\partial}{\partial \xi} - \frac{\sin \beta}{\xi} \frac{\partial}{\partial \beta}, \quad B_2 = \sin \beta \frac{\partial}{\partial \xi} + \frac{\cos \beta}{\xi} \frac{\partial}{\partial \beta}. \]

This part comes from the first order derivative terms (with respect to \(f_i\)) in (54).

Below we write out the reduced Schrödinger equations explicitly for those cases of particular interest.
(i) The case of $l = 0$:
\[- \frac{1}{2M} \left\{ \frac{\partial^2 \psi}{\partial \rho^2} + 5 \frac{\partial \psi}{\partial \rho} + \frac{4}{\rho^2} A^{(0)} \psi \right\} + V \psi = E \psi. \tag{67}\]

(ii) The case of $l = 1$ and of even parity:
\[- \frac{1}{2M} \left\{ \frac{\partial^2 \psi_0}{\partial \rho^2} + \frac{7}{\rho} \frac{\partial \psi_0}{\partial \rho} + \frac{4}{\rho^2} \left[ A^{(1)} \psi_0 + B_1 \psi_0 + B_2 \psi_1 \right] \right\} + V \psi_0 = E \psi_0, \tag{68}\]
\[- \frac{1}{2M} \left\{ \frac{\partial^2 \psi_1}{\partial \rho^2} + \frac{7}{\rho} \frac{\partial \psi_1}{\partial \rho} + \frac{4}{\rho^2} \left[ A^{(1)} \psi_1 - B_1 \psi_1 + B_2 \psi_0 \right] \right\} + V \psi_1 = E \psi_1. \tag{69}\]

3.4.2. Eigenfunctions of the angular differential operator $A^{(l)}$ Here we give the eigenfunctions for the following type of angular differential operator:
\[A^{(l)} \psi = (1 - \xi^2) \frac{\partial^2 \psi}{\partial \xi^2} + \frac{1 - (l + 3)\xi}{\xi} \frac{\partial \psi}{\partial \xi} + \frac{1}{\xi^2} \frac{\partial^2 \psi}{\partial \beta^2}. \tag{70}\]

Let $P_n^{(a,b)}(x)$ be the Jacobi polynomials, then the following set of functions constitutes a complete family of eigenfunctions of $A^{(l)}$:
\[J^{(l)}_{\pm m,n}(\xi, \beta) = e^{\pm im\beta} \xi^m P_n^{(\frac{a}{2}, \frac{b}{2})}(2\xi^2 - 1), \quad m, n \geq 0, \tag{71}\]
with their respective eigenvalues given by
\[\lambda^{(l)}_{m,n} = - \left\{ 4n \left(1 + \frac{l}{2} + m + n \right) + m(l + m + 2) \right\}. \tag{72}\]

The details and some properties of $J^{(l)}_{\pm m,n}$ are given in Appendix A.

3.4.3. Matrices $B_1$ and $B_2$ applied to the eigenfunctions of $A^{(l)}$ Applying $B_1$ and $B_2$ on the eigenfunctions of $A^{(l)}$, $\{J^{(l)}_{\pm m,n}(\xi, \beta), m, n \geq 0\}$, one obtains the following three cases.

(i) The case $m = 0$:
\[B_1 J^{(l)}_{0,n} = 2 \sum_{k=1}^{n} b^{(l)}_{0,n,k} \left\{ J^{(l)}_{1,n-k} + J^{(l)}_{-1,n-k} \right\}, \]
\[i B_2 J^{(l)}_{0,n} = 2 \sum_{k=1}^{n} b^{(l)}_{0,n,k} \left\{ J^{(l)}_{1,n-k} - J^{(l)}_{-1,n-k} \right\}. \tag{73}\]

(ii) The case of positive indices:
\[B_1 J^{(l)}_{m,n} = 2 \left( \sum_{k=1}^{m} b^{(l)}_{m,n,k} J^{(l)}_{m+1,n-k} + \sum_{k=0}^{n} \tilde{b}^{(l)}_{m,n,k} J^{(l)}_{m-1,n-k} \right), \]
\[i B_2 J^{(l)}_{m,n} = 2 \left( \sum_{k=1}^{m} b^{(l)}_{m,n,k} J^{(l)}_{m+1,n-k} - \sum_{k=0}^{n} \tilde{b}^{(l)}_{m,n,k} J^{(l)}_{m-1,n-k} \right). \tag{74}\]
(iii) The case of negative indices:

\[ B_1 J_{-m,n}^{(l)} = 2 \left( \sum_{k=1}^{n} b_{m,n,k}^{(l)} J_{-(m+1),n-k}^{(l)} + \sum_{k=0}^{n} \tilde{b}_{m,n,k}^{(l)} J_{-(m-1),n-k}^{(l)} \right) \]

\[ - i B_2 J_{-m,n}^{(l)} = 2 \left( \sum_{k=1}^{n} b_{m,n,k}^{(l)} J_{-(m+1),n-k}^{(l)} - \sum_{k=0}^{n} \tilde{b}_{m,n,k}^{(l)} J_{-(m-1),n-k}^{(l)} \right) \]  \hspace{1cm} (75)

In the above, the coefficients \( b_{m,n,k}^{(l)} \) and \( \tilde{b}_{m,n,k}^{(l)} \) are given by

\[
\begin{align*}
    b_{m,n,1}^{(l)} &= \frac{1}{2}(a + m) + n, \\
    b_{m,n,2}^{(l)} &= \frac{m + n}{a + m + n} \left( \frac{1}{2}(a + m) + n - 1 \right), \\
    b_{m,n,3}^{(l)} &= \frac{m + n}{a + m + n} \frac{m + n - 1}{a + m + n - 1} \left( \frac{1}{2}(a + m) + n - 2 \right), \text{etc.} \\
    \tilde{b}_{m,n,0}^{(l)} &= \frac{m + n}{a + m + n} \left( \frac{1}{2}(a + m) + n \right), \\
    \tilde{b}_{m,n,1}^{(l)} &= \frac{m + n}{a + m + n} \frac{m + n - 1}{a + m + n - 1} \left( \frac{1}{2}(a + m) + n - 1 \right), \\
    \tilde{b}_{m,n,2}^{(l)} &= \frac{m + n}{a + m + n} \frac{m + n - 1}{a + m + n - 1} \frac{m + n - 2}{a + m + n - 2} \left( \frac{1}{2}(a + m) + n - 2 \right), \text{etc.}
\end{align*}
\]  \hspace{1cm} (76)

where \( a = \frac{l}{2} \). The details of calculation can be found in Appendix A. Denote

\[ |m, n; l\rangle = C_{m,n}^{(l)} J_{m,n}^{(l)}, \quad (m \in \mathbb{Z}, n \in \mathbb{Z}^+) \]  \hspace{1cm} (77)

where \( C_{m,n}^{(l)} \) is the normalization constant of \( J_{m,n}^{(l)} \), \( B_1^{(l)} \) and \( B_2^{(l)} \) being the matrices of operators \( B_1 \) and \( B_2 \) on the function space \{ \( |m, n; l\rangle \), \( m \in \mathbb{Z}, n \in \mathbb{Z}^+ \) \}. \( B_1^{(l)} \) and \( B_2^{(l)} \) have two essential properties:

(i) For the index \( m \), both \( B_1^{(l)} \) and \( B_2^{(l)} \) are tridiagonal block matrices with zero diagonal blocks.

(ii) For a fixed \( m \), each none-zero sub-block matrix of \( B_1^{(l)} \) and \( B_2^{(l)} \) for the index \( n \) is an upper triangular matrix.

The above two properties will be used to advantage in designing the numerical scheme.

### 3.4.4. Coulomb potential expressed in Jacobi-spherical coordinates \((\rho, \xi, \beta)\)

From (19) and (39), it is easy to get the potential in the Jacobi-spherical coordinates

\[ V = \frac{U(\xi, \beta)}{\rho}, \]  \hspace{1cm} (78)

where

\[ U(\xi, \beta) = \frac{Z_2 Z_3 \left( \frac{2m_2 m_3}{1-m_1} \right)^{1/2}}{\sqrt{1 + \xi \cos \beta}} + \frac{Z_3 Z_1 \left( \frac{2m_1 m_2}{1-m_3} \right)^{1/2}}{\sqrt{1 + \xi \cos (\beta + 2\beta_3)}} + \frac{Z_1 Z_2 \left( \frac{2m_1 m_3}{1-m_2} \right)^{1/2}}{\sqrt{1 + \xi \cos (\beta + 2\beta_3)}}. \]  \hspace{1cm} (79)

From (25) and (39), one can see that
(i) The Coulomb potential is separable into $\rho$ and $(\xi, \beta)$ components, which is crucial for further reduction.

(ii) The potential has three singularities in the $(\xi, \beta)$ space: $(1, \pi)$, $(1, \pi - 2\beta_2)$, and $(1, \pi - 2\beta_3)$. These singularities affect the convergence of the numerical calculations.

3.4.5. Matrix elements of $U(\xi, \beta)$ with respect to the eigenfunctions of $A^{(l)}$

The matrix element of $U(\xi, \beta)$ in the space $\{|m, n; l\}, m \in \mathbb{Z}, n \in \mathbb{Z}^+\}$ is defined as

$$U_{mn, m'n'}^{(l)}(m, n) = \int_{-\pi}^{\pi} \int_{0}^{1} \exp(-i(m - m')\beta)U(\xi, \beta)T_{mn, m'n'}^{(l)}(\xi) \, d\xi \, d\beta,$$

(80)

where

$$T_{mn, m'n'}^{(l)}(\xi) = C_{m,n}^{(l)}C_{m',n'}^{(l)}\xi^{m + m' + 1}(1 - \xi^2)^{l/2}P_n^{(l/2,|m|)}(2\xi^2 - 1)P_{n'}^{(l/2,|m'|)}(2\xi^2 - 1).$$

(81)

Setting

$$U_0(\xi, \beta) = (1 + \xi \cos \beta)^{-1/2},$$

(82)

and denoting its matrix $U_0^{(l)}(mn, m'n')$ in the space $\{|m, n; l\}, m \in \mathbb{Z}, n \in \mathbb{Z}^+\}$ the “universal matrix”, one has

$$U^{(l)}(mn, m'n') = C(m - m')U_0^{(l)}(mn, m'n'),$$

(83)

where

$$C(n) = \sqrt{2m_2m_3}Z_2Z_3 + \sqrt{2m_3m_1}Z_3Z_1 \exp(i2n\beta_2) + \sqrt{2m_1m_2}Z_1Z_2 \exp(i2n\beta_3)$$

(84)

is denoted the “modulation factor”. A few properties of the matrix is noted below.

(i) The physical quantities, i.e., masses and charges, appear only in the modulation factor. For the special case of particle 2 and particle 3 being identical ($m_2 = m_3 = m_0$, $Z_2 = Z_3 = Z$ and $\beta_2 = -\beta_3 = \beta_0$), the modulation factor is a real number, given by

$$C(n) = \sqrt{m_0Z^2} + 2\sqrt{\frac{2m_0m_1}{1 - m_0}}ZZ_1 \cos(n\beta_0).$$

(85)

(ii) The universal matrix is independent of any specific system, which is the nature of three-body Coulomb system. In the numerical scheme, this property will be used to advantage.

In the particular case of helium-like ions with infinite nuclear mass, we would like to note that the Hamiltonian is

$$H = -\frac{1}{2} (\Delta_1 + \Delta_2) + \left( -\frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}} \right),$$

(86)

where $Z$ is the nuclear charge. In this case the modulation factor becomes

$$C(n) = 1 - 2\sqrt{2}Z \cos(n\pi/2).$$

(87)
3.5. Further reduction to a system of 1D ODEs

The “space-rotation reduction” enables us to completely remove the three rotational degrees of freedom, and reduce the Schrödinger equation to a system of PDEs solely in terms of the rotationally invariant parameters \((f_1, f_2, f_3)\). In terms of the Jacobi-spherical coordinates \((\rho, \xi, \beta)\), the above reduced system of PDEs becomes well-organized, in the sense that there can again be a separation of the angular component with the radial component. The angular component consists of the sum of \(A^{(l+\lambda)}\) and the integral multiples \(B_1\) and \(B_2\). The complete solutions of the eigen-functions of \(A^{(l)}\) in terms of the Jacobi polynomials, namely \(J_{l,m,n}^{(\lambda)}(\xi, \beta)\), can be explicitly obtained, as well as analytic formulas of the matrices of the linear differential operators \(B_1\) and \(B_2\) with respect to the above eigen-basis of \(A^{(l)}\). Furthermore, we provide a way of computing the matrix of \(U(\xi, \beta)\), which constitutes a separable part of the Coulomb potential. By combining all the above results, it is straightforward to further reduce the system of PDEs in \((\rho, \xi, \beta)\) to an infinite system of ODEs in terms of \(\rho\). By writing

\[
\psi_q^{(\lambda)} = \sum_{m=-\infty}^{\infty} \sum_{n=0}^{\infty} f_{q,m,n}^{(\lambda)}(\rho) |m, n; l + \lambda\rangle, \quad (\lambda = 0, 1; \lambda \leq q \leq l)
\]

and substituting the above into the system of PDEs (88), we obtain a set of ODEs on the expansion coefficients. That is, let \(F_q^{(\lambda)}(\rho)\) be the column vector with \(\{f_{q,m,n}^{(\lambda)}(\rho)\}\) as the components, and let \(B_1^{(l+\lambda)}, B_2^{(l+\lambda)}, U^{(l+\lambda)}\) be respectively the matrices of the linear operators \(B_1, B_2\) and \(U(\xi, \beta)\) with respect to the eigenfunctions of \(A^{(l+\lambda)}\). Then the set \(\{F_q^{(\lambda)}(\rho), \lambda \leq q \leq l\}\) satisfies the following system of coupled ODEs:

\[
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{5+2l+2\lambda}{\rho} \frac{\partial}{\partial \rho} \right) F_q^{(\lambda)} + \frac{4}{\rho^2} A^{(l+\lambda)} F_q^{(\lambda)} + \frac{1}{\rho} U^{(l+\lambda)} F_q^{(\lambda)} = E F_q^{(\lambda)}, \right. \tag{89}
\]

where \(\lambda = 0 \text{ or } 1, \lambda \leq q \leq l, \text{ and } A^{(l+\lambda)} \text{ is the diagonal matrix of the eigenvalues of } A^{(l+\lambda)}\). In particular, we note the following special cases.

