

The Three-Body Coulomb Potential Polynomials

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ABSTRACT

In this paper, we present a general analysis of the three-body Coulomb potential polynomials. We show why the three-body Coulomb wave functions expansion in a non-orthogonal Laguerre-type function basis gives two modified Pollaczek polynomials. The frozen-core model is used to examine the three-body Coulomb Hamiltonian. The resulting three-term recurrence relation is a special case of the Pollaczek polynomials which is a set of orthogonal polynomials having a nonempty continuous spectrum in addition to an infinite discrete spectrum. The completeness of the three-body Coulomb wave functions is further studied for different Laguerre basis size.

Keywords: three-body Coulomb, non-orthogonal Laguerre, Pollaczek polynomial, frozen-core model

INTRODUCTION

In atomic and nuclear scattering, it is often desirable to use Slater or oscillator function as a basis function. Heller and Yamani [1] have presented a new method for performing scattering calculations entirely with square-integrable (L^2) functions. They developed techniques in which they attempted to take full advantage of the analytic properties of a given Hamiltonian and also of the L^2 function basis which was used to describe the wave functions. They developed the basic theory using non-orthogonal Laguerre-type function basis appropriate for s -wave scattering.

An L^2 discretization of the radial two-body Coulomb problem has been given by Yamani and Reinhardt [2]. They presented the relationship between the matrix eigenvalues of the L^2 operator with a continuous spectrum, and the associated Gaussian quadrature was discussed for the radial kinetic energy and for the repulsive and attractive Coulomb Hamiltonians. It was shown that discretization of the radial kinetic energy in

a non-orthogonal Laguerre-type function basis gave an Ultraspherical (Gegenbauer) polynomial, while discretization in an oscillator-type basis generated a Laguerre polynomial. They showed that non-orthogonal Laguerre-type function basis discretization of the Coulomb problem gave a Pollaczek polynomial in the repulsive case and a new modified Pollaczek polynomial in the attractive case. The Coulomb problem, with an attractive potential, is known to have an infinite number of bound states as well as a nonempty continuous spectrum. These suggest that the polynomials corresponding to the attractive Coulomb potential will be orthogonal with respect to a distribution function having an absolutely continuous component and infinitely many discontinuities.

Board [3] proved that the equivalent quadrature Fredholm determinant and the J -matrix method are essentially equivalent, yielding the same result from the same appropriate treatment of the potential and exact treatment of kinetic energy operator. It was shown that relating the spacing of the pseudostate eigenvalues to the relative normalization of the pseudostate and actual continuum matrix elements provided an alternative to the Stieltjes imaging method. Board [4] has also applied the basis of Yamani and Reinhardt [2] and Gaussian quadrature based Pollaczek polynomials for calculating two-photon processes in hydrogen.

A new expansion of the radial two-body Coulomb wave functions in an orthogonal Laguerre-type function basis was later presented by Stelbovics [5]. It was shown [6, 7] that the orthogonal Laguerre-type function basis could be directly applied to the coupled-channels formulation of electron-hydrogen and electron-helium scattering.

The purpose of this paper is to present a new expansion of the three-body Coulomb wave functions in a non-orthogonal Laguerre-type function basis. The frozen-core model [6, 7] is used to calculate the three-body Coulomb Hamiltonian. It is shown that discretization of the radial kinetic energy and the Coulomb problem in the attractive case for the helium ground state ($1s$) give the modified Pollaczek polynomials of Yamani and Reinhardt [2], whereas the other discretization of the radial kinetic energy and the Coulomb problem in the attractive and electron-electron potential case for the helium excitation states give a new modified Pollaczek polynomial.

This paper is organized as follows. In section 2, we present the three-body Coulomb wave functions and non-relativistic Hamiltonian. Non-orthogonal Laguerre-type function basis discretization of the three-body Coulomb potential gives two modified Pollaczek polynomials and the

frozen-core model is used to examine the three-body Coulomb Hamiltonian are given in Section 3. The resulting three-term recurrence relation is shown to be a special case of the Pollaczek polynomials which is a set of orthogonal polynomials having a nonempty continuous spectrum in addition to an infinite discrete spectrum. In section 4, the completeness of the three-body Coulomb wave functions is then examined by Gaussian quadrature. The numerical results are given in Section 5. Finally in Section 6, we draw the concluding remarks from this work.

Accordingly, we introduce the fundamentals of orthogonality and the analytical study of orthogonal polynomials. A distribution function $\alpha(x)$ is a fixed non-decreasing function with infinitely many points of increase in the finite or infinite interval $[a, b]$, and the ‘moments’, $\int_a^b x^i d\alpha(x)$, exist and are finite for $i = 0, 1, 2, \dots$. A set of polynomials $\{P_i(x)\}$, where $P_i(x)$ is a polynomial of precise degree i , is called orthogonal with respect to α provided

$$\int_a^b P_i(x)P_j(x)d\alpha(x) = 0, \quad i \neq j. \tag{1}$$

With an interval $[a, b]$ and weight function, $w(x)$, we may associate Eq. (1)

$$\int_a^b w(x)P_i(x)P_j(x)dx = 0, \quad i \neq j \tag{2}$$

which is defined for all the orthogonal polynomials, that is, $\int_a^b w(x)|x|^n dx < \infty$ for all n . If $\alpha(x)$ is absolutely continuous, (1) reduces to

(2) with $w(x) = \frac{d\alpha(x)}{dx}$. On the other hand, if $\alpha(x)$ is a jump function, that is constant except for jumps of the magnitude w_i at $x = x_i$, then (1) reduces to sum

$$\sum_{n=1}^{\infty} w_n P_i(x_n)P_j(x_n) = 0, \quad \text{for } i \neq j \tag{3}$$

(where $\{x_n : n \geq 1\}$ is the set of jump discontinuities of $\alpha(x)$) which is the appropriate definition for functions of a discrete variable. A set of

orthogonal polynomials $\{P_i(x_n): n \geq 0\}$ will satisfy a three-term recurrence relation

$$P_i(x_n) = (A_i x_n + B_i) P_{i-1}(x_n) - C_i P_{i-2}(x_n), \quad i = 1, 2, \dots \quad (4)$$

