Convoluted Quasi-Sturmian Basis in Three-Body Coulomb Problems

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Abstract

A new type of basis functions is proposed to describe an $(e, 3e)$ process on helium. This is done in the framework of the first Born approximation approach presented in Ref. [1]. The basis functions used to expand the three-body solutions are calculated in terms of the recently introduced quasi-Sturmian (QS) functions [2]. The QS functions satisfy a non-homogeneous Schrödinger equation with Coulomb interactions and possess outgoing-wave boundary condition. By construction, the basis functions look asymptotically like a six-dimensional spherical wave. The transition amplitude for the $(e, 3e)$ process is obtained directly from the asymptotic part of the wave function. A fast convergence is achieved for the calculated wave function. An agreement in the shape of differential cross sections is obtained with the available experimental data. While the disagreement in magnitude is found with the experimental data, a reasonable agreement with other *ab initio* theories is found.

Keywords: *Quasi-Sturmian functions; Coulomb Green's function; driven equation*

1 Introduction

The Coulomb three-body scattering problem is one of the most fundamental outstanding problems in theoretical nuclear, atomic and molecular physics. The primary difficulty in description of three charged particles in the continuum is imposing appropriate asymptotic behaviors of the wave function.

In order to describe the Coulomb three-body continuum we propose a set of two-particle functions which are calculated by using the recently introduced so-called quasi-Sturmian (QS) functions [2]. The QS functions satisfy a two-body non-homogeneous Schrödinger equation with the Coulomb potential and an outgoing-wave boundary condition. Specifically, the two-particle basis functions are obtained, by an analogy with the Green's function of two non-interacting hydrogenic atomic systems, as a convolution integral of two one-particle QS functions. The QS functions have the merit that they are expressed in a closed form, which allows us to find an appropriate integration path that is useful for numerical calculations of such an integral representation. We name these basis functions Convoluted Quasi Sturmian (CQS). Note that by construction, the CQS function (unlike a simple product of two one-particle ones) looks asymptotically (as the hyperradius $\rho \to \infty$) like a six-dimensional outgoing spherical wave.

The atomic units are assumed throughout.

Proceedings of the International Conference 'Nuclear Theory in the Supercomputing Era — 2014' (NTSE-2014), Khabarovsk, Russia, June 23–27, 2014. Eds. A. M. Shirokov and A. I. Mazur. Pacific National University, Khabarovsk, Russia, 2016, p. 144.

http://www.ntse-2014.khb.ru/Proc/Zaytsev.pdf.

2 Quasi-Sturmian basis functions

2.1 Driven equation

In the approach of Ref. [1] to the (e, 3e) process, the four-body Schrödinger equation is reduced to the following driven equation for the three-body system $(e^-, e^-, \mathrm{He}^{++}) = (1, 2, 3)$:

$$\left[E - \hat{H}\right] \Phi_{sc}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2)\, \Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2). \tag{1}$$

$E = \frac{k_1^2}{2} + \frac{k_2^2}{2}$ is the energy of the two ejected electrons. The three-body helium Hamiltonian is given by

$$\hat{H} = -\frac{1}{2}\triangle_{r_1} - \frac{1}{2}\triangle_{r_2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}, \tag{2}$$

$\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2)$ represents the ground state of the helium atom. The perturbation operator $\hat{W}_{fi}$ is written as

$$\hat{W}_{fi}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{(2\pi)^3} \frac{4\pi}{q^2} (-2 + e^{i\mathbf{q}\cdot\mathbf{r}_1} + e^{i\mathbf{q}\cdot\mathbf{r}_2}), \tag{3}$$

where $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is the transferred momentum, $\mathbf{k}_i$ and $\mathbf{k}_f$ are the momenta of the incident and scattered electrons.

2.2 Two-particle quasi Sturmians

Our method of solving the driven equation (1) is to expand the solution in the series

$$\Phi_{sc}^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L,\ell,\lambda} \sum_{n,\nu=0}^{N-1} C_{n\nu}^{L(\ell\lambda)}\, |n\ell\nu\lambda; LM\rangle_Q, \tag{4}$$

where the basis

$$|n\ell\nu\lambda; LM\rangle_Q \equiv \frac{Q_{n\nu}^{\ell\lambda(+)}(E; r_1, r_2)}{r_1 r_2} \mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \tag{5}$$

$$\mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m\mu} (\ell m \lambda\mu \,|LM\,)\, Y_{\ell m}(\hat{\mathbf{r}}_1)\, Y_{\lambda\mu}(\hat{\mathbf{r}}_2). \tag{6}$$