(i) The case of \(l = 0\):

\[
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{5}{\rho} \frac{\partial}{\partial \rho} \right) F + \frac{4}{\rho^2} A^{(0)} F \right\} + \frac{1}{\rho} U^{(0)} F = E F. \tag{90}
\]

(ii) The case of \(l = 1\) and even parity:

\[
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{9}{\rho} \frac{\partial}{\partial \rho} \right) F + \frac{4}{\rho^2} A^{(2)} F \right\} + \frac{1}{\rho} U^{(2)} F = E F. \tag{91}
\]

(iii) The case of \(l = 1\) and odd parity:

\[
\begin{align*}
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{7}{\rho} \frac{\partial}{\partial \rho} \right) F_0 + \frac{4}{\rho^2} \left[ A^{(1)} F_0 + B_1^{(1)} F_0 + B_2^{(1)} F_1 \right] \right\} + \frac{1}{\rho} U^{(1)} F_0 &= E F_0, \tag{92} \\
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{7}{\rho} \frac{\partial}{\partial \rho} \right) F_1 + \frac{4}{\rho^2} \left[ A^{(1)} F_1 - B_1^{(1)} F_1 + B_2^{(1)} F_0 \right] \right\} + \frac{1}{\rho} U^{(1)} F_1 &= E F_1.
\end{align*}
\]
By using the following notations
\[
\mathcal{F} = \begin{pmatrix} \mathcal{F}_0 \\ \mathcal{F}_1 \end{pmatrix}, \quad \mathcal{A} = \begin{pmatrix} \mathcal{A}^{(1)} & \mathcal{O} \\ \mathcal{O} & \mathcal{A}^{(1)} \end{pmatrix},
\]
\[
\mathcal{B} = \begin{pmatrix} \mathcal{B}_1^{(1)} & \mathcal{B}_2^{(1)} \\ \mathcal{B}_2^{(1)} & -\mathcal{B}_1^{(1)} \end{pmatrix}, \quad \mathcal{U} = \begin{pmatrix} \mathcal{U}^{(1)} & \mathcal{O} \\ \mathcal{O} & \mathcal{U}^{(1)} \end{pmatrix},
\]
where \( \mathcal{O} \) represents the zero matrix, and \( \mathcal{A}, \mathcal{B} \) and \( \mathcal{U} \) are all block matrices, the two coupled equations (92) can be abbreviated as
\[
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{7}{\rho} \frac{\partial}{\partial \rho} \right) \mathcal{F} + \frac{4}{\rho^2} [\mathcal{A} \mathcal{F} + \mathcal{B} \mathcal{F}] \right\} + \frac{1}{\rho} \mathcal{U} \mathcal{F} = E \mathcal{F}.
\] (94)

In the general case of \( l \geq 2 \), we can use the block-matrix notations to write the system of ODEs in a more compact form:
\[
-\frac{1}{2M} \left\{ \left( \frac{\partial^2}{\partial \rho^2} + \frac{5+2l+2\lambda}{\rho} \frac{\partial}{\partial \rho} \right) \mathcal{F}^{[\lambda]} + \frac{4}{\rho^2} [\mathcal{A}^{[\lambda]} \mathcal{F}^{[\lambda]} + \mathcal{B}^{[\lambda]} \mathcal{F}^{[\lambda]}] \right\} + \frac{1}{\rho} \mathcal{U}^{[\lambda]} \mathcal{F}^{[\lambda]} = E \mathcal{F}^{[\lambda]},
\] (95)
where \( \lambda = 0 \) or 1, \( \mathcal{F}^{[\lambda]} \) is the collection of \( \{ \mathcal{F}^{(\lambda)}(\rho), \lambda \leq q \leq l \} \), \( \mathcal{A}^{[\lambda]} \) is the collection of the matrices \( \mathcal{A}^{(l+\lambda)} \), \( \mathcal{B}^{[\lambda]} \) is the collection of the matrices \( \mathcal{B}_1^{(l+\lambda)} \) and \( \mathcal{B}_2^{(l+\lambda)} \), and \( \mathcal{U}^{[\lambda]} \) is the collection of the matrices \( \mathcal{U}^{(l+\lambda)} \). All of \( \mathcal{A}^{[\lambda]}, \mathcal{B}^{[\lambda]} \) and \( \mathcal{U}^{[\lambda]} \) are \( (l+1-\lambda) \times (l+1-\lambda) \) block matrices. As it turns out, these block-matrix notations are not only convenient for analyzing the dependence of \( \mathcal{F}^{[\lambda]}(\rho) \) on \( \rho \), but they also provide more insight into the structure of the three-body system, which will greatly benefit the numerical calculations.

At this point it should be noted that while the starting point of the three-body problem is a nine-dimensional problem, in (95) the problem has been reduced to a one-dimensional problem, since \( \mathcal{F}^{[\lambda]}(\rho) \) depends only on \( \rho \). Below we provide a way to solve this one-dimensional coupled ODEs by converting them into a linear eigenvalue problem.

3.6. Conversion to a linear algebraic eigenvalue problem

In (95), there is a common differential operator, \( \frac{\partial^2}{\partial \rho^2} + \frac{5+2l+2\lambda}{\rho} \frac{\partial}{\partial \rho} \), for each component of the vector \( \mathcal{F}^{[\lambda]}(\rho) \). The energy level \( E \) of a stationary state should be negative, and if we analyze the “asymptotic behavior” of (95), the limiting equations are all reduced to the following single ODE:
\[
\left( -\frac{1}{2M} \frac{\partial^2}{\partial \rho^2} - E \right) \mathcal{F}^{[\lambda]} = 0 \quad (E < 0).
\] (96)

Equation (96) clearly implies the exponential asymptotic decay of the wave functions of stationary states and, moreover, the order of such exponential decay is given by
\[
k = \sqrt{-2ME}, \quad E < 0.
\] (97)

In other words,
\[
\mathcal{F}^{[\lambda]} \sim \exp(-k\rho), \quad \text{as} \ \rho \to \infty.
\] (98)
Setting $x = 2k \rho$, $F^{[\lambda]}(\rho) = e^{-k \rho} Y^{[\lambda]}(x)$ and

$$L^{(l)} = \left( \frac{\partial^2}{\partial \rho^2} + \frac{2l + 5}{\rho} \frac{\partial}{\partial \rho} - k^2 \right),$$

then

$$\rho e^{k \rho} L^{(l+\lambda)}(\rho) = 2k \left\{ x \frac{d^2}{dx^2} + (2l + 2\lambda + 5 - x) \frac{d}{dx} - (l + \lambda + \frac{5}{2}) \right\} Y^{[\lambda]}.$$  (100)

3.6.1. Expansion of the ODE system in terms of the Laguerre polynomials. If we substitute the above results into (103), the system is transformed into a system of ODEs with respect to the new independent variable $x$:

$$\bar{L}^{(l+\lambda)} Y^{[\lambda]} - \left( l + \lambda + \frac{5}{2} \right) Y^{[\lambda]} + \frac{4}{x} \left( A^{[\lambda]} Y^{[\lambda]} + B^{[\lambda]} Y^{[\lambda]} \right) = \frac{M}{k} U^{[\lambda]} Y^{[\lambda]},$$  (101)

where $\lambda = 0$ or 1, and

$$\bar{L}^{(l)} = x \frac{d^2}{dx^2} + (2l + 5 - x) \frac{d}{dx}.$$  (102)

These Laguerre polynomials $\{L_p^{(2l+4)}(x), p = 0, 1, 2, \ldots\}$ are the eigenfunctions of $\bar{L}^{(l)}$, i.e.,

$$\left( x \frac{d^2}{dx^2} + (2l + 5 - x) \frac{d}{dx} \right) L_p^{(2l+4)} = -p L_p^{(2l+4)}.$$  (103)

Equation (104) shows that it is advantageous to use the family of Laguerre polynomials $\{L_p^{(2l+2\lambda+4)}(x), p = 0, 1, 2, \ldots\}$ as the basis functions to solve (101).

3.6.2. Infinite linear equations for the coefficients. Let $v_p^{(\lambda)}$ be the undetermined coefficients in the expression of $Y^{[\lambda]}(x)$ as the linear combination of the Laguerre polynomials $\{L_p^{(2l+2\lambda+4)}(x), p = 0, 1, 2, \ldots\}$:

$$Y^{[\lambda]}(x) = \sum_{p=0}^{\infty} v_p^{(\lambda)} L_p^{(2l+2\lambda+4)}(x).$$  (104)

Here $v_p^{(\lambda)}$ is more precisely defined as the set $\{v_{q,p,m,n}^{(\lambda)}, \lambda \leq q \leq l\}$. By omitting the sub-indices $q, m$ and $n$ in the block-matrix notations, we obtain

$$\left\{ -\sum_{p=0}^{\infty} (p + l + \lambda + \frac{5}{2}) v_p^{(\lambda)} L_p^{(2l+2\lambda+4)} + \sum_{p=0}^{\infty} \frac{4}{x} v_p^{(\lambda)} L_p^{(2l+2\lambda+4)} [A^{[\lambda]} + B^{[\lambda]}] \right\} = \frac{M}{k} \sum_{p=0}^{\infty} v_p^{(\lambda)} L_p^{(2l+2\lambda+4)} U^{[\lambda]},$$  (105)

where $\lambda = 0$ or 1, and $I_{A^{[\lambda]}}$ is the identity matrix, with the same rank as $A^{[\lambda]}$. Multiplying the above equations by $kx$ and then making use of the recurrence relations of the Laguerre polynomials, we get the systems of linear relations in terms of the Laguerre polynomials. By applying the orthogonality relations of these polynomials, a system of algebraic linear equations for the coefficients $\{v_{q,p,m,n}^{(\lambda)}\}$ is obtained. In the block-matrix notations, they may be expressed as

$$k \left\{ \begin{bmatrix} p \left( p + l + \lambda + \frac{5}{2} \right) v_{p-1}^{(\lambda)} \\ -2 \left( p + l + \lambda + \frac{5}{2} \right) v_p^{(\lambda)} \\ + \left( p + l + \lambda + \frac{5}{2} \right) (p + 2l + 2\lambda + 5) v_{p+1}^{(\lambda)} \\ + 4v_p^{(\lambda)} (A^{[\lambda]} + B^{[\lambda]}) \end{bmatrix} \right\} I_{A^{[\lambda]}} = \begin{bmatrix} -p v_{p-1}^{(\lambda)} \\ + (2p + 2l + 2\lambda + 5) v_p^{(\lambda)} \\ - (p + 2l + 2\lambda + 5) v_{p+1}^{(\lambda)} \end{bmatrix} U^{[\lambda]}$$  (106)
where $\lambda = 0$ or $1$. Let $D_p^{(l)}$ and $G_p^{(l)}$ be the tridiagonal matrices related to the index $p$, and $I_p^{(l)}$ be the identity matrix with the same size of $D_p^{(l)}$ and $G_p^{(l)}$, where

\[
D_p^{(l)}(p,p-1) = p \left( p + l + \frac{3}{2} \right),
\]
\[
D_p^{(l)}(p,p) = -2 \left( p + l + \frac{5}{2} \right)^2,
\]
\[
D_p^{(l)}(p,p+1) = \left( p + l + \frac{7}{2} \right) (p + 2l + 5).
\]
\[
G_p^{(l)}(p,p-1) = -p,
\]
\[
G_p^{(l)}(p,p) = (2p + 2l + 5),
\]
\[
G_p^{(l)}(p,p+1) = -(p + 2l + 5).
\]

Equation (107) can be re-written into a compact form:

\[
k \left\{ D_p^{(l+\lambda)} \otimes I_p^{(l)} + 4I_p^{(l+\lambda)} \otimes (A^{[\lambda]} + B^{[\lambda]}) \right\} v^{(\lambda)} = M \left\{ G_p^{(l+\lambda)} \otimes U^{[\lambda]} \right\} v^{(\lambda)},
\]

where the symbol $\otimes$ denotes outer-product between two matrices. Three points should be noted.

(i) Equation (108) has a robust structure, mainly due to the fact that $\rho$ and $(\xi, \beta)$ are separable in the potential. $D_p^{(l+\lambda)}$ and $G_p^{(l+\lambda)}$ are unchanged when there are identical particles in the system.

