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The parabolic Sturmian-function basis representation of the six-dimensional Coulomb Green's function

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Abstract

The square integrable basis set representation of the resolvent of the asymptotic three-body Coulomb wave operator in parabolic coordinates is obtained. The resulting six-dimensional Green's function matrix is expressed as a convolution integral over separation constants.

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1. Introduction

The three-body Coulomb continuum problem has represented up till now a very difficult problem which is present in many areas of physics. The best known and widely used approximate solution is expressed in terms of a product of three Coulomb waves, the so-called C3 model [1–4] (also called the 3C or Brauner–Briggs–Klar (BBK) model). The C3 wavefunction satisfies the correct asymptotic conditions, when the three particles are far away from each other (the so-called region Ω_0). The C3 wavefunction has been, and is currently, successfully used as the final-state wavefunction for calculating cross sections for electron-impact double ionization of helium (so-called $(e, 3e)$ processes) [5–7], and the calculation results are in good agreement with the experimental [8] both in shape and in absolute value. On the other hand, the C3 wavefunction describes poorly the behavior at intermediate interparticle distances and when one particle is far away from the other two. The investigation of the role of the description of initial and final states in $(\gamma, 2e)$ and $(e, 2e)$ collisions allow the authors of [9] to conclude that collisional processes cannot be easily used as a conclusive test for the quality of approximated wavefunctions and the overall agreement with absolute $(e, 3e)$ experiment data is fortuitous.

The C3 wavefunction is obtained by neglecting all mixed derivatives of the three-body Hamiltonian written in generalized parabolic coordinates [1]. Many improvements to the C3 model have been developed by considering in some approximate way of the neglected terms of the kinetic energy. Most of them use the same form for the wavefunction, i.e. the

product of three two-body Coulomb wavefunctions. These modifications introduce position- or velocity-dependent effective charges (see, e.g., [10, 11]). Besides, modifications in the relative momenta of the particles have been introduced in [12] to describe the three-body Coulomb wavefunction in the regions Ω_α where the mutual distance between particles β and γ is much smaller than the distance between their center of mass and the particle α (see also [13] and references therein).

Some attempts to go beyond the C3 model have also been made. The author of [14] has suggested to express the three-body Coulomb continuum wavefunction in the ‘inner’ zone (where the potential energy dominates the kinetic one) as a linear superposition of C3 wavefunctions with different relative momenta between the particles. In [15–17] the Φ_2 model has been proposed and developed. Within this approach an approximate analytical wavefunction is expressed in terms of the hypergeometric function of two variables. Using the representation of the Φ_2 model wavefunction as a series expansion in powers of coordinates the authors of [15–17] have shown that the C3 wavefunction is included as a first order in this expansion. The authors of [17] have also pointed out that a Faddeev-type equation can be derived for the three-body Coulomb continuum wavefunction considering the Green’s function of the asymptotic separable Coulomb wave operator and taking an approximation to the non-orthogonal part of the kinetic energy as the components of the perturbed potential.

In the previous paper [18] we have attempted to apply the J -matrix method [19] (see also [20] and references therein) for solving numerically the three-body Coulomb continuum problem. Within this version of the J -matrix formalism, the three-body Coulomb continuum wavefunction is expanded in an infinite series of six-dimensional L^2 basis functions. Then the initial Schrödinger equation is transformed into a discrete analog of the Lippmann–Schwinger equation. However, the corresponding Green’s function was not derived in [18]. The goal of this paper is to obtain the expression for the six-dimensional Coulomb Green’s function matrix elements.

Below, we present some relations needed for understanding the separable approximation to the Schrödinger equation for the three-body Coulomb problem.

Consider the Schrödinger equation for a three-body Coulomb system with masses m_1, m_2, m_3 and charges Z_1, Z_2, Z_3 , respectively,

$$\left[-\frac{1}{2\mu_{12}} \Delta_{\mathbf{R}} - \frac{1}{2\mu_3} \Delta_{\mathbf{r}} + \frac{Z_1 Z_2}{r_{12}} + \frac{Z_2 Z_3}{r_{23}} + \frac{Z_1 Z_3}{r_{13}} \right] \Psi = E \Psi. \quad (1)$$

Here \mathbf{R} and \mathbf{r} are the Jacobi vectors

$$\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \quad \mathbf{r} = \mathbf{r}_3 - \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m_1 + m_2}, \quad (2)$$

$\mathbf{r}_{ls} = \mathbf{r}_l - \mathbf{r}_s$ is the relative position variable, $r_{ls} = |\mathbf{r}_{ls}|$. The reduced masses are

$$\mu_{12} = \frac{m_1 m_2}{m_1 + m_2}, \quad \mu_3 = \frac{(m_1 + m_2) m_3}{m_1 + m_2 + m_3}. \quad (3)$$

The eigenenergy E is given by $E = \frac{1}{2\mu_{12}} \mathbf{K}^2 + \frac{1}{2\mu_3} \mathbf{k}^2$. The ansatz

$$\Psi = e^{i(\mathbf{K} \cdot \mathbf{R} + \mathbf{k} \cdot \mathbf{r})} \bar{\Psi} \quad (4)$$

removes the eigenenergy giving the equation for $\bar{\Psi}$:

$$\left[-\frac{1}{2\mu_{12}} \Delta_{\mathbf{R}} - \frac{1}{2\mu_3} \Delta_{\mathbf{r}} - \frac{i}{\mu_{12}} \mathbf{K} \cdot \nabla_{\mathbf{R}} - \frac{i}{\mu_3} \mathbf{k} \cdot \nabla_{\mathbf{r}} + \frac{Z_1 Z_2}{r_{12}} + \frac{Z_2 Z_3}{r_{23}} + \frac{Z_1 Z_3}{r_{13}} \right] \bar{\Psi} = 0. \quad (5)$$

Let D denote the operator in the square braces in (5). This operator is considered in terms of parabolic coordinates introduced by Klar [1]

$$\begin{aligned}\xi_1 &= r_{23} + \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23}, & \eta_1 &= r_{23} - \hat{\mathbf{k}}_{23} \cdot \mathbf{r}_{23}, \\ \xi_2 &= r_{13} + \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13}, & \eta_2 &= r_{13} - \hat{\mathbf{k}}_{13} \cdot \mathbf{r}_{13}, \\ \xi_3 &= r_{12} + \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12}, & \eta_3 &= r_{12} - \hat{\mathbf{k}}_{12} \cdot \mathbf{r}_{12},\end{aligned}\quad (6)$$

where $\mathbf{k}_{ls} = \frac{\mathbf{k}_l m_s - \mathbf{k}_s m_l}{m_l + m_s}$ is the relative momentum vector between the particles l and s , $\hat{\mathbf{k}}_{ls}$ is the unit vector: $\hat{\mathbf{k}}_{ls} = \frac{\mathbf{k}_{ls}}{k_{ls}}$, $k_{ls} = |\mathbf{k}_{ls}|$. Then D is expressed as a sum of two parts

$$D = D_0 + D_1, \quad (7)$$

where D_0 is given by

$$D_0 = \sum_{j=1}^3 \frac{1}{\mu_{ls}(\xi_j + \eta_j)} [\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls}], \quad (8)$$

for $j \neq l, s$ and $l < s$. Here $t_{ls} = \frac{Z_l Z_s \mu_{ls}}{k_{ls}}$, $\mu_{ls} = \frac{m_l m_s}{m_l + m_s}$; the one-dimensional operators \hat{h}_{ξ_j} and \hat{h}_{η_j} are defined by

$$\hat{h}_{\xi_j} = -2 \left(\frac{\partial}{\partial \xi_j} \xi_j \frac{\partial}{\partial \xi_j} + ik_{ls} \xi_j \frac{\partial}{\partial \xi_j} \right), \quad \hat{h}_{\eta_j} = -2 \left(\frac{\partial}{\partial \eta_j} \eta_j \frac{\partial}{\partial \eta_j} - ik_{ls} \eta_j \frac{\partial}{\partial \eta_j} \right). \quad (9)$$

