Eur. Phys. J. D **28**, 307–315 (2004)
DOI: 10.1140/epjd/e2003-00321-4

THE EUROPEAN
PHYSICAL JOURNAL D

Study of non-orthogonal Laguerre-L^2 method for helium atom

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Received 12 May 2003 / Received in final form 20 August 2003

Abstract. We present a technique for describing solutions of the helium atom by using the non-orthogonal Laguerre-L^2 basis functions. The frozen-core approximation is used to calculate the helium energies. The completeness of helium wavefunctions obtained is studied in terms of weights of the Gaussian quadrature. The convergence of the energies is shown as the L^2 basis size increases and the completeness of the L^2 wave functions is also shown for different basis size.

PACS. 34.80.Bm Elastic scattering of electrons by atoms and molecules – 34.80.Dp Atomic excitation and ionization by electron impact

1 Introduction

The L^2 method which uses square integrable (L^2) functions has been the subject of considerable study for the solution of electron-atom scattering problems. Heller et al. [1] restricted the problem to that of understanding the process of extracting scattering information from approximations to the Fredholm determinant calculated in a finite L^2 basis. They showed that a calculation with an L^2 discretised matrix representation of an operator with a continuous spectrum was equivalent to a numerical quadrature approximation to the spectral representation of the operator. Heller et al. [2] further used the equivalent-quadrature relationship between the diagonalisation of the *s*-wave kinetic energy operator in a non-orthogonal Laguerre-type basis and a Chebyschev quadrature of the second kind to construct potential-scattering phase shifts from approximations to the Fredholm determinant using only L^2 functions. They produced highly accurate phase shifts over a continuous range of energies for electron-hydrogen scattering in the static approximation. Heller and Yamani [3] also used L^2 functions of a non-orthogonal Laguerre type to obtain phase shifts, wave functions, etc. for the full Hamiltonian in which the only approximation was made to the potential V. They worked out the method which has become known as the J-matrix method, to calculate the *s*-wave electron-hydrogen scattering model. Heller and Yamani [4] then developed a pseudostate model which is based on the L^2 functions and applied the model to elastic and inelastic scattering above and below the ionisation threshold. Yamani and Reinhardt [5] further generalised the techniques of Heller et al. [1,2] to higher partial waves for Coulomb interactions. They showed the convergence of the expansion for repulsive and attractive-Coulomb phase shifts, and the photoionisation cross-sections. Stelbovics and Slim [6] used the L^2 functions of Laguerre types to describe the scattering solutions of the Schrödinger equation for a variable coupling constant in a simple separable potential model which allows an exact solution. They found that the orthogonal polynomials which are generated by the L^2 solutions were positive definite only for a limited range of the coupling constant. Stelbovics and Winata [7] have studied and examined the convergence rates of the L^2 expansion of non-orthogonal Laguerre types. They showed that the L^2 wavefunctions converges to the exact Coulomb wavefunction in the coordinate representation. They used the Born approximation ionisation cross-section for electron-hydrogen collisions to further studies such as the convergence. It was shown that the convergence rate was rapid.

Konovalov and McCarthy [8] have worked on the Poet-Temkin model of electron-hydrogen scattering that can be solved to any required accuracy using the J-matrix method. The convergence in the basis size is achieved to an accuracy of better than 2% with the inclusion of 37 basis L^2 functions of a non-orthogonal Laguerre type. Previously observed pseudoresonances in the J-matrix calculation naturally disappear with an increase in basis size. For electron-helium excitation cross-sections in the energy region of the $n = 2$ and $n = 3$, the calculation using the J-matrix was later presented by Konovalov and McCarthy [9]. The calculation results were solved to

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an accuracy of better than 3% for $n = 2$ and 5% for $n = 3$ excitation cross-sections. The J-matrix method required wavefunctions of the whole system (He$^-$) target plus the scattering electron. They created the He$^-$ states by adding one more electron to the target configuration with the electron being in one-electron states with $n - l \leq N_l$. The total Hamiltonian of He$^-$ was diagonalized for each total spin S and orbital angular momentum L. More than 1000 configurations were used for various LS. They used the convenient formulae of Fano to calculate the He$^-$ matrix element.