(ii) The left-hand of (108) can be partitioned into two parts, namely

\[
M_0 = D_p^{(l+\lambda)} \otimes I_p^{(l)} + 4I_p^{(l+\lambda)} \otimes A^{[\lambda]}, \quad M_1 = 4I_p^{(l+\lambda)} \otimes B^{[\lambda]},
\]

where $M_0$ is a super-tridiagonal matrix that dominates the left. Consequently, we can solve the linear equation, $M_0x = y$, just like solving a tridiagonal equation. Furthermore, the equation $(M_0 + M_1)x = y$ can also be solved based on an iteration process, detailed in the next section.

(iii) The outer-product form provides a way to easily and efficiently get the matrix-on-vector product.

4. Numerical scheme

Schrödinger equation for the Coulomb three-body system has been reduced from a nine dimensional problem to a one dimensional problem and finally to a linear algebraic problem in section 3. Here we present a numerical scheme designed to solve the relevant linear equations. The core of the scheme is the iterative solution of the matrix-eigenvalue problem. The advantage of the iteration procedure is that it only requires the matrix-vector product, which can significantly facilitate the numerical calculations due to the sparse-block structure of the matrices in our problem. The general linear eigenvalue problem is written into a standard form, and by applying a special integration rule, presented in Appendix B, the calculation of the potential energy (Coulomb interaction)
matrix elements and the product of that matrix with a vector are combined together, to achieve a high degree of numerical accuracy with minimal computational resources. In present numerical calculations, the aim is to solve a system of sparse linear equations, and an iteration solver is adopted for that purpose. Since truncation is necessary, an extrapolation procedure is applied to accelerate the convergence.

4.1. Solution of the linear eigenvalue problem

After introducing the Jacobi polynomials, the system of PDEs is reduced to a system of ODEs, and the ODE system is further reduced to a linear eigenvalue problem through expansion in terms of the Laguerre polynomials. In the block-matrix notations, the linear algebraic equation can be expressed as

$$ k \left\{ D_{(l+\lambda)} \otimes I_{A[\lambda]} + 4I_{p(l+\lambda)} \otimes \left( A[\lambda] + B[\lambda] \right) \right\} v(\lambda) = M \left\{ G_{p(l+\lambda)} \otimes U[\lambda] \right\} v(\lambda), $$

(110)

where the symbols’ definitions can be found in section 3, and $k$ is related to the energy $E$ by

$$ k = \sqrt{-2ME}, $$

(111)

where $M$ is the total mass of three particles. Equation (110) may be compactly expressed as

$$ k_M \mathcal{M}_L v = \mathcal{M}_R v, $$

(112)

where $k_M = k/M$, and

$$ \mathcal{M}_L = D_{p(l+\lambda)} \otimes I_{A[\lambda]} + 4I_{p(l+\lambda)} \otimes \left( A[\lambda] + B[\lambda] \right), $$

$$ \mathcal{M}_R = G_{p(l+\lambda)} \otimes U[\lambda]. $$

(113)

In general, only the low-lying states are of interest, which implies only a few of the largest eigenvalues of (112) are needed. One can write this general eigenvalue problem in a standard form:

$$ \mathcal{M}_L^{-1} \mathcal{M}_R v = k_M v, $$

(114)

where $\mathcal{M}_L^{-1}$ means the inverse of $\mathcal{M}_L$. Hence, the task becomes to design a scheme to find a few of the largest eigenvalues of (114).

We use one of the software packages, such as ARPACK [64], designed to compute a few eigenvalues and their corresponding eigenvectors of a general n-by-n matrix $A$. It is most appropriate for large sparse or structured matrices where structured means that a matrix-vector product $w \leftarrow Av$ requires order $n$, rather than the usual order $n^2$, floating point operations. This particular software routine is based on an algorithmic variant of the Arnoldi process called the Implicitly Restarted Arnoldi Method. By using this package, only the operation of the matrix-vector product is needed. In our problem, the following two steps are used to calculate the matrix-vector product $\mathcal{M}_L^{-1} \mathcal{M}_R v$.

(i) First calculate $y \leftarrow \mathcal{M}_R v$. This step is the most time-consuming part, and the block-matrix structure of $\mathcal{M}_R$ is found to be suitable for distributed computing systems, such as PC clusters.
(ii) Calculate \( y \leftarrow M_L^{-1} y \). The difficult part of this step is to solve a large sparse equation, and a sparse solver is adopted.

Below we detail each of the two steps.

4.1.1. **Matrix-vector product \((M_Rv)\) evaluation** The matrix \(M_R\), derived from the Coulomb potential, is the tensor formed from the outer product of \(G_P^{(l+\lambda)}\) and \(U^{[\lambda]}\):

\[
M_R = G_P^{(l+\lambda)} \otimes U^{[\lambda]},
\]

where \(G_P^{(l+\lambda)}\) is a tridiagonal matrix, and \(U^{[\lambda]}\) is a block-diagonal matrix in which every sub-block is the same, denoted \(U^{(l+\lambda)}\).

The Kronecker tensor product, \(X \otimes Y\), of two matrices is a larger matrix formed from all possible products of the elements of \(X\) with those of \(Y\). If \(X\) is m-by-n and \(Y\) is p-by-q, then \(X \otimes Y\) is an mp-by-nq matrix. The elements are arranged in the following order:

\[
X \otimes Y = \begin{pmatrix}
X_{1,1} \ast Y & X_{1,2} \ast Y & \ldots & X_{1,n} \ast Y \\
X_{2,1} \ast Y & X_{2,2} \ast Y & \ldots & X_{2,n} \ast Y \\
\vdots & \vdots & \ddots & \vdots \\
X_{m,1} \ast Y & X_{m,2} \ast Y & \ldots & X_{m,n} \ast Y
\end{pmatrix},
\]

For the matrix-vector product \(\{X \otimes Y\}v\), where \(v\) is a vector, it is advantageous to reshape \(v\) to a q-by-n matrix \(V\), and to calculate \(R = (Y \ast V) \ast X^T\). The vector reshaped from the p-by-m matrix \(R\) is the final result.

The particular structure of \(M_R\) and \(U^{[\lambda]}\) makes it easy to calculate the matrix-vector product. The tensor form of \(M_R\) provides a straightforward way to calculate the matrix-vector product, and the block structure of \(U^{[\lambda]}\) lets one to focus on only the sub-block matrix \(U^{(l+\lambda)}\). The elements of matrix \(U^{(l)}\) are expressible as

\[
U^{(l)}(mn, m'n') = C(m - m')U_0^{(l)}(mn, m'n'),
\]

where both the “modulation factor” \(C(n)\) and \(U_0^{(l)}\) the “universal matrix” are given previously. From the definition

\[
U_0^{(l)}(mn, m'n') = 2 \int_{\beta=0}^{\pi} \int_{\xi=0}^{1} \frac{\cos (m - m') \beta}{\sqrt{1 + \xi \cos \beta}} w_l(\xi) P_{mn}^{(l)}(\xi) P_{m'n'}^{(l)}(\xi) \, d\xi \, d\beta, \tag{118}
\]

where

\[
w_l(\xi) = \xi (1 - \xi^2)^{l/2}, \quad P_{mn}^{(l)}(\xi) = C_{m,n}^{(l)}(\xi) P_{n}^{(l/2, |m|)}(2\xi^2 - 1),
\]

with \(\{P_{n}^{(l/2, |m|)}(x)\}\) being the set of Jacobi polynomials. Set

\[
u_m(\xi) = \int_0^\pi \cos m\beta \sqrt{\frac{1 - \xi}{1 + \xi \cos \beta}} \, d\beta, \tag{120}
\]

and

\[
U_0^{(l)}(\xi) = \frac{2C(m)w_l(\xi)u_m(\xi)}{\sqrt{1 - \xi}}, \tag{121}
\]
then (117) becomes
\[ U^{(l)}(mn, m'n') = \int_0^1 U^{(l)}_{m-m'}(\xi) P^{(l)}_{mn}(\xi) P^{(l)}_{m'n'}(\xi) \, d\xi. \] (122)
The integration implied by (122) is performed using the IMT integration scheme (see Appendix B).

4.1.2. Calculation of \( \mathcal{M}^{-1}_L \mathbf{v} \)

One needs to solve a linear algebraic equation to get the vector \( \mathcal{M}^{-1}_L \mathbf{v} \). From the previous discussion, it is known that \( \mathcal{M}_L \) is composed of two parts:
\[ \mathcal{M}_L = \mathcal{M}_0 + \mathcal{M}_1, \] (123)
where \( \mathcal{M}_0 = D_p^{(l+\lambda)} \otimes \mathcal{I}_A^{[\lambda]} + 4D_p^{(l+\lambda)} \otimes \mathcal{A}^{[\lambda]} \) is a super-tridiagonal matrix that dominates the matrix \( \mathcal{M}_L \), and \( \mathcal{M}_1 = 4D_p^{(l+\lambda)} \otimes \mathcal{B}^{[\lambda]} \) is relatively small. Because of the super-tridiagonal structure of \( \mathcal{M}_0 \), one can obtain the vector \( \mathcal{M}_0^{-1} \mathbf{v} \) exactly like solving a tridiagonal equation. Obtaining \( \mathcal{M}_L^{-1} \mathbf{v} \) may be implemented as
\[ \mathcal{M}^{-1}_L \mathbf{v} = (\mathcal{I} + \mathcal{M}^{-1}_0 \mathcal{M}_1)^{-1} \mathcal{M}_0^{-1} \mathbf{v}, \] (124)
where \( \mathcal{I} \) represents the identity matrix, through the following two steps.

(i) First solve for
\[ \mathbf{y} \leftarrow \mathcal{M}_0^{-1} \mathbf{v}. \] (125)
As described above, this step can be easily implemented.

(ii) Solve for
\[ \mathbf{y} \leftarrow (\mathcal{I} + \mathcal{M}_0^{-1} \mathcal{M}_1)^{-1} \mathbf{y}. \] (126)
Since the matrix \( \mathcal{M}_0 \) dominates, thus \( \mathcal{M}_0^{-1} \mathcal{M}_1 \) is small in some sense, so one can consider the matrix \( \mathcal{I} + \mathcal{M}_0^{-1} \mathcal{M}_1 \) to be close to the identity matrix, i.e.,
\[ \mathcal{I} + \mathcal{M}_0^{-1} \mathcal{M}_1 \sim \mathcal{I} + \epsilon. \] (127)
Thus an iteration solver should be efficient. In our calculations, the Conjugate-Gradients-Squared (CGS) [65] method is taken as the solver. The CGS method just requires the user to provide the matrix-vector product, i.e., one works out the vector
\[ (\mathcal{I} + \mathcal{M}_0^{-1} \mathcal{M}_1) \mathbf{v} \] (128)
during the intermediate iteration steps by first calculating \( \mathbf{t} \leftarrow \mathcal{M}_1 \mathbf{v} \), and then calculating \( \mathbf{t} \leftarrow \mathcal{M}_0^{-1} \mathbf{t} \). The final result is given by \( \mathbf{v} + \mathbf{t} \). In practice, after about 12 iterations, the relative error of the solution is reduced to \( 10^{-14} \).

Since the infinite matrices in the problem are truncated into finite matrices, the truncation is done by following a rule, specified below. Results obtained from smaller scale calculations, i.e., the eigenvalues and their eigenvectors, are taken as the initial guesses for the subsequent, increasingly larger cases. This process fully takes the advantage of the previous results, and significantly speeds up the calculation. It also provides a sequence of data from which one can apply the extrapolation procedure (see below) to obtain a few more digits of accuracy.
4.2. Truncation and extrapolation procedures

In our numerical calculations, the expansion of the partial wave function $\psi_{q}^{(\lambda)}$ has to be truncated, i.e.,

$$\psi_{q}^{(\lambda)} = e^{-kp} \sum_{m=-M}^{M} \sum_{n=0}^{N} \sum_{p=0}^{P} u_{q,m,n,p}^{(\lambda)} J_{m,n}^{(l+\lambda)}(\xi, \beta) L_{p}^{(2l+2\lambda+4)}(2kp),$$  \hspace{1cm} (129)

where $M$, $N$ and $P$ represent the three truncation indices for the $m$, $n$ and $p$, respectively. One solves the finite dimensional algebraic eigenvalue equation to obtain the lowest order eigenvalues and their corresponding eigenvectors. These eigenvalues are functions of $M$, $N$ and $P$, i.e.,

$$E = E(M, N, P),$$  \hspace{1cm} (130)

where the desired answer is the limiting value

$$E_{\infty} = E(\infty, \infty, \infty).$$  \hspace{1cm} (131)

4.2.1. Truncation path  We have carefully checked the dependence of $E$ on the three numbers $M$, $N$ and $P$. In our procedure, we chose a “path” in the \{M, N, P\} space to approach the limit $E_{\infty}$. First, it was found that for sufficiently large $P$ (typically $P \sim 70$), increase in $P$ does not provide any significant improvement on $E$. This behavior owes to the fact that $P$ controls how many terms in the Laguerre polynomials are included in the expansion, but there is a direct relation between the spatial extend of the system and the spherical variable $\rho$, so for large enough $P$ the terms of Laguerre polynomials in the expansion are sufficient to delineate the spatial domain. Different states have different “appropriate” $P$ values, and after that value is determined, denoted $P_{0}$, the following “path” in \{M, N\} space is taken:

$$M = M_{0} + 20K, \quad N = N_{0} + 10K, \quad K = 0, 1, \ldots,$$  \hspace{1cm} (132)

where $M_{0}$ and $N_{0}$ are the initial truncations for $m$ and $n$, generally in the range of 70 and 50, respectively. The three-dimensional sequence $E(M, N, P)$ is thus mapped to a one-dimensional sequence:

$$E(K) = E(M_{0} + 20K, N_{0} + 10K, P_{0}).$$  \hspace{1cm} (133)