Each function $Q_{n\nu}^{\ell\lambda(+)}$ is assumed to satisfy the radial equation

$$\left[E - \hat{h}_1^{\ell} - \hat{h}_2^{\lambda}\right] Q_{n\nu}^{(\ell\lambda_2)(+)}(E; r_1, r_2) = \frac{\psi_n^{\ell}(r_1)\, \psi_\nu^{\lambda}(r_2)}{r_1 r_2}, \tag{7}$$

where

$$\hat{h}_i^{\ell} = -\frac{1}{2}\frac{\partial^2}{\partial r_i^2} + \frac{1}{2}\frac{\ell(\ell+1)}{r_i^2} - \frac{2}{r_i}, \tag{8}$$

ψ_n^{ℓ} are the Laguerre basis functions (b is a real scale parameter),

$$\psi_n^{\ell}(r) = \left[(n+1)_{2\ell+1}\right]^{-\frac{1}{2}} (2br)^{\ell+1} e^{-br} L_n^{2\ell+1}(2br), \tag{9}$$

which are orthogonal with the weight $\frac{1}{r}$:

$$\int_0^{\infty} dr\; \psi_n^{\ell}(r)\, \frac{1}{r}\, \psi_m^{\ell}(r) = \delta_{nm}. \tag{10}$$

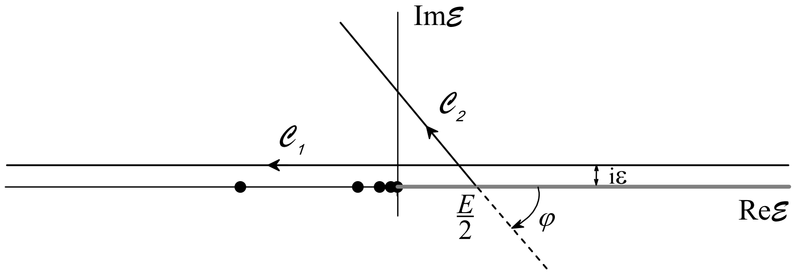

Figure 1: $\mathcal{C}_1$ is the straight-line path of integration of the convolution integral (11). The rotated contour $\mathcal{C}_2$ penetrates into the region of unphysical energies.

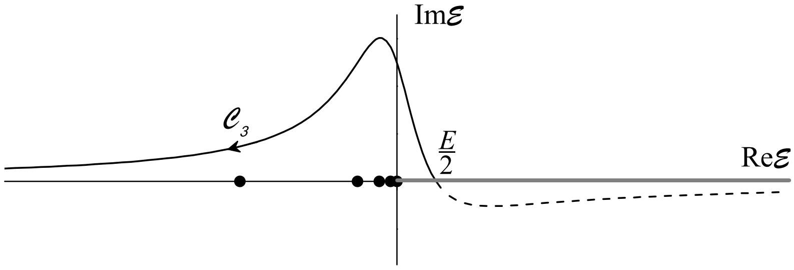

Figure 2: The deformed contour $\mathcal{C}_3$ asymptotically approaches the real energy axis.

In order to obtain the $Q_{n\nu}^{\ell\lambda(+)}$ with the outgoing-wave boundary condition, we use the Green's function $\hat{G}^{(\ell\lambda)(+)}(E)$ [which is the inverse of the operator in the left-hand-side of Eq. (7)] which can be expressed in the form of the convolution integral [3, 4],

$$\hat{G}^{(\ell\lambda)(+)}(E) = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_1} d\mathcal{E}\, \hat{G}^{\ell(+)}(\sqrt{2\mathcal{E}})\, \hat{G}^{\lambda(+)}(\sqrt{2(E-\mathcal{E})}), \tag{11}$$

where the path of integration $\mathcal{C}_1$ in the complex energy plane $\mathcal{E}$ runs slightly above the branch cut and bound-state poles of $\hat{G}^{\ell(+)}$ (see Fig. 1). In order to avoid these singularities we, following the method of Ref. [3], rotate the contour about the point $\frac{E}{2}$ by an angle φ, $-\pi < \varphi < 0$. A part of the rotated straight-line contour $\mathcal{C}_2$ indicated by a dashed line in Fig. 1, lies on the unphysical energy sheet, $-2\pi < \arg(\mathcal{E}) < 0$. Note that $\hat{G}^{\ell(+)}$ grows exponentially for large $|\mathcal{E}|$ in the lower half-plane. In order to ensure a rapid convergence of the integral in Eq. (11), we deform the contour $\mathcal{C}_2$ in such a way that the resulting path $\mathcal{C}_3$ shown in Fig. 2 asymptotically approaches the real axis.