Here A_i , B_i , and C_i are constants, $A_i > 0$ and $C_i > 0$, and the positivity conditions

$$A_{i-1} A_i C_i > 0, \quad i = 1, 2, \dots, \quad (5)$$

are satisfied. For many of the classical polynomials there are analytic relations between function and its first and/or second derivatives

$\left\{ \left[\frac{dP_i(x)}{dx} \right]_{x=x_n} : n \geq 0 \right\}$ which may be used to generate the derivatives if

needed. In the absence of such relationships, it is trivial to differentiate the recursion any number of times to obtain equations useful for computing derivatives. For example,

$$\left[\frac{dP_i(x)}{dx} \right]_{x=x_n} = (A_i x_n + B_i) \left[\frac{dP_{i-1}(x)}{dx} \right]_{x=x_n} - C_i \left[\frac{dP_{i-2}(x)}{dx} \right]_{x=x_n} + A_i P_{i-1}(x_n), \quad (6)$$

may be used for the first derivative once the functions are known. Starting from a three-term recurrence relation it is possible to determine two linearly independent sets of polynomials with initial conditions

$$P_0(x_n) = 1, \quad P_1(x_n) = A_0 x_n + B_0, \quad \left[\frac{dP_0(x)}{dx} \right]_{x=x_n} = 0, \quad (7)$$

$$\left[\frac{dP_1(x)}{dx} \right]_{x=x_n} = A_0.$$

The recurrence relation (4) and the positivity condition (5) imply orthogonality [8].

The Pollaczek polynomials are defined by three-term recurrence relation

$$iP_i^\lambda(x; a, b) - 2[(i-1+\lambda+a)x+b]P_{i-1}^\lambda(x; a, b) + (i+2\lambda-2)P_{i-2}^\lambda = 0$$

$$i = 1, 2, \dots, \quad (8)$$

with initial conditions: $P_{-1}^\lambda(x; a, b) = 0$ and $P_0^\lambda(x; a, b) = 1$. They have the generating function

$$\sum_{i=0}^{\infty} P_i^\lambda(x; a, b) z^i = (1 - ze^{i\theta})^{-\lambda+i\phi(\theta)} (1 - ze^{-i\theta})^{-\lambda-i\phi(\theta)}, \quad |z| < 1, \quad (9)$$

where $x = \cos \theta$, $0 \leq \theta \leq \pi$, and $\phi(\theta) = \frac{a \cos \theta + b}{2 \sin \theta}$. When a and b real, $a \geq |b|, \lambda > -1$, the Pollaczek polynomials satisfy the orthogonality relation in the interval $-1 \leq x \leq 1$

$$\int_{-1}^{+1} P_i^\lambda(x; a, b) P_j^\lambda(x; a, b) w^\lambda(x; a, b) dx = \lambda_j \delta_{i,j}, \quad \lambda_i = \frac{\Gamma(i+2\lambda)}{(i+\lambda+a/2)i!}, \quad (10)$$

with the weight function [9, 10]

$$w^\lambda(x; a, b) = \frac{2^{2\lambda-1}}{\pi} \exp\{(2\theta - \pi)\phi(\theta)\} (1-x^2)^{\lambda-1/2} |\Gamma(\lambda+i\phi(\theta))|^2. \quad (11)$$

THE THREE-BODY COULOMB WAVE FUNCTIONS AND HAMILTONIAN

We consider first a system of two electrons in *LS* coupling. We define the orbital functions in radial, ϕ_l , spherical harmonic, $Y_{lm}(\hat{r})$, and spin function, $\chi(\sigma)$, for a single-electron as

$$\varphi(x) = \frac{1}{r} \phi_l(r) Y_{lm}(\hat{r}) \chi(\sigma). \quad (12)$$

Here x is used to denote both the spatial and spin coordinates. The radial part of the single-particle functions, can then be written using the non-orthogonal Laguerre-type function basis (see Yamani and Reinhardt [2])

$$\phi_{il}(r) = (\lambda_i r)^{l+1} \exp(-\lambda_i r/2) L_i^{2l+1}(\lambda_i r), \quad (13)$$

where the $L_i^{2l+1}(\lambda_i r)$ are the associated Laguerre polynomials, λ_i is the interaction parameter and i ranges from 1 to the basis size n . The two-particle space is written in terms of the product of these orbital for coordinates r_1 and r_2 . We may rearrange these products into linear combinations which are eigenvalues of the total orbital angular momentum and total spin

$$|\varphi_\alpha(x_1)\varphi_\beta(x_2):\pi l m s v\rangle = \frac{1}{r_1 r_2} \phi_{i_\alpha l_\alpha}(r_1)\phi_{i_\beta l_\beta}(r_2)|l_\alpha l_\beta:lm\rangle X(sv), \quad (14)$$

the notation α and β are used to denote the first and second electron, where

$$|l_\alpha l_\beta:lm\rangle = \sum_{m_\alpha, m_\beta} \langle l_\alpha l_\beta m_\alpha m_\beta | lm \rangle Y_{l_\alpha m_\alpha}(\hat{r}_1) Y_{l_\beta m_\beta}(\hat{r}_2), \quad (15)$$

and the two-electron spin function is defined by

$$X(sv) = \sum_{\sigma_1, \sigma_2} \left\langle \frac{1}{2} \frac{1}{2} \mu_\alpha \mu_\beta \middle| sv \right\rangle \chi_{\frac{1}{2}\mu_\alpha}(\sigma_1) \chi_{\frac{1}{2}\mu_\beta}(\sigma_2). \quad (16)$$

The three-body Coulomb wave functions in configuration interaction form are

$$\Phi_{\pi l m s v}(x_1, x_2) = \sum_{i_\alpha, i_\beta} C_{i_\alpha i_\beta}^{(\alpha\beta)} \frac{1}{r_1 r_2} \phi_{i_\alpha l_\alpha}(r_1)\phi_{i_\beta l_\beta}(r_2)|l_\alpha l_\beta:lm\rangle X(sv), \quad (17)$$

where the configuration interactions are chosen so that the selection rules are satisfied for the combination $(\alpha\beta)$ and they are correctly anti-symmetrized two-electron states of parity $(-1)^{l_\alpha+l_\beta}$ and with total orbital angular momentum eigenvalues l, m and spin eigenvalues s, v . Here the configuration interaction coefficients $C_i^{(\alpha\beta)}$ satisfy the symmetry property

$$C_i^{(\alpha\beta)} = (-1)^{l_\alpha+l_\beta-l-s} C_i^{(\beta\alpha)}, \quad (18)$$

to ensure anti-symmetry of the two-electron system states.

