Electron Correlations in the Framework of the Quasi Sturmian Approach

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Abstract

In the asymptotic region Ω_0 (large hyperradius), the two-electron continuum wave function presents formally a logarithmic phase term corresponding to the electron-electron interaction. The idea of this contribution is to include this phase into a Convoluted Quasi Sturmian (CQS) basis whose elements already behave asymptotically as an outgoing (incoming) six-dimensional spherical wave. With an appropriately introduced phase factor, the new CQS possess an asymptotic form very close to the formal one, and hopefully constitute a suitable set of basis functions for the three-body Coulomb continuum wave function representation in the entire space. As demonstrated numerically by solving a first order $(e, 3e)$ non-homogeneous Schrödinger equation in a two-channel case, a considerable improvement of the convergence rate is observed with a simple two-parameter form of the introduced phase factor.

Keywords: *Ionization of atoms; three-body Coulomb continuum; three-body wave function asymptotic behavior*

1 Introduction

The continuum spectrum of three charged particles is notoriously difficult to describe. In atomic or molecular ionization problems imposing cumbersome boundary conditions, the wave function should obey constituents of these conditions of primary mathematical and numerical difficulties. Besides, the long range nature of the Coulomb interaction implies solving Schrödinger equation on relatively large spatial domains and hence requires to use large basis sets and a high computational cost. Ideally, such a domain should be extended up to the boundary of the asymptotic region where all three particles are well separated. In real calculations, however, the domain size is not known in advance, even though the general boundary condition form has been obtained in Ref. [1]. As a general rule, the convergence rate of basis function expansion reflects its capacity in building up adequately the intricate asymptotic behavior.

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For the sake of simplicity, hereafter we consider the two-electron continuum associated with the problem of two electrons with coordinates r_1 and r_2 escaping in the field of a nucleus of charge Z. Such a state may arise as a results of a single or double ionization of atoms or molecules by a charged projectile or by a photon.

A few *ab initio* methods (see, e. g., the review [2] and Introduction of Ref. [3]) have been and are being developed for constructing numerically three-body continuum wave functions. Two of them convert the ionization problem into an inhomogeneous differential equation with a spatially confined driven term, equation that is solved within a finite size box. The exterior complex scaling (ECS) method [4] makes it possible to solve the problem without explicit use of the asymptotic form of the wave function by recasting the original problem into a boundary problem with zero boundary conditions. An interesting extension of ECS to the case of long-range Coulomb interaction has been proposed in Refs. [5–7]. The generalized Sturmian approach [8, 9] makes use of an expansion in terms of products of two single-particle generalized Sturmian functions with Coulomb outgoing-wave boundary conditions set at the box border; the angular coupling builds up a three-body scattering solution with a hyperspherical wave front in the Ω_0 region where all inter-particle distances are large. On the other hand, within the convergent close coupling method [10–12], the ionization problem is treated using a finite set of square integrable single-particle functions; in this case, accurate boundary conditions need not be imposed. Alternative approaches are provided by the Coulomb–Sturmian separable expansion [13, 14] and the J-matrix [15, 16] methods which deal with the wave function in the entire space using the Laguerre basis representation; the two-electron continuum problem is transformed in this case into a Lippmann–Schwinger equation with a kernel which is generally non-compact, and thus the validity of these approaches may be questionable.

In this contribution, we would like to put forward an alternative approach to the two-electron continuum representation in the entire space. The key idea is to use a basis set of functions with asymptotic behavior as close as possible to the formal one in the Ω_0 region [1, 17]. Our principal goal is to show that the adequate asymptotic property leads to an acceptable convergence rate for expansions in such a basis.