There is a reason why we increase $M$ twice as fast as $N$. It is known that the eigenvalues of operator $A^{(l)}$ have the form

$$\lambda_{l,m,n}^{(l)} = -\left\{4n \left(1 + \frac{l}{2} + m + n\right) + m(l + m + 2)\right\}.$$  \hspace{1cm} (134)

As $m$ and $n$ approach infinity, $\lambda_{l,m,n}^{(l)}$ has the asymptotic form

$$\lambda_{l,m,n}^{(l)} \propto -(m + 2n)^{2},$$  \hspace{1cm} (135)

so that the stipulated sequence is designed to coincide with this asymptotic behavior.
4.2.2. Extrapolation procedure  For extrapolation, an auxiliary variable $x$, defined as

$$x = \frac{100}{M + 2N} = \frac{100}{M_0 + 2N_0 + 40K}, \quad (136)$$

is used to determine the form of $E(x)$ as provided by the data sequence. A power law form is assumed, such that

$$E(x) = E_{\infty} - c_0 x^a (1 + c_1 x + c_2 x^2 + \cdots). \quad (137)$$

The task is to identify the leading term $x^a$. Sequences of $E(k)$ ($E(x)$) are collected in the numerical calculations. The leading term is identified by studying the relation of $E(x)$ versus $x^a$, where $a_k$ is an estimated value of $a$. If the plot is a straight line, the leading term can be immediately identified. The process of Richardson extrapolation is then performed on the sequence \{\(E(x_i), i = 0, 1, \cdots\)\} to estimate the limiting value $E_{\infty}$. The Richardson extrapolation utilizes the following sequences:

$$E(x_0) = E_{\infty} - c_0 x_0^a - c_1 x_0^{a+1} - c_2 x_0^{a+2} - \cdots$$
$$E(x_1) = E_{\infty} - c_0 x_1^a - c_1 x_1^{a+1} - c_2 x_1^{a+2} - \cdots$$
$$E(x_2) = E_{\infty} - c_0 x_2^a - c_1 x_2^{a+1} - c_2 x_2^{a+2} - \cdots$$
\[\vdots\]
$$E(x_n) = E_{\infty} - c_0 x_n^a - c_1 x_n^{a+1} - c_2 x_n^{a+2} - \cdots, \quad (138)$$

to approach $E_{\infty}$. By defining

$$g_1(n) = x_n^a, \quad g_2(n) = x_n^{a+1}, \quad g_3(n) = x_n^{a+2}, \cdots, \quad (139)$$

and denoting $E(x_n)$ as $E_n$, (138) becomes

$$E_n = E_{\infty} - c_0 g_1(n) - c_1 g_2(n) - c_2 g_3(n) - \cdots, \quad n = 0, 1, 2, \cdots. \quad (140)$$

Then the recursive $E - algorithm$ declares that the limiting value $E_{\infty}$ can be approached by the following rule. Let

$$E_{0}^{(n)} = E_n, \quad n = 0, 1, \cdots$$
$$g_{0,i}^{(n)} = g_i(n), \quad n = 0, 1, \cdots \text{ and } i = 1, 2, \cdots. \quad (141)$$

For $k = 1, 2, \cdots$ and $n = 0, 1, \cdots$ one has

$$E_k^{(n)} = E_{k-1}^{(n)} - \frac{E_{k-1}^{(n+1)} - E_{k-1}^{(n)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}} \cdot g_{k-1,k}^{(n)}, \quad (142)$$

where the $g_{k-1,k}^{(n)}$’s are auxiliary quantities recursively computed by

$$g_{k,i}^{(n)} = g_{k-1,i}^{(n)} - \frac{g_{k-1,i}^{(n+1)} - g_{k-1,k}^{(n)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}} \cdot g_{k-1,k}^{(n)}, \quad i = k + 1, k + 2, \cdots. \quad (143)$$

The sequences \{\(E_k^{(n)}, n = 0, 1, \cdots, \text{ and } k \geq 1\)\} are more convergent than the initial sequence \{\(E_0^{(n)}, n = 0, 1, \cdots\)\}. From the convergence pattern of \{\(E_k^{(n)}\)\}, one may determine the limiting value with high accuracy.
5. Results on three-body systems

In this section we present results on some three-body systems, and discuss the properties of their relevant wave functions. In order to display the data in physical space, we first give a description of the relevant angles, as well as the procedure by which the wave functions are re-constituted from numerical data.

5.1. Euler angles and wave functions

5.1.1. Euler angles and the distribution function

The three-body wave function depends upon the shape of the triangle formed by three particles and the three Euler angles \([58]\), such that

\[
\Psi = \Psi(\Delta; \Omega),
\]

where \(\Delta\) represents the triangle which can be described by the three spherical variables \((\rho, \xi, \beta)\), or its three edges \((r_1, r_2, r_3)\), or \((r_2, r_3, \cos \theta)\) as shown in figure and \(\Omega\) denotes the Euler angles that depict the rotational orientation of the triangle in space. Here \(r_2\) and \(r_3\) denote the distances of particles 2 and 3 from particle 1, respectively, and \(r_1\) denotes the distance between the two identical particles 2 and 3. The \(\cos \theta\) is between particles 2 and 3 (the identical pair). For a six-dimensional function, visualization is an issue. The Euler angles are noted to take part in the wave function through the angular momentum eigenfunctions, but do not enter in the rotation-invariant functions, which indicates that in order to deal with the Euler angles, we just need to focus on the angular momentum eigenfunctions \(\{l^{(\lambda)}_{l-q+\lambda,q}(x, y), \lambda \leq q \leq l\}\). After the Euler angles are integrated out from the wave function, a three-variable probability distribution

![Figure 1. The triangle formed by three particles.](image-url)
function is obtained, i.e.,
\[ P(\Delta) \equiv \int_\Omega |\Psi(\Delta; \Omega)|^2 d\Omega, \]  
which can be easier to visualize. Let \( P(\Delta) = g(r_1, r_2, r_3) \). In order to display
the information contained in \( g(r_1, r_2, r_3) \), we propose to use the following probability
distribution functions (PDF).

(i) One-variable PDF, e.g., the distribution of \( r_1 \):
\[ P(r_1) dr_1 \equiv \int_{r_2} \int_{r_3} g(r_1, r_2, r_3) d\tau, \]  
where \( d\tau \) is the volume element.

(ii) Two-variable PDF, e.g., the radial correlation function:
\[ P(r_2, r_3) dr_2 dr_3 \equiv \int_{r_1} g(r_1, r_2, r_3) d\tau, \]  
or the conditional distribution
\[ P(r_2, r_3; r_1 = a) dr_2 dr_3 \equiv g(r_1 = a, r_2, r_3) d\tau/dr_1, \]  
where \( a \) is a given value, and a PDF is obtained for each given \( a \).

We noted that the volume element \( dxdy \) in different coordinate systems has the following
explicit form:
\[ dxdy \propto \rho^5 \xi d\rho d\xi d\beta d\Omega \propto r_1^2 r_2^2 r_3 d\rho d\xi d\beta d\Omega = r_1 r_2 r_3 dr_1 dr_2 dr_3 d\Omega. \]  
In calculations, we always normalize the wave function, i.e.,
\[ \int |\Psi|^2 \rho^5 \xi d\rho d\xi d\beta d\Omega = 1. \]  
If there are two identical particles in the three-body system, we identify them as particles
2 and 3.

5.2. Negative hydrogen ion

The negative hydrogen ion \( H^- \) is an interesting special case of helium-like ions (\( Z=1 \)).
It is marginally stable against dissociation into a neutral hydrogen atom plus a free
electron. The dissociation energy \( J \) of \( H^- \) ground state is only about 0.75\( eV \) and this
ion possesses no other bound state [67, 68].

The negative hydrogen ion has been found to be of great importance for the opacity
of sun’s atmosphere. The ionization potential of \( H^- \) ground state is only about 0.75\( eV \) and this
ion possesses no other bound state [67, 68].

As free electrons are released by the ionization of the metal elements present in the
gas, and since neutral hydrogen is by far the main constituent of the solar atmosphere,
many of these electrons will be captured to form an abundant source of \( H^- \). The
radiation flux coming from the sun’s interior would be absorbed by the \( H^- \) ions,
accompanied by their dissociation. The electrons released can again be captured by
\( H^- \) atoms with the emission of radiation, and so on. The process \( H^- \leftrightarrow H + e^- \) is the
main source of observed opacity in the solar atmosphere. The absorption coefficient of H− has been studied extensively and used in the theory of the solar atmosphere. In fact, discrepancies between early calculations and observational evidence on the sun’s radiation have pointed out the inaccuracies of the calculated H− wave functions available then. Calculation of the wave function and energy of H− is also of purely methodological interest, since this most loosely-bound of all Helium-like ions provides a severe test for the various approximation schemes.

5.2.1. The ground state

Bethe was the first to give an unambiguous proof of this ion as a bound system [69]. Using the Hylleraas variational wave functions, Bethe concluded that the resulting Rayleigh-Ritz upper bound on the energy lies below -0.5 a.u.. In 1944, Chandrasekhar introduced a two-parameter trial wave function,

$$\Psi = \exp(-\alpha r_2 - \beta r_3) + \exp(-\alpha r_2 - \beta r_3),$$ (151)

and showed that the energy minimum at $\alpha = 1.03925$ and $\beta = 0.28309$ is sufficient to provide binding for H−. The function shown in (151) exhibits the specific nature of electron-electron correlation in the ground state. The two electrons are on very different footings, one bound much closer to the nucleus than the other, which is weakly held at a distance $\simeq 4 - 5$ from the nucleus, and this electron can be regarded as weakly

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure2.pdf}
\caption{Distributions of $r_1$, $r_2$ (or $r_3$) and $\cos \theta$ of the ground state of $^\infty$H−. The solid line is the distribution of $r_2$ or $r_3$ (same), and the dashed line is the distribution of $r_1$. Inset is the distribution of $\cos \theta$.}
\end{figure}
bound in a short-range attractive potential well. In modern variational calculations, many $r^j_1$ terms are necessary in the trial wave function in order to fully account for the electron-electron correlation. While many-parameter variational calculations can give great accuracy for the ground state energy, the best experimental values come from a high resolution (0.03cm$^{-1}$) laboratory photodetachment laser experiment. The binding energy has been determined to be $6082.99 \pm 0.15$cm$^{-1}$ for $\infty$H$^-$ and $6086.2 \pm 0.6$cm$^{-1}$ for the similar D states [70]. In table 1, our results on the ground states of $\infty$H$^-$ and H$^-$ are compared with other calculations. In general, all our results have $10 \sim 12$ significant figures when double precision programming is used. The accuracy in this case is less than those obtained variationally. It is well known that the precision of the operator expectation values in the variational calculations usually has two less significant figures than that for the energy. Thus much more efforts is required to obtain the wave function expectation values to the same accuracy. In our case the wave function is calculated at the same time as the eigenvalues. No extra effort is required.

Figure 2 shows the distributions of $r_1$, $r_2$, $r_3$ and $\cos \theta$ of the ground state of $\infty$H$^-$. The distribution of $\cos \theta$ is a curve that shows a maximum at $\theta = \pi$. If the shell model is valid, the curve of the $\cos \theta$ distribution should be close to a horizontal line at 0.5. For comparison, we also plot the radial density distribution $P(r)$, for $\infty$H$^-(^3S)$, H(1s) and H(2s) in figure 3. A long tail is seen in the distribution of $r_1$, $r_2$ (or $r_3$). In
Figure 4. Distributions of \( r_1 \), \( r_2 \) (or \( r_3 \)) and \( \cos \theta \) of the \( ^3P^e \) state of \( ^\infty H^- \). The solid line is the distribution of \( r_2 \) or \( r_3 \) (same), and the dashed line is the distribution of \( r_1 \). Inset is the distribution of \( \cos \theta \).

Figure 5: the electron distribution of \( ^\infty H^- \) is seen to be very different from the neutral 1s or 2s state. Thus the electron-electron correlation plays an important role in H\(^-\), and independent-electron model can not give an accurate picture.

5.2.2. The \( ^3P^e \) state  The even-parity \( ^3P^e \) state of \( ^\infty H^- \) and H\(^-\) is quasi-stable, and its energy is just below the n=2 threshold (-0.125 a.u.) of the hydrogen atom. For the \( ^\infty H^- \) ion, the existence of the even-parity \( ^3P^e \) state was predicted computationally nearly 40 years ago, followed by many variational calculations. Jáuregui and Bunge \[71\] used a configuration-interaction(CI)-expansion of 108 configuration terms and obtained the energy -0.125 354 716 6 a.u.. They analyzed the convergence pattern of their computations and extrapolated to -0.125 355 08(10) a.u.. The largest Hylleraas-type computation for this state, done by Drake and then repeated by \[73\] gave only -0.125 335 6 a.u., though they used about 50 thousand terms containing powers of \( r_1 \) up to 82. The best result, as we know, was obtained by Bylicki and Bednarz \[72\] who applied the Hyllerasse configuration-interaction correlated expansions and used 1442 terms to give -0.125 355 451 24 a.u.. More efforts are needed than that for the ground state. In our approach, this problem is reconsidered from a new viewpoint, and the finite mass of proton is naturally taken into account.
We compare our results with other calculations in table 2. The convergence is just as good in this case as for the ground state, and the leading term of all the sequences is estimated to be $x^5$. Our energy eigenvalue is $0.125355451242$ a.u. for $\infty$H$, better than most of previous calculations.