A new expansion of the Coulomb eigenfunctions in an orthogonal Laguerre L^2 basis function was later presented by Stelbovics [10]. It was shown that the new expansion can be directly applied to the coupled-channels formulation of electron-hydrogen scattering. The close-coupling formalism studied by expanding the target states in the orthogonal L^2 Laguerre basis was shown by Bray and Stelbovics [11]. Their theory is without approximation, and convergence is established by increasing the basis size. They present convergent elastic, $2s$, and $2p$ differential electron-hydrogen cross-section, spin asymmetries, and angular-correlation parameters for the $2p$ excitation at 35, 54.4, and 100 eV. The summary of convergent close-coupling theory for the calculation of electron-helium scattering was presented by Fursa and Bray [12]. They demonstrated its applicability for projectile energies in the range of 1.5 to 500 eV to the scattering from the ground state to $n \leq 3$ states. The extensive review and discussion of the convergent close-coupling method can be seen for example in other papers [13–15].

Basis sets of the B-splines type have been tried by Bachau et al. [16] in a new development of the wavefunction of the atomic and molecular physics. B-splines have the property of being "complete enough" with a relatively small number of basis functions and, since linear dependences are negligible, even for a large basis, it is possible for such a basis set to compete with the finite-difference methods. This accounts for the recent swing towards the use of B-splines in atomic calculations, while also for molecular problems, B-splines have considerable advantages over earlier basis sets. B-splines have been used in many other types of calculation of various properties for both bound and continuum states and this is the main subject of the physics part in their review. In particular, B-splines are able to provide a very accurate representation of continuum states, which makes them superior to more conventional L^2 basis sets.

In atomic physics, one approach to describing electron scattering from atomic targets is to use pseudostate coupled-channel equations [17]. In this model one uses a finite basis of L^2 functions to diagonalize the target Hamiltonian thus giving both negative and positive energy states. The basis is usually chosen so that the lowest-lying channels are described adequately while the other bound states are collectively approximated by the remaining energy eigenvectors. The positive energy eigenstates and associated L^2 eigenvector in some way approximate the target continuum. The target states cannot all be included in any practical implementation of the electron scattering equations. A pragmatic way to approach such a calculation is to include the effects of the target states which are liable to be most important, for example in the helium target to choose just the ^{1,3}S and ^{1,3}P levels. Unfortunately it has been observed that such expansions are inadequate at all but the lowest energies; there is considerable evidence that the coupling to all open channels must be included in some way. Above the ionisation threshold this means that allowance for coupling to continuum channels must be made. An efficient way to include such coupling is by means of taking a subspace of the one-body Hilbert space of the target. A convenient basis for the one-body Hilbert space is that provided by the Laguerre functions. In this work we discuss this method in some detail, with the primary purpose being to elucidate the sense in which these finite-basis expansions of the target approximate the true target states so that the convergence of the close-coupling equations of the electron scattering equations can be studied.

Since the ground work of Yamani and Reinhardt [5], Stelbovics and Winata [7] and Stelbovics [10] who developed a systematic approach to illustrate the mathematical sense in which the L^2 functions would approximate electron scattering solutions, the L^2 functions of the non-orthogonal Laguerre-type and the orthogonal Laguerre-type have been widely applied to describe the scattering processes. The L^2 expansion methods with an orthogonal Laguerre basis function has been successfully applied to electron-helium scattering by Fursa and Bray [12,13] and Bray et al. [14] for which they used the frozen-core representation of the helium target. They were interested solely in numerical calculations and did not investigate the completeness of the helium target. They made the assumption that the completeness of the helium target using the frozen-core approximation was similar to the hydrogen target with which Bray and Stelbovics [11] applied to electron-hydrogen scattering. Therefore, we focus on extending the use of non-orthogonal Laguerre basis function using the frozen-core approximation which is a relatively new development in the completeness of a two-electron atom system. Since non-orthogonal Laguerre basis functions have the property of being "complete enough" with a relatively small number of basis functions, it is possible to also apply such a basis set in the electron-helium system.