D_0 is the leading term which provides a three-body continuum wavefunction that satisfies exact asymptotic boundary conditions for Coulomb systems in the limit of all particles being far from each other [1]. The operator D_1 , which contains all mixed second derivatives $\frac{\partial^2}{\partial \xi_j \partial \xi_j}$, $\frac{\partial^2}{\partial \eta_j \partial \eta_j}$, $j \neq l$ and $\frac{\partial^2}{\partial \xi_j \partial \eta_l}$ (see, e.g., [21]), is regarded as a small perturbation which does not violate the boundary conditions [1].

Further, if we neglect D_1 from equation (5) we obtain the approximate equation

$$D_0 \bar{\Psi} = 0, \quad (10)$$

which is separable with an infinite number of solutions [1]

$$\bar{\Psi} = \prod_{j=1}^3 f_j(\xi_j, \eta_j) \quad (11)$$

and each of the functions $f_j(\xi_j, \eta_j)$ is a solution of equation [1]:

$$\frac{1}{\mu_{ls}(\xi_j + \eta_j)} [\hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls}] f_j(\xi_j, \eta_j) = -C_j f_j(\xi_j, \eta_j). \quad (12)$$

The separation constant C_j satisfy the constraints [1]

$$C_1 + C_2 + C_3 = 0. \quad (13)$$

The solution f_j is represented in the form $f_j(\xi_j, \eta_j) = u_j(\xi_j)v_j(\eta_j)$, and the functions $u_j(\xi_j)$ and $v_j(\eta_j)$ satisfy the equations

$$\begin{aligned}[\hat{h}_{\xi_j} + 2k_{ls}A_j + \mu_{ls}C_j \xi_j] u_j(\xi_j) &= 0, \\ [\hat{h}_{\eta_j} + 2k_{ls}B_j + \mu_{ls}C_j \eta_j] v_j(\eta_j) &= 0,\end{aligned}\quad (14)$$

with the constraint

$$A_j + B_j = t_{ls}. \quad (15)$$

The general solutions of (14) can be obtained by transforming the confluent hypergeometric equation (see, e.g., [21]). Thus, the general solution of (10) is expressed in terms of a product of six Kummer hypergeometric functions (the so-called C6 model wavefunction Ψ_{C6} [21]). By setting specific values for separation constants A_j , B_j , C_j solutions with a particular asymptotic behavior can be obtained. For instance, putting $C_j = B_j = 0$ and $A_j = t_{ls}$, the

C3 wavefunction with pure outgoing behavior is obtained [1]:

$$\Psi_{C3} = \prod_{j=1}^3 {}_1F_1(it_{ls}, 1; -ik_{ls}\xi_j). \quad (16)$$

The exact three-body Coulomb continuum wavefunction $\bar{\Psi}$ satisfies the six-dimensional differential equation

$$[D_0 + D_1]\bar{\Psi} = 0. \quad (17)$$

Then, multiplying (17) by $\prod_{j=1}^3 \mu_{ls}(\xi_j + \eta_j)$ yields [18]

$$[\hat{h} + \hat{V}]\bar{\Psi} = 0 \quad (18)$$

where

$$\begin{aligned} \hat{h} = \prod_{j=1}^3 \mu_{ls}(\xi_j + \eta_j) D_0 &= \mu_{13}(\xi_2 + \eta_2) \mu_{12}(\xi_3 + \eta_3) \hat{h}_1 \\ &+ \mu_{23}(\xi_1 + \eta_1) \mu_{12}(\xi_3 + \eta_3) \hat{h}_2 + \mu_{23}(\xi_1 + \eta_1) \mu_{13}(\xi_2 + \eta_2) \hat{h}_3, \end{aligned} \quad (19)$$

$$\hat{h}_j = \hat{h}_{\xi_j} + \hat{h}_{\eta_j} + 2k_{ls}t_{ls} \quad (20)$$

and

$$\hat{V} = \prod_{j=1}^3 \mu_{ls}(\xi_j + \eta_j) D_1. \quad (21)$$

In turn, equation (18), in view of the boundary condition

$$\bar{\Psi} \rightarrow \Psi_{C3} \quad \text{or} \quad \bar{\Psi} \rightarrow \Psi_{C6}, \quad (22)$$

is transformed [18] into the following Lippmann–Schwinger-type equation:

$$\bar{\Psi} = \Psi_{C3} + \hat{\mathcal{G}}\hat{V}\bar{\Psi} \quad \text{or} \quad \bar{\Psi} = \Psi_{C6} + \hat{\mathcal{G}}\hat{V}\bar{\Psi}, \quad (23)$$

where $\hat{\mathcal{G}}$ is the resolvent of the operator \hat{h} (19). It has been suggested in [18] to treat the equation (23) within the context of L^2 parabolic Sturmian basis set [22]

$$|\mathcal{N}\rangle = \prod_{j=1}^3 \phi_{n_j m_j}(\xi_j, \eta_j), \quad (24)$$

$$\phi_{n_j m_j}(\xi_j, \eta_j) = \psi_{n_j}(\xi_j) \psi_{m_j}(\eta_j), \quad (25)$$

$$\psi_n(x) = \sqrt{2b} e^{-bx} L_n(2bx), \quad (26)$$

where b is the scaling parameter. Thus, the wavefunction $\bar{\Psi}$ is expanded in basis function series

$$\bar{\Psi} = \sum_{\mathcal{N}} a_{\mathcal{N}} |\mathcal{N}\rangle. \quad (27)$$

Then, the projection of (23) onto functions $|\mathcal{N}\rangle$ yields an infinite set of equations in the coefficients $a_{\mathcal{N}}$

$$\underline{a} = \underline{a}^{(0)} - \underline{\mathcal{G}}\underline{V}\underline{a}, \quad (28)$$

where $\underline{\mathcal{G}}$ and \underline{V} are the matrices with elements $\langle \mathcal{N} | \hat{\mathcal{G}} | \mathcal{N}' \rangle$ and $\langle \mathcal{N} | \hat{V} | \mathcal{N}' \rangle$, respectively, \underline{a} is the vector with components $a_{\mathcal{N}}$, $a_{\mathcal{N}}^{(0)} = \langle \mathcal{N} | \Psi_{C3} \rangle$ or $a_{\mathcal{N}}^{(0)} = \langle \mathcal{N} | \Psi_{C6} \rangle$.

The problem of calculation of the matrix elements $\langle \mathcal{N} | \widehat{V} | \mathcal{N}' \rangle$ of the operator \widehat{V} (which contains very involved algebraic functions of the parabolic variables) is beyond the scope of the present paper. At this stage it will suffice to consider that the short-range operator \widehat{V} can be approximated by a finite-order matrix V .