The one-particle Green's function operator $\hat{G}^{\ell(\pm)}$ kernel satisfies the equation

$$\left[\mathcal{E} - \hat{h}^{\ell}\right] G^{\ell(\pm)}(\sqrt{2\mathcal{E}}; r, r') = \delta(r - r') \tag{12}$$

and can be expressed, e. g., in terms of the Whittaker functions [5]:

$$G^{\ell(\pm)}(k; r, r') = \pm\frac{1}{ik}\frac{\Gamma(\ell \pm i\alpha)}{(2\ell+1)!}\,\mathcal{M}_{\mp i\alpha;\ell+1/2}(\mp 2ikr_<)\,\mathcal{W}_{\mp i\alpha;\ell+1/2}(\mp 2ikr_>), \tag{13}$$

where $\alpha = \frac{\mu Z}{k} = -\frac{2}{k}$. From the formulae above one deduces that $Q_{n\nu}^{\ell\lambda(+)}$ can be written as

$$Q_{n\nu}^{(\ell\lambda)(+)}(E; r_1, r_2) = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_3} d\mathcal{E}\, Q_n^{\ell_1(+)}(\sqrt{2\mathcal{E}}; r_1)\, Q_\nu^{\lambda(+)}(\sqrt{2(E-\mathcal{E})}; r_2), \tag{14}$$

where the one-particle QS functions $Q_{n_j}^{\ell_j(+)}$ are defined by [2]

$$Q_n^{\ell(\pm)}(k;r) = \int_0^\infty dx'\, G^{\ell(\pm)}(k;r,r')\, \frac{1}{r'}\, \psi_n^\ell(r'). \tag{15}$$

2.3 Asymptotic behavior

It follows from the asymptotic behavior of the irregular Whittaker function $\mathcal{W}$ that

$$\begin{aligned} Q_n^{\ell(\pm)}(k;r) &\underset{r\to\infty}{\sim} \mp 2\frac{i}{k}\, S_{n\ell}(k)\, (-2kr)^{\ell+1} e^{\pi\alpha/2}\, e^{\pm i(kr+\sigma_\ell(k))}\, U(\ell+1\pm i\alpha, 2\ell+2, \mp 2ikr) \\ &\underset{r\to\infty}{\sim} -\frac{2}{k}\, S_{n\ell}(k)\, e^{\pm i\left(kr-\alpha\ln(2kr)-\frac{\pi\ell}{2}+\sigma_\ell(k)\right)}, \end{aligned} \tag{16}$$

where $\sigma_\ell(k) = \arg\Gamma(\ell+1+i\alpha)$ is the Coulomb phase. Here $S_{n\ell}$ is the sine-like J-matrix solution [6],

$$\begin{aligned} S_{n\ell}(k) = \frac{1}{2}\left[(n+1)_{(2\ell+1)}\right]^{1/2} (2\sin\xi)^{\ell+1}\, e^{-\pi\alpha/2}\, \omega^{-i\alpha} \frac{|\Gamma(\ell+1+i\alpha)|}{(2\ell+1)!} \\ \times (-\omega)^n\, {}_2F_1\!\left(-n, \ell+1+i\alpha; 2\ell+2; 1-\omega^{-2}\right), \end{aligned} \tag{17}$$

where

$$\omega \equiv e^{i\xi} = \frac{b+ik}{b-ik}, \quad \sin\xi = \frac{2bk}{b^2+k^2}, \tag{18}$$

$U(a,b,z)$ is the Kummer function. Recall that $S_{n\ell}$ are formally defined as the coefficients of the expansion

$$\Psi_\ell^C(k,r) = \sum_{n=0}^\infty S_{n\ell}(k)\psi_n^\ell(r) \tag{19}$$

of the regular Coulomb solution Ψ_ℓ^C [7]

$$\Psi_\ell^C(k,r) = \frac{1}{2}(2kr)^{\ell+1}\, e^{-\pi\alpha/2}\, e^{ikr} \frac{|\Gamma(\ell+1+i\alpha)|}{(2\ell+1)!}\, {}_1F_1(\ell+1+i\alpha; 2\ell+2; -2ikr), \tag{20}$$

i. e.,

$$S_{n\ell}(k) = \int_0^\infty dr\, \frac{1}{r}\, \psi_n^\ell(r)\, \Psi_\ell^C(k,r). \tag{21}$$