As a negative ion, the extra electron is significantly affected by the other electron. Figure 4 shows the distribution of $r_1$, $r_2$, $r_3$ and $\cos \theta$ of the $\infty$H$. The radial distribution has a very long tail; even at $r = 60$ the probability does not vanish. If the electron-electron interaction is ignored so as to approximate this state by two $2p$-state electrons, the charge distribution of the $2p$ state would to vanish at about $r = 15$ (see figure 5), very far from $r = 60$. This long tail exponentially decays with a decay length $l \sim 18.3$, with a form $r^a \exp (-r/l)$ with $a \approx 0.5$. In this case, the independent-electron picture is very far removed from the present excited state. The variational method is observed to be less accurate for this state due to the very strong electron-electron correlation. For some of the expectation values, such as $< r_i >$, comparable results can not be found in the literature. To our knowledge, our calculated result on this state is probably the most accurate so far.

It is interesting to observe that in this state, the two electrons form nearly an angle of $\pi/2$ relative to the nucleus (the value of $< \cos(r_{12}, r_{13}) > \approx 0$). Also, the value of...
< \textit{r}_1 > \text{ is nearly twice that of the ground state.}

5.3. \textit{Helium and helium-like ions}

Except for the hydrogen atom, helium atom (or helium-like ions) is perhaps the simplest system in quantum mechanics. However, the calculation of its properties is not trivial and represents a real challenge. It has been 80 years since the beginning of quantum mechanics, and there are still efforts trying to understand the system from some new perspectives.

In atomic theory, the shell model is the starting point to understand complex atoms. This model is an independent-electron picture, and the interaction between electrons are averaged by a mean field. For helium, we denote one of the electrons as the inner-electron, and the other as the outer-electron. But when the correlation of two electrons is strong, this picture fails. For example, in the shell model language the two electrons in the ground state are in the same orbit. Interaction would thus become important, which would make the independent-electron picture not suitable. For the doubly excited states in which both electrons are not in the ground state, interaction can affect the slow-moving electrons very significantly.

5.3.1. \textit{The S states of helium}  
These states have been extensively studied, and there are many methods used to treat the \( S \) states. For extrapolation, we estimate the leading term of \( E(x) \) (for all of the \( S \) states) to be \( x^3 \), and a list of the limiting values are given in table 3 after performing the Richardson extrapolation. Except for the ground state \( 1S^e \), the other states are close to the independent-electron picture. In tables 5 and 6, some of expectation values are given for the \( 1^3S^e \) states of \( \infty \text{He} \).

5.3.2. \textit{The odd parity P states}  
The leading term of \( E(x) \) of all of these states is estimated to be \( x^2 \). Table 4 shows the convergence for the three low-lying \( 1^3P^o \) states of \( \infty \text{He} \).

5.3.3. \textit{The parity-unfavorable 1^3P^e, 1^3D^o, 1^3F^e states}  
The doubly excited states \( 1^3P^e \) and \( 1^3D^o \) have been observed in experiments long ago. Dolye \textit{et al} \cite{77} calculated the positions of the \( 1^3P^e \) and \( 1^3D^o \) states of the helium isoelectronic sequence using the 1/Z expansion method. By using a variational scheme Bhatia \cite{74} had calculated the \( 1^3D^o \) states of helium again and obtained a few higher-precision results. The best results for the states of helium were obtained by Goodson \textit{et al} \cite{78}, who took the advantage of the interdimensional degeneracies of the problem and used the variational method in the five-dimensional space to obtain the results. The observation of the \( 1^3F^e \) states is rarely reported, and its energies had been computed by Galán and Bunge \cite{79}. In this subsection, we report the energies re-calculated by our approach.

For the \( 1^3P^e \) states, we compare our results with other calculations in table 9. As a non-variational method, the performance of our approach is excellent. The distributions
Figure 6. Distributions of $r_1$, $r_2$ (or $r_3$) of the five low-lying $^3P^e$ states of $^\infty$He (ground state plus four excited states). The solid line is the distribution of $r_2$ or $r_3$ (same), and the dashed line is the distribution of $r_1$. For comparison, we also plot the radial density distribution of the neutral He(2p), H(2p) and H(3p) states in (5) (normalized to 1/2).
of \( r_1, r_2, r_3 \) and \( \cos \theta \) are shown in figure 6 for \( \infty \)He. Some properties of these states are given in tables 7 and 8. It should be mentioned that only in the case of \( E_2 \) of the \( ^1P_e \) state is our result higher in energy than the variational approach, but has more significant figures. We think that in this case our result is correct, because our excited states’ eigen-energies and their related wavefunctions were all obtained simultaneously with the ground state properties. Hence the accuracy of our excited states’ properties are insured by the demonstrated accuracy of the ground state eigenvalue. For helium-like ions (\( Z = 3 \sim 6 \)), the eigen-energies are summarized in table 10.

We have also calculated four low-lying \( ^1S_0 \), \( ^1D_0 \) states of \( \infty \)He. We compare our results with Bathia’s in table 11. The three low-lying states \( ^1F_e \) states of Li\(^+\) ion are given in table 12. It is seen that our results are better than those obtained by other methods.

5.4. \( H_2^+ \) and Ps\(^-\)

In order to obtain a better understanding of the underlying dynamical property of the Coulomb three-body system with two identical particles, three typical systems are the most interesting: (1) where the mass ratio \( m_1 \) is large compared to \( m_2, m_3 \) in the identical particles pair, e.g., for a helium atom or a helium-like ion (such as the H\(^-\) ion), (2) where \( m_1 = m_2 = m_3 \) for a positronium negative ion Ps\(^-\), and (3) where \( m_1 \) is very small, e.g., for a hydrogen molecular ion H\(_2^+\). It should be noted that the case of hydrogen molecular ion is very close to a one-body system in which the single electron moves in the field of two heavy protons.

5.4.1. The hydrogen molecular ion H\(_2^+\)

We have calculated 15 low-lying \( S \) states for this ion, the most achieved so far, and the numerical results are summarized in table 13. For exploring the properties of H\(_2^+\), the coordinate system \((X, Y, R)\) as shown in figure 7.
Figure 8. Distributions of $R$ for the five low-lying $S$ states of $H_2^+$. Similarity to oscillator is noted.
Figure 9. The function $|\Psi(X, Y, R = R_0)|$ for the ground state of $H_2^+$, where $R_0 = 0.5, 1.0$. The electron density is noted to peak directly above the positions of the protons, with a sharp cusp.

is used, and the wave function has the form:

$$\Psi = \Psi(X, Y, R).$$  \hspace{1cm} (152)

Here $R$ is the distance between the two protons, and $X, Y$ denote the coordinate of the electron relative to the two protons. Figure 9 shows the distribution of $R$ for the calculated states. It is obvious that there is vibrational motion between the two protons, similar to an anharmonic oscillator. In this case the attraction between the two protons is clearly mediated by the electron. Figures 9 and 10 show the function $|\Psi(X, Y, R)|$ of the ground state when $R = 0.5, 1.0, 1.5, 2.0$. It is clear from these pictures that the electron probability density is the highest directly above each of the protons, with a sharp cusp at the proton locations.

5.4.2. The positronium negative ion $Ps^-$ The experimental and theoretical studies of the positronium negative ion $Ps^-$, consisting of two electrons and one positron, have attracted considerable interest since the work of Wheeler [84], who proved $Ps^-$ to be
The formation of $\text{Ps}^-$ has been discussed in the $e^+ - \text{He}$ [85] and $\text{Ps} - \text{H}$ [86] scattering calculations. The binding energy has been calculated variationally by several authors. Recent interests include the calculations of autoionizing doubly-excited states and the investigations of the possible existence of the so-called second bound state $^3P^e$. These positronium negative ions have been observed in the laboratory by Mills [87, 88]. A large number of the doubly-excited states of a positronium negative ion were calculated by the method of complex-coordinate rotations [89].

We compare our results with other calculations in table 14. Figure 11 shows the distributions for $r_1$, $r_2$ (or $r_3$) and $\cos \theta$ between the two electrons. It is seen that the two electrons plus the positron form a triangle in which the angle formed by $r_2$ and $r_3$ is greater than 60 degrees, consistent with the fact that the separation between the two electrons is larger than their respective distances to the positron. It should be noted that the curve of the $\cos \theta$ distribution is very different from that of the $^\infty\text{H}^-$ (see figure 2). Since the only difference between the two systems lies in the mass of the positive charge, the comparison is useful to delineate the importance of mass ratio.
the present case, the mass of the positive charge is the same as that of the electron, so the positron is envisioned to be much more mobile, whereas in the case of H\(^-\) the proton is more localized. This comparison is perhaps helpful in answering the question [90]: Is the positronium system a molecule or an atom?

6. Further developments

The kinetic energy operator approach is noted to have applications potential for a number of interesting problems. The approach is obviously applicable to the three-body problem in two dimensions. The addition of a perpendicular magnetic field plus a circularly symmetric potential is noted to be possible in this case, without breaking the symmetry that is essential to the solution approach. Thus it would be particularly interesting to examine the interaction of three electrons under a strong magnetic field, a configuration which might be relevant to a fractional quantum Hall state.

The fact that we can reduce the dimensionality of the three-body problem also promises numerical efficiency in the case of three-body scattering, which requires very extensive computational resources at present [5]. There is also the possibility of carrying out time-dependent calculations, with implications to the enumeration of doubly excited
states in the continuum.

Appendix A. Eigenfunctions of $A^{(l)}$

Appendix A.1. Eigenfunctions of $A^{(l)}$

In this appendix, we give the details for computing the eigenfunctions of the operator

$$A^{(l)} = (1 - \xi^2) \frac{\partial^2}{\partial \xi^2} + \frac{1 - (l + 3)\xi^2}{\xi} \frac{\partial}{\partial \xi} + \frac{1}{\xi^2} \frac{\partial^2}{\partial \beta^2},$$

and list some useful properties of the Jacobi polynomials.

Let $x = 2\xi^2 - 1$ and $\psi = e^{\pm im\beta} \xi^m F(x)$, where $m = 0, 1, 2, \cdots$. Straightforward computation shows that

$$A^{(l)} \psi = e^{\pm im\beta} \xi^m \left\{ L_m^{(l)} F(x) - m(l + m + 2) F(x) \right\},$$

where

$$L_m^{(l)} F(x) = 4 \left\{ (1 - x^2) F''(x) + \left( m - \frac{l}{2} \right) - \left( 2 + \frac{l}{2} + m \right) x \right\} F'(x).$$

The Jacobi polynomial $P_n^{(a,b)}(x)$ satisfies the following differential equation $(D := \frac{d}{dx})$:

$$(1 - x^2) D^2 P_n^{(a,b)}(x) + [b - a - (2 + a + b)x] D P_n^{(a,b)}(x) + n(1 + a + b + n) P_n^{(a,b)}(x) = 0.$$  \hspace{1cm} (A.4)

The orthogonal relations of Jacobi polynomials $\{P_n^{(a,b)}(x), n = 0, 1, 2, \cdots\}$ are given by

$$\int_{-1}^{1} (1 - x)^a (1 + x)^b P_n^{(a,b)}(x) P_{n'}^{(a,b)}(x) dx = \frac{2^{1+a+b} \Gamma(1 + a + n) \Gamma(1 + b + n)}{n!(1 + a + b + 2n) \Gamma(1 + a + b + n)} \delta_{n,n'}.$$ \hspace{1cm} (A.5)

From (A.3) and (A.4), we can see that the following set of functions constitute a complete family of eigenfunctions of $A^{(l)}$, i.e.,

$$\left\{ J_{\pm m,n}^{(l)}(\xi, \beta) = e^{\pm im\beta} \xi^m P_n^{(\frac{l}{2},m)}(2\xi^2 - 1), \; m,n \geq 0 \right\},$$

with their eigenvalues given by

$$\lambda_m^{(l)} = - \left\{ 4n \left( 1 + \frac{l}{2} + m + n \right) + m(l + m + 2) \right\}. \hspace{1cm} (A.6)$$

The orthogonal relations become

$$\int_{-\pi}^{\pi} \int_{0}^{1} J_{m_1,n_1}^{(l)} J_{m_2,n_2}^{(l)} \xi (1 - \xi)^{1/2} d\xi d\beta = \frac{\pi \Gamma(1 + \frac{l}{2} + n) \Gamma(1 + m + n)}{n!(1 + \frac{l}{2} + m + 2n) \Gamma(1 + \frac{l}{2} + m + n)} \delta_{m_1,m_2} \delta_{n_1,n_2}. \hspace{1cm} (A.7)$$
Appendix A.2. Recurrence relations of the Jacobi polynomials and the matrices of $B_1$ and $B_2$

Appendix A.2.1. Matrices of $B_1$ and $B_2$  For the two linear differential operators

\[ B_1 = \cos \beta \frac{\partial}{\partial \xi} - \sin \beta \frac{\partial}{\partial \beta}, \quad \text{and} \quad B_2 = \sin \beta \frac{\partial}{\partial \xi} + \cos \beta \frac{\partial}{\partial \beta}, \]

we have

(i) The case of $m = 0$:

\[ B_1 J_{0,n}^{(l)} = (2ie^{i\beta} \xi + 2ie^{-i\beta} \xi) DP_n^{(\frac{l}{2},0)}(x), \]
\[ B_2 J_{0,n}^{(l)} = (-2ie^{i\beta} \xi + 2ie^{-i\beta} \xi) DP_n^{(\frac{l}{2},0)}(x). \]