In this paper, we present a thorough study of the L^2 expansion methods for the helium atom. The non-orthogonal Laguerre basis will be used and the related expansions for discrete and continuum states will be considered. The finite-basis expansions, considered as approximations to the infinite expansion will be studied and their convergence will be shown. The manner in which the L^2 approximated wavefunctions are related to the true eigenstates is examined through the underlying Gaussian quadrature. The frozen-core [12,18] approximation will be used.

This paper is written in the following way. In Section 2, we present the helium configuration. The details of the frozen-core approximation and its L^2 solution of helium atom are given in Section 3. In Section 4 we examine the finite basis solution and the standard presentations of the Gaussian quadrature approximations and their convergence properties. Finally in Section 5, we draw conclusions from this work and indicate future directions for our research.

2 Helium configurations

We consider first a system of two electrons in LS coupling. We define the orbital functions in radial, spherical harmonic and spin functions for a single-electron as:

$$\varphi(x) = \frac{1}{r}\phi_{nl}(r)\,Y_{lm}(\hat{r})\,\chi(\sigma). \tag{1}$$

Here x is used to denote both the spatial and spin coordinates. The radial part of the single-particle functions, we take to be the non-orthogonal Laguerre basis:

$$\phi_{nl}(r) = (\lambda_l r)^{l+1}\exp(-\lambda_l r/2)L_n^{2l+1}(\lambda_l r), \tag{2}$$

where the $L_n^{2l+1}(\lambda_l r)$ are the associated Laguerre polynomials, λ_l is the interaction parameter and n ranges from 1 to the basis size N. The two-particle space is written in terms of the product of these orbitals 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:

$$\begin{aligned}\Phi_{lms\mu}^{(\alpha\beta)}(x_1,x_2) = {}& \frac{1}{r_1 r_2}\phi_{n_\alpha l_\alpha}(r_1)\\ &\times \phi_{n_\beta n_\beta}(r_2)\,|l_\alpha l_\beta : lm\rangle\, X(sv),\end{aligned} \tag{3}$$

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

$$|l_\alpha l_\beta : lm\rangle = \sum_{m_\alpha,m_\beta}\langle l_\alpha l_\beta m_\alpha m_\beta \mid lm\rangle\, Y_{l_\alpha m_\alpha}(\hat{r}_1)Y_{l_\beta m_\beta}(\hat{r}_2), \tag{4}$$

and the two-electron spin function is defined by:

$$X(sv) = \sum_{\sigma_1,\sigma_2}\left\langle \frac{1}{2}\frac{1}{2}\mu_\alpha\mu_\beta \,\middle|\, sv\right\rangle \chi_{\frac{1}{2}\mu_\alpha}(\sigma_1)\,\chi_{\frac{1}{2}\mu_\beta}(\sigma_2). \tag{5}$$

The helium atom states in configuration interaction form are:

$$\Psi_{n\pi lmsv}(x_1,x_2) = \sum_{n_\alpha,n_\beta}^{\infty} C_{n\pi}^{(\alpha\beta)}\Phi_{nlmsv}^{(\alpha\beta)}, \tag{6}$$

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

$$C_n^{(\alpha\beta)} = (-1)^{l_\alpha+l_\beta-l-s}\,C_n^{(\beta\alpha)}, \tag{7}$$

to ensure antisymmetry of the two-electron system states.

3 The L^2 solution of helium atom

The non-relativistic helium atom Hamiltonian can be written as:

$$H = H_1 + H_2 + V_{12}, \tag{8}$$

where:

$$H_i = K_i + V_i = -\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}, \tag{9}$$

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

$$V_{12} = \frac{1}{r_{12}}, \tag{10}$$

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

Whereas the above Hamiltonian formalism is general and includes two-electron excitation, in practice we have found that it is sufficient to make the frozen-core approximation, where one of the electrons is in a fixed orbital 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 [12,18].