The proposed basis set contains two ingredients. First, it uses two-particle functions named Convoluted Quasi Sturmians (CQS) in Ref. [3] behaving asymptotically as a six-dimensional outgoing (incoming) spherical wave. This means that, contrary to pure products of single-particle functions, the basis functions already possess intrinsically some three-body features. However truncated expansions in CQS functions fail to converge satisfactorily. The reason behind that is the lack of an important term in the large hyperradius $\left(\rho = \sqrt{r_1^2 + r_2^2}\right)$ domain, the Coulomb logarithmic phase corresponding to the inter-electronic interaction. This brings us to the second ingredient, which is the introducing — from the outset — of an appropriate phase factor into the basis set. The modified CQS functions possess an asymptotic behavior closer to the formal one, and lead to a considerable convergence improvement in numerical results. We have already mentioned that, when dealing with the Coulomb three-body scattering problem, we do not know *a priori* the size of the finite domain in which one needs to solve the corresponding driven Schrödinger equation. With the modified CQS basis, we know however that the functions satisfy the equation in the asymptotic region Ω_0, and thus the size of this domain is determined by the range of the 'perturbation' operator (at least of its basis-independent part) induced by the phase factor.

As we focus on the region Ω_0, we consider as a numerical test case the double ionization channel of helium atom in kinematical conditions measured experimentally [18]. In our previous paper [3] we analyzed the feasibility of the proposed approach within the Temkin–Poet framework. Here we extend the study by including higher partial waves. We first investigate the compatibility of introducing the phase factor when using truncated expansions to solve the Schrödinger driven equation in the entire space. Then, we use a simple two-parameters form of the introduced phase factor to demonstrate that a satisfactory convergence rate can be achieved indeed.

Atomic units ($\hbar = e = m_e = 1$) are used throughout unless otherwise stated.

2 Problem statement

The first order treatment of ionization of atoms can be recast into a driven differential equation with a square integrable inhomogeneity. For example, in the case of the double ionization of helium by photon impact or by impact of a fast charged projectile, the inhomogeneous Schrödinger equation takes the form

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

where $E = \frac{k_1^2}{2} + \frac{k_2^2}{2}$ is the energy of the two ejected electrons with coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$, $\Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2)$ represents the ground state of the helium atom, and the three-body helium Hamiltonian is given by

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{1}{r_{12}}, \tag{2}$$

$$\hat{H}_j = -\frac{1}{2}\triangle_{r_j} - \frac{2}{r_j}, \qquad j = 1, 2; \tag{3}$$

$r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ denotes the relative inter-electronic distance. In the case of high incident electron impact energy, the perturbation operator is given by [9, 19]

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

where $\mathbf{k}_i$ and $\mathbf{k}_f$ are the momenta of the incident and scattered electrons, and $\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f$ is the transferred momentum. The solution $\Phi^{(+)}$ with outgoing wave boundary condition, contains all information on the scattering dynamics.

In this section we examine the solution of Eq. (1) for given quantum numbers (L, M) in the space of CQS functions $Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}$ [3],

$$|n_1 \ell_1 n_2 \ell_2; LM\rangle_Q \equiv \frac{Q_{n_1 n_2}^{\ell_1 \ell_2 (+)}(E; r_1, r_2)}{r_1 r_2}\, \mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2), \tag{5}$$

where the bispherical harmonics are given by

$$\mathcal{Y}_{LM}^{\ell_1 \ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \sum_{m_1 + m_2 = M} (\ell_1 m_1 \ell_2 m_2 \,|LM)\, Y_{\ell_1 m_1}(\hat{\mathbf{r}}_1)\, Y_{\ell_2 m_2}(\hat{\mathbf{r}}_2). \tag{6}$$

The radial CQS functions $Q_{n_1 n_2}^{\ell_1 \ell_2 (\pm)}$ satisfy the inhomogeneous equation

$$\left[E - \hat{h}_1^{\ell_1} - \hat{h}_2^{\ell_2}\right] Q_{n_1 n_2}^{\ell_1 \ell_2 (\pm)}(E; r_1, r_2) = \frac{\psi_{n_1}^{\ell_1}(r_1)\, \psi_{n_2}^{\ell_2}(r_2)}{r_1 r_2}, \tag{7}$$

where

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

and

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

are square integrable Laguerre basis functions with a scaling parameter b. A number of properties of these CQS functions have been obtained in Ref. [3]. For example, they can be expressed as a convolution integral of two single-particle Quasi Sturmian functions [20]; using Green's function, the radial CQS can be expressed through a contour integral which is useful for deducing the leading asymptotic behavior at large hyperradius ρ:

$$Q_{n_1 n_2}^{\ell_1\ell_2(+)}(E; r_1, r_2) \simeq \sqrt{\frac{8}{\pi}}\, e^{\frac{i\pi}{4}} S_{n_1\ell_1}(p_1)\, S_{n_2\ell_2}(p_2)\, \frac{1}{\sqrt{k\rho}} \times \exp\left\{ i\left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2) + \sigma_{\ell_1}(p_1) + \sigma_{\ell_2}(p_2) - \frac{\pi(\ell_1+\ell_2)}{2}\right]\right\}, \tag{10}$$

where α is the hyperangle, $\tan(\alpha) = r_2/r_1$; $k = \sqrt{2E}$, $p_1 = k\cos(\alpha)$, $p_2 = k\sin(\alpha)$, $\beta_1 = \frac{-2}{p_1}$, $\beta_2 = \frac{-2}{p_2}$, and $\sigma_\ell(p) = \mathrm{Arg}\left[\Gamma(\ell+1+\mathrm{i}\beta)\right]$ is the Coulomb phase shift. $S_{n\ell}(p)$ is the sine-like J-matrix solution [21] [an explicit expression can be found, e. g., in Ref. [3], Eq. (14a)].

Assuming that the outgoing solution of Eq. (1) can be expanded as

$$\Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\ell_1,\,\ell_2=0}^{\infty} \sum_{n_1,\,n_2=0}^{\infty} C_{n_1 n_2}^{L(\ell_1\ell_2)}\, |n_1\ell_1 n_2\ell_2; LM\rangle_Q, \tag{11}$$

we find the formal asymptotic expression

$$\Phi^{(+)}(\mathbf{r}_1, \mathbf{r}_2) \simeq A(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)\, \frac{1}{\rho^{5/2}} \exp\left\{ i\left[k\rho - \beta_1 \ln(2p_1 r_1) - \beta_2 \ln(2p_2 r_2)\right]\right\}, \tag{12}$$

$$A(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \frac{2}{E\sin(2\alpha)} \sqrt{\frac{2}{\pi}}\, (2E)^{3/4} e^{\frac{i\pi}{4}} \times \sum_{\ell_1\ell_2=0}^{\infty} \mathcal{Y}_{LM}^{\ell_1\ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \exp\left\{ i\left[\sigma_{\ell_1}(p_1) + \sigma_{\ell_2}(p_2) - \frac{\pi(\ell_1+\ell_2)}{2}\right]\right\} \times \sum_{n_1,n_2=0}^{\infty} C_{n_1 n_2}^{L(\ell_1\ell_2)}\, S_{n_1\ell_1}(p_1)\, S_{n_2\ell_2}(p_2). \tag{13}$$

The leading asymptotic behavior of the two-electron continuum wave function is known [1, 17] to include the Coulomb phase corresponding to the inter-electronic interaction $1/r_{12}$,

$$W_3(\mathbf{r}_1, \mathbf{r}_2) = -\frac{\rho}{k}\frac{1}{r_{12}} \ln(2k\rho)\,. \tag{14}$$

Expression (12) clearly does not contain such a phase. As observed within a Temkin–Poet framework [3], this failure leads to a lack of convergence for the proposed CQS basis. The remedy proposed in Ref. [3] for the S-wave case is extended here to higher partial waves.

3 Two-electron continuum representation

In order to describe better the two-electron correlation in the continuum, in particular, in the Ω_0 region, we propose a solution of the form

$$\Phi^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = e^{i\mathcal{W}(\mathbf{r}_1,\mathbf{r}_2)}\,\widetilde{\Phi}^{(+)}(\mathbf{r}_1,\mathbf{r}_2), \tag{15}$$

where the leading asymptotic form of the phase $\mathcal{W}$ is given by Eq. (14). Assuming $\widetilde{\Phi}^{(+)}$ to be properly expandable in terms of the CQS functions (5),

$$\widetilde{\Phi}^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{\ell_1,\ell_2=0}^{\infty}\sum_{n_1,n_2=0}^{\infty} \widetilde{C}^{L(\ell_1\ell_2)}_{n_1n_2}\,|n_1\ell_1n_2\ell_2;LM\rangle_Q, \tag{16}$$

the expression (15) is hereafter referred to as a *two-electron continuum* (TEC) representation of the solution.