The non-relativistic three-body Coulomb Hamiltonian can be written as

$$H = H_1 + H_2 + V_{12}, \quad (19)$$

where

$$H_i = K_i + V_i = -\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}, \quad (20)$$

for $i = 1, 2$, is the one-electron Hamiltonian of the He^+ ion ($Z = 2$), and

$$V_{12} = \frac{1}{|r_1 - r_2|}, \quad (21)$$

is the electron-electron potential. Atomic units (a.u.) are assumed throughout.

THE THREE-BODY COULOMB POTENTIAL POLYNOMIALS

We consider first a system of two electrons in LS coupling. Whereas the general Hamiltonian formalism in Eq. (19) includes two-electron excitation, in practice we have found that it is sufficient to use the frozen-core model, where one of the electrons is in a fixed orbital (the ground state) while the second electron is described by a set of independent L^2 functions, thus permitting it to span the discrete and continuum excitations, in which all configurations have one of the electrons occupying the lowest orbital.

In order to get a good description of the ground state ($1s$) polynomial, we must diagonalized the ground state Hamiltonian in $\Phi(x_1, x_2)$

$$\langle \Phi_m | -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} - \mathcal{E}_{i_\alpha} | \Phi_n \rangle = 0, \quad (22)$$

where \mathcal{E}_{i_α} is the energy associated with the $1s$ state of He^+ ion. By using the recurrence relations, orthogonality relation and differentiation formula of the Laguerre polynomial [8, 10], Eq. (22) finally becomes

$$i_\alpha P_{i_\alpha}^{l_\alpha+1}(x_\alpha) = 2 \left[\left(i_\alpha + l_\alpha - 2\frac{Z}{\lambda_{l_\alpha}} \right) x_\alpha + 2\frac{Z}{\lambda_{l_\alpha}} \right] P_{i_\alpha-1}^{l_\alpha+1}(x_\alpha) - (i_\alpha + 2l_\alpha) P_{i_\alpha-2}^{l_\alpha+1}(x_\alpha), \quad (23)$$

$$i_\alpha = 1, 2, \dots$$

To initialize the recurrence one sets

$$P_{-1}^{l_\alpha+1}(x_\alpha) = 0; \quad P_0^{l_\alpha+1}(x_\alpha) = 1, \quad (24)$$

where

$$P_{i_\alpha}^{l_\alpha+1}(x_\alpha) = \frac{\Gamma(i_\alpha + 2l_\alpha + 1)}{\Gamma(i_\alpha + 1)} C_{i_\alpha}^\alpha(x_\alpha), \quad (25)$$

and

$$x_{i_\alpha} = \frac{\mathcal{E}_{i_\alpha} - \frac{\lambda_{i_\alpha}^2}{8}}{\mathcal{E}_{i_\alpha} + \frac{\lambda_{i_\alpha}^2}{8}}. \quad (26)$$

The energy \mathcal{E}_{i_α} which are obtained from (26) are given by

$$\mathcal{E}_{i_\alpha} = \frac{\lambda_{i_\alpha}^2}{8} \left[\frac{1 + x_{i_\alpha}}{1 - x_{i_\alpha}} \right]. \quad (27)$$

The excitation states polynomial for $\Phi(x_1, x_2)$ can now be obtained by solving the equation

$$\langle \Phi_m | -\frac{1}{2} \nabla^2 - \frac{Z}{r_2} + \frac{1}{|r_1 - r_2|} - \mathcal{E}_{i_\beta} | \Phi_n \rangle = 0, \quad (28)$$

where \mathcal{E}_{i_β} is the energy associated with the excitation states of the helium atom.

The matrix elements of the electron-electron potential interaction for states where the orbital angular momenta of the two non-equivalent electrons (different n and l) are coupled to a specific l and the spins to a specific s . The expectation value of the electron-electron potential interaction for this state consists of two direct terms for which the ordering of the quantum numbers is the same on both sides and two exchange terms for which the order is reversed. The electron-electron potential matrix elements may then be written as the difference of a direct and an exchange matrix element, for an LS configuration ($l_\alpha = 0, l = l_\beta$), this reduces to the simple expression

$$\begin{aligned} & \left\langle \Phi_{lmsv}^{(\alpha\beta)} \left| \frac{1}{|r_1 - r_2|} \right| \Phi_{lmsv}^{(\alpha\beta)} \right\rangle = \\ & \left\langle \phi_\alpha(r_1) \left| \phi_\alpha(r_1) \right\rangle \left\langle \phi_\beta(r_2) \left| \frac{2}{r_2} \right| \phi_\beta(r_2) \right\rangle \quad (29) \\ & + \frac{(-1)^s}{(2l_\beta + 1)} \int_0^\infty \int_0^\infty \frac{r_{<}^{l_\beta}}{r_{>}^{l_\beta+1}} \phi_\alpha(r_2) \phi_\beta(r_1) \phi_\alpha(r_1) \phi_\beta(r_2) dr_1 dr_2 \end{aligned}$$

in which $r_{<}$ stands for the smaller of the two distances $|r_1|$ and $|r_2|$, $r_{>}$ is greater of the two distances $|r_1|$ and $|r_2|$. This configuration has two *LS* terms: a *triplet* term with $s = 1$ (3l) and a *singlet* term with $s = 0$ (1l). These two terms are split by the exchange part of the electron-electron potential interaction. Thus, this splitting of the two spin states is a consequence of the anti-symmetry of functions. In order to use this formula for a real system, made up of indistinguishable particles, we must, of course, use properly anti-symmetrized functions.