In the previous paper [18] the resolvent \widehat{G}_j for the two-dimensional operator

$$\widehat{h}_j + \mu_{l_s} C_j (\xi_j + \eta_j) \tag{29}$$

has been treated within the context of the basis set (25). In particular, a matrix representation \mathbf{G}_j of the Green's function \widehat{G}_j has been obtained which is formally the matrix inverse to the infinite matrix $[\mathbf{h}_j + \mu_{l_s} C_j \mathbf{Q}_j]$ of the operator (29):

$$[\mathbf{h}_j + \mu_{l_s} C_j \mathbf{Q}_j] \mathbf{G}_j(t_{l_s}; \mu_{l_s} C_j) = \mathbf{I}_j. \tag{30}$$

Here

$$\mathbf{h}_j = \mathbf{h}_{\xi_j} \otimes \mathbf{I}_{\eta_j} + \mathbf{I}_{\xi_j} \otimes \mathbf{h}_{\eta_j} + 2k_{l_s} t_{l_s} \mathbf{I}_j \tag{31}$$

is the matrix of the operator \widehat{h}_j (20) in the basis (25), \mathbf{I}_{ξ_j} , \mathbf{I}_{η_j} and $\mathbf{I}_j = \mathbf{I}_{\xi_j} \otimes \mathbf{I}_{\eta_j}$ are the unit matrices. $\mathbf{Q}_j = \mathbf{Q}_{\xi_j} \otimes \mathbf{I}_{\eta_j} + \mathbf{I}_{\xi_j} \otimes \mathbf{Q}_{\eta_j}$, where \mathbf{Q}_{ξ_j} and \mathbf{Q}_{η_j} are the matrices of ξ_j and η_j in basis (26), respectively.

In this paper, we consider a Green's function $\widehat{\mathfrak{G}}$ associated with the six-dimensional operator \widehat{h} (19). Namely, we construct a matrix $\underline{\mathfrak{G}}$ which is formally inverse to the long-range operator (19) infinite matrix

$$\underline{h} = \mu_{13} \mu_{12} \mathbf{h}_1 \otimes \mathbf{Q}_2 \otimes \mathbf{Q}_3 + \mu_{23} \mu_{12} \mathbf{Q}_1 \otimes \mathbf{h}_2 \otimes \mathbf{Q}_3 + \mu_{23} \mu_{13} \mathbf{Q}_1 \otimes \mathbf{Q}_2 \otimes \mathbf{h}_3. \tag{32}$$

As we pointed out in [18], the six-dimensional Green's function matrix $\underline{\mathfrak{G}}$ is expressed as the convolution integral

$$\underline{\mathfrak{G}} = \aleph \iint dC_1 dC_2 \mathbf{G}_1(t_{23}; \mu_{23} C_1) \otimes \mathbf{G}_2(t_{13}; \mu_{13} C_2) \otimes \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2)), \tag{33}$$

where \mathbf{G}_j are the two-dimensional Green's functions \widehat{G}_j matrices, \aleph is a normalizing factor. Thus, our problem now is to determine the paths of integration over the separation constants C_1 and C_2 in (33) and to find the corresponding normalizing factor \aleph such that the condition

$$\underline{h} \underline{\mathfrak{G}} = \mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{I}_3 \tag{34}$$

holds. For this purpose consider the product $\underline{h} \underline{\mathfrak{G}}$. From the relation (30) we obtain

$$\begin{aligned} \underline{h} \underline{\mathfrak{G}} = \aleph \left\{ \iint dC_1 dC_2 [\mathbf{I}_1 - \mu_{23} C_1 \mathbf{Q}_1 \mathbf{G}_1(t_{23}; \mu_{23} C_1)] \otimes \mu_{13} \mathbf{Q}_2 \mathbf{G}_2(t_{13}; \mu_{13} C_2) \right. \\ \otimes \mu_{12} \mathbf{Q}_3 \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2)) + \iint dC_1 dC_2 \mu_{23} \mathbf{Q}_1 \mathbf{G}_1(t_{23}; \mu_{23} C_1) \\ \otimes [\mathbf{I}_2 - \mu_{13} C_2 \mathbf{Q}_2 \mathbf{G}_2(t_{13}; \mu_{13} C_2)] \\ \otimes \mu_{12} \mathbf{Q}_3 \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2)) + \iint dC_1 dC_2 \mu_{23} \mathbf{Q}_1 \mathbf{G}_1(t_{23}; \mu_{23} C_1) \\ \left. \otimes \mu_{13} \mathbf{Q}_2 \mathbf{G}_2(t_{13}; \mu_{13} C_2) \otimes [\mathbf{I}_3 + \mu_{12}(C_1 + C_2) \mathbf{Q}_3 \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2))] \right\}, \tag{35} \end{aligned}$$

and hence

$$\begin{aligned} \underline{h}\mathcal{G} = \aleph \left\{ \iint dC_1 dC_2 [\mathbf{I}_1 \otimes \mu_{13} \mathbf{Q}_2 \mathbf{G}_2(t_{13}; \mu_{13} C_2) \otimes \mu_{12} \mathbf{Q}_3 \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2)) \right. \\ \left. + \mu_{23} \mathbf{Q}_1 \mathbf{G}_1(t_{23}; \mu_{23} C_1) \otimes \mathbf{I}_2 \otimes \mu_{12} \mathbf{Q}_3 \mathbf{G}_3(t_{12}; -\mu_{12}(C_1 + C_2))] \right. \\ \left. + \left[\mu_{23} \mathbf{Q}_1 \int dC_1 \mathbf{G}_1(t_{23}; \mu_{23} C_1) \right] \otimes \left[\mu_{13} \mathbf{Q}_2 \int dC_2 \mathbf{G}_2(t_{13}; \mu_{13} C_2) \right] \otimes \mathbf{I}_3 \right\}. \end{aligned} \tag{36}$$

As a first step toward our goal we consider the integrals

$$\int dC_j \mathbf{G}_j(t_{ls}; \mu_{ls} C_j) \tag{37}$$

inside the figure brackets on the right-hand side of (36).

In section 2 completeness of the eigenfunctions of the two-dimensional operator (29) is considered. In particular, an integral representation of the matrix **A** which is inverse to the infinite matrix **Q** of the operator $(\xi + \eta)$ in the basis (25) is obtained. In section 3 it is demonstrated that the integral (37) taken along an appropriate contour is proportional to the matrix **A** obtained in the previous section. Finally, section 4 presents a convolution integral representation of the six-dimensional Coulomb Green's function matrix.