The asymptotic behavior of the QS function (14) for $r_1\to\infty$ and $r_2\to\infty$ simultaneously (in the constant ratio $\tan(\phi) = r_2/r_1$, where ϕ is the hyperangle) is obtained by replacing $Q_n^{\ell(+)}$ and $Q_\nu^{\lambda(+)}$ by their asymptotic approximation (16) and making use of the stationary phase method to evaluate the resulting integral along the contour $\mathcal{C}_1$:

$$\begin{aligned} Q_{n\nu}^{(\ell\lambda)(+)}(E;r_1,r_2) &\underset{\rho\to\infty}{\sim} \frac{1}{E}\sqrt{\frac{2}{\pi}}(2E)^{3/4} e^{\frac{i\pi}{4}}\, S_{n\ell}(p_1)\, S_{n\lambda}(p_2) \frac{1}{\sqrt{\rho}} \\ &\times \exp\left\{ i\left[\sqrt{2E}\rho - \alpha_1\ln(2p_1r_1) - \alpha_2\ln(2p_2r_2) + \sigma_\ell(p_1) + \sigma_\lambda(p_2) - \frac{\pi(\ell+\lambda)}{2}\right]\right\}, \end{aligned} \tag{22}$$

where $\rho = \sqrt{r_1^2+r_2^2}$ is the hyperradius, $p_1 = \cos(\phi)\sqrt{2E}$, $p_2 = \sin(\phi)\sqrt{2E}$, $\alpha_1 = -\frac{2}{p_1}$, $\alpha_2 = -\frac{2}{p_2}$. Notice that on the left part of the contour $\mathcal{C}_3$ where $k \sim i|k|$ and $|k|\to\infty$, the function $Q_n^{\ell(+)}$ behaves like e^{-br} for large r (rather than e^{ikr}). Thus, for larger scale parameter b, the QS function (14) reaches its asymptotic form of Eq. (22) faster.

Finally, by inserting Eq. (22) into the Eq. (4), we find the following asymptotic expression:

$$\Phi_{sc}^{(+)}(\mathbf{r}_1,\mathbf{r}_2) \approx \frac{2}{E\sin(2\phi)}\sqrt{\frac{2}{\pi}}(2E)^{3/4}e^{\frac{i\pi}{4}}\frac{\exp\left\{i\left[\sqrt{2E}\rho-\alpha_1\ln(2p_1r_1)-\alpha_2\ln(2p_2r_2)\right]\right\}}{\rho^{5/2}} \times\sum_{\ell\lambda L}\mathcal{Y}_{LM}^{\ell\lambda}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\exp\left\{i\left[\sigma_\ell(p_1)+\sigma_\lambda(p_2)-\frac{\pi(\ell+\lambda)}{2}\right]\right\} \times\sum_{n,\nu=0}^{N-1}C_{n\nu}^{L(\ell\lambda)}S_{n\ell}(p_1)\,S_{\nu\lambda}(p_2). \quad (23)$$

2.4 Transition amplitude

On the other hand, the asymptotic limit of the Green's function of the three-body Coulomb system ($e^-, e^-, \mathrm{He}^{++}$) (for $\rho\to\infty$ while ρ' is finite) reads [1, 8]

$$G^{(+)}(E;\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2') \approx \frac{(2E)^{3/4}e^{\frac{i\pi}{4}}}{(2\pi)^{5/2}}\frac{\exp\left\{i\left[\sqrt{2E}\rho+W_0(\mathbf{r}_1,\mathbf{r}_2)\right]\right\}}{\rho^{5/2}}\Psi_{\mathbf{k}_1',\mathbf{k}_2'}^{(-)*}(\mathbf{r}_1',\mathbf{r}_2'), \quad (24)$$

where the Coulomb phase W_0 is given by

$$W_0(\mathbf{r}_1,\mathbf{r}_2) = -\frac{\rho}{\sqrt{2E}}\left(-\frac{2}{r_1}-\frac{2}{r_2}+\frac{1}{r_{12}}\right)\ln 2\sqrt{2E}\rho, \quad (25)$$