After the same step as the ground states equation and the electron-electron potential interaction calculation of a two-electron system, Eq. (28) can be written as

$$\begin{aligned} & 2 \left[\left(i_\beta + l_\beta - \left(2 \frac{Z}{\lambda_{l_\beta}} - \frac{2}{\lambda_{l_\beta}} - V_{exc} \right) \right) x_\beta + \left(2 \frac{Z}{\lambda_{l_\beta}} - \frac{2}{\lambda_{l_\beta}} - V_{exc} \right) \right] P_{i_\beta-1}^{l_\beta+1}(x_\beta) \\ & - (i_\beta + 2l_\beta) P_{i_\beta-2}^{l_\beta+1}(x_\beta) = i_\beta P_{i_\beta+1}^{l_\beta+1}(x_\beta), \quad i_\beta = 1, 2, \dots, \quad (30) \end{aligned}$$

to initialize the recurrence one sets

$$P_{-1}^{l_\beta+1}(x_\beta) = 0; \quad P_0^{l_\beta+1}(x_\beta) = 1, \quad (31)$$

where

$$P_{i_\beta}^{l_\beta+1}(x_\beta) = \frac{\Gamma(i_\beta + 2l_\beta + 1)}{\Gamma(i_\beta + 1)} C_{i_\beta}^\beta(x_\beta), \quad (32)$$

$$V_{exc} = \frac{2 \left(\frac{\lambda_{l_\beta}}{\lambda_{l_\alpha}} \right)^{l_\beta} \frac{(-1)^s}{(2l_\beta + 1)} \int_0^\infty \int_0^\infty \frac{r_{<}^{l_\beta}}{r_{>}^{l_\beta+1}} \phi_\alpha(r_2) \phi_\beta(r_1) \phi_\alpha(r_1) \phi_\beta(r_2) dr_1 dr_2}{\left\langle \phi_\alpha(r_1), \phi_\alpha(r_1) \right\rangle \left\langle \phi_\beta(r_2), \phi_\beta(r_2) \right\rangle}, \quad (33)$$

and

$$x_{i_\beta} = \frac{\mathcal{E}_{i_\beta} - \frac{\lambda_{i_\beta}^2}{8}}{\mathcal{E}_{i_\beta} + \frac{\lambda_{i_\beta}^2}{8}}. \quad (34)$$

The energy \mathcal{E}_{i_β} which is obtained from equation (34) is given by

$$\mathcal{E}_{i_\beta} = \frac{\lambda_{i_\beta}^2}{8} \left[\frac{1 + x_{i_\beta}}{1 - x_{i_\beta}} \right]. \quad (35)$$

It is clear that the resulting three-term recurrence relation (23) and (30) are a special case of recurrence relation (8) satisfied by the Pollaczek polynomials.

The three-term recurrence relation (23) and (30) are defined by the generality three-term recurrence relation

$$iP_i^\lambda(x) - 2[(i-1+\lambda-a)x+a]P_{i-1}^\lambda(x) + (i+2\lambda-2)P_{i-2}^\lambda(x) = 0, \quad (36)$$

$$i = 1, 2, \dots,$$

where (the subscript of α and β for (23) and (30) respectively),

$$a_\alpha = \frac{2Z}{\lambda_{i_\alpha}}; \quad a_\beta = \frac{2Z}{\lambda_{i_\beta}} - \frac{2}{\lambda_{i_\beta}} - V_{exc}, \quad (37)$$

and

$$\lambda_\alpha = l_\alpha + 1; \quad \lambda_\beta = l_\beta + 1, \quad (38)$$

are orthogonal polynomials when the positivity condition (5) holds. The following sequence of inequalities must be valid

$$0 < (i-2+\lambda-a)(i-1+\lambda-a)(i+2\lambda-2), \quad i = 1, 2, \dots \quad (39)$$

Case A: $\lambda > 0$. The inequality in (39) with $i = 1$ is

$$(\lambda - a - 1)(\lambda - a)(2\lambda - 1) > 0. \quad (40)$$

This inequality will be satisfied if $(\lambda - a) > 0$. Moreover, the remaining inequalities in (39) for $i = 2, 3, \dots$ will also be satisfied. On the other hand, if $(\lambda - a) < 0$, then there will be a smallest integer k such that $(k + \lambda - a) > 0$. The k th inequality in (39) will fail, since $(k + \lambda - a - 1) \leq 0$. This shows that if $\lambda > 0$, then the polynomials generated by the recurrence relation (36) are orthogonal with respect to a positive measure if and only if $(\lambda - a) > 0$.

Case B: $-\frac{1}{2} < \lambda < 0$. Since λ is negative, (40) holds when $(\lambda - a - 1)$ and $(\lambda - a)$ have opposite signs. In particular, (40) holds when $(\lambda - a) > 0$ and $(\lambda - a - 1) < 0$. It follows that $(\lambda - a) > 0$ and $(1 + \lambda - a) > 0$. The inequality in (39) for $i = 2$ is

$$(\lambda - a)(1 + \lambda - a)(2\lambda) > 0. \tag{41}$$

This holds because $-\frac{1}{2} < \lambda$, so $(2\lambda) > 0$ in this case. Moreover, each of the terms in (39) will be positive for the remaining inequalities when $i = 3, 4, \dots$. When either $(\lambda - a) < 0$ or $(\lambda - a - 1) > 0$, (40) fails. This shows that for $-\frac{1}{2} < \lambda < 0$ the polynomials generated by recurrence (36) are orthogonal with respect to a positive measure if and only if $-1 < \lambda - a < 0$.

Case C: $\lambda < -\frac{1}{2}$. In this case $(2\lambda - 1) < 0$ and $(2\lambda) < 0$. The validity of (40) would require $(\lambda - a - 1)$ and $(\lambda - a)$ to have opposite signs. Now (41) requires $(\lambda - a)$ and $(1 + \lambda - a)$ to have opposite signs. This is impossible. This shows that when $\lambda < -\frac{1}{2}$ the recurrence (36) will never generate an infinite set of polynomials orthogonal with respect to a positive measure.