2. Completeness relations

2.1. The continuous spectrum

Of particular interest are the regular solutions

$$f(\gamma, \tau, \xi, \eta) = u(\gamma, \tau, \xi)v(\gamma, \tau, \eta) \tag{38}$$

of the system

$$[\hat{h}_\xi + 2kt + \mu C \xi]u(\gamma, \tau, \xi) = 0, \tag{39}$$

$$[\hat{h}_\eta + 2k(t_0 - t) + \mu C \eta]v(\gamma, \tau, \xi) = 0. \tag{40}$$

Obviously, the regular solutions u and v are proportional to confluent hypergeometric functions (see, e.g., [21])

$$u(\gamma, \tau, \xi) = e^{\frac{1}{2}(\gamma-k)\xi} {}_1F_1\left(\frac{1}{2} + i\tau, 1, -i\gamma\xi\right) \tag{41}$$

and

$$\begin{aligned} v(\gamma, \tau, \eta) &= e^{-\frac{1}{2}(\gamma-k)\eta} {}_1F_1\left(\frac{1}{2} + i(\tau - \tau_0), 1, i\gamma\eta\right) \\ &= e^{\frac{1}{2}(\gamma+k)\eta} {}_1F_1\left(\frac{1}{2} + i(\tau_0 - \tau), 1, -i\gamma\eta\right), \end{aligned} \tag{42}$$

where

$$\mu C = \frac{k^2}{2} - \frac{\gamma^2}{2}, \quad \tau = \frac{k}{\gamma} \left(t + \frac{i}{2}\right), \quad \tau_0 = \frac{k}{\gamma} t_0. \tag{43}$$

It should be noted that since the representation of the two-dimensional Coulomb Green's functions matrix elements [18] involves an integration over τ from $-\infty$ to ∞ , in the subsequent discussion we assume that τ is real. With this assumption it is readily seen that the solutions (41) and (42) coincide, except for normalization and the phase factors $e^{-\frac{1}{2}k\xi}$ and $e^{\frac{1}{2}k\eta}$, with parabolic Coulomb Sturmians treated in [24]. In this case γ plays the role of the momentum

and $\mathcal{E} = \frac{\gamma^2}{2}$ is the energy. From this we conclude that for $\gamma > 0$ the solutions (41) and (42) correspond to the continuous spectrum of \mathcal{E} .

It is readily verified that the solutions $u(\gamma, \tau, \xi)$ and $v(\gamma, \tau, \eta)$ are expressed by basis set (26) expansions

$$u(\gamma, \tau, \xi) = \frac{2\sqrt{2b}}{2b - i(\gamma - k)} \left(\frac{2b - i(\gamma - k)}{2b + i(\gamma + k)} \right)^{i\tau + \frac{1}{2}} \sum_{n=0}^{\infty} \theta^n p_n(\tau; \zeta) \psi_n(\xi), \quad (44)$$

$$v(\gamma, \tau, \eta) = \frac{2\sqrt{2b}}{2b - i(\gamma + k)} \left(\frac{2b - i(\gamma + k)}{2b + i(\gamma - k)} \right)^{i(\tau_0 - \tau) + \frac{1}{2}} \sum_{n=0}^{\infty} \lambda^{-n} p_n(\tau_0 - \tau; \zeta) \psi_n(\eta), \quad (45)$$

where

$$\theta = \frac{2b + i(\gamma - k)}{2b - i(\gamma - k)}, \quad \lambda = \frac{2b - i(\gamma + k)}{2b + i(\gamma + k)}, \quad \zeta = \frac{\lambda}{\theta}. \quad (46)$$

The expansion (44) and (45) coefficients contain the polynomials [18]

$$p_n(\tau; \zeta) = \frac{(-1)^n \Gamma(n + \frac{1}{2} - i\tau)}{n! \Gamma(\frac{1}{2} - i\tau)} {}_2F_1\left(-n, \frac{1}{2} + i\tau; -n + \frac{1}{2} + i\tau; \zeta\right). \quad (47)$$

The basis set (26) representation of the equation (39) is the three-term recursion relation [18]

$$a_n y_{n-1} + b_n y_n + d_{n+1} y_{n+1} = 0, \quad n \geq 1 \quad (48)$$

where

$$b_n = \left(b + \frac{\mu C}{2b} + ik \right) + 2 \left(b + \frac{\mu C}{2b} \right) n + 2kt, \quad (49)$$

$$a_n = \left(b - \frac{\mu C}{2b} - ik \right) n, \quad d_n = \left(b - \frac{\mu C}{2b} + ik \right) n.$$

The functions

$$s_n(t; \mu C) = \theta^n p_n(\tau; \zeta) \quad (50)$$

are the ‘regular’ solutions of (48) with the initial conditions: $s_0 \equiv 1, s_{-1} \equiv 0$. The polynomials p_n (47) of degree n in τ are orthogonal with respect to the weight function [18]

$$\rho(\tau; \zeta) = \frac{\Gamma(\frac{1}{2} - i\tau) \Gamma(\frac{1}{2} + i\tau)}{2\pi i} (-\zeta)^{i\tau + \frac{1}{2}}, \quad (51)$$

where it is considered that $|\arg(-\zeta)| < \pi$. The corresponding orthogonality relation reads

$$\frac{i}{\zeta^m} \left(\frac{\zeta - 1}{\zeta} \right) \int_{-\infty}^{\infty} d\tau \rho(\tau; \zeta) p_n(\tau; \zeta) p_m(\tau; \zeta) = \delta_{nm}. \quad (52)$$

2.2. The discrete spectrum

For $t_0 < 0$ the eigenfunctions of (39) corresponding to the discrete spectrum $\mathcal{E}^{(\ell)} = \frac{\gamma_\ell^2}{2}, \gamma_\ell = i\kappa_\ell, \kappa_\ell = -\frac{k\ell_0}{\nu}, \ell = 1, 2, \dots, \infty$ are [25]

$$f_{\ell,m}(\xi, \eta) = u_{\ell,m}(\xi) v_{\ell,\ell-m-1}(\eta), \quad m = 0, 1, \dots, \ell - 1, \quad (53)$$

where

$$u_{\ell,m}(\xi) = e^{-\frac{i}{2}k\xi} e^{-\frac{\kappa_\ell \xi}{2}} {}_1F_1(-m, 1; \kappa_\ell \xi) = e^{-\frac{i}{2}k\xi} e^{-\frac{\kappa_\ell \xi}{2}} L_m(\kappa_\ell \xi) \quad (54)$$

and

$$v_{\ell,m}(\eta) = e^{\frac{i}{2}k\eta} e^{-\frac{\kappa_\ell\eta}{2}} {}_1F_1(-m, 1; \kappa_\ell\eta) = e^{\frac{i}{2}k\eta} e^{-\frac{\kappa_\ell\eta}{2}} L_m(\kappa_\ell\eta). \quad (55)$$

The solutions $f_{\ell,m}$ meet the orthogonality relation

$$\frac{\kappa_\ell^3}{2\ell} \int_0^\infty \int_0^\infty (\xi + \eta) d\xi d\eta f_{\ell,m}(\xi, \eta) [f_{\ell',m'}(\xi, \eta)]^* = \delta_{\ell,\ell'} \delta_{m,m'}. \quad (56)$$

It is readily verified that the expansions of $u_{\ell,m}(\xi)$ and $v_{\ell,m}(\eta)$ in a basis function (26) series are

$$u_{\ell,m}(\xi) = \sum_{n=0}^\infty S_n^{(\ell,m)} \psi_n(\xi) \quad (57)$$

and

$$v_{\ell,m}(\eta) = \sum_{n=0}^\infty [S_n^{(\ell,m)}]^* \psi_n(\eta), \quad (58)$$

where the coefficients are given by

$$S_n^{(\ell,m)} = 2\sqrt{2b}(-)^n \frac{(m+1)_n (2b - \kappa_\ell - ik)^n (2b - \kappa_\ell + ik)^m}{n! (2b + \kappa_\ell + ik)^{n+m+1}} \times {}_2F_1\left(-n, -m, -n - m; \frac{(2b + \kappa_\ell)^2 + k^2}{(2b - \kappa_\ell)^2 + k^2}\right). \quad (59)$$