In order to get a good description of the He$^+$ ion state, we must diagonalize the ground state ($1s$) Hamiltonian in $\Psi(x_1, x_2)$:

$$\langle\Psi_m| - \frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} - \varepsilon_{n_\alpha}|\Psi_n\rangle = 0, \tag{11}$$

where ε_{n_α} is the energy associated with the $1s$ state of He$^+$ ion. By using equations (1–6) and applying the recurrence formulas of the Laguerre polynomials, the differentiation formula and orthogonality relations [19], equation (11) finally becomes:

$$\begin{aligned}&2\left[\left(n_\alpha + l_\alpha + 1 - 2\frac{Z}{\lambda_{l_\alpha}}\right)X^\alpha + 2\frac{Z}{\lambda_{l_\alpha}}\right]P_{n_\alpha}^{l_\alpha+1}(X^\alpha)\\ &-(n_\alpha+2l_\alpha+1)\,P_{n_\alpha-1}^{l_\alpha+1}(X^\alpha) - (n_\alpha+1)\,P_{n_\alpha+1}^{l_\alpha+1}(X^\alpha) = 0,\end{aligned} \tag{12}$$

where:

$$P_{n_\alpha}^{l_\alpha+1}(X^\alpha) = \frac{\Gamma(n_\alpha+2l_\alpha+1)}{\Gamma(n_\alpha+1)}C_{n_\alpha}^{\alpha}(X^\alpha), \tag{13}$$

to initialize the recurrence one sets:

$$P_{-1}^{l_\alpha+1}(X^\alpha) = 0;\quad P_0^{l_\alpha+1}(X^\alpha) = 1, \tag{14}$$

and:

$$X^\alpha = \frac{\varepsilon_{n_\alpha} - \dfrac{\lambda_{l_\alpha}^2}{8}}{\varepsilon_{n_\alpha} + \dfrac{\lambda_{l_\alpha}^2}{8}}, \tag{15}$$

the energy ε_{n_α} which is obtained from equation (15) and is given by

$$\varepsilon_{n_\alpha} = \frac{\lambda_{l_\alpha}^2}{8}\left[\frac{1+X^\alpha}{1-X^\alpha}\right]. \tag{16}$$

The excitation states for $\Psi(x_1,\ x_2)$ can be obtained by solving the equation:

$$\left\langle \Psi_m \right| -\frac{1}{2}\nabla_2^2 - \frac{Z}{r_2} + \frac{1}{r_{12}} - \varepsilon_{n_\beta} \left| \Psi_n \right\rangle = 0, \tag{17}$$

where ε_{n_β} is the energy associated with the excitation states of the helium atom. After the same step as the ground state equation, equation (17) can be written as:

$$\begin{aligned} &2\left[\left(n_\beta + l_\beta + 1 - \left(2\frac{Z}{\lambda_{l_\beta}} - \frac{2}{\lambda_{l_\beta}} - V_{exc}\right)\right) X^\beta \right. \\ &\qquad \left. + \left(2\frac{Z}{\lambda_{l_\beta}} - \frac{2}{\lambda_{l_\beta}} - V_{exc}\right)\right] P_{n_\beta}^{l_\beta+1}\left(X^\beta\right) \\ &- \left(n_\beta + 2l_\beta + 1\right) P_{n_\beta-1}^{l_\beta+1}\left(X^\beta\right) - \left(n_\beta + 1\right) P_{n_\beta+1}^{l_\beta+1}\left(X^\beta\right) = 0, \end{aligned} \tag{18}$$

where:

$$P_{n_\beta}^{l_\beta+1}\left(X^\beta\right) = \frac{\Gamma\left(n_\beta + 2l_\beta + 1\right)}{\Gamma\left(n_\beta + 1\right)} C_{n_\beta}^{\beta}\left(X^\beta\right), \tag{19}$$

and:

$$\begin{aligned} V_{exc} &= 2\left(\frac{\lambda_{l_\beta}}{\lambda_{l_\alpha}}\right)^{l_\beta} \\ &\times \frac{\dfrac{(-1)^s}{(2l_\beta+1)} \int\limits_0^\infty \int\limits_0^\infty \dfrac{r_<^{l_\beta}}{r_>^{l_\beta+1}} \phi_\alpha(r_2)\phi_\beta(r_1)\phi_\alpha(r_1)\phi_\beta(r_2) dr_1 dr_2}{\langle\phi_\alpha(r_1)|\phi_\alpha(r_1)\rangle\langle\phi_\beta(r_2)|\phi_\beta(r_2)\rangle}, \end{aligned} \tag{20}$$