In summary, the positivity condition for (5) holds if and only if

$$\lambda > 0 \text{ and } (\lambda - a) > 0 \tag{42a}$$

or

$$-\frac{1}{2} < \lambda < 0 \text{ and } -1 < \lambda - a < 0. \tag{42b}$$

THE COMPLETENESS OF THE THREE-BODY COULOMB WAVE FUNCTIONS

With the aid of the recurrence relations and orthogonality relation of Laguerre polynomial and Christoffel-Darboux relation [8] satisfied by the Pollaczek polynomial, the normalization configuration interaction constants $C_{i_\alpha}^\alpha$ and $C_{i_\beta}^\beta$ can be expressed as follows

$$\left[C_{ni_\alpha}^\alpha \right]^2 = \frac{\lambda_\alpha}{1 - x_{ni_\alpha}^{l_\alpha}} \frac{\Gamma(i_\alpha + 2l_\alpha + 1)}{\Gamma(i_\alpha + 1)} \left[P_{n_\alpha - 1}^{l_\alpha} \left(x_{ni_\alpha}^{l_\alpha} \right) \left\{ \frac{d}{dx} P_{n_\alpha}^{l_\alpha} \right\}_{x=x_{ni_\alpha}^{l_\alpha}} \right]^{-1} \tag{43a}$$

and

$$\left[C_{ni_\beta}^\beta \right]^2 = \frac{\lambda_\beta}{1 - x_{ni_\beta}^{l_\beta}} \frac{\Gamma(i_\beta + 2l_\beta + 1)}{\Gamma(i_\beta + 1)} \left[P_{n_\beta - 1}^{l_\beta} \left(x_{ni_\beta}^{l_\beta} \right) \left\{ \frac{d}{dx} P_{n_\beta}^{l_\beta} \right\}_{x=x_{ni_\beta}^{l_\beta}} \right]^{-1}. \tag{43b}$$

The observation that for the Laguerre basis (13) in the three-body Coulomb wave functions have L^2 expansion coefficients proportional to the Pollaczek polynomial can be exploited further to show a connection with Gaussian quadrature rules. Consider the completeness relation for the true eigenfunctions folded between two arbitrary L^2 wave functions $|f\rangle$ and $|g\rangle$

$$\sum_i \langle f | \Phi_{ii} \rangle \langle \Phi_{ii} | g \rangle + \int_0^\infty \langle f | \Phi_{Ei} \rangle \langle \Phi_{Ei} | g \rangle dE = \langle f | g \rangle \tag{44}$$

and a finite basis representation in the space spanned by the first n basis states of Eq. (13) type

$$\sum_i^n \langle f | \Phi_{ni} \rangle \langle \Phi_{ni} | g \rangle = \langle f | g \rangle_n. \tag{45}$$

Generally $|f\rangle$ and $|g\rangle$ may be chosen to possess an infinite number of non-zero Fourier coefficients so

$$\langle f|g\rangle_n \neq \langle f|g\rangle, \tag{46}$$

but

$$\langle f|g\rangle_n \rightarrow \langle f|g\rangle \quad \text{as } n \rightarrow \infty. \tag{47}$$

To derive an equivalent quadrature rule for this convergence we write (44) as

$$\langle f|g\rangle_n = \sum_{i_\alpha, i_\beta}^n (C_{ni}^{(\alpha\beta)})^2 \langle f|\Phi_n(x_{ni}^{(\alpha\beta)})\rangle \langle \Phi_n(x_{ni}^{(\alpha\beta)})|g\rangle. \tag{48}$$

We see that the implied quadrature rule for a function $f(x)$ is

$$\int_a^b w(x)f(x)dx = \sum_{i=1}^n (C_{ni}^{(\alpha\beta)})^2 f(x_{ni}^{(\alpha\beta)}). \tag{49}$$

The interval limit $[a, b]$ comprise any interval which covers the point and continuum mapped into x variable. The quadrature rule (49) can be identified as a special case of Gaussian quadrature based Pollaczek polynomials. This can be seen by noting some standard results that for general orthogonal polynomial there exists a Gaussian quadrature formula given by Chihara [11]. The associated quadrature weights, w_{ni} , are given by

$$w_{ni}^{(\alpha\beta)} = \frac{\pi\Gamma(n+2l+1)}{2^{2l}\Gamma(n+1)} \frac{1}{P_{n-1}^{l+1}(x_{ni}^{(\alpha\beta)}) \frac{d}{dx} P_n^l(x_{ni}^{(\alpha\beta)})}. \tag{50}$$

The configuration interaction coefficient $C_{ni}^{(\alpha\beta)}$ in Eq. (43) which are then determined using (50) is given by

$$(C_{ni}^{(\alpha\beta)})^2 = \frac{2^{2l(\alpha\beta)}}{\pi} \frac{\lambda_{l(\alpha\beta)}}{(1-x_{ni}^{(\alpha\beta)})} w_{ni}^{(\alpha\beta)}. \tag{51}$$

NUMERICAL RESULTS

We state a number of results that can be obtained by choosing subsets of the basis we have truncated the Fourier expansion. This is equivalent to imposing the boundary condition that the $(n+1)$ th coefficient is zero, namely that

$$P_n^{l+1}(x_{ni}) = 0, \quad i = 0, 1, \dots, n-1 \quad (52)$$

as the notation implies there are n real roots to the Eqs. (23) and (30).

A good description of the ground state ($\epsilon_{i\alpha} = -2.00$ a.u.), we take $\lambda_{i\alpha} = 4.0$ for $n_\alpha = 1$ in (23). The second electron can be in any nl state $n_\beta \geq 1$, we use the set of $n_\beta = 5, 10, 15$ and 20 with $\lambda_{i\beta} = 0.93$ for the 1^3S states to obtain an approximation of negative and positive states in (30). All of the roots and resulting eigenvalues are presented in Table 1. All excited-state energies are described to an accuracy of better than 0.1% and are presented in Table 2. We obtained the energy of -2.862345 a.u. for 1^1S in the basis size 5. It is shown by increasing the number of basis size up to 20 we obtained the convergence number of -2.870211 a.u. while the experiment measured -2.903386 a.u. [12, 13]. The discrepancy between the calculated and the experiment is 0.988%. In order to increase the convergence for 1^1S one can slightly change $\lambda_{i\beta}$ and results are presented in Table 3. The values of the configuration interaction coefficient C_1^α and weight w_1^α which belong to the ground state ($1s$) are 1.4141959 and -1.62830282×10^4 . The values of $w_{ni\beta}^\beta$ and $C_{ni\beta}^\beta$ are tabulated in Tables 4 and 5 for singlet and triplet S -states with different basis size and $\lambda_{i\beta} = 0.93$ respectively.