2.3. One-dimensional completeness relations

The eigensolution $u(\gamma, \tau, \xi)$ of (39) corresponding to the continuous spectrum ($\gamma > 0$) for large ξ behaves as

$$u(\gamma, \tau, \xi) \underset{\xi \rightarrow \infty}{\sim} \frac{e^{-\frac{i}{2}k\xi} e^{\frac{\pi\tau}{2}}}{|\Gamma(\frac{1}{2} + i\tau)| \sqrt{\gamma\xi}} \frac{2i}{\sqrt{\gamma\xi}} \sin\left(\frac{\gamma\xi}{2} - \tau \ln(\gamma\xi) + \frac{\pi}{4} + \sigma\right), \quad (60)$$

where $\sigma = \arg \Gamma(\frac{1}{2} + i\tau)$. Therefore (see, e.g., [24, 26]),

$$\frac{\gamma}{4} \left| \Gamma\left(\frac{1}{2} + i\tau\right) \right|^2 e^{-\pi\tau} \int_0^\infty \xi d\xi u(\gamma, \tau, \xi) [u(\gamma', \tau, \xi)]^* = \pi \delta(\gamma - \gamma'), \quad (61)$$

and for $\tau > 0$ ($\tau = \frac{Z_0}{\gamma}$ with fixed $Z_0 > 0$)

$$\xi \int_0^\infty \gamma d\gamma \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{4\pi} e^{-\pi\tau} u(\gamma, \tau, \xi) [u(\gamma, \tau, \xi')]^* = \delta(\xi - \xi'). \quad (62)$$

On the other hand, if the functions $u(\gamma, \tau, \xi)$ are regarded as charge Sturmians [24], i.e. the parameter τ is considered as the eigenvalue of the problem, whereas the momentum γ remains constant, the corresponding orthogonality and completeness relations are given by [24]

$$\gamma \left| \Gamma\left(\frac{1}{2} + i\tau\right) \right|^2 e^{-\pi\tau} \int_0^\infty d\xi u(\gamma, \tau, \xi) [u(\gamma, \tau', \xi)]^* = 2\pi \delta(\tau - \tau') \quad (63)$$

and

$$\gamma \int_{-\infty}^\infty d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} e^{-\pi\tau} u(\gamma, \tau, \xi) [u(\gamma, \tau, \xi')]^* = \delta(\xi - \xi'). \quad (64)$$

Taking matrix elements of the completeness relation (64) we find

$$\frac{8b\gamma\theta^{n-m}}{\sqrt{[4b^2 + (\gamma + k)^2][4b^2 + (\gamma - k)^2]}} \int_{-\infty}^{\infty} d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} (-\zeta)^{i\tau} p_n(\tau; \zeta) [p_n(\tau; \zeta)]^* = \delta_{n,m}. \tag{65}$$

It may be noted that (65) is closely related to (52). To see this, let $\gamma > 0$. Then, it follows from the definitions (46) that

$$\frac{(\zeta - 1)}{\zeta} (-\zeta)^{\frac{1}{2}} = \frac{8b\gamma}{\sqrt{[4b^2 + (\gamma + k)^2][4b^2 + (\gamma - k)^2]}}. \tag{66}$$

Further, the regular solution $\theta^n p_n(\tau; \zeta)$ of the three-term recursion relation (48) is an even function of γ , since the coefficients a_n, b_n and d_n depend on γ only through $\mu C = \frac{1}{2}(k^2 - \gamma^2)$. Thus, replacing γ by $-\gamma$, and hence τ by $-\tau$ ($\theta \rightarrow \lambda$ and $\lambda \rightarrow \theta$) and ζ by ζ^{-1} in equation (47) gives

$$\theta^n p_n(\tau; \zeta) = \lambda^n \frac{(-1)^n \Gamma(n + \frac{1}{2} + i\tau)}{n! \Gamma(\frac{1}{2} + i\tau)} {}_2F_1\left(-n, \frac{1}{2} - i\tau; -n + \frac{1}{2} - i\tau; \zeta^{-1}\right). \tag{67}$$

Comparing equations (47) and (67) then yields the relation

$$\theta^n p_n(\tau; \zeta) = \lambda^n [p_n(\tau; \zeta)]^*, \tag{68}$$

and hence

$$[p_n(\tau; \zeta)]^* = \zeta^{-n} p_n(\tau; \zeta). \tag{69}$$

From the argument above, we conclude that for $\gamma > 0$ the orthogonality relation (52) reduces to (65).

2.4. The two-dimensional completeness relation

It follows from the relations (61) and (63) and analogous relations for $v(\gamma, \tau, \xi)$ that the two-dimensional orthogonality relation for $\gamma > 0$ is given by

$$e^{-\pi\tau_0} \frac{\gamma^2}{4} \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} \frac{|\Gamma(\frac{1}{2} + i(\tau_0 - \tau))|^2}{2\pi} \int_0^\infty \int_0^\infty (\xi + \eta) d\xi d\eta \{f(\gamma, \tau, \xi, \eta) \times [f(\gamma', \tau', \xi, \eta)]^*\} = \delta(\gamma - \gamma')\delta(\tau - \tau'). \tag{70}$$

In turn, in the case $t_0 > 0$ (where there are no bound states) it would appear reasonable that the two-dimensional completeness relation would be given by

$$(\xi + \eta) \left\{ \alpha \int_0^\infty d\gamma \gamma^2 e^{-\pi\tau_0} \int_{-\infty}^\infty d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} \frac{|\Gamma(\frac{1}{2} + i(\tau_0 - \tau))|^2}{2\pi} \times f(\gamma, \tau, \xi, \eta) [f(\gamma, \tau, \xi', \eta')]^* \right\} = \delta(\xi - \xi')\delta(\eta - \eta'). \tag{71}$$

The integration over τ in (71) is performed on the assumption that τ is independent of γ . To test this hypothesis and determine the normalizing factor α , we carried out the following numerical experiments. First with some parameters $t_0 > 0, k > 0$ and b we calculate the matrix elements $A_{n_1, n_2; m_1, m_2}$ for the expression in the figure braces on the left-hand side of

(71) in the basis (25):

$$\begin{aligned}
 A_{n_1, n_2; m_1, m_2} &= \alpha \int_0^\infty d\gamma \frac{64b^2 \gamma^2 (-\zeta)^{i\tau_0}}{[4b^2 + (\gamma + k)^2][4b^2 + (\gamma - k)^2]} \theta^{n_1 - m_1} \lambda^{m_2 - n_2} \\
 &\times \int_{-\infty}^\infty d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} \frac{|\Gamma(\frac{1}{2} + i(\tau_0 - \tau))|^2}{2\pi} \\
 &\times p_{n_1}(\tau; \zeta) p_{n_2}(\tau_0 - \tau; \zeta) [p_{m_1}(\tau; \zeta) p_{m_2}(\tau_0 - \tau; \zeta)]^*. \tag{72}
 \end{aligned}$$