Substituting $\Phi^{(+)}(\mathbf{r}_1,\mathbf{r}_2)$ in Eq. (1) by Eq. (15), we obtain

$$\left[E-\hat{H}_1-\hat{H}_2+\hat{\mathcal{L}}\right]\widetilde{\Phi}^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = e^{-i\mathcal{W}(\mathbf{r}_1,\mathbf{r}_2)}\,\hat{W}_{fi}\,\Phi^{(0)}(\mathbf{r}_1,\mathbf{r}_2), \tag{17}$$

where the operator

$$\widehat{\mathcal{L}} = \frac{i}{2}\left[\triangle_{r_1}\mathcal{W}+\triangle_{r_2}\mathcal{W}\right] - \frac{1}{2}\left[(\nabla_{r_1}\mathcal{W})^2+(\nabla_{r_2}\mathcal{W})^2\right] + i\left[(\nabla_{r_1}\mathcal{W})\cdot\nabla_{r_1}+(\nabla_{r_2}\mathcal{W})\cdot\nabla_{r_2}\right] - \frac{1}{r_{12}}, \tag{18}$$

can be eventually treated as a perturbation. Using the gradient operator expression [22],

$$\nabla_r = \frac{\mathbf{r}}{r}\frac{\partial}{\partial r}+\frac{1}{r}\nabla_\Omega, \tag{19}$$

we present the operator (18) as

$$\widehat{\mathcal{L}} = \widehat{\mathcal{U}}+\widehat{\mathcal{V}}, \tag{20}$$

where

$$\widehat{\mathcal{U}} = \frac{i}{2}\left[\triangle_{r_1}\mathcal{W}+\triangle_{r_2}\mathcal{W}\right] - \frac{1}{2}\left[(\nabla_{r_1}\mathcal{W})^2+(\nabla_{r_2}\mathcal{W})^2\right] + i\left[\frac{1}{r_1}(\nabla_{r_1}\mathcal{W})\cdot\nabla_{\Omega_1}+\frac{1}{r_2}(\nabla_{r_2}\mathcal{W})\cdot\nabla_{\Omega_2}\right], \tag{21}$$

$$\widehat{\mathcal{V}} = i\left[(\nabla_{r_1}\mathcal{W})\cdot\frac{\mathbf{r}_1}{r_1}\frac{\partial}{\partial r_1}+(\nabla_{r_2}\mathcal{W})\cdot\frac{\mathbf{r}_2}{r_2}\frac{\partial}{\partial r_2}\right] - \frac{1}{r_{12}}. \tag{22}$$

The operator $\widehat{\mathcal{U}}$ acts only on the bispherical harmonics, and it can be easily verified that it is a short-range potential. Concerning the operator $\widehat{\mathcal{V}}$, the phase $\mathcal{W}$ in the asymptotic region is given by Eq. (14), an hence at large ρ

$$\nabla_{r_1}\mathcal{W} \simeq -\frac{1}{k}\left\{\frac{\mathbf{r}_1}{r_{12}\rho}\left[1+\ln(2k\rho)\right]-\frac{\mathbf{r}_{12}}{r_{12}^3}\rho\ln(2k\rho)\right\}, \tag{23}$$

$$\nabla_{r_2}\mathcal{W} \simeq -\frac{1}{k}\left\{\frac{\mathbf{r}_2}{r_{12}\rho}\left[1+\ln(2k\rho)\right]+\frac{\mathbf{r}_{12}}{r_{12}^3}\rho\ln(2k\rho)\right\}. \tag{24}$$

Moreover, using the asymptotics of the radial CQS functions (10), we obtain ($j = 1, 2$):

$$\frac{\partial}{\partial r_j} |n_1\ell_1 n_2\ell_2; LM\rangle_Q \simeq ik\frac{r_j}{\rho} |n_1\ell_1 n_2\ell_2; LM\rangle_Q. \tag{25}$$

Finally, by applying the operator (22) to Eq. (5) and taking into account Eqs. (23) and (25), we conclude that $\widehat{\mathcal{V}}$ acts upon these basis functions as a short-range potential that vanishes faster than ρ^{-1} in the limit $\rho \to \infty$. Thus the operator (18) may be treated as a perturbation and therefore the expansion (16) of the solution in our TEC representation is expected to converge.