CONCLUDING REMARKS

As we indicated in the Introduction, the general Pollaczek polynomials $\{P_i^\lambda(x; a, b)\}$ are orthogonal with respect to an absolutely distribution function if

$$a \geq |b|, \quad \lambda > -1. \quad (53)$$

Note that

$$P_i^\lambda(-x; a, -b) = (-1)^i P_i^\lambda(x; a, b), \quad (54)$$

which easily follows from the generating function (9), indicates that there is no loss of generality in considering only one of the cases $b \geq 0$ or $b \leq 0$. The positivity condition (5) in the case of $\{P_i^\lambda(x; a, b)\}$ is independent of b , since b appears neither in A_i nor in C_i . This means that $\{P_i^\lambda(x; a, b)\}$ are orthogonal if and only if (42a) or (42b) holds.

Using the restricted basis for the three-body Coulomb states in which one of the electrons is in fixed orbital ($1s$) while the second electron is described by a set of independent L^2 functions, we are able to produce the complete helium atom energies which agree well with the experimental results of references [12, 13] and other calculations of Konovalov and McCarthy [14] and Accad et al. [15]. The convergence of the energies is shown as the Laguerre basis size increases. For example, we obtained the energy of -2.174905 a.u. for 1^3S in the basis size 5. It is shown by increasing the number of basis size up to 20 we obtained the convergence number of -2.174940 a.u. while the experiment measured -2.175028 a.u. [12, 13].

The completeness relation of the three-body Coulomb wave functions is calculated in terms of the configuration interaction coefficient via the Gaussian quadrature. It is shown that the weights and configuration interaction coefficients converge to certain number for different basis size.

ACKNOWLEDGMENTS

The authors like to thank Prof. Andris Stelbovics and Prof. Igor Bray for their helpful references they supplied.

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TABLE 1: The roots and pseudo-states energies ($\epsilon_{i_\alpha} + \epsilon_{i_\beta}$) which are produced from non-orthogonal Laguerre- L^2 expansions are shown for the ground states, $\lambda_\alpha = 4.0$ for $n_\alpha = 1, {}^1, {}^3S$ excited states, $\lambda_\beta = 0.93$ for $n_\beta = 5, 10, 15$ and 20. Powers of ten are denoted by the number in brackets.

N_β	i	x_{i_β}	1S	x_{i_β}	3S
5	1	0.66808090(+1)	-2.145	0.13282618(+1)	-2.175
	2	-0.35185507(+1)	-2.060	0.41686718(+1)	-2.068
	3	-0.16628586(+1)	-2.027	-0.50627876(+1)	-2.024
	4	-0.35362914	-1.949	-0.15819399(+1)	-2.022
	5	0.68283608	-1.430	0.38607842	-1.757
10	1	0.66808089(+1)	-2.145	0.13250302(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18855244(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14455480(+1)	-2.020	-0.21120690(+1)	-2.022
	5	-0.10519270(+1)	-2.003	-0.15184051(+1)	-2.001
	6	-0.57415939	-1.971	-0.10145974(+1)	-1.956
	7	-0.77645763(-1)	-1.908	-0.42011142	-1.851
	8	0.37253183	-1.765	0.16170720	-1.521
	9	0.72269176	-1.333	0.63352830	-1.150
	10	0.93569806	1.234	0.92129230	0.622
15	1	0.66808089(+1)	-2.145	0.13250260(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18857648(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14816654(+1)	-2.021	-0.21123202(+1)	-2.024
	5	-0.12887558(+1)	-2.014	-0.15654176(+1)	-2.015
	6	-0.10902887(+1)	-2.005	-0.13298493(+1)	-2.005
	7	-0.84176699	-1.991	-0.10998427(+1)	-1.989
	8	-0.56057641	-1.970	-0.81221773	-1.963
	9	-0.26506416	-1.938	-0.48953736	-1.922
	10	0.27839887(-1)	-1.886	-0.15626455	-1.850
	11	0.30247889	-1.799	0.16520870	-1.714
	12	0.54481143	-1.635	0.45456512	-1.405
	13	0.74294921	-1.272	0.69410085	-0.462
	14	0.88776305	-0.193	0.86942456	5.279
	15	0.97358844	6.027	0.97091398	7.258

TABLE 1 (continued) : The roots and pseudo-states energies ($\epsilon_{i_\alpha} + \epsilon_{i_\beta}$) which are produced from non-orthogonal Laguerre- L^2 expansions are shown for the ground states, $\lambda_{i_\alpha} = 4.0$ for $n_\alpha = 1, {}^1, {}^3S$ excited states, $\lambda_{i_\beta} = 0.93$ for $n_\beta = 5, 10, 15$ and 20. Powers of ten are denoted by the number in brackets.