It should be noted that the value of $(-\zeta)^{i\tau_0}$ in this formula is determined by the condition $|\arg(-\zeta)| < \pi$. Then the resulting matrix **A** is multiplied by the matrix

$$\mathbf{Q} = \mathbf{Q}_\xi \otimes \mathbf{I}_\eta + \mathbf{I}_\xi \otimes \mathbf{Q}_\eta \tag{73}$$

of the operator $(\xi + \eta)$. Finally, using the condition

$$\mathbf{Q}\mathbf{A} = \mathbf{I}_\xi \otimes \mathbf{I}_\eta \tag{74}$$

we have obtained that $\alpha = \frac{1}{2}$. Note that the infinite symmetric matrices \mathbf{Q}_ξ and \mathbf{Q}_η are tridiagonal [18]:

$$Q_{n, n'}^{\xi, \eta} = \begin{cases} -\frac{1}{2b}n, & n' = n - 1, \\ \frac{1}{2b}(2n + 1), & n' = n, \\ -\frac{1}{2b}(n + 1), & n' = n + 1, \end{cases} \tag{75}$$

therefore the normalization condition (74) can be rewritten in the form

$$\begin{aligned}
 &\frac{1}{2b} \delta_{n_2 m_2} \{-n_1 A_{n_1 - 1, n_2; m_1, m_2} + (2n_1 + 1) A_{n_1, n_2; m_1, m_2} - (n_1 + 1) A_{n_1 + 1, n_2; m_1, m_2}\} \\
 &+ \frac{1}{2b} \delta_{n_1 m_1} \{-n_2 A_{n_1, n_2 - 1; m_1, m_2} + (2n_2 + 1) A_{n_1, n_2; m_1, m_2} \\
 &- (n_2 + 1) A_{n_1, n_2 + 1; m_1, m_2}\} = \delta_{n_1 m_1} \delta_{n_2 m_2}. \tag{76}
 \end{aligned}$$

For $t_0 < 0$ the completeness relation (71) transforms into

$$\begin{aligned}
 (\xi + \eta) &\left\{ \frac{1}{2} \int_0^\infty d\gamma \gamma^2 e^{-\pi\tau_0} \int_{-\infty}^\infty d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} \frac{|\Gamma(\frac{1}{2} + i(\tau_0 - \tau))|^2}{2\pi} \right. \\
 &\times f(\gamma, \tau, \xi, \eta) [f(\gamma, \tau, \xi', \eta')]^* \\
 &\left. + \sum_{\ell=1}^\infty \frac{\kappa_\ell^3}{2\ell} \sum_{m=0}^{\ell-1} f_{\ell, m, \ell - m - 1}(\xi, \eta) [f_{\ell, m, \ell - m - 1}(\xi', \eta')]^* \right\} = \delta(\xi - \xi') \delta(\eta - \eta'). \tag{77}
 \end{aligned}$$

In this case the matrix **A** with elements

$$\begin{aligned}
 A_{n_1, n_2; m_1, m_2} &= \int_0^\infty d\gamma \frac{32b^2 \gamma^2 (-\zeta)^{i\tau_0}}{[4b^2 + (\gamma + k)^2][4b^2 + (\gamma - k)^2]} \theta^{n_1 - m_1} \lambda^{m_2 - n_2} \\
 &\times \int_{-\infty}^\infty d\tau \frac{|\Gamma(\frac{1}{2} + i\tau)|^2}{2\pi} \frac{|\Gamma(\frac{1}{2} + i(\tau_0 - \tau))|^2}{2\pi} \\
 &\times p_{n_1}(\tau; \zeta) p_{n_2}(\tau_0 - \tau; \zeta) [p_{m_1}(\tau; \zeta) p_{m_2}(\tau_0 - \tau; \zeta)]^* \\
 &+ \sum_{\ell=1}^\infty \frac{\kappa_\ell^3}{2\ell} \sum_{m=0}^{\ell-1} S_{n_1}^{(\ell, m)} S_{m_2}^{(\ell, \ell - m - 1)} [S_{n_2}^{(\ell, \ell - m - 1)} S_{m_1}^{(\ell, m)}]^* \tag{78}
 \end{aligned}$$

is also inverse to the matrix \mathbf{Q} (73). The expression (78) can be rewritten, in view of (66) and (69), as

$$A_{n_1, n_2; m_1, m_2} = -\frac{1}{2} \int_0^\infty d\gamma \left\{ \left(\frac{\zeta - 1}{\zeta} \right)^2 \frac{\theta^{n_1+m_2}}{\lambda^{n_2+m_1}} \int_{-\infty}^\infty d\tau \rho(\tau; \zeta) \rho(\tau_0 - \tau; \zeta) \right. \\ \left. \times p_{n_1}(\tau; \zeta) p_{n_2}(\tau_0 - \tau; \zeta) p_{m_1}(\tau; \zeta) p_{m_2}(\tau_0 - \tau; \zeta) \right\} \\ + \sum_{\ell=1}^\infty \frac{\kappa_\ell^3}{2\ell} \sum_{m=0}^{\ell-1} \mathcal{S}_{n_1}^{(\ell, m)} \mathcal{S}_{m_2}^{(\ell, \ell-m-1)} [\mathcal{S}_{n_2}^{(\ell, \ell-m-1)} \mathcal{S}_{m_1}^{(\ell, m)}]^*. \quad (79)$$

To illustrate the accuracy which can be obtained with the help of a standard FORTRAN numerical integration over an infinite interval code, the matrix elements $A_{n_1, n_2; m_1, m_2}$ (79) and the corresponding left-hand side of (76) in some (diagonal and nondiagonal) cases have been calculated. Here we put $b = 0.3, k = 0.15$ and $t_0 = \pm 0.5$. The results are presented in table 1.

3. Contour integrals

Note that expressing the resolvent of the one-dimensional operator $[\hat{h}_\xi + 2kt + \mu C\xi]$ requires two linearly independent solutions of (39). Irregular solutions of (39) are expressed in terms of the confluent hypergeometric function [23]

$$w^{(\pm)}(\gamma, \tau, \xi) = e^{\frac{i}{2}(\pm\gamma-k)\xi} U\left(\frac{1}{2} \pm i\tau, 1; \mp\gamma\xi\right). \quad (80)$$

The corresponding solutions of the three-term recursion relation (48) are

$$c_n^{(+)}(t; \mu C) = \theta^{n+1} q_n^{(+)}(\tau; \zeta), \quad c_n^{(-)}(t; \mu C) = \lambda^{n+1} q_n^{(-)}(\tau; \zeta), \quad (81)$$

where

$$q_n^{(+)}(\tau; \zeta) = (-)^n \frac{n! \Gamma(\frac{1}{2} + i\tau)}{\Gamma(n + \frac{3}{2} + i\tau)} {}_2F_1\left(\frac{1}{2} + i\tau, n + 1; n + \frac{3}{2} + i\tau; \zeta^{-1}\right), \\ q_n^{(-)}(\tau; \zeta) = (-)^n \frac{n! \Gamma(\frac{1}{2} - i\tau)}{\Gamma(n + \frac{3}{2} - i\tau)} {}_2F_1\left(\frac{1}{2} - i\tau, n + 1; n + \frac{3}{2} - i\tau; \zeta\right). \quad (82)$$

In particular, the functions

$$\tilde{w}^{(\pm)}(\gamma, \tau, \xi) = \frac{2i\sqrt{2b}}{2b - i(\gamma - k)} \left(-\frac{2b + i(\gamma - k)}{2b - i(\gamma + k)} \right)^{i\tau + \frac{1}{2}} \frac{e^{-\pi\tau}}{\theta \Gamma(\frac{1}{2} \pm i\tau)} \sum_{n=0}^\infty c_n^{(\pm)}(t; \mu C) \psi_n(\xi) \quad (83)$$

tend to $w^{(\pm)}(\gamma, \tau, \xi)$ as $\xi \rightarrow \infty$.