$\mathbf{k}_1' = p_1\hat{\mathbf{r}}_1$, $\mathbf{k}_2' = p_2\hat{\mathbf{r}}_2$. Therefore, from Eq. (1) we obtain that in this region [1]

$$\Phi_{sc}^{(+)}(\mathbf{r}_1,\mathbf{r}_2) \approx \frac{(2E)^{3/4}e^{\frac{i\pi}{4}}}{(2\pi)^{5/2}}\frac{\exp\left\{i\left[\sqrt{2E}\rho+W_0(\mathbf{r}_1,\mathbf{r}_2)\right]\right\}}{\rho^{5/2}}T_{\mathbf{k}_1',\mathbf{k}_2'}, \quad (26)$$

where the transition amplitude

$$T_{\mathbf{k}_1',\mathbf{k}_2'} = \left\langle\Psi_{\mathbf{k}_1',\mathbf{k}_2'}^{(-)}\right|\hat{W}_{fi}\left|\Phi^{(0)}\right\rangle. \quad (27)$$

Then, comparing two asymptotic expressions (23) and (26), we find

$$T_{\mathbf{k}_1',\mathbf{k}_2'} = \frac{(4\pi)^2}{E\sin(2\phi)}\exp\left\{-i\left[W_0(\mathbf{r}_1,\mathbf{r}_2)+\alpha_1\ln(2p_1r_1)+\alpha_2\ln(2p_2r_2)\right]\right\} \times\sum_{\ell\lambda L}\left(\left[\sum_{n,\nu=0}^{N-1}C_{n\nu}^{L(\ell\lambda)}S_{n\ell}(p_1)S_{\nu\lambda}(p_2)\right] \times\exp\left\{i\left[\sigma_\ell(p_1)+\sigma_\lambda(p_2)-\frac{\pi(\ell+\lambda)}{2}\right]\right\}\mathcal{Y}_{\ell\lambda}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)\right). \quad (28)$$

Obviously, the differential cross section is expressed in terms of the 'reduced' transition amplitude:

$$\frac{d^5\sigma}{d\Omega_1 d\Omega_2 d\Omega_f dE_1 dE_2} = \frac{1}{(2\pi)^2}\frac{k_f k_1 k_2}{k_i}\left|T_{\mathbf{k}_1',\mathbf{k}_2'}\right|^2. \quad (29)$$

3 Solving driven equation

The QS approach is based on the assumption that the asymptotic behavior of the basis Sturmian functions is correct. Hence there remains a problem of finding the wave function in the finite 'inner' spatial region. This calculation can be performed in the context of a set of square integrable basis functions. In this case, the left-hand-side of Eq. (1) decreases sufficiently fast to zero as $\rho \to \infty$ and therefore can be approximated by a finite linear combination of L^2 basis functions. In this work, we have tried to apply the method for obtaining the solution of the equation (1) by expanding it into a set of the pure CQS functions (14).

Inserting Eq. (4) into Eq. (1) and having in mind Eq. (7), yields

$$\sum_{L,\ell',\lambda'} \sum_{n',\nu'=0}^{N-1} C^{L(\ell'\lambda')}_{n'\nu'} \left[|\, \widetilde{n'\ell'\nu'\lambda'; LM}\, \rangle_L + \hat{V}^C_3 \, |n'\ell'\nu'\lambda'; LM\rangle_Q \right] = \hat{W}_{fi} \left| \Phi^{(0)} \right\rangle, \quad (30)$$

where

$$|\, \widetilde{n\ell\nu\lambda; LM}\, \rangle_L \equiv \frac{\psi^\ell_n(r_1)\, \psi^\lambda_\nu(r_2)}{r_1^2 r_2^2}\, \mathcal{Y}^{\ell\lambda}_{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \quad (31)$$

The method of obtaining the expansion coefficients $C^{L(\ell\lambda)}_{n\nu}$ is to multiply Eq. (30) by

$$|n\ell\nu\lambda; LM\rangle_L \equiv \frac{\psi^\ell_n(r_1)\, \psi^\lambda_\nu(r_2)}{r_1 r_2}\, \mathcal{Y}^{\ell\lambda}_{LM}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \quad (32)$$

(see, e. g., Refs. [9–11]), integrate over $\mathbf{r_1}$ and $\mathbf{r_2}$, and utilize the orthogonality condition

$$_L\, \langle n\ell\nu\lambda; LM|\, \widetilde{n'\ell'\nu'\lambda'; LM}\, \rangle_L = \delta_{n,n'}\, \delta_{\nu,\nu'}\, \delta_{\ell,\ell'}\, \delta_{\lambda,\lambda'}. \quad (33)$$

As a result, we obtain the following matrix equation:

$$\sum_{L,\ell',\lambda'} \sum_{n',\nu'=0}^{N-1} \left[\delta_{n,n'}\, \delta_{\nu,\nu'}\, \delta_{\ell,\ell'}\, \delta_{\lambda,\lambda'} - U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} \right] C^{L(\ell'\lambda')}_{n'\nu'} = R^{L(\ell\lambda)}_{n\nu}. \quad (34)$$