The following issue has to be taken into account. Although the use of the phase factor allows one to take care of the Coulomb potential $1/r_{12}$, we cannot employ Eq. (14) directly because singular terms $1/r_{12}^3$ and $1/r_{12}^4$ appear in Eq. (21). However, this difficulty can be easily circumvented by using in both the Hamiltonian and the phase factor a truncated multipole expansion,

$$V_{12} = \sum_{\lambda=0}^{\lambda_{max}} \left(\frac{r_<^\lambda}{r_>^{\lambda+1}}\right) P_\lambda(x), \tag{26}$$

$$x = \frac{r_1^2 + r_2^2 - r_{12}^2}{2r_1\, r_2}, \tag{27}$$

instead of $1/r_{12}$. In Ref. [3] we considered only the $\lambda = 0$ case (Temkin–Poet model).

4 Two-channel case

As an illustration, we compare below the functions $\Phi^{(+)}$ and $\widetilde{\Phi}^{(+)}$ by solving the inhomogeneous Eq. (1). More precisely, we consider the truncated expansions of $\Phi_N^{(+)}$ and $\widetilde{\Phi}_N^{(+)}$ containing $N \times N$ terms and compare their convergence rate as N increases. For test purposes, we consider the case of zero total angular momentum, $L = M = 0$, and, for simplicity, we retain in the partial-wave expansions in Eqs. (11) and (16) only two bispherical terms $\mathcal{Y}_{00}^{00}$ and $\mathcal{Y}_{00}^{11}$. Hence it is sufficient to retain the first three multipole terms in Eq. (26).

We solve Eq. (1) with the initial helium ground state wave function in the driven term given by the product of hydrogen functions (with $Z_e = 2 - 5/16$), and we set $E = 0.791$ (i. e., 20 eV) and $q = 0.24$, as in one of the Orsay experiments [18] (see also Ref. [19]). The scale parameter of the CQS basis is chosen to be $b = 0.6$.

Consider first the expansion

$$\Phi_N^{(+)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\ell=0,1} \sum_{n_1,n_2=0}^{N-1} C_{n_1 n_2}^{\ell} |n_1\ell n_2\ell; 00\rangle_Q. \tag{28}$$

With the help of Eq. (7) we rewrite Eq. (1) as

$$\sum_{\ell=0,1} \sum_{n_1,n_2=0}^{N-1} C_{n_1 n_2}^{\ell} \left[\frac{1}{r_1 r_2} |n_1\ell n_2\ell; 00\rangle_L - \frac{1}{r_{12}} |n_1\ell n_2\ell; 00\rangle_Q\right] = \hat{W}_{fi}\, \Phi^{(0)}(\mathbf{r}_1, \mathbf{r}_2), \tag{29}$$