The matrix elements of the resolvent of $[\hat{h}_\xi + 2kt + \mu C\xi]$ can be written in the form [18]

$$g_{n, m}^{(+)}(t; \mu C) = \frac{i}{2\gamma} \left(\frac{\zeta - 1}{\zeta} \right) \frac{\theta^{n-m}}{\zeta^m} p_{n_<}(\tau; \zeta) q_{n_>}^{(+)}(\tau; \zeta) \quad (84)$$

and

$$g_{n, m}^{(-)}(t; \mu C) = \frac{i}{2\gamma} \left(\frac{\zeta - 1}{\zeta} \right) \frac{\theta^{n-m}}{\zeta^m} p_{n_<}(\tau; \zeta) \zeta^{n_>+1} q_{n_>}^{(-)}(\tau; \zeta), \quad (85)$$

where $n_>$ and $n_<$ are the greater and lesser of n and m . Note that $c_n^{(+)}$ ($c_n^{(-)}$) are defined in the upper (lower) half of the complex γ -plane where $|\zeta| \geq 1$ ($|\zeta| \leq 1$). To analytically continue $c_n^{(+)}$ onto the lower half of the γ -plane the relation [18]

$$c_n^{(+)}(t; \mu C) = c_n^{(-)}(t; \mu C) + 2\pi i \rho(\tau; \zeta) \theta^{n+1} p_n(\tau; \zeta) \quad (86)$$

can be used.

Table 1. $A_{n'_1, n'_2; m_1, m_2}$ involved into the normalization condition (76) and the left-hand side of (76) values. We put the following values of parameters: $b = 0.3, k = 0.15, t_0 = \pm 0.5$. The matrix elements were evaluated numerically by using (a) equation (79) and (b) the integral representation (92) with the parameters $\mathcal{E}_0 = 50$ and $\varphi = -\pi/3$. These calculations were performed with FORTRAN standard code.

$n_1 = m_1 = 3, n_2 = m_2 = 2$							
		$A_{22;32}$	$A_{32;32}$	$A_{42;32}$	$A_{31;32}$	$A_{33;32}$	the lhs of (76)
$t_0 > 0$	(a)	0.122 857 1428	0.164 502 1645	0.112 705 6277	0.118 095 2380	0.106 147 1861	1.000 000 0000
	(b)	0.122 857 2055	0.164 502 3080	0.112 705 5134	0.118 095 2862	0.106 148 0934	0.999 998 6214
$t_0 < 0$	(a)	0.122 857 1432	0.164 502 1641	0.112 705 6279	0.118 095 2386	0.106 147 1862	0.999 999 9877
	(b)	0.122 857 1040	0.164 502 1610	0.112 705 3228	0.118 095 2743	0.106 147 2855	1.000 001 5392
$n_1 = m_1 = 3, n_2 = 3, m_2 = 2$							
		$A_{23;32}$	$A_{33;32}$	$A_{43;32}$	$A_{32;32}$	$A_{34;32}$	the lhs of (76)
$t_0 > 0$	(a)	0.100 259 7402	0.106 147 1861	0.090 469 5304	0.164 502 1645	0.082 474 1924	$-0.555 111 5123 \times 10^{-15}$
	(b)	0.100 259 7440	0.106 148 0934	0.090 468 3789	0.164 502 3080	0.082 471 8107	$0.439 896 4458 \times 10^{-4}$
$t_0 < 0$	(a)	0.100 259 7401	0.106 147 1862	0.090 469 5303	0.164 502 1641	0.082 474 1924	$0.538 181 0552 \times 10^{-8}$
	(b)	0.100 259 5989	0.106 147 2855	0.090 466 9943	0.164 502 1610	0.082 478 2355	$-0.700 351 3032 \times 10^{-5}$
$n_1 = 3, m_1 = 2, n_2 = 3, m_2 = 2$							
		$A_{23;22}$	$A_{33;22}$	$A_{43;22}$	$A_{32;22}$	$A_{34;22}$	the lhs of (76)
$t_0 > 0$	(a)	0.122 857 1428	0.100 259 7402	0.083 311 6883	0.122 857 1428	0.083 311 6883	$-0.854 871 7289 \times 10^{-14}$
	(b)	0.122 857 5807	0.100 259 7454	0.083 312 1690	0.122 857 5170	0.083 311 0148	$-0.265 367 4140 \times 10^{-5}$
$t_0 < 0$	(a)	0.122 857 1432	0.100 259 7400	0.083 311 6883	0.122 857 1432	0.083 311 6883	$-0.851 979 5091 \times 10^{-8}$
	(b)	0.122 857 3492	0.100 259 6377	0.083 311 9210	0.122 857 2818	0.083 311 8111	$-0.648 893 0841 \times 10^{-5}$

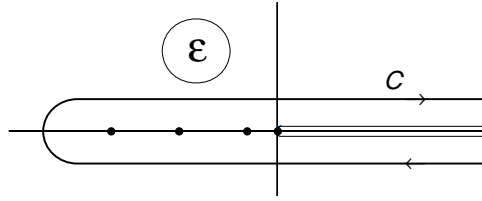


Figure 1. The path of integration C in (90).

In [18] we obtained the basis set (25) representation of the resolvent for the two-dimensional operator $[\hat{h}_\xi + 2kt + \mu C\xi] + [\hat{h}_\eta + 2k(t_0 - t) + \mu C\eta]$. In particular, the matrix elements of the two-dimensional Green's function can be expressed as the convolution integral

$$G_{n_1, n_2; m_1, m_2}^{(\pm)}(t_0; \mu C) = i \left(\frac{\zeta - 1}{\zeta} \right) \frac{\lambda^{m_2 - n_2}}{\zeta^{m_2}} \int_{-\infty}^{\infty} d\tau \rho(\tau_0 - \tau; \zeta) \times g_{n_1, m_1}^{(\pm)}(t; \mu C) p_{n_2}(\tau_0 - \tau; \zeta) p_{m_2}(\tau_0 - \tau; \zeta). \tag{87}$$

Note that in this case only the regular solutions of (40) discrete analogues $\lambda^{-n} p_n(\tau_0 - \tau; \zeta)$ are used.

Let us consider the integral

$$\mathcal{I}_1 = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \gamma d\gamma G_{n_1, n_2; m_1, m_2}^{(+)}(t_0; \mu C). \tag{88}$$

Note that by replacing $\gamma \rightarrow -\gamma$ (and hence $\theta \rightarrow \lambda, \lambda \rightarrow \theta, \zeta \rightarrow 1/\zeta, \tau \rightarrow -\tau$ and $\tau_0 \rightarrow -\tau_0$) in equation (87) $G_{n_1, n_2; m_1, m_2}^{(+)}(t_0; \mu C)$ is transformed to $G_{n_1, n_2; m_1, m_2}^{(-)}(t_0; \mu C)$. Thus, for the integral \mathcal{I}_1 we obtain

$$\mathcal{I}_1 = \frac{1}{2\pi i} \int_0^{\infty} \gamma d\gamma \{ G_{n_1, n_2; m_1, m_2}^{(+)}(t_0; \mu C) - G_{n_1, n_2; m_1, m_2}^{(-)}(t_0; \mu C) \}. \tag{89}$$

Inserting equations (87), (84) and (85) into equation (89), we find, in view of (86), that \mathcal{I}_1 coincides with the integral on the right-hand side of (79).