to initialize the recurrence one sets:

$$P_{-1}^{l_\beta+1}\left(X^\beta\right) = 0; \quad P_0^{l_\beta+1}\left(X^\beta\right) = 1, \tag{21}$$

and:

$$X^\beta = \frac{\varepsilon_{n_\beta} - \dfrac{\lambda_{l_\beta}^2}{8}}{\varepsilon_{n_\beta} + \dfrac{\lambda_{l_\beta}^2}{8}}, \tag{22}$$

the energy ε_{n_β} which is obtained from equation (22) is given by:

$$\varepsilon_{n_\beta} = \frac{\lambda_{l_\beta}^2}{8}\left[\frac{1+X^\beta}{1-X^\beta}\right]. \tag{23}$$

It is clear that equations (12, 18) are just the recurrence relation of Pollaczek polynomials in the variable X.

We state a number of results that can be obtained, by choosing a subset 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:

$$P_N^{l+1}\left(X_{nl}^N\right) = 0, \quad n = 0, 1, ..., N-1 \tag{24}$$

as the notation implies there are N real roots to equations (12, 18). We associate a pseudoenergy ε_{n_α} and ε_{n_β} through the mapping equations (16, 23).

The behavior of the non-orthogonal Laguerre basis in equation (2) is oscillations and dependent upon the number of basis size N and interaction parameter λ_l, therefore the convergence of the resulting eigenvalues in equations (12, 18) are dependent upon the number of the basis size N and interaction parameter λ_l. A good description of the ground state is obtained if we take $\lambda_{l_\alpha} = 4.0$ for $N_\alpha = 1$ in equation (12). 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. In this work, we take $\lambda_{l_\beta} = 0.93$ for the ^{1,3}S states and we take $\lambda_{l_\beta} = 0.72$ (*triplet*) and 0.73 (*singlet*) for the ^{1,3}P states to obtain the number of coupled bound and continuum helium states which are in convergence with the results of other calculations [9,22] and the observations [20,21] in equation (18) except for the 1^1S state. We obtained the energy of −2.862345 a.u. for 1^1S in the basis size 5. It is shown that by increasing the number of the basis size up to 20 the convergence number obtained is −2.870211 a.u. while the experiment gives −2.903386 a.u. [20,21]. The discrepancy between the calculated and the experiment is 0.988%. In order to increase the accuracy for the 1^1S state one can slightly change the interaction parameter λ_{l_β}. For example by choosing $\lambda_{l_\beta} = 1.09$ for $N_\beta = 5$ and $\lambda_{l_\beta} = 1.06$ for $N_\beta = 10, 15$ and 20, we obtain −2.903376 a.u. The resulting eigenvalues are presented in Table 1. All excited-state energies are described to an accuracy of better than 0.1%.

4 Finite basis and equivalent quadrature

The idea that energy pseudostates are connected to the true functions in the manner discussed has been developed in several papers with varying degrees of rigour. The normalisation of the pseudostates is for example required to calculate spectral integrals involving Green's functions constructed for the target Hamiltonian. For example suppose it is necessary to evaluate:

$$\begin{aligned} \langle f|\left(z - H_l\right)^{-1}|f\rangle &= \sum_{n=l+1}^{\infty} \left(z - \varepsilon_{nl}\right)^{-1} \langle f \mid U_{nl}\rangle \langle U_{nl} \mid f\rangle \\ &+ \int\limits_0^\infty dE' \left(z - E'\right) \langle f \mid U_{E'l}\rangle \langle U_{E'l} \mid f\rangle, \end{aligned} \tag{25}$$

for some L^2 function $|f\rangle$ where:

$$\langle U_{E'l} \mid U_{E'l}\rangle = \delta\left(E - E'\right). \tag{26}$$

If we diagonalize H_l in a finite Laguerre basis of dimension N we have:

$$\langle f|(z - \overline{H}_l)^{-1}|f\rangle = \sum_{i=0}^{N-1} (z - \varepsilon_{Ni}^l)^{-1} \langle f|\Psi_{Ni}^{\alpha\beta}\rangle\langle\Psi_{Ni}^{\alpha\beta}|f\rangle. \tag{27}$$