Here $R^{L(\ell\lambda)}_{n\nu}$ is the projection of the right-hand-side of Eq. (30):

$$R^{L(\ell\lambda)}_{n\nu} = {}_L\langle n\ell\nu\lambda; LM|\hat{W}_{fi} \left| \Phi^{(0)} \right\rangle. \quad (35)$$

Due to the definition

$$|n\ell\nu\lambda; LM\rangle_Q \equiv \hat{G}^{(\ell\lambda)(+)} \left| \widetilde{n\ell\nu\lambda; LM} \right\rangle_L, \quad (36)$$

the matrix element

$$U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = {}_L\langle n\ell\nu\lambda; LM| \frac{1}{r_{12}}\, |n'\ell'\nu'\lambda'; LM\rangle_Q \quad (37)$$

can be written as

$$U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = {}_L\langle n\ell\nu\lambda; LM| \frac{1}{r_{12}} \hat{G}^{(\ell'\lambda')(+)} \left| \widetilde{n'\ell'\nu'\lambda'; LM} \right\rangle_L. \quad (38)$$

Then using the Laguerre basis (32) completeness, we obtain

$$U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = \sum_{n'',\nu''=0} {}_L\langle n\ell\nu\lambda; LM| \frac{1}{r_{12}} |n''\ell'\nu''\lambda'; LM\rangle_L$$
$$\times\, {}_L\left\langle \widetilde{n''\ell'\nu''\lambda'; LM} \right| \hat{G}^{(\ell'\lambda')(+)} \left| \widetilde{n'\ell'\nu'\lambda'; LM} \right\rangle_L. \quad (39)$$

In order to calculate the matrix elements of the Green's function in the basis of functions (31)

$$G^{(\ell\lambda)(+)}_{n\nu,n'\nu'} = {}_L\left\langle \widetilde{n\ell\nu\lambda; LM} \right| \hat{G}^{(\ell\lambda)(+)} \left| \widetilde{n'\ell\nu'\lambda; LM} \right\rangle_L, \quad (40)$$

we use the convolution integral [9–11]

$$G^{(\ell\lambda)(+)}_{n\nu,n'\nu'} = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_3} d\mathcal{E}\, G^{\ell(+)}_{nn'}(\sqrt{2\mathcal{E}})\, G^{\lambda(+)}_{\nu\nu'}(\sqrt{2(E-\mathcal{E})}). \tag{41}$$

The matrix elements of the one-particle Green's function $G^{\ell(+)}$ (13)

$$G^{\ell(+)}_{nm}(k) = \int\limits_0^\infty\int\limits_0^\infty drdr'\,\frac{1}{r}\,\psi^\ell_n(r)\,G^{\ell(+)}(k;r,r')\,\frac{1}{r'}\,\psi^\ell_m(r') \tag{42}$$

are expressed in terms of the two independent J-matrix solutions [12]:

$$G^{\ell(+)}_{nm}(k) = -\frac{2}{k}\,S_{n_<\ell}(k)\,C^{(+)}_{n_>\ell}(k), \tag{43}$$

$$C^{(+)}_{n\ell}(k) = -\sqrt{n!(n+2\ell+1)}\,\frac{e^{\pi\alpha/2}\,\omega^{i\alpha}}{(2\sin\xi)^\ell}$$
$$\times\,\frac{\Gamma(\ell+1+i\alpha)}{|\Gamma(\ell+1+i\alpha)|}\,\frac{(-\omega)^{n+1}}{\Gamma(n+\ell+2+i\alpha)}\,{}_2F_1\big(-\ell+i\alpha,n+1;n+\ell+2+i\alpha;\omega^2\big). \tag{44}$$

Our numerical calculations showed that the values of the convolution integrals (41) along the contour $\mathcal{C}_3$ are equal to those on the straight-line path $\mathcal{C}_2$. Note that the integrand in Eq. (41) does not have exponentially divergent factors unlike that of Eq. (11).

We approximate $U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'}$ by a finite sum

$$U^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = \sum_{n''\nu''=0}^{N-1} V^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n''\nu''}\,G^{(\ell'\lambda')(+)}_{n''\nu'',n'\nu'}. \tag{45}$$

Here $V^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'}$ are the matrix elements of $\frac{1}{r_{12}}$ in the basis (32):

$$V^{L(\ell\lambda)(\ell'\lambda')}_{n\nu,n'\nu'} = {}_L\langle n\ell\nu\lambda;LM|\frac{1}{r_{12}}\,|n'\ell'\nu'\lambda';LM\rangle_L. \tag{46}$$

In our calculations we take N in Eq. (45) to be equal to the number of QS functions (for each of the coordinates r_1 and r_2). In order to examine the applicability of the QS approach, in conjunction with the approximation (45), we study the convergence of the cross section with increasing N.