N_β	i	x_{i_β}	1S	x_{i_β}	3S
20	1	0.66808089(+1)	-2.145	0.13250260(+1)	-2.175
	2	-0.35195686(+1)	-2.060	0.41686005(+1)	-2.068
	3	-0.18857648(+1)	-2.033	-0.50659650(+1)	-2.036
	4	-0.14819681(+1)	-2.021	-0.21123202(+1)	-2.024
	5	-0.13084548(+1)	-2.014	-0.15656459(+1)	-2.016
	6	-0.11979999(+1)	-2.010	-0.13501023(+1)	-2.011
	7	-0.10705412(+1)	-2.004	-0.12233178(+1)	-2.004
	8	-0.91232049	-1.995	-0.10829059(+1)	-1.995
	9	-0.73101700	-1.983	-0.90766420	-1.982
	10	-0.53401026	-1.967	-0.70670226	-1.963
	11	-0.32808692	-1.946	-0.48919027	-1.937
	12	-0.11972151	-1.916	-0.26355659	-1.900
	13	0.84878801(-1)	-1.873	-0.37805456(-1)	-1.845
	14	0.27982937	-1.809	0.18045213	-1.759
	15	0.45966677	-1.710	0.38408549	-1.612
	16	0.61946674	-1.543	0.56657397	-1.334
	17	0.75496825	-1.231	0.72214597	-0.713
	18	0.86269873	-0.543	0.84592530	1.156
	19	0.94010779	1.480	0.93416906	12.146
	20	0.98575646	12.975	0.98492723	13.250

TABLE 2: The ground and excited-states eigenvalues ($\epsilon_{i_\alpha} + \epsilon_{i_\beta}$) of the non-relativistic Hamiltonian of the three-body Coulomb wave functions (in a.u.) are shown as a function of number of L^2 basis functions $n_\beta = 5, 10, 15$ and 20. The observation results by references [12, 13]. Highly accurate non-relativistic energy levels of the helium atom by Konovalov and McCarthy (KM) [14] and by Accad et al. [15].

n_β	5	10	15	20	Observation	KM	Accad et al.
State		[Present work]			[12, 13]	[14]	[15]
1^1S	-2.862345	-2.868680	-2.868880	-2.870211	-2.903386	-2.87247	-2.90372
2^3S	-2.174905	-2.174918	-2.174940	-2.174988	-2.175028	-2.1742	-2.17523
2^1S	-2.145175	-2.145385	-2.145575	-2.145678	-2.145770	-2.1434	-2.14597
3^3S	-2.068295	-2.068320	-2.068358	-2.068399	-2.068497	-2.0684	-2.06869
3^1S	-2.060760	-2.060798	-2.060860	-2.060952	-2.061079	-2.0605	-2.06127
4^3S	-2.024980	-2.035111	-2.035326	-2.035420	-2.036323		
4^1S	-2.027555	-2.032980	-2.033290	-2.033307	-2.033398		

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TABLE 3: Convergence of the ground states (1^1S) eigenvalues ($\epsilon_{i_\alpha} + \epsilon_{i_\beta}$) for the three-body Coulomb wave functions (in a.u.) are shown as a function of number of L^2 basis functions $n_\beta = 5, 10, 15$ and 20 and λ_{i_β} .

$\lambda_{i_\beta} \backslash n_\beta$	5	10	15	20
0.63	-2.537891	-2.538022	-2.538223	-2.538300
0.73	-2.624580	-2.624789	-2.625024	-2.625432
0.83	-2.756891	-2.757022	-2.757202	-2.757348
0.93	-2.862345	-2.868680	-2.868880	-2.870211
1.03	-2.899875	-2.903346	-2.903356	-2.903366
1.13	-3.024432	-3.024502	-3.024555	-3.024588
1.23	-3.103346	-3.103368	-3.103389	-3.103402

TABLE 4: The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{i_\beta} = 0.93$, $I_\beta = 0$ (singlet) and different basis sizes n_β . Powers of ten are denoted by the number in brackets.

n_β	I_β	x_{ni_β}	w_{ni_β}	$\sum_{i_\beta}^{n_\beta} w_{ni_\beta}$	$C_{ni_\beta}^\beta$
1	1	0.73493151(+1)	-0.99734808(+1)	-0.99734808(+1)	0.68080834
5	1	0.66808090(+1)	-0.10774258(+2)	-0.99734808(+1)	0.74808942
	2	-0.35185507(+1)	0.31493798		0.14340948
	3	-0.16628586(+1)	0.14155879		0.12524468
	4	-0.35362914	0.20171034		0.20969070
	5	0.68283608	0.14256958		0.36419709
10	1	0.66808089(+1)	-0.10772700(+2)	-0.99734808(+1)	0.74803536
	2	-0.35195686(+1)	0.31248160		0.14283304
	3	-0.18855244(+1)	0.71324684(-1)		0.85402873(-1)
	4	-0.14455480(+1)	0.41947328(-1)		0.71142478(-1)
	5	-0.10519270(+1)	0.58201515(-1)		0.91485259(-1)
	6	-0.57415939	0.73797063(-1)		0.11761430
	7	-0.77645763(-1)	0.81947100(-1)		0.14979376
	8	0.37253183	0.78209674(-1)		0.19177824
	9	0.72269176	0.57963768(-1)		0.24834868
	10	0.93569806	0.23346650(-1)		0.32731445

TABLE 4 (continued): The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{i\beta} = 0.93$, $l_{\beta} = 0$ (singlet) and different basis sizes n_{β} . Powers of ten are denoted by the number in brackets.

n_{β}	I_{β}	$x_{ni_{\beta}}$	$w_{ni_{\beta}}$	$\sum_{i_{\beta}}^{n_{\beta}} w_{ni_{\beta}}$	$C_{ni_{\beta}}^{\beta}$
15	1	0.66808089(+1)	-0.10772700(+2)	-0.99734808(+1)	0.74803535
	2	-0.35195686(+1)	0.31248160		0.14283304
	3	-0.18857648(+1)	0.71114521(-1)		0.85273406(-1)
	4	-0.14816654(+1)	0.29140499(-1)		0.58862921(-1)
	5	-0.12887558(+1)	0.21661697(-1)		0.52845917(-1)
	6	-0.10902887(+1)	0.29261407(-1)		0.64270162(-1)
	7	-0.84176699	0.36994743(-1)		0.76987035(-1)
	8	-0.56057641	0.43252889(-1)		0.90433632(-1)
	9	-0.26506416	0.47777777(-1)		0.10556541
	10	0.27839887(-1)	0.49986514(-1)		0.12317497
	11	0.30247889	0.49081183(-1)		0.14409329
	12	0.54481143	0.44233034(-1)		0.16933340
	13	0.74294921	0.34947410(-1)		0.20029170
	14	0.88776305	0.21760215(-1)		0.23918206
	15	0.97358844	0.75257880(-2)		0.28996389
20	1	0.66808089(+1)	-0.10772700(+2)	-0.99734808(+1)	0.74803534
	2	-0.35195686(+1)	0.31248160		0.14283303
	3	-0.18857648(+1)	0.71114521(-1)		0.85273406(-1)
	4	-0.14819681(+1)	0.28915174(-1)		0.58631329(-1)
	5	-0.13084548(+1)	0.15296600(-1)		0.44218265(-1)
	6	-0.11979999(+1)	0.14098964(-1)		0.43505554(-1)
	7	-0.10705412(+1)	0.18763174(-1)		0.51710191(-1)
	8	-0.91232049	0.23190347(-1)		0.59818871(-1)
	9	-0.73101700	0.27023846(-1)		0.67871562(-1)
	10	-0.53401026	0.30294044(-1)		0.76336005(-1)
	11	-0.32808692	0.32924161(-1)		0.85528142(-1)
	12	-0.11972151	0.34764632(-1)		0.95714721(-1)
	13	0.84878801(-1)	0.35613715(-1)		0.10716038
	14	0.27982937	0.35236562(-1)		0.12015559
	15	0.45966677	0.33394312(-1)		0.13504246
	16	0.61946674	0.29894102(-1)		0.15225143
	17	0.75496825	0.24671680(-1)		0.17236660
	18	0.86269873	0.17921714(-1)		0.19625351
	19	0.94010779	0.10305502(-1)		0.22532756
	20	0.98575646	0.33143435(-2)		0.26203222