Table 1. The ground and excited-states eigenvalues ($\varepsilon_{n_\alpha} + \varepsilon_{n_\beta}$) of the non-relativistic Hamiltonian of the helium atom (in a.u.) are shown as a function of number of L^2 basis functions N_β = 5, 10, 15 and 20. The observation results by references [20,21]. Highly accurate non-relativistic energy levels of helium by Konovalov and McCarthy (KM) [9] and by Accad et al. [22].

N_β	5	10	15	20	Observation	KM	Accad et al.
State		[Present work]			[20,21]	[9]	[22]
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
2^3P	−2.132880	−2.132900	−2.132918	−2.132970	−2.132969	−2.1312	−2.13316
2^1P	−2.122890	−2.122956	−2.123211	−2.123545	−2.123637	−2.1223	−2.12384
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
3^3P	−2.057260	−2.057350	−2.057560	−2.057784	−2.057891	−2.0575	−2.05808
3^1P	−2.054297	−2.054580	−2.054750	−2.054835	−2.054953	−2.0546	−2.05515
4^3S	−2.024980	−2.035111	−2.035326	−2.035420	−2.036323		
4^1S	−2.027555	−2.032980	−2.033290	−2.033307	−2.033398		
4^3P	−2.031576	−2.031950	−2.032002	−2.032046	−2.032136		
4^1P	−2.030322	−2.030425	−2.030650	−2.030790	−2.030880		

Table 2. The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{l_\beta} = 0.93$, $l_\beta = 0$ (singlet) and different basis sizes N. Powers of ten are denoted by the number in brackets.

N	i	X_{Ni}	W_{Ni}	$\sum W_{Ni}$	C^β_{Ni}
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		−0.99734808(+1)
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
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

Table 3. The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{l_\beta} = 0.93$, $l_\beta = 0$ (triplet) and different basis sizes N. Powers of ten are denoted by the number in brackets.

N	i	X_{Ni}	W_{Ni}	$\sum W_{Ni}$	C^{β}_{Ni}
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

The observation that for the Laguerre basis (2) in the helium target eigenstates have L^2 expansion coefficients proportional to the Pollaczek polynomials 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 wavefunctions $|f\rangle$ and $|g\rangle$:

$$\sum_{n}^{\infty} \langle f \mid \Psi_{nl}\rangle \langle \Psi_{nl} \mid g\rangle + \int_{0}^{\infty} \langle f \mid \Psi_{El}\rangle \langle \Psi_{El} \mid g\rangle \, dE = \langle f \mid g\rangle \tag{28}$$

and a finite basis representation in the space spanned by the first N basis states of type (2):

$$\sum_{i}^{N} \langle f \mid \Phi_{ni}\rangle \langle \Phi_{ni} \mid g\rangle = \langle f \mid g\rangle_N \,. \tag{29}$$

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

$$\langle f \mid g\rangle_N \neq \langle f \mid g\rangle \,, \tag{30}$$

but:

$$\langle f \mid g\rangle_N \to \langle f \mid g\rangle \quad \text{as} \quad N \to \infty. \tag{31}$$

To derive an equivalent quadrature rule for this convergence we write equation (28) as:

$$\langle f \mid g\rangle_N = \sum_{i_\alpha, i_\beta}^{N} \left(C^{(\alpha\beta)}_{Ni}\right)^2 \left\langle f \,\middle|\, \Phi_N\left(X^{(\alpha\beta)}_{Ni}\right)\right\rangle \times \left\langle \Phi_N\left(X^{(\alpha\beta)}_{Ni}\right) \,\middle|\, g\right\rangle . \tag{32}$$

We see that the quadrature rule implied is for a function $F(X)$ just:

$$\int d\mu\,(X) F\,(X) = \sum_{i=1}^{N} \left(C^{(\alpha\beta)}_{Ni}\right)^2 F\left(X^{(\alpha\beta)}_{Ni}\right) . \tag{33}$$

Table 4. The weights of Gaussian quadrature and configuration interaction coefficient are shown for λ_{l_β}= 0.73, l_β= 1 (singlet) and different basis sizes N. Powers of ten are denoted by the number in brackets.