Now, we consider the integral

$$\frac{1}{2\pi i} \int_C d\mathcal{E} \mathbf{G}^{(+)} \left(t_0; \frac{k^2}{2} - \mathcal{E} \right), \tag{90}$$

taken along the contour in the complex \mathcal{E} -plane shown in figure 1. The contour C passes in a negative direction (clockwise) round all the points $\mathcal{E}^{(\ell)} = -\frac{\kappa_\ell^2}{2}$ (filled circles in figure 1 which accumulate at the origin) and the cut along the right-half of the real axis and is closed at infinity (see, e.g., [27]). The corresponding matrix element of the integral along the two sides of the cut is equal to \mathcal{I}_1 (88) (this is circumstantial evidence that the normalizing factor α in the completeness relation (71) is equal to $\frac{1}{2}$). On the other hand, the integration along a contour enclosing $\mathcal{E}^{(\ell)}$ reduces to (-1) times the double sum of the residues of the integrand at the points $\tau^{(m)} = i(m + \frac{1}{2}), m = 0, 1, \dots$ and $\mathcal{E}^{(\ell)} = -\frac{(kt_0)^2}{2\ell^2}, \ell = 1, 2, \dots$, which are the poles of the gamma functions $\Gamma(\frac{1}{2} + i\tau)$ and $\Gamma(\frac{1}{2} + i(\tau_0 - \tau)) = \Gamma(m + 1 + \frac{kt_0}{\sqrt{-2\mathcal{E}^{(\ell)}}})$, respectively. It is readily shown that the matrix element of this part of the integral (90) coincides with the double sum in (79). Thus, the integral (90) is equal to the matrix \mathbf{A} . The contour C can be deformed, for instance, into a straight line parallel to the real axis. The resulting path C_1 shown in figure 2 runs above the cut and the bound-state poles of $\mathbf{G}^{(+)}(t_0; \frac{k^2}{2} - \mathcal{E})$. The contour C_1 can be rotated about some point \mathcal{E}_0 on the right-half of the real axis through an angle φ in the

is proportional to the unit matrix:

$$\left[\mathbf{Q}_1 \int_{C_2} d\mathcal{E}_1 \mathbf{G}_1^{(+)} \left(t_{23}; \frac{k_{23}^2}{2} - \mathcal{E}_1 \right) \right] \otimes \left[\mathbf{Q}_2 \int_{C_2} d\mathcal{E}_2 \mathbf{G}_2^{(+)} \left(t_{13}; \frac{k_{13}^2}{2} - \mathcal{E}_2 \right) \right] \otimes \mathbf{I}_3 = (2\pi i)^2 \mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{I}_3. \tag{94}$$

Consider the first two terms in the figure braces in (36). For the energy $\mathcal{E}_3 = \frac{k_{12}^2}{2} + \mu_{12}(C_1 + C_2)$ we have

$$\mathcal{E}_3 = \frac{k_{12}^2}{2} + \frac{\mu_{12}}{\mu_{23}} \left(\frac{k_{23}^2}{2} - \mathcal{E}_1 \right) + \frac{\mu_{12}}{\mu_{13}} \left(\frac{k_{13}^2}{2} - \mathcal{E}_2 \right). \tag{95}$$

On the other hand, on the contours C_2 the energy variables $\mathcal{E}_j, j = 1, 2$ are given by

$$\mathcal{E}_j = \mathcal{E}_{0j} + E_j e^{i\varphi}, \tag{96}$$

where $\varphi < 0, \mathcal{E}_{0j}$ is an arbitrary positive parameter, E_j is real and runs from $-\infty$ to ∞ . Hence, for the energy \mathcal{E}_3 (95) we obtain

$$\mathcal{E}_3 = \left[\frac{k_{12}^2}{2} + \frac{\mu_{12}}{\mu_{23}} \left(\frac{k_{23}^2}{2} - \mathcal{E}_{01} \right) + \frac{\mu_{12}}{\mu_{13}} \left(\frac{k_{13}^2}{2} - \mathcal{E}_{02} \right) \right] + \left(-\frac{\mu_{12}}{\mu_{23}} E_1 - \frac{\mu_{12}}{\mu_{13}} E_2 \right) e^{i\varphi}. \tag{97}$$

Thus, \mathcal{E}_3 can be expressed in the form

$$\mathcal{E}_3 = \mathcal{E}_{03} + E_3 e^{i\varphi}, \tag{98}$$

where \mathcal{E}_{03} and E_3 denote the term in the square braces and the real factor in front of the exponent in (97), respectively. Since \mathcal{E}_{03} should be positive, therefore the positive parameters \mathcal{E}_{01} and \mathcal{E}_{02} have to satisfy the constraint

$$\frac{\mu_{12}}{\mu_{23}} \mathcal{E}_{01} + \frac{\mu_{12}}{\mu_{13}} \mathcal{E}_{02} < \frac{k_{12}^2}{2} + \frac{\mu_{12}}{\mu_{23}} \frac{k_{23}^2}{2} + \frac{\mu_{12}}{\mu_{13}} \frac{k_{13}^2}{2}. \tag{99}$$

Now, we consider the integral

$$\mathcal{I}_2 = \int_{C_2} d\mathcal{E}_1 \mathbf{G}_3^{(+)} \left(t_{12}; \frac{k_{12}^2}{2} - \mathcal{E}_3 \right). \tag{100}$$

With fixed \mathcal{E}_2 , in view (97), (98) and (92), we see that

$$\begin{aligned} \mathcal{I}_2 &= e^{i\varphi} \int_{-\infty}^{\infty} dE_1 \mathbf{G}_3^{(+)} \left(t_{12}; \frac{k_{12}^2}{2} - \mathcal{E}_3 \right) = -\frac{\mu_{23}}{\mu_{12}} e^{i\varphi} \int_{-\infty}^{\infty} dE_3 \mathbf{G}_3^{(+)} \left(t_{12}; \frac{k_{12}^2}{2} - \mathcal{E}_3 \right) \\ &= -\frac{\mu_{23}}{\mu_{12}} \int_{C_2} d\mathcal{E}_3 \mathbf{G}_3^{(+)} \left(t_{12}; \frac{k_{12}^2}{2} - \mathcal{E}_3 \right) = -2\pi i \frac{\mu_{23}}{\mu_{12}} \mathbf{Q}_3^{-1}. \end{aligned} \tag{101}$$

Similarly, we obtain

$$\int_{C_2} d\mathcal{E}_2 \mathbf{G}_3^{(+)} \left(t_{12}; \frac{k_{12}^2}{2} - \mathcal{E}_3 \right) = -2\pi i \frac{\mu_{13}}{\mu_{12}} \mathbf{Q}_3^{-1}. \tag{102}$$

Inserting (101), (102) and (94) into (36) then yields

$$\underline{\mathfrak{h}\mathcal{G}} = \aleph 4\pi^2 \mathbf{I}_1 \otimes \mathbf{I}_2 \otimes \mathbf{I}_3. \tag{103}$$

Thus, from (103) we conclude that

$$\aleph = \frac{1}{4\pi^2}. \tag{104}$$

5. Conclusion

The Sturmian basis set representation of the resolvent for the asymptotic three-body Coulomb wave operator is obtained, which can be used in the discrete analog of the Lippmann–Schwinger equation for the three-body continuum wavefunction. The six-dimensional Green’s function matrix is expressed as a convolution integral over separation constants. The integrand of this contour integral involves Green’s function matrices corresponding to the two-dimensional operators which are constituents of the full six-dimensional wave operator. The completeness relation of the eigenfunctions of these two-dimensional operators is used to define the appropriate paths of integration of the convolution integral.

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