4 Results and discussion

We have applied the method outlined above to the problem of electron-impact double ionization of He. The corresponding fully resolved fivefold differential cross sections (FDCS) measurements have been performed by the Orsay group [13]. The geometry of the $(e,3e)$ process is coplanar with an incident energy $E_0 = 5599$ eV and a small momentum transfer $q = 0.24$ a.u. For a fixed value of one of the ejected electron angles, say, θ_1, the FDCS is measured as function of the other angle θ_2.

The energies of the two ejected electrons are $E_1 = E_2 = 10$ eV, so that $E = 0.737$ a.u. Hence for $\phi = \frac{\pi}{4}$ we have $p_1 = p_2 = k_1 = k_2 = 0.859$. As for the scale parameter b, note that the sine-like J-matrix solution (17) depends on the wave number k through its dependence on ω [see Eq. (18)]. Thus, it seems intuitively obvious that the parameter b must be chosen in such a way that the value of ω is far from its limits $\omega_0 = \pm 1$. In other words, b should be comparable to $k_{1,2}$. In our calculations we set $b = 0.78$.

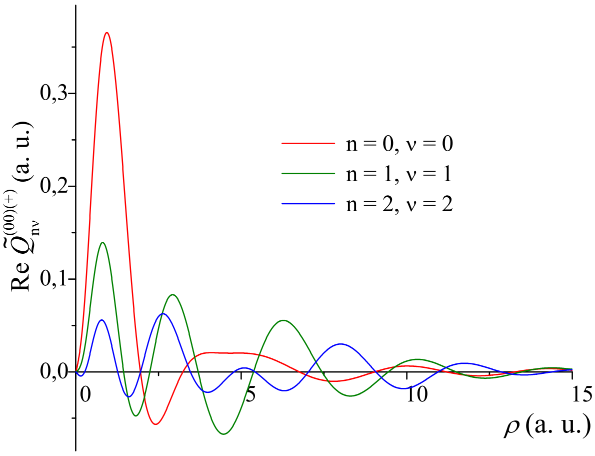

Figure 3: The real parts of the first three QS functions.

Note that the asymptotic behavior (22) of the two-particle QS functions (14) depends upon the indices n and ν. It follows from Eq. (17) that this dependence can be eliminated by dividing Eq. (14) by $A^{\ell}_{n}(p_1)\, A^{\lambda}_{\nu}(p_2)$, where

$$A^{\ell}_{n}(k) = [(n+1)_{2\ell+1}]^{1/2}(-\omega)^{n}\, {}_2F_1\big(-n, \ell+1+i\alpha; 2\ell+2; 1-\omega^{-2}\big). \tag{47}$$

The same result can be obtained using modified one-particle QS functions

$$\widetilde{Q}^{\ell(+)}_{n}(k;\ r) = \frac{Q^{\ell(+)}_{n}(k;\ r)}{A^{\ell}_{n}(k)} \tag{48}$$

in the integral in Eq. (14). To illustrate the use of the convolution integral representation (14), we present in Figs. 3 and 4 a few modified CQS functions

$$\widetilde{Q}^{(\ell\lambda)(+)}_{n\nu}(E; r_1, r_2) = \frac{1}{2\pi i}\int\limits_{\mathcal{C}_3} d\mathcal{E}\, \widetilde{Q}^{\ell(+)}_{n}(\sqrt{2\mathcal{E}}; r_1)\, \widetilde{Q}^{\lambda(+)}_{\nu}(\sqrt{2(E-\mathcal{E})}; r_2) \tag{49}$$

for $\ell = \lambda = 0$ on the diagonal $r_1 = r_2 = \rho/\sqrt{2}$. The energy $\mathcal{E}$ on the contour $\mathcal{C}_3$ is parametrized in the form