N	i	X_{Ni}	W_{Ni}	$\sum W_{Ni}$	C^β_{Ni}
1	1	0.37412764(+1)	−0.53824836	−0.53824836	0.42720019
5	1	0.33163164(+1)	−0.69247911	−0.53824836	0.52713383
	2	−0.10872138(+2)	0.72221779(−1)		0.75194511(−1)
	3	−0.26953315(+1)	0.19776099(−1)		0.70527762(−1)
	4	−0.10017035(+1)	0.30593764(−1)		0.11918815
	5	0.42493210	0.31639105(−1)		0.22613564
10	1	0.33163066(+1)	−0.69254346	−0.53824836	0.52715943
	2	−0.10872138(+2)	0.72221779(−1)		0.75194508(−1)
	3	−0.27621050(+1)	0.16482855(−1)		0.63814190(−1)
	4	−0.18521338(+1)	0.68742118(−2)		0.47330708(−1)
	5	−0.14079582(+1)	0.71727296(−2)		0.52617990(−1)
	6	−0.89939382	0.10482557(−1)		0.71621365(−1)
	7	−0.33961324	0.13261339(−1)		0.95922494(−1)
	8	0.18642161	0.13966144(−1)		0.12631504
	9	0.60920327	0.10434779(−1)		0.15753703
	10	0.88329485	0.33987000(−2)		0.16452349
15	1	0.33163066(+1)	−0.69254346	−0.53824836	0.52715943
	2	−0.10872138(+2)	0.72221779(−1)		0.75194508(−1)
	3	−0.27621061(+1)	0.16482980(−1)		0.63814422(−1)
	4	−0.18568357(+1)	0.65489316(−2)		0.46159286(−1)
	5	−0.15242802(+1)	0.34794911(−2)		0.35793616(−1)
	6	−0.13145464(+1)	0.35360621(−2)		0.37682827(−1)
	7	−0.10684716(+1)	0.48868371(−2)		0.46860362(−1)
	8	−0.77524503	0.61981290(−2)		0.56966251(−1)
	9	−0.45748953	0.73469580(−2)		0.68449069(−1)
	10	−0.13617966	0.81724991(−2)		0.81765562(−1)
	11	0.16970592	0.83898340(−2)		0.96911921(−1)
	12	0.44336218	0.76436242(−2)		0.11297434
	13	0.67080942	0.57196210(−2)		0.12707977
	14	0.84180300	0.29807388(−2)		0.13233640
	15	0.95096966	0.68762244(−3)		0.11417185

The quadrature rule (33) can be identified as a special case of Gaussian quadrature based Pollaczek polynomials. This can be seen by noting some standard results that for a general orthogonal polynomial there exists a Gauss quadrature formula given by:

$$\int_a^b F(X)\, d\mu(X) \approx \sum_{i=1}^{N} W_{Ni} F(X_{Ni}). \tag{34}$$

The limits a and b comprise any interval which covers the point and continuum spectrum mapped into the X variable. W_{Ni} are the associated quadrature weights which are given by:

$$W_{Ni}^{(\alpha\beta)} = \frac{\pi\Gamma(N+2l+1)}{2^{2l}\Gamma(N+1)} \frac{1}{P_{N-1}^{l+1}\left(X_{Ni}^{(\alpha\beta)}\right)\frac{d}{dx}P_N^l\left(X_{Ni}^{(\alpha\beta)}\right)}. \tag{35}$$

The configuration interaction coefficient $C_{Ni}^{(\alpha\beta)}$ which are then determined using (35) is given by

$$\left(C_{Ni}^{(\alpha\beta)}\right)^2 = \frac{2^{2l}}{\pi} \frac{\lambda_l}{\left(1 - X_{Ni}^{(\alpha\beta)}\right)} W_{Ni}^{(\alpha\beta)}. \tag{36}$$