(ii) The case of positive indices:

\[ B_1 J_{m,n}^{(l)} = 2e^{i(m+1)\beta} \xi^{m+1} DP_n^{(\frac{l}{2},m)}(x) \]
\[ + e^{i(m-1)\beta} \xi^{-m-1} \left[ mP_n^{(\frac{l}{2},m)}(x) + (1 + x) DP_n^{(\frac{l}{2},m)}(x) \right], \]
\[ B_2 J_{m,n}^{(l)} = -2ie^{i(m+1)\beta} \xi^{m+1} DP_n^{(\frac{l}{2},m)}(x) \]
\[ + ie^{i(m-1)\beta} \xi^{-m-1} \left[ mP_n^{(\frac{l}{2},m)}(x) + (1 + x) DP_n^{(\frac{l}{2},m)}(x) \right]. \]

(iii) The case of negative indices:

\[ B_1 J_{-m,n}^{(l)} = 2e^{-i(m+1)\beta} \xi^{m+1} DP_n^{(\frac{l}{2},m)}(x) \]
\[ + e^{-i(m-1)\beta} \xi^{-m-1} \left[ mP_n^{(\frac{l}{2},m)}(x) + (1 + x) DP_n^{(\frac{l}{2},m)}(x) \right], \]
\[ B_2 J_{-m,n}^{(l)} = 2ie^{-i(m+1)\beta} \xi^{m+1} DP_n^{(\frac{l}{2},m)}(x) \]
\[ - ie^{-i(m-1)\beta} \xi^{-m-1} \left[ mP_n^{(\frac{l}{2},m)}(x) + (1 + x) DP_n^{(\frac{l}{2},m)}(x) \right]. \]

Therefore, we need explicit formulas which express $DP_n^{(\frac{l}{2},m)}(x)$ ($mP_n^{(\frac{l}{2},m)}(x)$ ($1 + x) DP_n^{(\frac{l}{2},m)}(x)$) as linear combination of $P_k^{(\frac{l}{2},m+1)}(x)$($P_k^{(\frac{l}{2},m-1)}(x)$). Here, the existence of a collection of recurrence relations among Jacobi polynomials provides a handy tool for such a purpose.

Appendix A.2.2. Recurrence relations of the Jacobi polynomials  We recall some of the mixed-type ones from §138 of Rainville [44]:

\[ DP_n^{(a,b)}(x) = \frac{1}{2} (1 + a + b + n) P_{n-1}^{(a+1,b+1)}(x) \]
\[ = \frac{1}{2} (b + n) P_{n-1}^{(a+1,b)}(x) + \frac{1}{2} (a + n) P_{n-1}^{(a,b+1)}(x) \]
\[ (1 + x) DP_n^{(a,b)}(x) = nP_n^{(a,b)}(x) + (b + n) P_{n-1}^{(a+1,b)}(x) \]
\[ (a + b + 2n) P_n^{(a,b-1)}(x) = (a + b + n) P_n^{(a,b)}(x) + (a + n) P_{n-1}^{(a,b)}(x) \]
(a + b + 2n)P_{n}^{(a, b)}(x) = (a + b + n)P_{n}^{(a, b)}(x) - (b + n)P_{n-1}^{(a, b)}(x)
\quad P_{n}^{(a, b-1)}(x) - P_{n}^{(a-1, b)}(x) = P_{n-1}^{(a, b)}(x).

We have the following specific recurrence relations:
\[ DP_{n}^{(a, b)}(x) = \left[ \frac{1}{2}(a + b) + n \right] P_{n-1}^{(a, b+1)}(x) + \frac{b + n}{a + b + n} DP_{n-1}^{(a, b)}(x), \]
\[ (bP_{n}^{(a, b)}(x) + (1 + x)DP_{n}^{(a, b)}(x)) = (b + n)P_{n}^{(a+1, b-1)}(x) \]
\[ = \frac{b + n}{a + b + n} \left[ bP_{n-1}^{(a, b)}(x) + (1 + x)DP_{n-1}^{(a, b)}(x) \right] \]
\[ + \frac{(b + n)(a + b + 2n)}{a + b + n} P_{n}^{(a, b-1)}(x). \]

By using the above formulas, we get the explicit expressions for the matrices of \( B_1 \) and \( B_2 \). The results are given in section 3.

**Appendix B. IMT Integration Scheme**

Consider the real value function \( f(x) \) defined on the interval \([0, 1]\), which is continuous and differentiable sufficiently many times on \([0, 1]\). For the \( N \)-point trapezoidal rule, there is the Euler-Maclaurin formula
\[
\int_{0}^{1} f(x) \, dx = \frac{1}{N} \sum_{n=1}^{N-1} f(n/N) + \frac{1}{2} f(0) + f(1) + \sum_{r=1}^{m-1} \frac{B_r}{(2r)!} N^{2r} \left[ f^{(2r-1)}(1) - f^{(2r-1)}(0) \right] + R_m, \tag{B.1}
\]
where \( B_r \) is the \( r \)-th Bernoulli number and \( R_m \) is the reminder term. Noting that the expression for the truncation error depends only on values of the functional derivatives at the integration end points, we design a change of variable, so that
\[
f^{(2r-1)}(1) = f^{(2r-1)}(0) \quad \text{for} \quad r = 1, 2, \ldots. \tag{B.2}
\]
It follows from (B.1) that all error terms will vanish, and high precision can be achieved.

The IMT-rule [95, 96], also denoted the “double-exponential formula”, is one type of integration technique. Consider
\[
Q = \int_{0}^{1} \exp \left( -\frac{1}{t} - \frac{1}{1-t} \right) \, dt = 0.00702 98584 06609 65623 92412 70530 \ldots. \tag{B.3}
\]
Define the function \( \varphi(t) \) by
\[
\varphi(t) = \int_{0}^{t} \varphi'(\tau) \, d\tau, \quad \varphi'(t) = \frac{1}{Q} \exp \left( -\frac{1}{t} - \frac{1}{1-t} \right). \tag{B.4}
\]
The transformation \( x = \varphi(t) \) maps the variable \( x \in [0, 1] \) into the variable \( t \in [0, 1] \), and we have a new expression for the integration of \( f(x) \) over \([0, 1]\):
\[
\int_{0}^{1} f(x) \, dx = \int_{0}^{1} g(t) \, dt, \quad \text{with} \quad g(t) = f(\varphi(t))\varphi'(t). \tag{B.5}
\]
If the function $f(x)$ is differentiable infinitely many times on $(0, 1)$ and has an algebraic singularity such as $x^\alpha$ or $(1 - x)^\beta$ $(\alpha, \beta > -1)$, then the function $g(t)$ also can be differentiable many times and all its derivatives vanish at the two ends of the interval $[0, 1]$ due to the strong singularity of $\varphi'(t)$, so that

$$g^{(m)}(0) = g^{(m)}(1) = 0, \quad \text{for } m = 0, 1, 2, \cdots. \quad (B.6)$$

Applying the trapezoidal rule on (B.5), we get the approximation for the integration:

$$S_N = \frac{1}{N} \sum_{n=1}^{N-1} w_n^{(N)} f(x_n^{(N)}), \quad \text{and} \quad x_n^{(N)} = \varphi(n/N), \; w_n^{(N)} = \varphi'(n/N). \quad (B.7)$$

If we define

$$c_k = \int_0^1 g(t) \exp(i2\pi kt) \, dt,$$

then obviously

$$g(t) = \sum_{k=-\infty}^{\infty} c_k \exp(-i2\pi kt)$$

and

$$\int_0^1 f(x) \, dx = \int_0^1 g(t) \, dt = c_0.$$

The approximation $S_N$ is given by

$$S_N = \frac{1}{N} \sum_{n=0}^{N-1} g(n/N) = c_0 + \sum_{p=1}^{\infty} (c_p N + c_{-p} N). \quad (B.8)$$

The truncation error $\varepsilon_N$ is estimated as:

$$\varepsilon_N = S_N - \int_0^1 g(t) \, dt$$

$$= \sum_{p=1}^{\infty} (c_p N + c_{-p} N)$$

$$= 2 \sum_{p=1}^{\infty} \text{Re} c_p N$$

$$\sim 2 \text{Re} c_N. \quad (B.9)$$

For $f(x)$ with singularity $x^\alpha$ or $(1 - x)^\alpha$, an estimate of $\varepsilon(N, \alpha)$ is given by

$$\varepsilon(N, \alpha) = \frac{\sqrt{4\pi}}{(e\xi)^{\alpha+1}} \frac{(\alpha + 1)^{1/4 + \alpha}}{(2\pi N)^{3/4 + \alpha}}$$

$$\cdot \exp \left[ -\sqrt{4\pi(\alpha + 1)N} \right] \cdot \cos \left[ \sqrt{4\pi(\alpha + 1)N} + \frac{3 + 4\alpha}{8\pi} \right]. \quad (B.10)$$

References

[1] Bether H A and Salpeter E E 1977 Quantum Mechanics of One- and Two-Electron Atoms (Plenum, New York)

[2] Madden R P and K Codding 1963 Phys. Rev. Lett. 10 516

[3] Levin F S and Shertzer J 1988 Phys. Rev. Lett. 61 1089
[4] Botero J and Shertzer J 1992 Phys. Rev. A 46 1155
[5] Rescigno T N, Baertschy M, Issaacs W A and McCurdy C W 1999 Science 286 2474
[6] Baertschy M, Rescigno T N, Isaacs W A, Li X and McCurdy C W 2001 Phys. Rev. A 63 022712
[7] Hsiang W T and Hsiang W Y 1996 Center for Pure and Applied Mathematics, Univ. of California, Berkeley PAM-636 preprint
[8] Hsiang W Y 1997 Proc. Natl. Acad. Sci. USA 94 8936
[9] Hsiang W T and Hsiang W Y 1997 Center for Pure and Applied Mathematics, Univ. of California, Berkeley PAM-697 preprint
[10] Hsiang W T and Hsiang W Y 1997 Center for Pure and Applied Mathematics, Univ. of California, Berkeley PAM-699 preprint
[11] Kellner G W 1927 Z. Phys. 44 91
[12] Hylleraas E A 1928 Z. Phys. 48 469
[13] Hylleraas E A 1929 Z. Phys. 54 347
[14] Kinoshita T 1959 Phys. Rev. 115 366
[15] Frankowski K and Pekeris C L 1966 Phys. Rev. 146 46
[16] Frolov A M and Bishop D M 1992 Phys. Rev. A 45 6236
[17] Frolov A M, Smith V H and Bishop D M 1993 Phys. Rev. A 49 1686
[18] Bishop D M 1994 Phys. Rev. A 51 3636
[19] Bürgers A, Wintgen D and Rost J M 1995 J. Phys. B: At. Mol. Phys. 28 3163
[20] Frolov A M 1998 Phys. Rev. A 56 4479
[21] Drake G W F, Cassar M M and Nistor R A 2002 Phys. Rev. A 65 054501
[22] Aguilar J and Combes J M 1971 Commun. Math. Phys. 22 269
[23] Balslev E and Combes J M 1971 Commun. Math. Phys. 22 280
[24] Simmon B 1972 Commun. Math. Phys. 27 1
[25] Ho Y K 1979 J. Phys. B: At. Mol. Phys. 12 387
[26] Reinhardt W 1982 Annu. Rev. Phys. Chem. 33 223
[27] Ho Y K 1983 Phys. Rep. 99 1
[28] Ho Y K 1986 Phys. Rev. A 34 34
[29] Ho Y K and Bhatia A K 1994 Phys. Rev. A 50 2155
[30] Grounwall T H 1937 Phys. Rev. 51 655
[31] Knirk D L 1974 J. Chem. Phys. 60 760
[32] Haftel M I and Mandelzweig V B 1983 Ann. Phys., NY 150 48
[33] Frey G and Howard B J 1987 Chem. Phys. 111 33
[34] Jerjian K A and Macek J 1987 Phys. Rev. A 36 2667
[35] Haftel M I and Mandelzweig V B 1987 Phys. Rev. A 120 232
[36] Haftel M I and Mandelzweig V B 1988 Phys. Rev. A 38 5995
[37] Haftel M I and Mandelzweig V B 1988 Phys. Rev. A 39 2813
[38] Haftel M I and Mandelzweig V B 1990 Phys. Rev. A 42 6324
[39] Haftel M I and Mandelzweig V B 1993 Phys. Rev. A 49 3344
[40] Krivec R, Mandelzweig V B and Varga K 2000 Phys. Rev. A 61 062503
[41] Macek J 1968 J. Phys. B: At. Mol. Phys. 1 831
[42] Fano U 1969 Atomic Physics 1 209
[43] Fano U 1983 Rep. Prog. Phys. 46 97
[44] Fano U and Rau A 1986 Atomic Collisions and Spectra (Academic Press, Orlando)
[45] Ram-Mohan L R 2002 Finite Element and Boundary Element Applications in Quantum Mechanics (University Press, Oxford)
[46] Levin F S and Shertzer J 1985 Phys. Rev. A 32 3285
[47] Braun M, Schweizer W and Herold H 1993 Phys. Rev. A 48 1916
[48] Bottcher C D, Shultz D R and Madison D H 1994 Phys. Rev. A 49 1714
[49] Scrinzi A 1995 Comput. Phys. Commun. 86 67
[50] Ackermann J and Shertzer J 1995 Phys. Rev. A 54 365
[51] Laaksonen L, Pyykö P and Sundholm D 1983 *Int. J. Quantum Chem.* **23** 309
[52] Ford W K and Levin F S 1984 *Phys. Rev.* A **29** 43
[53] Schulze W and Kolb D 1985 *Chem. Phys. Lett.* **122** 271
[54] Yang L, Heinemann D and Kolb D 1991 *Chem. Phys. Lett.* **178** 213
[55] Ackermann J and Roitzsch R 1993 *Chem. Phys. Lett.* **214** 106
[56] Ackermann J and Roitzsch R 1994 *J. Chem. Phys.* **101** 7463
[57] Ackermann J 1995 *Phys. Rev.* A **52** 1968
[58] Zare R N 1998 *Angular Momentum: Understanding Spatial Aspects in Chemistry and Physics* (Wiley, New York)
[59] Simonov Y A 1969 *Sov. J. Nucl. Phys.* **3** 461
[60] Whitten R C 1969 *J. Math. Phys.* **10** 1631
[61] Haftel M I and Mandelzweig V B 1989 *Ann. Phys., NY* **189** 29
[62] Haftel M I and Mandelzweig V B 1991 *Phys. Rev.* A **46** 142
[63] Barnea N and Mandelzweig V B 1990 *Phys. Rev.* A **46** 142
[64] ARPACK [http://www.caam.rice.edu/software/ARPACK](http://www.caam.rice.edu/software/ARPACK)
[65] Sonneveld P 1989 *SIAM J. Sci. Statist. Comput.* **10** 36
[66] Brezinski C and Zaglia M R 1991 *Extrapolation Methods: Theory and Practice* (Amsterdam, NORTH-HOLLAND)
[67] Hill R N 1977 *Phys. Rev. Lett.* **38** 643
[68] Hill R N 1977 *J. Math. Phys.* **18** 2316
[69] Bethe H A 1929 *Z. Phys.* **57** 815
[70] Lykke K R, Murray K K and Lineberger W C 1991 *Phys. Rev.* A **43** 6104
[71] Jăuregui R and Bunge C F 1979 *J. Chem. Phys.* **71** 4611
[72] Banyard K E, Keeble D and Drake G W K 1992 *J. Phys. B: At. Mol. Phys.* **25** 3405
[73] Bhatia A K 1972 *Phys. Rev.* A **6** 6
[74] Hesse M and Baye D 2001 *J. Phys. B: At. Mol. Phys.* **34** 1425
[75] Dolye H, Oppenheimer M and Drake G W F 1971 *Phys. Rev.* A **5** 5
[76] Goodson D Z, Watson D K, Loeser J G and Herschbach D R 1990 *Phys. Rev.* A **44** 97
[77] Galán M and Bunge C 1981 *Phys. Rev.* A **23** 1624
[78] Mukherjee T K and Mukherjee P 1965 *Phys. Rev.* **140** 1104
[79] Mills A P 1981 *Phys. Rev. Lett.* **69** 064501
[80] Duan B, Gu X and Ma Z Q 2001 *Eur. Phys. J. D* **19** 9
[81] Lipsky L, Anania R and Conneeley M J 1977 *Atomic Data and Nuclear Data Tables* **20** 127
[82] Wheeler E A 1946 *Ann. NY Acad.Sci.* **46** 219
[83] Ferrante G and Geracitano R 1969 *Phys. Rev.* **182** 215
[84] Mills A P 1983 *Phys. Rev. Lett.* **50** 671
[85] Lin C D 1995 *Phys. Rev.* **1** 257
[86] Rost J M and Wintgen D 1992 *Phys. Rev. Lett.* **69** 2499
[87] Petelenz P and Smith V H 1987 *Phys. Rev.* A **36** 5125
[88] Lin C D 1995 *Phys. Rev. A* **48** 4780
[89] Frolov A M 1999 *Phys. Rev.* A **60** 2834
[90] Rainville E D 1960 *Special Functions* (MacMillan, New York)
[91] Ooura T and Mori M 1974 *Pub. RIMS Kyoto Univ.* **9** 721
[92] Davis P J and Rabinowitz P 1984 *Methods of Numerical Integration* (Academic Press, New York)
Table 1. Comparison of the ground state of $\infty{H^{-}}$ and $H^{-}$ ($m_p = 1836.152701$) with other theoretical calculations.