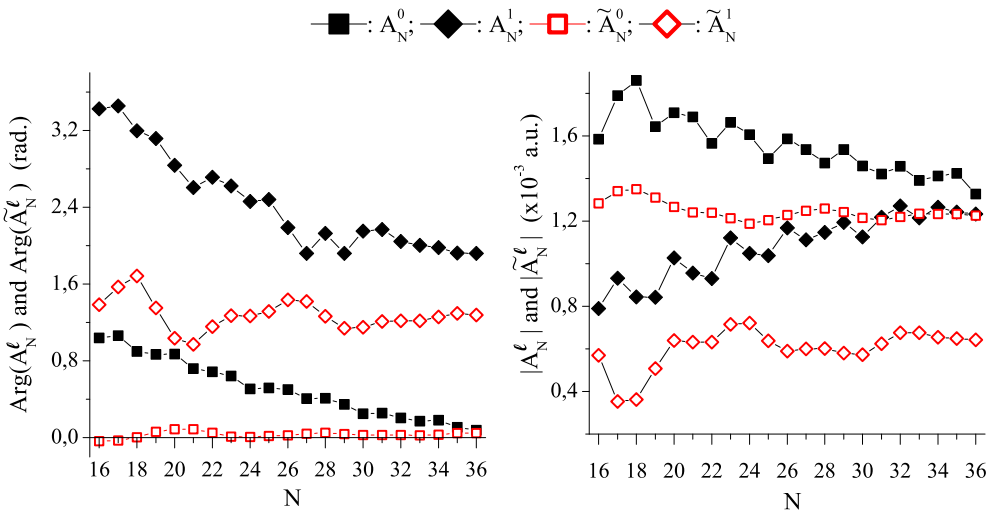

Figure 1: Convergence of the amplitudes A_N^ℓ (filled symbols) and $\widetilde{A}_N^\ell$ (open symbols) for $\alpha = \frac{\pi}{4}$ and $\ell = 0, 1$. We present separately the results for the arguments $\mathrm{Arg}\left(A_N^\ell\right)$ and $\mathrm{Arg}\left(\widetilde{A}_N^\ell\right)$ (left panel) and absolute values $\left|A_N^\ell\right|$ and $\left|\widetilde{A}_N^\ell\right|$ (right panel).

where the coupled Laguerre basis functions

$$|n_1\ell_1 n_2\ell_2; LM\rangle_L \equiv \frac{\psi_{n_1}^{\ell_1}(r_1)\,\psi_{n_2}^{\ell_2}(r_2)}{r_1\,r_2}\,\mathcal{Y}_{LM}^{\ell_1\ell_2}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2). \tag{30}$$

We obtain a matrix equation for the coefficients $C_{n_1 n_2}^\ell$ (see, e. g., Ref. [23]) by projecting Eq. (29) onto the basis set (30) and making use of the orthogonality relation

$${}_L\langle n_1'\ell_1' n_2'\ell_2'; LM| \frac{1}{r_1 r_2} |n_1\ell_1 n_2\ell_2; LM\rangle_L = \delta_{n_1' n_1}\,\delta_{n_2' n_2}\,\delta_{\ell_1'\ell_1}\,\delta_{\ell_2'\ell_2}. \tag{31}$$

The asymptotic behavior of the proposed solution is given by Eq. (12) where the amplitude

$$A\left(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2\right) = \sum_{\ell=0,1} A_N^\ell\,\mathcal{Y}_{00}^{\ell\ell}(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) \tag{32}$$

is expressed in terms of partial amplitudes

$$A_N^\ell = \frac{2}{\sin(2\alpha)}\sqrt{\frac{8}{\pi}}\,e^{\frac{i\pi}{4}}\,k^{-1/2}\exp\left\{i\left[\sigma_\ell(p_1) + \sigma_\ell(p_2) - \pi\ell\right]\right\} \times \sum_{n_1, n_2=0}^{N-1} C_{n_1 n_2}^\ell\,S_{n_1\ell}(p_1)\,S_{n_2\ell}(p_2). \tag{33}$$

The amplitudes A_N^ℓ for $\alpha = \frac{\pi}{4}$ and $\ell = 0, 1$ are shown in Fig. 1 as functions of N (filled symbols). A poor convergence of both the argument $\mathrm{Arg}\left(A_N^\ell\right)$ and the absolute value $\left|A_N^\ell\right|$ clearly demonstrates a limited practical usefulness of the expansion (28).

Consider now the solution $\widetilde{\Phi}^{(+)}$ in the TEC representation given by the truncated expansion

$$\widetilde{\Phi}_N^{(+)}(\mathbf{r}_1,\mathbf{r}_2) = \sum_{\ell=0,1} \sum_{n_1,n_2=0}^{N-1} \widetilde{C}^{\ell}_{n_1 n_2} |n_1 \ell n_2 \ell; 00\rangle_Q. \tag{34}$$

Upon substitution into Eq. (17) we find

$$\sum_{\ell=0,1} \sum_{n_1,n_2=0}^{N-1} \left[\frac{1}{r_1 r_2} |n_1 \ell n_2 \ell; 00\rangle_L + \widehat{\mathcal{L}} |n_1 \ell n_2 \ell; 00\rangle_Q \right] \widetilde{C}^{\ell}_{n_1 n_2} = e^{-i\mathcal{W}(\mathbf{r}_1,\mathbf{r}_2)} \hat{W}_{fi} \Phi^{(0)}(\mathbf{r}_1,\mathbf{r}_2). \tag{35}$$

This equation should be solved in the same manner as Eq. (29) to obtain the expansion coefficients $\widetilde{C}^{\ell}_{n_1 n_2}$.