$$\mathcal{E} = t + i\frac{\frac{E}{2} - t}{1 + t^2}, \tag{50}$$

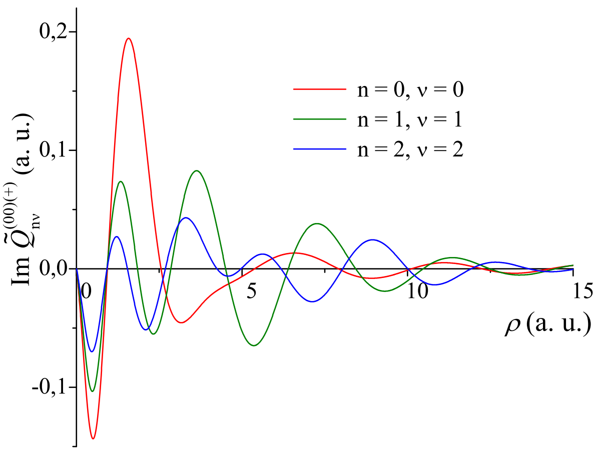

Figure 4: The same as Fig. 3 but for the imaginary parts.

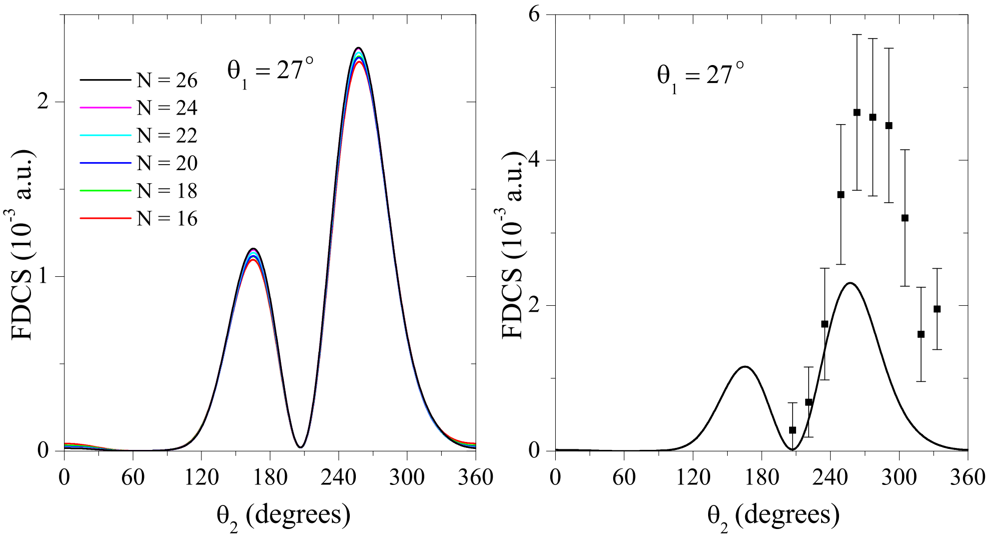

Figure 5: Convergence of FDCS for the He$(e, 3e)$He^{++} reaction with increasing N and comparison with experimental data [13].

where t runs from ∞ to $-\infty$.

To find the helium ground-state function $\Phi^{(0)}$, we diagonalize the matrix of the Hamiltonian (2) in the basis

$$|n\nu\ell\rangle \equiv \frac{\chi_n^\ell(r_1)\,\chi_\nu^\ell(r_2)}{r_1 r_2}\,\mathcal{Y}_{00}^{\ell\ell}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \tag{51}$$

where

$$\chi_n^\ell(r) = \sqrt{2b_0}\,[(n+1)_{2\ell+2}]^{-\frac{1}{2}}\,(2b_0 r)^{\ell+1} e^{-b_0 r} L_n^{2\ell+2}(2b_0 r). \tag{52}$$

In doing this, we limit ourselves to $\ell_{max} = 5$ and $n_{max} = \nu_{max} = 20$. Choosing the basis parameter $b_0 = 1.688$, we obtain $E_0 = -2.903542$ a. u. for the ground state energy.

We restrict ourselves to the maximal value of the total angular momentum $L_{\max} = 2$ and set the maximal angular momentum quantum numbers ℓ and λ to be 3 in the expansion (4). We examine the differential cross section convergence with increasing number N of the one-particle QS functions $Q_n^{\ell(+)}$ and $Q_\nu^{\lambda(+)}$, $n, \nu = 0, \ldots, N-1$ [see Eq. (15)] employed in the basis. A very good convergence of our numerical procedure is displayed in Fig. 5 where the FDCS (29) for $\theta_1 = 27^\circ$ calculated with different N are plotted. This result is surprising keeping in mind the aforementioned shortcoming of the CQS basis functions (14) asymptotic behavior, which results in noncompactness of Eq. (1). In Fig. 5 we show results for FDCS (29) in comparison with the experimental data [13]. The results are in agreement in shape, but not in magnitude, with the experiment.

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