|                  | $\infty{H^{-}}$                  | $H^{-}$                  |
|------------------|----------------------------------|--------------------------|
| $-E$             | 0.527 751 016 54                 | 0.527 445 881 1          |
|                  | 0.527 751 016 544 302 $^a$        | 0.527 445 881 114 104 $^a$|
|                  | 0.527 751 016 532 $^b$           | 0.527 445 881 110 $^c$   |
| $< 1/r_2 >=< 1/r_3 >$ | 0.683 261 767                   | 0.682 853 385            |
|                  | 0.683 261 767 654 0 $^a$         | 0.682 853 384 854 $^a$   |
|                  | 0.683 261 768 $^b$               | 0.682 853 384 96 $^c$    |
| $< 1/r_1 >$      | 0.311 021 502 2                 | 0.310 815 007            |
|                  | 0.311 021 502 219 1 $^a$         | 0.310 815 007 479 $^a$   |
|                  | 0.311 021 503 $^b$              | 0.310 815 007 66 $^c$    |
| $< r_2 >=< r_3 >$| 2.710 178 27                    | 2.712 095 6              |
|                  | 2.710 178 278 34 $^a$            | 2.712 095 626 51 $^a$    |
|                  | 2.710 178 263 $^b$               | 2.712 095 621 4 $^c$     |
| $< r_1 >$        | 4.412 694 50                    | 4.415 692 6              |
|                  | 4.412 694 497 79 $^a$            | 4.415 692 603 31 $^a$    |
|                  |                                   | 4.415 692 593 4 $^c$     |
| $< r_2^2 >=< r_3^2 >$ | 11.913 699 6                    | 11.931 747 7             |
|                  | 11.913 699 681 6 $^a$            | 11.931 747 760 $^a$      |
|                  | 11.913 699 235 $^b$              | 11.931 747 62 $^c$       |
| $< r_1^2 >$      | 25.202 025 2                    | 25.237 175               |
|                  | 25.202 025 298 2 $^a$            | 25.237 175 614 $^a$      |
|                  |                                   | 25.237 175 34 $^c$       |
| $< \cos(r_{12}, r_{13}) >$ | $-0.105 147 693 7$              | $-0.104 996 606$         |
|                  | $-0.105 147 693 566 0 $^a$       | $-0.104 996 606 303 $^a$ |
| $< \cos(r_{12}, r_{32}) >$ | 0.649 871 581                   | 0.694 795 647            |
|                  | 0.649 871 581 199 9 $^a$         | 0.694 795 646 586 $^a$   |

$^a$Ref. [20] $^b$Ref. [57] $^c$Ref. [50]
Table 2. Comparison of the $^3P^e$ state of $\infty\text{H}^-$ and $\text{H}^-$ ($m_p = 1836.152701$) with other theoretical calculations.

|       | $\infty\text{H}^-$ | $\text{H}^-$ |
|-------|---------------------|--------------|
| $-E$  | 0.125 355 451 242   | 0.125 283 157 034 |
|       | 0.125 354 7$^a$    | 0.125 354 7$^a$ |
|       | 0.125 355 451 24$^b$ | 0.125 355 451 24$^b$ |
|       | 0.125 354 705$^c$ | 0.125 282 391 9$^c$ |
|       | 0.125 351 3$^d$    | 0.125 279 0$^d$ |
|       | 0.125 355 08$^e$   |                |
| $<1/r_2>$ | 0.160 520 878 4 | 0.160 397 165 |
| $<1/r_1>$ | 0.0703 308 548   | 0.0702 280 17 |
|       | 0.0706 30$^a$    |                |
| $<1/r_3>$ | 11.657 657 7     | 11.683 161 8 |
| $<r_1>$   | 19.585 091      | 19.632 096 8 |
|       | 19.237$^a$    |                |
| $<r_2>$ $<$ $r_3>$ | 271.263 4 | 273.015 9 |
| $<r_1^2>$ | 557.259 2      | 560.744 |
|       | 517.09$^a$    |                |
| $<\cos(r_{12},r_{13})>$ | $-0.093 867 209 4$ | $-0.093 625 370$ |
| $<\cos(r_{12},r_{32})>$ | 0.651 280 257 | 0.651 086 687 |

$^a$Ref. [73], $^b$Ref. [72], $^c$Ref. [75], $^d$Ref. [76], $^e$Ref. [71].

Table 3. Comparison for the energies of the five low-lying $^1S^e$ states of $\infty\text{He}$ and $\text{He}$ with others calculations.

|       | $-E(^1S^e)$ | $-E(^3S^e)$ |
|-------|-------------|-------------|
| This work | Ref. [19] | This work | Ref. [19] |
| $\infty\text{He}$ | | |
| 2.903 724 377 03 | 2.903 724 377 034 119 | 2.175 229 378 2 | 2.175 229 378 236 |
| 2.145 974 046 | 2.145 974 046 054 | 2.068 689 067 | 2.068 689 067 47 |
| 2.061 271 98 | 2.061 271 989 7 | 2.036 512 0 | 2.036 512 083 |
| 2.033 586 | 2.033 586 7 | 2.022 6 | 2.022 618 |
| 2.021 17 | 2.021 17 | 2.015 | 2.015 377 |
| $\text{He}(m_\alpha = 7294.299507)$ | | |
| 2.903 304 557 7 | 2.174 930 190 6 | 2.174 930 190 6 |
| 2.145 678 587 | 2.068 405 243 | 2.068 405 243 |
| 2.060 989 07 | 2.036 232 73 | 2.036 232 73 |
| 2.033 307 6 | 2.022 280 | 2.022 280 |
| 2.020 77 | 2.013 34 | 2.013 34 |
Table 4. Convergence study for the three low-lying $^1^3P_o$ states of $\infty$He.

| $(M, N, P)$      | $-E_0$     | $-E_1$     | $-E_2$     |
|------------------|------------|------------|------------|
|                  | $^1P_o$    |            |            |
| (290,160,60)     | 2.121 781 471 934 | 2.045 206 888 028 | 2.007 282 642 688 |
| (310,170,60)     | 2.122 001 335 701 | 2.046 159 516 026 | 2.009 274 234 036 |
| (330,180,60)     | 2.122 187 837 151 | 2.046 981 326 187 | 2.011 018 748 522 |
| (350,190,60)     | 2.122 347 396 423 | 2.047 695 333 577 | 2.012 556 633 845 |
| (370,200,60)     | 2.122 484 960 882 | 2.048 319 671 610 | 2.013 920 175 194 |
| (390,210,60)     | 2.122 604 392 689 | 2.048 868 793 171 | 2.015 435 817 |
| (410,220,60)     | 2.122 708 742 385 | 2.049 354 337 962 | 2.016 223 670 874 |
| (430,230,60)     | 2.122 800 445 240 | 2.049 785 768 826 | 2.017 202 374 649 |
| Extrap.          | 2.123 842 8    | 2.055 149   | 2.031 0    |
| Ref. [80]        | 2.123 843 085 800 | 2.055 146 355 4 | 2.031 069 591 |
|                  | $^3P_o$    |            |            |
| (290,160,60)     | 2.131 433 366 926 | 2.049 022 358 625 | 2.009 815 747 062 |
| (310,170,60)     | 2.131 618 811 233 | 2.049 898 916 341 | 2.011 718 260 682 |
| (330,180,60)     | 2.131 775 987 950 | 2.050 654 119 626 | 2.013 383 329 203 |
| (350,190,60)     | 2.131 910 360 569 | 2.051 309 458 014 | 2.014 849 959 935 |
| (370,200,60)     | 2.132 026 134 097 | 2.051 881 840 210 | 2.016 149 272 454 |
| (390,210,60)     | 2.132 126 587 511 | 2.052 384 725 339 | 2.017 306 376 122 |
| (410,220,60)     | 2.132 214 308 072 | 2.052 828 939 042 | 2.018 341 737 893 |
| (430,230,60)     | 2.132 291 359 280 | 2.053 223 271 537 | 2.019 272 194 566 |
| Extrap.          | 2.133 164 06   | 2.058 081   | 2.032 36   |
| Ref. [80]        | 2.133 164 190 534 | 2.058 081 081 6 | 2.032 324 325 |

Table 5. Properties of the five low-lying $^1^S_e$ states of $\infty$He.

| State     | $^1^1S_e$     | $^2^1S_e$     | $^3^1S_e$     | $^4^1S_e$     | $^5^1S_e$     |
|-----------|---------------|---------------|---------------|---------------|---------------|
| $<1/r_2>$ | 1.688 316 800 71 | 1.135 407 686 | 1.058 514 75  | 1.032 484 8   | 1.021 298    |
| $<1/r_1>$ | 0.945 818 448 80 | 0.249 682 652 | 0.111 514 95  | 0.062 760 2   | 0.041 429    |
| $<r_2>$   | 0.929 472 294 87 | 2.973 061 12  | 6.511 676    | 11.550 6      | 17.573       |
| $<r_1>$   | 1.422 070 255 5 | 5.269 696 20  | 12.304 521   | 22.368 1      | 34.407       |
| $<r_2^2>$ | 1.193 482 995 0 | 16.089 233 2  | 85.890 18    | 281.33        | 660.7        |
| $<r_1^2>$ | 2.516 439 312 9 | 32.302 380 3  | 171.838 66   | 562.71        | 132.14       |
| $<\cos(r_{12}, r_{13})>$ | -0.064 202 614 217 | -0.014 657 043 3 | -0.004 317 036 7 | -0.001 795 63 | -0.000 958 99 |
| $<\cos(r_{12}, r_{32})>$ | 0.648 017 667 47 | 0.557 144 578 | 0.526 466 53 | 0.515 120     | 0.510 057    |
Table 6. Properties of the five low-lying $^3S_e$ states of $\infty$He.