We have seen how the leading asymptotic form of the phase $\mathcal{W}$ given by Eq. (14) determines the features of the operator (18) acting on the CQS basis functions in the region Ω_0. There is no need to reproduce precisely the r.h.s of Eq. (14) since it is asymptotical. On the other hand, we have to ensure the regularity at the origin of the $\widehat{\mathcal{L}}$ operator representation. Apart from this constraint, we are free to modify properties of $\widehat{\mathcal{L}}$ at moderate distances by including higher order terms in $\mathcal{W}$ with the aim to optimize the basis set. We use the following phase parametrization (note, various other parametrizations can be also explored):

$$\mathcal{W}(\mathbf{r}_1,\mathbf{r}_2) = -\frac{s}{k}\left[\ln(2ks) + d\right] \left(\frac{1}{u} + \frac{r_1 r_2}{u^3} P_1(x) + \frac{(r_1 r_2)^2}{u^5} P_2(x) \right), \tag{36}$$

$$u = \sqrt{a^2 + r_>^2}, \quad s = \sqrt{c^2 + \rho^2}, \tag{37}$$

where real positive parameters a and c are introduced to avoid singularities at the origin (for simplicity we set $c^2 = a$). We have also introduced a real parameter d that allows one to improve the convergence rate of expansion (34). The results presented below are obtained with $a = 5$ and $d = -4.75$.

Let us now come back to the proposed truncated expansion (34). The asymptotic behavior of $\widetilde{\Phi}_N^{(+)}$ is still given by Eq. (12) with the amplitude $A(\hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2)$ which should be calculated using Eq. (32) where the partial amplitudes A_N^{ℓ} should be replaced by

$$\widetilde{A}_N^{\ell} = \frac{2}{\sin(2\alpha)} \sqrt{\frac{8}{\pi}}\, e^{\frac{i\pi}{4}}\, k^{-1/2} \exp\left\{ i\left[\sigma_\ell(p_1) + \sigma_\ell(p_2) - \pi\ell\right]\right\} \times \sum_{n_1,n_2=0}^{N-1} \widetilde{C}^{\ell}_{n_1 n_2}\, S_{n_1 \ell}(p_1)\, S_{n_2 \ell}(p_2). \tag{38}$$

The convergence behavior of $\widetilde{A}_N^{\ell}$ is shown in Fig. 1 (open symbols). As expected, the rate and smoothness of convergence are considerably improved by the TEC representation. This result demonstrates numerically that the inclusion of an appropriate phase factor into the basis functions is able to adequately absorb the leading asymptotic effect of the electron-electron interaction.

5 Summary

In our previous publication [3], we have proposed the phase factor method as a new approach to double ionization problems represented by the three-body driven equation with a square integrable inhomogeneity. Specifically, we tried to solve the S-model equation describing the fast electron impact double ionization of helium by expanding the solution in terms of the so-called Convoluted Quasi Sturmian functions. Since the asymptotic behavior of these functions is inconsistent with that of formal Coulomb three-body continuum states, the CQS basis cannot represent the solution in the entire space. Even worse, we have found out that our solution diverges as the basis size increases. In order to circumvent this failure, and thus to improve the convergence rate, we have suggested equipping the basis CQS functions with the phase factor corresponding to the inter-electronic interaction. Within the S-wave framework, this strategy has been demonstrated to be successful.

In this paper an extension of the phase factor approach of Ref. [3] to arbitrary angular momenta is proposed. Since the phase factor is intended to account for the inter-electronic Coulomb interaction, it is natural to use the same truncated multipole expansion of $1/r_{12}$ in the generalized phase as employed to approximate this potential in the Hamiltonian. We examine the validity of our modified CQS approach in a two-channel case by constructing a suitable formula for the phase. The inclusion of higher order terms in $1/\rho$ in the leading asymptotic behavior, results in a significant convergence acceleration of the calculated amplitudes. We also demonstrate the convergence rate of the solution expansion to be rather sensitive to the phase behavior at moderate distances; optimized parameters (only two in our case) can therefore improve the efficiency of the basis. We expect the CQS basis combined with the proposed phase method to provide an efficient tool for the studies of full $(e, 3e)$ processes as well.

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