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TABLE 5: The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{i_\beta} = 0.93$, $l_\beta = 0$ (triplet) and different basis sizes n_β . Powers of ten are denoted by the number in brackets.

n_β	I_β	x_{ni_β}	w_{ni_β}	$\sum_{i_\beta}^{n_\beta} w_{ni_\beta}$	$C_{ni_\beta}^\beta$
1	1	0.15689909(+1)	-0.89376884	-0.89376884	0.68080835
5	1	0.13282618(+1)	-0.84345818	-0.89376884	0.87073610
	2	0.41686718(+1)	-0.68175809(-1)		0.79678560(-1)
	3	-0.50627876(+1)	0.43604365(-3)		0.46067410(-2)
	4	-0.15819399(+1)	0.11690549(-2)		0.11558710(-1)
	5	0.38607842	0.16260060(-1)		0.88403520(-1)
10	1	0.13250302(+1)	-0.85510609	-0.89376884	0.88107540
	2	0.41686005(+1)	-0.67731395(-1)		0.79419330(-1)
	3	-0.50659650(+1)	0.30828950(-3)		0.38725260(-2)
	4	-0.21120690(+1)	0.31064874(-3)		0.54271910(-2)
	5	-0.15184051(+1)	0.26082688(-3)		0.55281310(-2)
	6	-0.10145974(+1)	0.56576811(-3)		0.91031150(-2)
	7	-0.42011142	0.13634289(-2)		0.16831390(-1)
	8	0.16170720	0.35159590(-2)		0.35179440(-1)
	9	0.63352830	0.90251728(-2)		0.85245700(-1)
	10	0.92129230	0.13718550(-1)		0.22678300
15	1	0.13250260(+1)	-0.85512987	-0.89376884	0.88109330
	2	0.41686005(+1)	-0.67731395(-1)		0.79419330(-1)
	3	-0.50659650(+1)	0.30828950(-3)		0.38725260(-2)
	4	-0.21123202(+1)	0.28380453(-3)		0.51871930(-2)
	5	-0.15654176(+1)	0.17210788(-3)		0.44492450(-2)
	6	-0.13298493(+1)	0.14342999(-3)		0.42620740(-2)
	7	-0.10998427(+1)	0.23698094(-3)		0.57706970(-2)
	8	-0.81221773	0.39983448(-3)		0.80686310(-2)
	9	-0.48953736	0.67198745(-3)		0.11537710(-1)
	10	-0.15626455	0.11518934(-2)		0.17145200(-1)
	11	0.16520870	0.20196838(-2)		0.26718840(-1)
	12	0.45456512	0.35650010(-2)		0.43916050(-1)
	13	0.69410085	0.60127339(-2)		0.76157350(-1)
	14	0.86942456	0.83331104(-2)		0.13722640
	15	0.97091398	0.57935694(-2)		0.24243530

TABLE 5: The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{i_\beta} = 0.93$, $l_\beta = 0$ (triplet) and different basis sizes n_β . Powers of ten are denoted by the number in brackets.

n_β	I_β	x_{ni_β}	w_{ni_β}	$\sum_{i_\beta}^{n_\beta} w_{ni_\beta}$	$C_{ni_\beta}^\beta$
20	1	0.13250260(+1)	-0.85512987	-0.89376884	0.88109330
	2	0.41686005(+1)	-0.67731395(-1)		0.79419330(-1)
	3	-0.50659650(+1)	0.30828950(-3)		0.38725260(-2)
	4	-0.21123202(+1)	0.28380453(-3)		0.51871930(-2)
	5	-0.15656459(+1)	0.17115898(-3)		0.44367650(-2)
	6	-0.13501023(+1)	0.10206099(-3)		0.35797390(-2)
	7	-0.12233178(+1)	0.97126148(-4)		0.35903120(-2)
	8	-0.10829059(+1)	0.14709215(-3)		0.45648320(-2)
	9	-0.90766420	0.21703996(-3)		0.57940710(-2)
	10	-0.70670226	0.31319220(-3)		0.73585380(-2)
	11	-0.48919027	0.45165529(-3)		0.94600490(-2)
	12	-0.26355659	0.65678171(-3)		0.12384490(-1)
	13	-0.37805456(-1)	0.96599589(-3)		0.16572750(-1)
	14	0.18045213	0.14353021(-2)		0.22732620(-1)
	15	0.38408549	0.21409900(-2)		0.32026690(-1)
	16	0.56657397	0.31601392(-2)		0.46383180(-1)
	17	0.72214597	0.44773248(-2)		0.68955020(-1)
	18	0.84592530	0.57077487(-2)		0.10455180
	19	0.93416906	0.56444177(-2)		0.15905950
	20	0.98492723	0.28123047(-2)		0.23463870