| State          | $^2^3S_e$ | $^3^3S_e$ | $^4^3S_e$ | $^5^3S_e$ | $^6^3S_e$ |
|----------------|----------|----------|----------|----------|----------|
| $< 1/r_2 >$    | 1.154 663 198 4 | 1.063 661 050 | 1.034 491 5 | 1.021 740 | 1.019 08 |
| $< 1/r_1 >$    | 0.268 197 633 6 | 0.117 316 73 7 | 0.065 253 6 | 0.042 086 | 0.037 343 |
| $< r_2 >$      | 2.550 464 78 2 | 5.856 041 6 | 10.661 70 | 16.702 8 | 19.945 |
| $< r_1 >$      | 4.447 538 89 | 10.998 910 1 | 20.592 6 | 32.666 8 | 39.150 |
| $< r_2^2 >$    | 11.464 340 5 | 68.710 08 | 238.596 5 | 70.702 8 | 870.56 |
| $< r_1^2 >$    | 23.046 235 5 | 137.478 4 | 477.225 | 119.220 | 174.13 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{13}) >$ | -0.015 839 217 1 | -0.004 245 085 8 | -0.001 686 96 | -0.000 853 68 | 0.000 753 55 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{32}) >$ | 0.562 788 947 4 | 0.528 301 29 | 0.515 917 | 0.510 32 | 0.509 16 |

Table 7. Properties of the five low-lying $^1P_e$ states of $\infty$He.

| State          | $^3^1P_e$ | $^4^1P_e$ | $^5^1P_e$ | $^6^1P_e$ | $^7^1P_e$ |
|----------------|----------|----------|----------|----------|----------|
| $< 1/r_2 >$    | 0.320 101 054 07 | 0.286 233 304 00 | 0.272 597 920 5 | 0.265 345 943 5 | 0.261 119 621 |
| $< 1/r_1 >$    | 0.119 911 271 50 | 0.066 410 151 50 | 0.045 587 471 8 | 0.032 033 447 1 | 0.021 194 314 |
| $< r_2 >$      | 5.678 437 023 5 | 10.289 515 048 | 16.391 632 59 | 23.993 012 6 | 33.043 005 |
| $< r_1 >$      | 9.383 100 140 0 | 18.332 172 25 | 30.436 532 33 | 45.587 471 6 | 63.658 480 |
| $< r_2^2 >$    | 48.197 972 382 | 187.544 430 1 | 517.827 867 8 | 1160.997 52 | 2260.938 |
| $< r_1^2 >$    | 97.935 626 136 | 376.133 444 1 | 1036.363 473 | 2322.499 92 | 4522.255 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{13}) >$ | -0.031 985 135 41 | -0.012 745 156 27 | -0.006 214 829 38 | -0.003 469 611 28 | -0.002 133 310 32 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{32}) >$ | 0.608 746 828 961 | 0.527 235 307 6 | 0.503 973 838 7 | 0.528 046 351 7 | 0.520 635 797 |

Table 8. Properties of the five low-lying $^3P_e$ states of $\infty$He.

| State          | $^2^3P_e$ | $^3^3P_e$ | $^4^3P_e$ | $^5^3P_e$ | $^6^3P_e$ |
|----------------|----------|----------|----------|----------|----------|
| $< 1/r_2 >$    | 0.148 098 166 677 7 | 0.312 484 187 824 | 0.284 034 111 28 | 0.271 400 549 88 | 0.264 691 916 1 |
| $< 1/r_1 >$    | 0.251 392 355 540 | 0.143 109 538 48 | 0.064 402 067 59 | 0.041 093 048 12 | 0.028 447 092 |
| $< r_2 >$      | 3.089 879 331 46 | 6.460 150 723 | 11.307 445 32 | 17.670 872 20 | 25.539 291 0 |
| $< r_1 >$      | 4.676 371 886 38 | 10.831 799 73 | 20.337 436 31 | 32.980 000 76 | 48.672 531 0 |
| $< r_2^2 >$    | 11.790 987 877 61 | 65.499 664 26 | 232.269 920 | 609.030 026 0 | 1325.763 8 |
| $< r_1^2 >$    | 25.068 197 316 2 | 132.737 982 45 | 465.625 639 3 | 1220.528 804 | 2652.039 2 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{13}) >$ | -0.071 403 717 508 2 | -0.031 229 607 724 0 | -0.013 396 063 21 | -0.006 806 335 01 | -0.003 898 879 99 |
| $< \cos(\mathbf{r}_{12}, \mathbf{r}_{32}) >$ | 0.680 042 940 389 3 | 0.603 424 804 436 | 0.560 482 902 42 | 0.539 239 063 10 | 0.527 421 792 |
Table 9. Comparison for the energies of the five low-lying $^{1,3}P_e$ states of $\infty\text{He}$ and He with other calculations.

| $-E(1P_e)$ | $-E(3P_e)$ |
|------------|------------|
| This work  | other results | This work  | other results |
| $\infty\text{He}$ | | $\infty\text{He}$ | | |
| 0.580 246 472 594 | 0.580 246 472 594 392 \textsuperscript{a} | 0.710 500 155 678 3 | 0.710 500 155 678 334 3 \textsuperscript{a} |
| 0.580 246 472 594 388 \textsuperscript{b} | | 0.710 500 155 678 23 \textsuperscript{b} | |
| 0.540 041 590 93 | 0.540 041 590 938 1 \textsuperscript{a} | 0.567 812 898 725 1 | 0.567 812 898 725 31 \textsuperscript{a} |
| 0.540 041 590 938 52 \textsuperscript{b} | | 0.567 812 898 725 16 \textsuperscript{b} | |
| 0.524 178 981 8 | 0.524 179 01 \textsuperscript{a} | 0.535 867 188 767 | 0.535 867 188 71 \textsuperscript{a} |
| 0.516 208 609 4 | 0.516 03 \textsuperscript{b} | 0.522 254 575 706 | 0.522 253 \textsuperscript{a} |
| 0.511 624 834 | | 0.515 160 203 83 | |

He ($m_\alpha = 7294.299507$)

| $-E(1P_e)$ | $-E(3P_e)$ |
|------------|------------|
| This work  | other results | This work  | other results |
| $Z=3$ | | $Z=4$ | | |
| 0.580 165 768 725 | 0.580 165 768 308 4 \textsuperscript{b} | 0.710 396 457 557 | 0.710 396 457 021 81 \textsuperscript{b} |
| 0.580 165 768 \textsuperscript{d} | | 0.710 396 457 \textsuperscript{d} | |
| 0.539 967 178 01 | 0.539 967 177 633 \textsuperscript{b} | 0.567 733 870 122 | 0.567 733 869 714 03 \textsuperscript{b} |
| 0.539 967 2 \textsuperscript{d} | | 0.567 733 87 \textsuperscript{d} | |
| 0.524 106 954 1 | | 0.535 793 284 74 | |
| 0.516 137 755 4 | | 0.522 182 770 7 | |
| 0.511 554 646 4 | | 0.515 089 462 | |

\textsuperscript{a}Ref. \[78\], \textsuperscript{b}Ref. \[76\], \textsuperscript{c}Ref. \[81\], \textsuperscript{d}Ref. \[82\]

Table 10. The eigen-energies for the $^{1,3}P_e$ states of helium-like ions ($Z = 3 \sim 6$).

| $-E(1P_e)$ | $-E(3P_e)$ |
|------------|------------|
| $Z=3$ | | $Z=4$ | | |
| 1.401 410 927 020 | 1.796 648 099 720 | 2.583 994 187 432 | 3.382 712 420 777 |
| 1.269 787 972 287 | 1.373 589 535 176 | 2.312 232 549 880 | 2.540 768 798 391 |
| 1.214 520 958 34 | 1.260 545 265 63 | 2.194 982 661 13 | 2.298 106 658 34 |
| 1.185 881 076 3 | 1.210 287 247 90 | 2.133 407 126 0 | 2.188 554 817 30 |
| 1.169 099 559 | 1.183 580 072 8 | 2.097 031 380 | 2.129 923 592 6 |

| $Z=5$ | | $Z=6$ | | |
| 4.127 776 355 386 | 5.468 730 984 923 | 6.032 706 408 00 | 8.054 724 273 276 |
| 3.667 237 481 32 | 4.069 185 038 025 | 5.334 768 645 76 | 5.958 774 148 469 |
| 3.465 482 470 00 | 3.648 310 490 768 | 5.025 999 284 37 | 5.311 076 536 74 |
| 3.358 735 604 6 | 3.456 902 285 67 | 4.861 852 996 5 | 5.015 282 040 9 |
| 3.295 388 021 8 | 3.354 092 319 0 | 4.764 160 404 | 4.856 057 141 |
Table 11. Comparison for the energies of the five low-lying $^{1,3}D_o$ states of $\infty$He with Bhatia's

| $-E^{(1}D_o)$ | $-E^{(3}D_o)$ |
|---------------|---------------|
| This work     | Bhatia        | This work     | Bhatia        |
| 0.563 800 420 4 | 0.563 800 405 | 0.559 328 263 0 | 0.559 328 25  |
| 0.534 576 384 | 0.534 576 015 | 0.532 678 600 | 0.532 678 075 |
| 0.521 659 00 | 0.521 642 77 | 0.520 703 44 | 0.520 693 865 |
| 0.514 833 4 | 0.514 269 06 | 0.514 288 2 | 0.514 235 78 |

Table 12. Convergence study for the three low-lying $^{1}F_e$ states of Li$^+$ ion.

| $(M,N,P)$     | $-E_0$     | $-E_1$     | $-E_2$     |
|---------------|------------|------------|------------|
| (310,170,40)  | 1.252 443 716 475 54 | 1.206 193 104 449 | 1.181 010 621 655 |
| (330,180,40)  | 1.252 445 059 532 88 | 1.206 204 195 186 | 1.181 059 878 109 |
| (350,190,40)  | 1.252 446 091 667 05 | 1.206 212 775 544 | 1.181 098 378 639 |
| (370,200,40)  | 1.252 446 895 466 84 | 1.206 219 497 607 | 1.181 128 811 337 |
| (390,210,40)  | 1.252 447 529 007 27 | 1.206 224 824 200 | 1.181 153 115 955 |
| Extrap.       | 1.252 450 636 | 1.206 251 57 | 1.181 279 1 |

1.252 445 1 Ref. [79]  
1.252 258 Ref. [80]

Table 13. 15 low-lying S states of H$_2^+$

| n  | $-E_n$ | n  | $-E_n$ | n  | $-E_n$ |
|----|--------|----|--------|----|--------|
| 0  | 0.597 139 | 5  | 0.552 841 | 10 | 0.521 699 |
| 1  | 0.587 156 | 6  | 0.545 593 | 11 | 0.517 002 |
| 2  | 0.577 752 | 7  | 0.538 858 | 12 | 0.512 827 |
| 3  | 0.568 909 | 8  | 0.532 631 | 13 | 0.509 189 |
| 4  | 0.560 609 | 9  | 0.526 911 | 14 | 0.506 11 |
Table 14. Comparison of the ground state of Ps$^-$ with other theoretical calculations.

| $-E$         | $<1/r_2> = <1/r_3>$ | $<1/r_1>$       |
|--------------|---------------------|-----------------|
| 0.262 005 070 2 | 0.339 821 023       | 0.155 631 905 7 |
| 0.262 004 857$^a$ | 0.339 831 3$^a$   | 0.155 654 3$^a$ |
| 0.262 005 070 0$^b$ | 0.339 821 02$^b$ | 0.155 631 90$^b$ |
| 0.262 005 070 232 94$^c$ | 0.339 821 023 06$^c$ | 0.155 631 905 653$^c$ |
| 0.262 005 070 232 978$^d$ | 0.339 821 023 059 27$^d$ | 0.155 631 905 652 66$^d$ |
| $<r_2> = <r_3>$ | $<r_1>$           | $<r_2^2> = <r_3^2>$ |
| 5.489 633 2   | 8.548 580 6         | 48.418 936      |
| 5.488 352$^a$ | 8.546 111 29$^a$   | 48.379 317$^a$  |
| 5.489 633 3$^b$ | 8.548 580 8$^b$    | 48.418 936$^b$ |
| 5.489 633 252$^c$ | 8.548 580 655$^c$ | 48.418 937 2$^c$ |
| 5.489 633 252 38$^d$ | 8.548 580 655 16$^d$ | 48.418 937 230$^d$ |
| $<r_1^2>$     | $<\cos(r_{12}, r_{13})>$ | $<\cos(r_{12}, r_{32})>$ |
| 93.178 63     | 0.019 769 632 8     | 0.591 981 70     |
| 93.100 697 0$^a$ |                  |                 |
| 93.100 633$^b$ |                  |                 |
| 93.178 633 80$^c$ |              |                 |
| 93.178 633 855$^d$ | 0.019 769 632 816 7$^d$ | 0.591 981 701 149 2$^d$ |

$^a$Ref. [37] $^b$Ref. [31] $^c$Ref. [32] $^d$Ref. [33]