The values of the configuration interaction coefficient C_1^α and weight W_1^α which belong to the ground state are 1.4141959 and -1.62830282×10^4. The values of W_{Ni}^β and C_{Ni}^β are shown in Tables 2 and 3 for singlet and triplet S-states with different basis size and $\lambda_{l_\beta} = 0.93$. We also show the results for P-states calculated using the assumption that the convergence behavior of the configuration interaction coefficient and weight which the orbital angular momentum is not zero ($l_\beta \neq 0$). The values of W_{Ni}^β and C_{Ni}^β for p-states for $\lambda_{l_\beta} = 0.72$ (*triplet*) and 0.73 (*singlet*) with different basis size is shown in Tables 4 and 5 respectively.

Table 5. The weights of Gaussian quadrature and configuration interaction coefficient are shown for $\lambda_{l_\beta}= 0.72$, $l_\beta= 1$ (triplet) and different basis sizes N. Powers of ten are denoted by the number in brackets.

N	i	X_{Ni}	W_{Ni}	$\sum W_{Ni}$	C^β_{Ni}
1	1	0.37412764(+1)	−0.44737870	−0.44737870	0.38679651
5	1	0.28868042(+1)	−0.55322787	−0.44737870	0.51845362
	2	−0.15981694(+2)	0.42277639(−1)		0.47773401(−1)
	3	−0.28654172(+1)	0.13608096(−1)		0.56809610(−1)
	4	−0.10845255(+1)	0.22113873(−1)		0.98616618(−1)
	5	0.40488989	0.27849554(−1)		0.20712464
10	1	0.28867808(+1)	−0.55175847	−0.44737870	0.51776786
	2	−0.15981694(+2)	0.42277639(−1)		0.47773401(−1)
	3	−0.29189870(+1)	0.10188871(−1)		0.48819960(−1)
	4	−0.19025399(+1)	0.49457039(−2)		0.39522669(−1)
	5	−0.14447971(+1)	0.49827350(−2)		0.43224880(−1)
	6	−0.93291512	0.76078886(−2)		0.60068528(−1)
	7	−0.36480534	0.10209363(−1)		0.82810476(−1)
	8	0.17140160	0.11548178(−1)		0.11303319
	9	0.60291796	0.93449200(−2)		0.14688214
	10	0.88201378	0.32744685(−2)		0.15950565
15	1	0.28867808(+1)	−0.55175847	−0.44737870	0.51776787
	2	−0.15981694(+2)	0.42277639(−1)		0.47773401(−1)
	3	−0.29189875(+1)	0.10189336(−1)		0.48821071(−1)
	4	−0.19059833(+1)	0.47739343(−2)		0.38807259(−1)
	5	−0.15493787(+1)	0.25275221(−2)		0.30147522(−1)
	6	−0.13353269(+1)	0.24725384(−2)		0.31154371(−1)
	7	−0.10898995(+1)	0.34857377(−2)		0.39102629(−1)
	8	−0.79552582	0.45488820(−2)		0.48192318(−1)
	9	−0.47513313	0.55689910(−2)		0.58829337(−1)
	10	−0.15030607	0.64293695(−2)		0.71581170(−1)
	11	0.15943127	0.68846533(−2)		0.86651429(−1)
	12	0.43676915	0.65699504(−2)		0.10340919
	13	0.66728260	0.51599192(−2)		0.11923534
	14	0.84040398	0.28165033(−2)		0.12719364
	15	0.95066943	0.67479605(−3)		0.11198233

5 Conclusions and future work

Using the restricted basis for the helium state in which one of the electrons is in a 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 energies which agree well with the results of the observations [20,21] and other calculations of Konovalov and McCarthy [9] and Accad et al. [22].

The completeness relation of the helium eigenfunctions is calculated in term of the configuration interaction coefficient via the Gaussian quadrature. It is shown that the weights and configuration interaction coefficients converge to the same number for different basis size. It is therefore our next goal to apply these results to the electron-helium cross-section calculation.

The authors acknowledge the support from the DGHE Indonesian Government through the Hibah Bersaing Research grant and BPPS scholarship. The authors would like to thank Prof. Andris Stelbovics and Prof. Igor Bray for their comments on this paper and helpful references they supplied.

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